



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 18, 2017 – 04:43 PM EDT

PDB ID : 4V5H  
EMDB ID: : EMD-1657  
Title : E.Coli 70s Ribosome Stalled During Translation Of Tnac Leader Peptide.  
Authors : Seidelt, B.; Innis, C.A.; Wilson, D.N.; Gartmann, M.; Armache, J.; Villa, E.;  
Trabuco, L.G.; Becker, T.; Mielke, T.; Schulten, K.; Steitz, T.A.; Beckmann,  
R.  
Deposited on : unknown  
Resolution : 5.80 Å(reported)  
Based on PDB ID : 3FIH, 3FIK

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

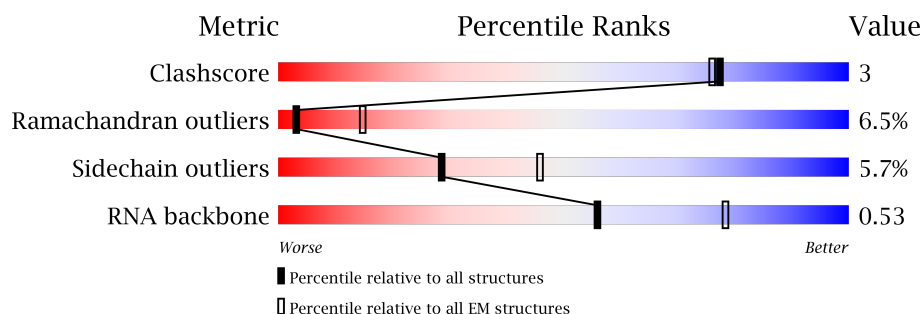
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




























| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 125131                      | 1336                        |
| Ramachandran outliers | 121729                      | 1120                        |
| Sidechain outliers    | 121581                      | 1026                        |
| RNA backbone          | 3398                        | 335                         |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | AA    | 1530   | 35% 47% 18%      |
| 2   | AB    | 218    | 68% 28% .        |
| 3   | AC    | 206    | 65% 25% 9% .     |
| 4   | AD    | 205    | 67% 24% 8%       |
| 5   | AE    | 150    | 65% 28% 7% .     |
| 6   | AF    | 100    | 65% 28% 6% .     |
| 7   | AG    | 150    | 67% 25% 7% .     |
| 8   | AH    | 129    | 71% 26% .        |









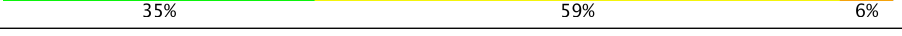

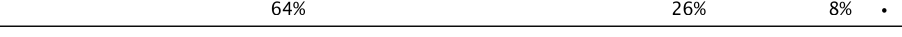
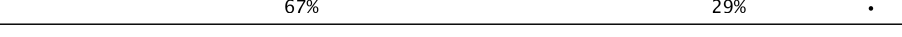

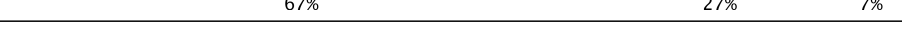




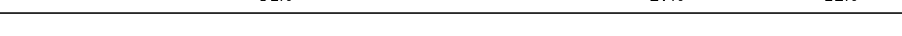



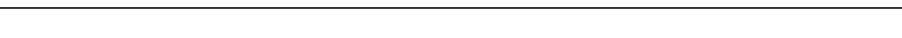
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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 9   | AI    | 127    |    |
| 10  | AJ    | 98     |    |
| 11  | AK    | 117    |    |
| 12  | AL    | 123    |    |
| 13  | AM    | 113    |    |
| 14  | AN    | 96     |    |
| 15  | AO    | 88     |    |
| 16  | AP    | 80     |    |
| 17  | AQ    | 80     |    |
| 18  | AR    | 55     |    |
| 19  | AS    | 79     |    |
| 20  | AT    | 85     |    |
| 21  | AU    | 51     |  |
| 22  | AV    | 77     |  |
| 23  | AX    | 11     |  |
| 24  | AZ    | 20     |  |
| 25  | B0    | 77     |  |
| 26  | B1    | 63     |  |
| 27  | B2    | 58     |  |
| 28  | B3    | 56     |  |
| 29  | B4    | 50     |  |
| 30  | B5    | 234    |  |
| 31  | B6    | 46     |  |
| 32  | B7    | 64     |  |
| 33  | B8    | 38     |  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 34  | BA    | 117    |  42% 43% 14% .    |
| 35  | BB    | 2903   |  38% 45% 17%      |
| 36  | BC    | 271    |  68% 25% 6% .     |
| 37  | BD    | 209    |  67% 23% 8% .     |
| 38  | BE    | 201    |  66% 27% 6%       |
| 39  | BF    | 178    |  63% 26% 10% .    |
| 40  | BG    | 176    |  72% 22% 6% .     |
| 41  | BH    | 149    |  74% 21% 5%       |
| 42  | BI    | 141    |  35% 59% 6%       |
| 43  | BJ    | 142    |  69% 21% 8% .     |
| 44  | BK    | 121    |  64% 26% 8% .     |
| 45  | BL    | 143    |  67% 29% .       |
| 46  | BM    | 136    |  68% 29% . .    |
| 47  | BN    | 120    |  67% 27% 7%     |
| 48  | BO    | 116    |  74% 22% .      |
| 49  | BP    | 114    |  68% 25% 7%     |
| 50  | BQ    | 117    |  60% 31% 7% .   |
| 51  | BR    | 103    |  59% 32% 7% .   |
| 52  | BS    | 110    |  61% 27% 12%    |
| 53  | BT    | 93     |  56% 39% 5%     |
| 54  | BU    | 102    |  62% 26% 6% . . |
| 55  | BW    | 94     |  61% 31% 7% .   |
| 56  | BY    | 79     |  63% 27% 6% .   |



## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 145960 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | AA    | 1530     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32831 | 14642 | 6024 | 10635 | 1530 |         |       |

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | AB    | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1704  | 1081 | 305 | 311 | 7 |         |       |

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | AC    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |       |

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | AD    | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | AE    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1105  | 687 | 211 | 201 | 6 |         |       |

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | AF    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 817   | 515 | 148 | 148 | 6 |         |       |

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | AG    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1174  | 730 | 226 | 214 | 4 |         |       |

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | AH    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | AI    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | AJ    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |       |

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | AK    | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |       |

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | AL    | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |       |

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | AM    | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 541 | 177 | 155 | 3 |         |       |

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | AN    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 774   | 483 | 160 | 128 | 3 |         |       |

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | AO    | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 716   | 440 | 146 | 129 | 1 |         |       |

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | AP    | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 638   | 400 | 126 | 111 | 1 |         |       |

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | AQ    | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |       |

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 18  | AR    | 55       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 455   | 288 | 86 | 81 |         |       |

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | AS    | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 637   | 408 | 120 | 107 | 2 |         |       |

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | AT    | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |       |

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S21.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 21  | AU    | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 425   | 265 | 86 | 73 | 1 |         |       |

- Molecule 22 is a RNA chain called P-SITE TRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 22  | AV    | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1649  | 733 | 297 | 542 | 77 |         |       |

- Molecule 23 is a RNA chain called MRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 23  | AX    | 11       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 236   | 106 | 46 | 73 | 11 |         |       |

- Molecule 24 is a protein called POLY-ALA NASCENT CHAIN.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 24  | AZ    | 20       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 100   | 60 | 20 | 20 |         |       |

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | B0    | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26  | B1    | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |       |

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 27  | B2    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28  | B3    | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L33.

| Mol | Chain | Residues | Atoms |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 29  | B4    | 50       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 409   | 263 | 75 | 71 |  |         |       |

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 30  | B5    | 234      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1733  | 1081 | 315 | 330 | 7 |         |       |

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31  | B6    | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 32  | B7    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 33  | B8    | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 34 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 34  | BA    | 115      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2464  | 1097 | 451 | 801 | 115 |         |       |

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 35  | BB    | 2903     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62321 | 27801 | 11467 | 20150 | 2903 |         |       |

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36  | BC    | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | BD    | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |       |

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | BE    | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | BF    | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1420  | 905 | 251 | 258 | 6 |         |       |

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | BG    | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1316  | 827 | 242 | 245 | 2 |         |       |

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | BH    | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |       |

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | BI    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |       |

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | BJ    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | BK    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 930   | 582 | 179 | 163 | 6 |         |       |

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | BL    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |       |

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | BM    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |       |

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | BN    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 960   | 593 | 196 | 166 | 5 |         |       |

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 48  | BO    | 116      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |  |         |       |

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | BP    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L20.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 50  | BQ    | 117      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |  |         |       |

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | BR    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | BS    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | BT    | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |       |

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 54  | BU    | 99       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 755   | 479 | 140 | 136 |  |         |       |

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | BW    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L27.

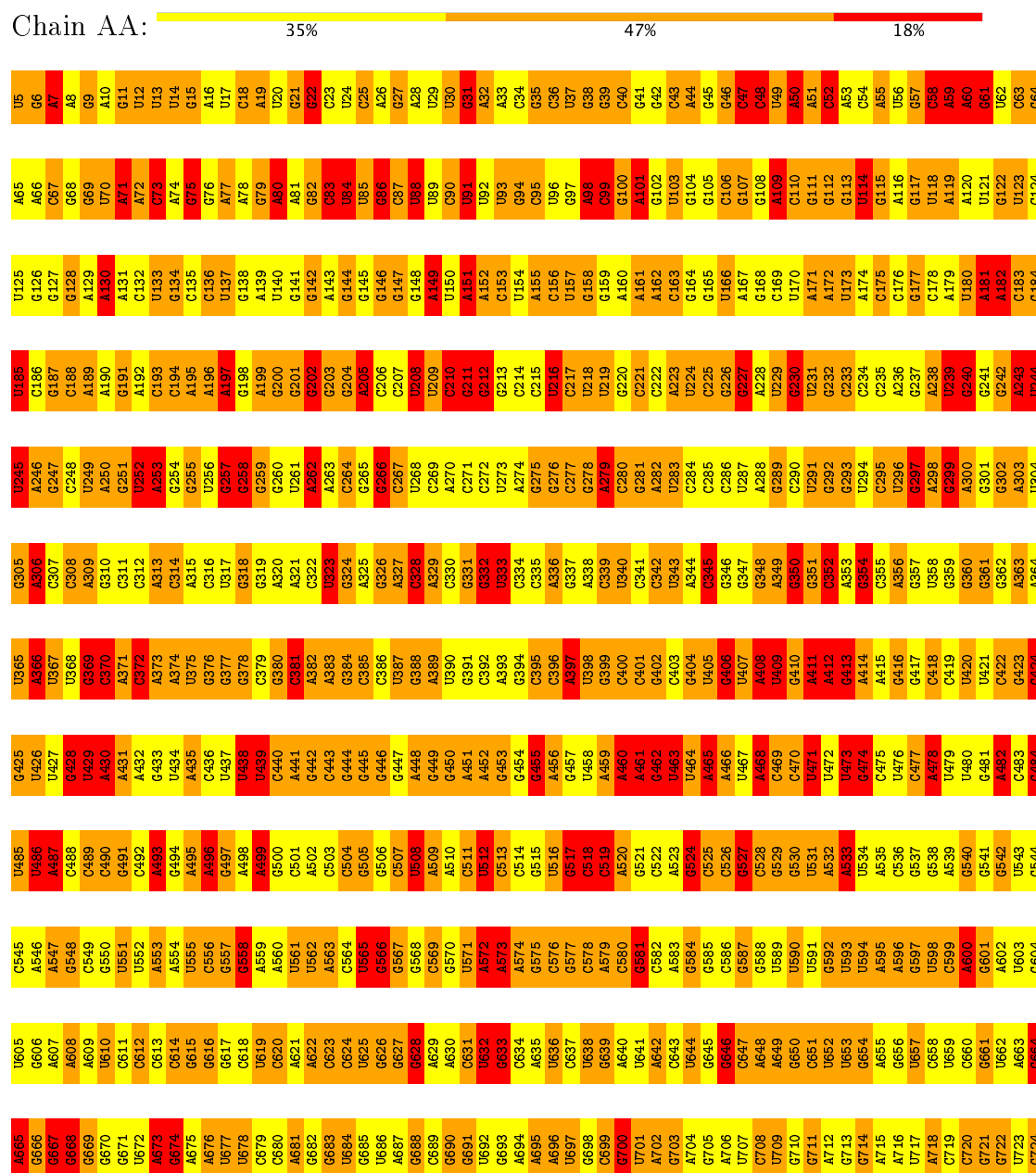


| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 56  | BY    | 79       | 596   | 367 | 120 | 108 | 1 | 0       | 0     |

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

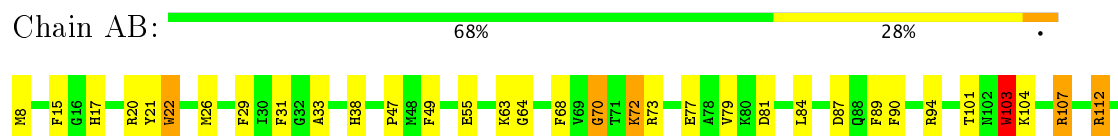
#### • Molecule 1: 16S RIBOSOMAL RNA

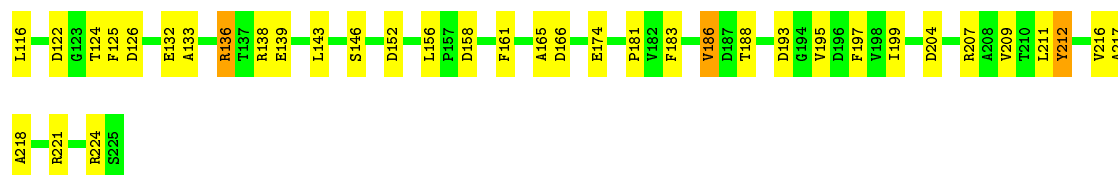


|       |       |       |       |       |       |      |      |      |      |
|-------|-------|-------|-------|-------|-------|------|------|------|------|
| G1505 | U1445 | C1325 | C1265 | U1025 | U965  | U905 | A845 | G785 | G725 |
| U1506 | A1446 | U1326 | G1266 | G1026 | G966  | A906 | G846 | G786 | G726 |
| A1507 | A1447 | C1327 | G1267 | G1027 | C1027 | A907 | G847 | A787 | G727 |
| A1508 | C1448 | C1328 | G1268 | C1028 | A968  | A908 | C948 | U788 | A728 |
| C1509 | C1449 | A1329 | A1269 | C1029 | G1089 | A909 | G849 | U789 | A729 |
| C1510 | U1330 | G1330 | G1270 | U1030 | C970  | C910 | U850 | A790 | G730 |
| U1511 | U1331 | G1331 | A1271 | C1031 | G971  | U911 | G851 | G791 | G731 |
| U1512 | C1332 | A1332 | G1272 | G1032 | G972  | C912 | G852 | A792 | C732 |
| A1513 | G1453 | G1333 | G1273 | G1033 | G973  | A913 | C853 | U793 | G733 |
| G1514 | G1454 | G1334 | A1274 | G1034 | A974  | A914 | U854 | A794 | G734 |
| G1515 | C1335 | U1335 | G1275 | A1035 | A975  | A915 | U855 | G795 | C735 |
| G1516 | A1456 | G1336 | A1276 | C1036 | G976  | U916 | C856 | G796 | C736 |
| C1517 | G1457 | G1337 | G1277 | C1037 | A977  | G917 | C857 | G797 | C737 |
| A1518 | G1458 | G1338 | G1278 | C1038 | A978  | A918 | G858 | U798 | C738 |
| C1519 | G1459 | A1339 | G1279 | G1039 | G979  | A919 | G859 | G799 | C739 |
| C1520 | C1460 | A1340 | A1280 | C1100 | C980  | U920 | A860 | G800 | U740 |
| C1521 | G1461 | U1341 | C1281 | G1041 | U981  | U921 | G861 | U801 | G741 |
| U1522 | C1462 | C1342 | G1282 | A1042 | U982  | G922 | C862 | A802 | G742 |
| G1523 | G1463 | G1343 | U1283 | G1043 | A983  | A923 | U863 | G803 | A743 |
| G1524 | U1464 | C1344 | C1284 | A1044 | C984  | G924 | A864 | U804 | C744 |
| G1525 | A1465 | U1345 | A1285 | A1105 | C985  | G925 | A865 | C805 | G745 |
| C1526 | C1466 | A1346 | U1286 | C1046 | U986  | G926 | C866 | C806 | A746 |
| U1527 | C1467 | G1347 | A1287 | G1047 | G987  | G927 | G867 | A807 | A747 |
| A1528 | A1468 | U1348 | A1288 | G1048 | G988  | G928 | C868 | C808 | G748 |
| G1529 | C1469 | A1349 | A1289 | U1049 | U989  | G929 | G869 | G809 | A749 |
| G1530 | U1470 | A1350 | G1290 | C1050 | C990  | C930 | U870 | C810 | C750 |
| A1531 | U1471 | U1351 | U1291 | C1051 | U991  | C931 | U871 | C811 | U751 |
| C1532 | U1472 | C1352 | G1292 | C1172 | U992  | C932 | A872 | G812 | G752 |
| C1533 | G1473 | G1353 | C1293 | C1173 | G993  | G933 | A873 | U813 | A753 |
| A1534 | U1474 | U1354 | G1294 | C1054 | A994  | C934 | G874 | A814 | C754 |
|       | G1475 | G1355 | U1295 | A1055 | C995  | A935 | U875 | A815 | G755 |
|       | A1476 | G1356 | C1296 | U1056 | A996  | C936 | G876 | A816 | C756 |
|       | U1477 | A1357 | G1297 | G1057 | U997  | A937 | G877 | C817 | U757 |
|       | U1478 | U1358 | U1298 | C1058 | C998  | A938 | A878 | G818 | C758 |
|       | C1479 | C1359 | A1299 | C1059 | C999  | G939 | C879 | A819 | A759 |
|       | A1480 | U1420 | A1360 | U1060 | A1000 | C940 | C880 | U820 | G760 |
|       | U1481 | G1361 | U1301 | G1061 | G1001 | G941 | G881 | G821 | G761 |
|       | G1482 | A1362 | C1302 | G1242 | U1002 | G942 | C882 | U822 | U762 |
|       | A1483 | A1363 | C1303 | C1063 | G1003 | G943 | C883 | C823 | G763 |
|       | C1484 | U1364 | G1304 | G1064 | U884  | G944 | G884 | G824 | C764 |
|       | U1485 | G1365 | G1305 | U1065 | A1005 | G945 | G885 | A825 | G765 |
|       | G1486 | C1366 | A1306 | C1066 | G1006 | A946 | G886 | C826 | A766 |
|       | G1487 | C1367 | U1307 | A1067 | U1007 | G947 | G887 | U827 | A767 |
|       | G1488 | A1368 | U1308 | C1068 | U1008 | C948 | G888 | U828 | A768 |
|       | G1489 | C1369 | G1309 | G1069 | U1009 | A949 | A889 | G829 | G769 |
|       | U1490 | G1370 | U1310 | U1070 | U1010 | U950 | G890 | A830 | C770 |
|       | A1491 | G1371 | A1311 | C1071 | C1011 | G951 | U891 | A831 | G771 |
|       | A1492 | G1372 | G1312 | G1072 | A1012 | U952 | A892 | G832 | U772 |
|       | A1493 | G1373 | U1313 | U1073 | G1013 | G953 | C893 | G833 | G773 |
|       | G1494 | A1374 | C1314 | G1074 | A1014 | G954 | G894 | U834 | G774 |
|       | U1495 | A1375 | G1315 | U1075 | G1015 | U955 | G895 | U835 | G775 |
|       | C1496 | U1376 | G1316 | U1076 | U1016 | U956 | C896 | G836 | G776 |
|       | G1497 | A1377 | A1257 | G1077 | U1017 | U957 | C897 | U837 | A777 |
|       | U1498 | C1378 | G1318 | U1078 | G1018 | A958 | G898 | G838 | G778 |
|       | A1499 | G1379 | A1319 | G1079 | U1019 | A959 | C899 | C839 | C779 |
|       | U1500 | U1380 | C1320 | A1080 | G1020 | U960 | A900 | C840 | A780 |
|       | C1501 | U1381 | A1261 | A1081 | A1021 | U961 | A901 | C841 | A781 |
|       | A1502 | C1382 | C1262 | A1082 | A1022 | C962 | G902 | U842 | A782 |
|       | A1503 | G1383 | C1263 | G1143 | U1023 | G963 | G903 | U843 | C783 |
|       | G1504 | C1384 | A1324 | G1144 | G1024 | A964 | U904 | G844 | A784 |

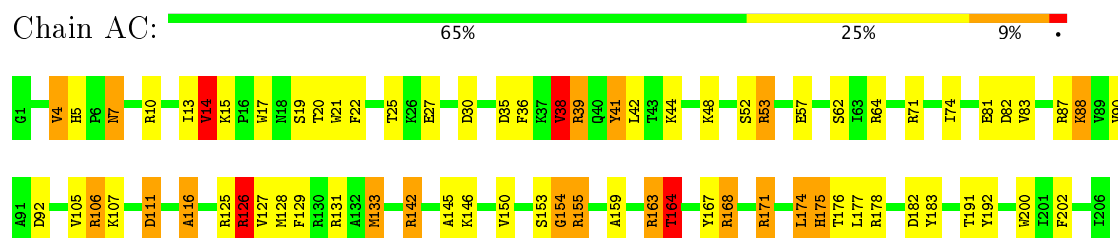
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB:

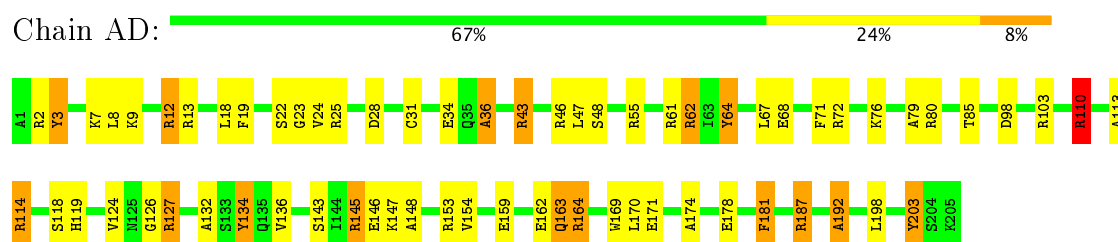




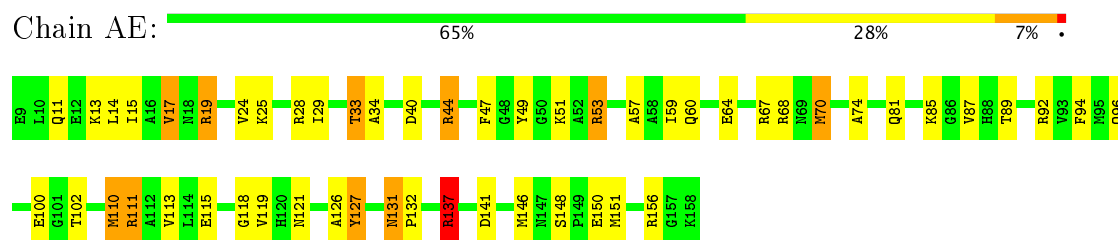
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



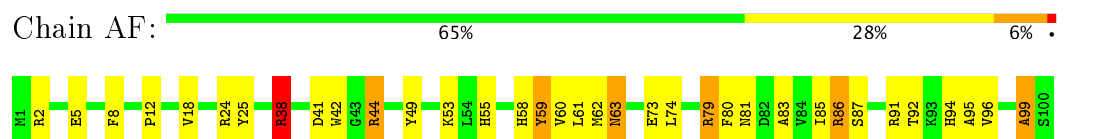
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



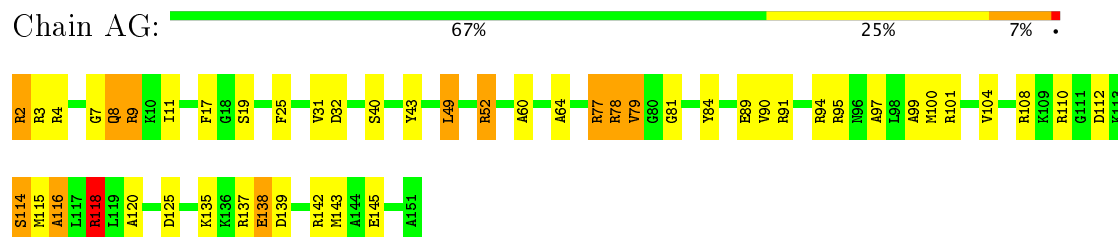
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



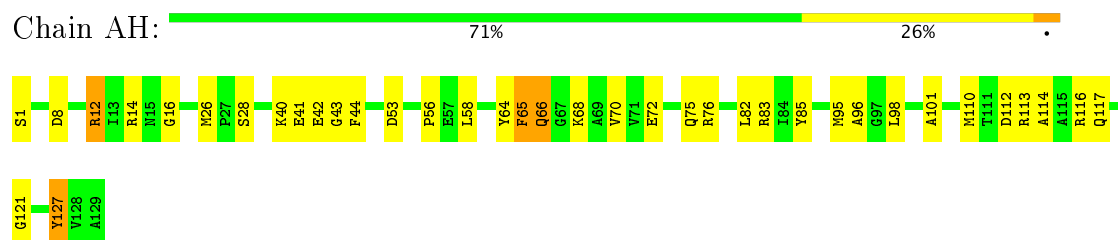
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



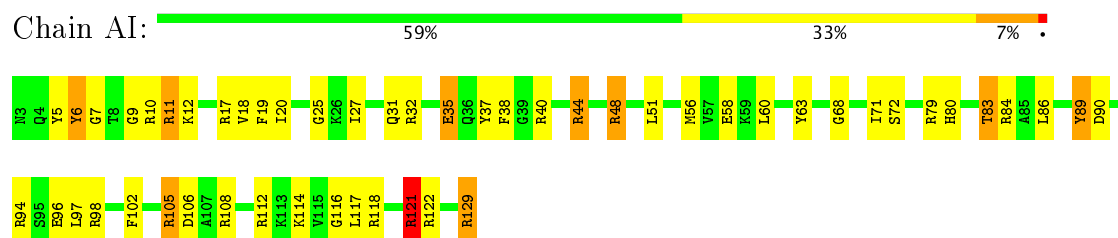
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



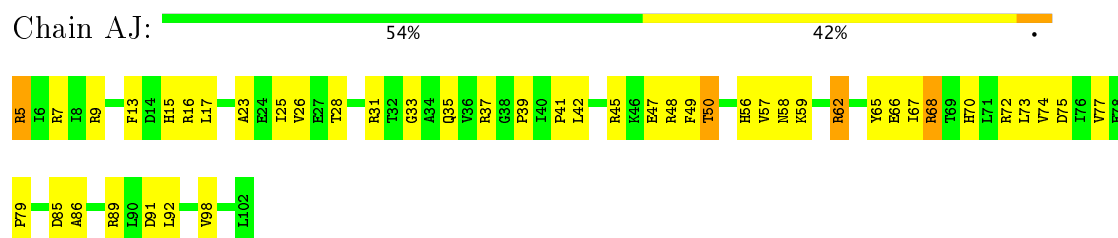
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



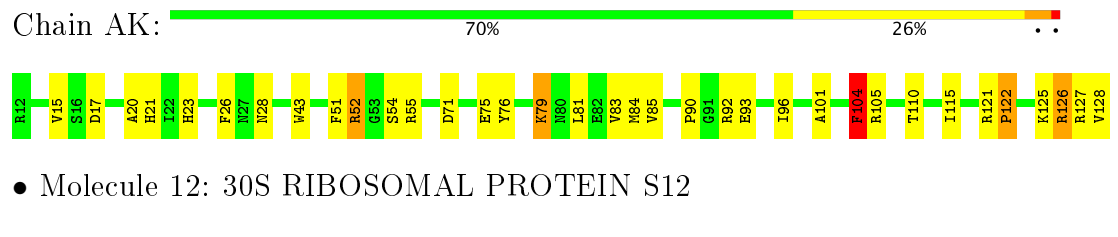
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



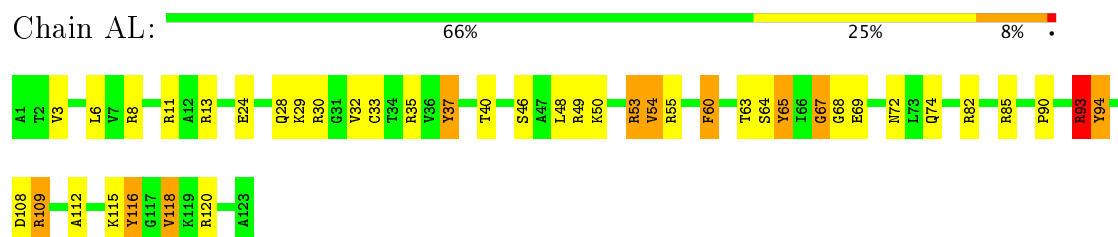
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



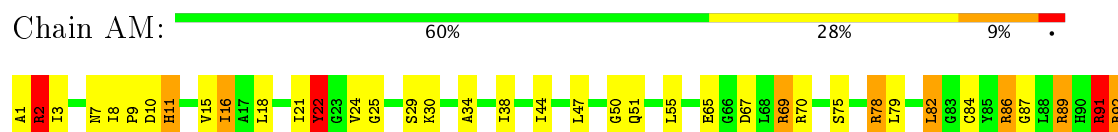
- Molecule 11: 30S RIBOSOMAL PROTEIN S11




- Molecule 12: 30S RIBOSOMAL PROTEIN S12

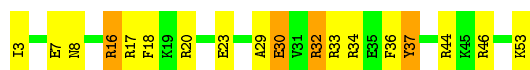


- Molecule 13: 30S RIBOSOMAL PROTEIN S13



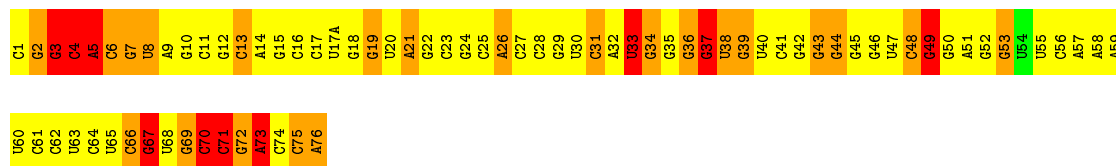


Chain AU:  65% 27% 8%




- Molecule 22: P-SITE TRNA

Chain AV:  57% 29% 13%




- Molecule 23: MRNA

Chain AX:  9% 18% 27% 45%



- Molecule 24: POLY-ALA NASCENT CHAIN

Chain AZ:  80% 20%



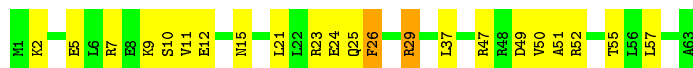
- Molecule 25: 50S RIBOSOMAL PROTEIN L28

Chain B0:  70% 25% 5%




- Molecule 26: 50S RIBOSOMAL PROTEIN L29

Chain B1:  65% 32% 3%



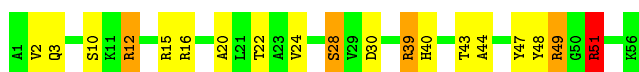
- Molecule 27: 50S RIBOSOMAL PROTEIN L30

Chain B2:  76% 24%



- Molecule 28: 50S RIBOSOMAL PROTEIN L32

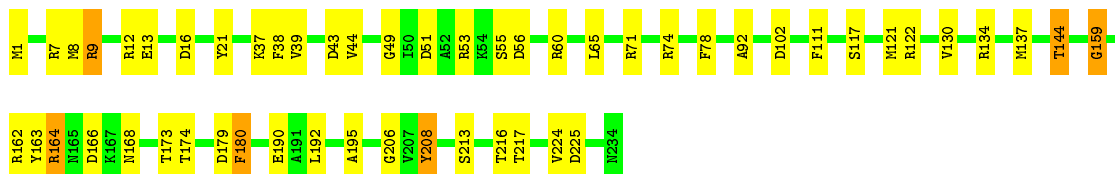
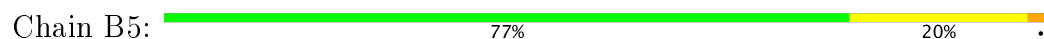
Chain B3:  66% 25% 7% 2%



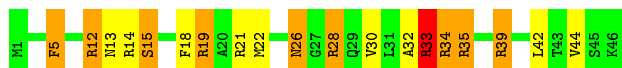
- Molecule 29: 50S RIBOSOMAL PROTEIN L33



- Molecule 30: 50S RIBOSOMAL PROTEIN L1



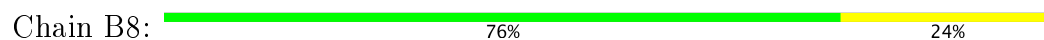
- Molecule 31: 50S RIBOSOMAL PROTEIN L34



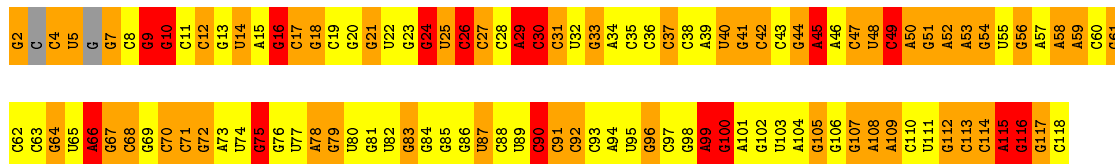
- Molecule 32: 50S RIBOSOMAL PROTEIN L35



- Molecule 33: 50S RIBOSOMAL PROTEIN L36



- Molecule 34: 5S RIBOSOMAL RNA



- Molecule 35: 23S RIBOSOMAL RNA



Chain BB:

38%

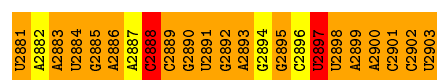
45%

17%

|     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| G1  | C61  | G121 | A181 | A241 | G301 | G361 | C421 | G481 | A541 | C601 | A661 | A721 | A781 | G841 | C901 |
| G2  | U62  | G122 | A182 | G242 | G302 | A362 | A422 | A482 | C542 | A602 | G662 | A722 | A782 | G842 | C902 |
| U3  | A63  | G123 | C183 | U243 | G303 | G363 | G423 | A483 | G543 | A603 | G663 | C723 | A783 | G843 | C903 |
| U4  | A64  | G124 | C184 | A244 | U304 | G364 | A244 | C484 | C544 | A604 | G664 | U724 | A784 | A844 | G904 |
| A5  | U65  | A125 | G185 | G245 | C305 | U365 | G245 | C485 | U545 | G605 | U665 | G725 | G785 | A845 | A905 |
| A6  | C66  | A126 | G186 | C246 | U306 | C366 | C246 | C486 | U546 | G606 | A666 | G726 | G786 | U846 | U906 |
| G7  | U67  | A127 | G187 | G247 | G307 | G367 | U247 | C487 | A547 | U607 | U667 | A727 | A787 | U847 | G907 |
| C8  | G68  | C128 | G188 | G248 | G308 | A368 | A428 | C488 | G548 | A608 | A668 | G728 | A788 | C848 | C908 |
| G9  | C69  | C129 | G189 | C249 | A309 | U369 | A429 | G489 | G549 | A609 | G669 | G729 | A789 | C849 | A909 |
| G70 | A71  | C130 | A191 | G250 | A310 | G370 | A430 | C490 | C550 | G610 | A670 | A730 | A790 | U850 | A910 |
| C11 | U72  | A131 | A191 | A251 | A311 | G371 | U431 | G491 | C551 | G611 | C671 | C731 | C791 | C851 | A911 |
| U12 | A73  | G132 | C192 | G252 | G312 | G372 | A432 | A492 | U552 | G612 | G672 | G732 | A792 | U852 | C912 |
| A13 | A74  | U133 | G193 | C263 | G313 | U373 | C433 | C493 | G553 | A613 | C673 | G733 | A793 | C853 | U913 |
| G15 | G75  | A135 | A195 | A255 | G315 | G375 | C435 | G495 | G555 | U615 | A675 | A735 | A795 | C854 | G914 |
| C16 | C76  | U136 | A196 | A256 | C316 | G376 | A436 | G496 | A556 | A616 | A676 | A736 | C796 | G856 | C916 |
| G17 | U77  | U137 | A197 | G257 | G317 | G377 | U437 | A497 | C557 | G617 | A677 | G737 | G797 | G858 | A917 |
| U18 | G78  | U138 | C198 | G258 | C318 | G378 | U438 | G498 | U558 | G618 | C678 | G738 | A798 | G859 | A918 |
| A19 | C79  | U139 | A199 | G259 | G319 | G379 | A439 | U499 | G559 | G619 | C679 | A739 | G799 | G859 | U919 |
| C20 | G80  | C140 | U200 | G260 | A320 | G380 | C440 | U500 | C560 | G620 | G680 | C740 | A800 | U860 | A920 |
| A21 | G81  | G141 | C201 | G261 | U321 | G381 | U441 | A501 | G561 | A621 | C681 | U741 | G801 | U861 | C921 |
| G22 | U82  | C143 | A203 | A262 | C323 | C383 | A443 | A503 | A563 | C623 | G683 | A743 | A803 | G863 | G923 |
| C23 | A83  | C143 | A203 | C264 | A324 | A384 | C444 | A504 | C564 | G624 | G684 | U744 | A804 | G864 | G924 |
| G24 | A84  | C145 | G205 | A265 | G325 | C385 | C445 | A505 | C565 | G625 | A685 | G745 | G805 | C865 | A925 |
| U25 | G85  | C146 | G206 | G266 | G326 | G386 | G446 | G506 | U566 | A626 | U686 | U746 | C806 | A866 | G926 |
| G26 | G86  | A146 | U207 | C267 | G327 | U387 | A447 | A507 | U567 | A627 | C687 | U747 | U807 | G867 | A927 |
| G27 | U87  | C147 | C208 | G268 | U328 | G388 | U448 | A508 | U568 | G628 | U688 | G748 | A808 | U868 | A928 |
| A28 | U88  | U148 | C209 | C269 | G329 | C389 | A449 | C509 | U569 | G629 | A689 | A749 | A809 | G869 | U929 |
| U29 | A89  | U149 | G210 | A270 | A330 | U390 | G450 | C510 | U570 | G630 | G690 | A750 | A810 | U870 | G930 |
| G30 | U90  | U150 | C211 | G271 | C331 | U391 | U451 | U511 | U571 | A631 | C691 | A751 | U811 | U871 | U931 |
| C31 | A91  | A151 | G212 | A272 | A332 | U392 | A452 | G512 | A572 | A632 | C692 | A752 | C812 | U872 | U932 |
| G32 | U92  | U153 | A213 | G273 | G333 | C393 | A453 | A513 | U573 | A633 | C693 | A753 | U813 | U873 | A933 |
| C33 | G93  | C154 | G214 | C274 | C334 | C394 | A454 | A514 | A574 | G634 | U694 | U754 | C814 | G874 | U934 |
| U34 | A94  | A155 | G215 | C275 | C335 | U395 | C455 | A515 | A575 | G635 | G695 | U755 | C815 | G875 | C935 |
| G35 | C95  | A156 | A216 | U276 | C336 | G396 | C456 | C516 | U576 | G636 | G696 | A756 | C816 | C876 | A936 |
| G36 | G96  | C157 | A217 | G277 | C337 | U397 | A457 | C517 | G577 | A637 | C697 | A757 | C817 | A877 | G937 |
| C37 | U97  | U158 | A218 | A278 | G338 | C398 | G458 | G518 | G578 | G638 | C698 | A758 | C818 | A878 | G938 |
| A38 | G98  | U159 | A219 | G279 | U339 | U399 | U459 | U519 | U579 | U639 | A699 | G759 | A819 | G879 | G939 |
| G39 | U99  | A160 | G220 | U280 | A340 | G400 | A460 | G520 | U580 | U640 | G700 | A760 | A820 | G880 | G940 |
| U40 | A101 | C161 | A221 | C281 | C341 | A401 | C461 | U521 | C581 | U641 | G701 | A761 | A821 | G881 | A941 |
| C41 | U102 | U162 | A222 | A282 | A342 | A402 | C462 | A522 | A582 | U642 | U702 | A762 | G822 | G882 | G942 |
| A42 | U103 | C163 | A223 | G283 | C343 | U403 | G463 | C523 | G583 | A643 | G703 | G763 | G823 | G883 | A943 |
| G43 | A104 | C164 | U224 | U284 | C344 | A404 | U464 | C524 | G584 | A644 | U704 | A764 | U824 | U884 | C944 |
| A44 | C105 | U166 | C225 | G285 | A345 | U405 | G465 | U525 | G585 | C645 | A705 | C765 | A825 | C885 | A945 |
| G45 | C106 | U166 | A226 | U286 | A346 | A406 | A466 | A526 | A586 | U646 | A706 | U766 | U826 | A886 | C946 |
| U46 | G107 | A167 | A227 | G287 | A347 | G407 | G467 | C527 | C587 | U647 | G707 | A767 | U827 | U887 | A947 |
| C48 | G108 | C168 | C228 | U288 | A348 | G408 | G468 | A528 | U588 | U648 | G708 | G768 | U828 | C888 | C948 |
| A49 | G109 | G169 | C229 | G289 | U349 | A409 | G469 | A529 | U589 | U649 | U709 | U769 | A829 | C889 | G949 |
| U50 | G110 | U170 | G230 | U290 | G350 | G410 | A470 | G530 | A590 | U650 | U710 | G770 | G830 | C890 | G950 |
| G51 | A111 | U171 | A231 | G291 | C351 | G411 | A471 | C531 | U591 | G651 | G711 | G771 | G831 | C891 | C951 |
| A52 | U112 | A172 | G232 | U292 | A352 | A412 | A472 | A532 | A592 | U652 | G712 | C772 | U832 | A892 | G952 |
| G53 | U113 | A173 | A233 | U293 | C353 | C413 | G473 | C533 | U593 | G653 | G713 | U773 | A833 | C893 | G953 |
| A54 | U114 | U174 | U234 | A294 | A354 | C414 | G474 | U534 | U594 | A654 | U714 | G774 | G834 | U894 | G954 |
| G55 | C115 | G175 | U235 | G295 | G355 | A415 | C475 | G535 | C595 | A655 | A715 | G775 | C835 | U895 | U955 |
| A56 | G116 | U176 | C236 | U296 | U356 | U416 | G476 | G536 | U596 | A656 | U716 | G776 | G836 | A896 | G956 |
| C57 | G117 | C177 | C237 | G297 | C357 | C417 | A477 | G537 | G597 | U657 | C717 | G777 | C837 | C897 | C957 |
| G58 | A118 | G178 | C238 | G298 | U358 | C418 | A478 | A538 | U598 | U658 | A718 | G778 | C838 | U898 | G958 |
| U59 | C119 | C179 | C239 | A299 | G359 | U419 | A479 | G539 | A599 | U659 | C719 | G779 | U839 | A899 | A959 |
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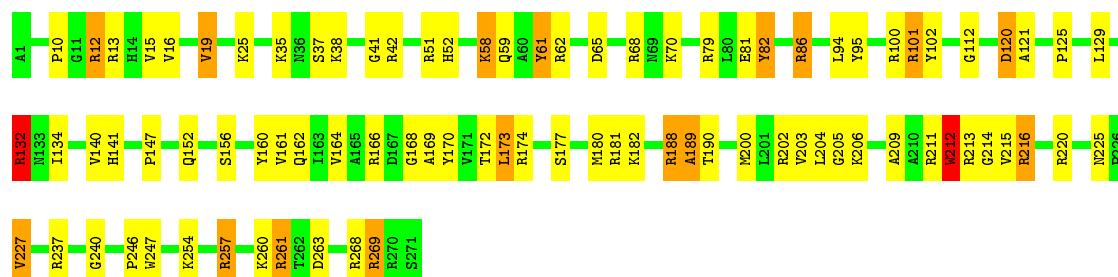
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| G1861 | A1801 | C1741 | G1681 | U1621 | C1561 | G1501 | G1441 | G1381 | A1321 | C1261 | U1201 | U1141 | U1081 | A1021 | C961  |
| G1862 | A1802 | U1742 | G1682 | G1622 | U1562 | A1502 | U1442 | G1382 | A1322 | A1262 | G1202 | A1142 | U1082 | G1022 | G962  |
| G1863 | A1803 | G1743 | G1683 | G1623 | U1563 | A1503 | U1443 | G1383 | C1323 | A1263 | U1203 | A1143 | U1083 | G1023 | U963  |
| G1864 | C1804 | A1744 | G1684 | U1624 | C1564 | A1504 | G1444 | A1384 | G1324 | A1264 | A1204 | A1144 | A1084 | G1024 | C964  |
| U1865 | A1805 | A1745 | C1685 | C1625 | U1565 | U1505 | G1445 | A1385 | U1325 | A1265 | G1205 | C1145 | A1085 | G1025 | C965  |
| A1866 | A1806 | A1746 | C1686 | A1626 | A1566 | U1506 | C1446 | C1386 | U1326 | G1266 | G1206 | C1146 | A1086 | G1026 | G966  |
| G1867 | G1807 | U1747 | G1687 | G1627 | G1567 | C1507 | C1447 | A1387 | A1327 | U1267 | G1207 | A1147 | G1087 | A1027 | U967  |
| C1868 | A1808 | C1748 | U1688 | G1628 | G1568 | A1508 | G1448 | G1388 | A1328 | A1268 | C1208 | U1148 | A1088 | A1028 | C968  |
| C1869 | A1809 | A1749 | A1689 | U1629 | A1569 | A1509 | G1449 | G1389 | U1329 | A1269 | U1209 | U1149 | A1089 | A1029 | G969  |
| A1870 | A1810 | U1750 | A1690 | A1630 | A1570 | G1510 | G1450 | U1390 | C1330 | G1270 | G1210 | A1150 | A1090 | C1030 | U970  |
| A1871 | G1811 | U1751 | G1691 | G1631 | A1571 | C1511 | C1451 | U1391 | G1331 | G1271 | C1211 | A1151 | G1091 | G1031 | G971  |
| A1872 | U1812 | G1752 | U1692 | A1632 | A1572 | C1512 | G1452 | A1392 | G1332 | U1272 | G1212 | C1152 | C1092 | A1032 | A972  |
| G1873 | G1813 | G1753 | U1693 | G1633 | G1573 | U1513 | A1463 | A1393 | G1333 | U1273 | A1213 | C1153 | G1093 | U1033 | A973  |
| C1874 | G1814 | A1754 | C1694 | A1634 | C1574 | G1514 | C1454 | U1394 | G1334 | A1274 | A1214 | G1154 | U1094 | G1034 | G974  |
| G1875 | A1815 | A1755 | G1695 | A1635 | C1575 | A1515 | G1455 | U1395 | A1335 | A1275 | G1215 | A1155 | A1095 | A975  | A975  |
| A1876 | C1816 | G1756 | G1696 | U1636 | U1576 | G1516 | G1456 | U1396 | A1336 | A1276 | G1216 | A1156 | A1096 | G1036 | G976  |
| A1877 | A1817 | U1757 | G1697 | A1637 | C1577 | A1517 | U1457 | U1397 | G1337 | G1277 | U1217 | G1157 | U1097 | G1037 | G977  |
| G1878 | U1818 | U1758 | A1698 | C1638 | U1578 | C1518 | U1458 | G1398 | G1338 | G1278 | G1218 | C1158 | A1098 | G1038 | G978  |
| C1879 | A1819 | A1759 | G1699 | C1639 | A1579 | G1519 | G1459 | C1399 | G1339 | G1279 | U1219 | U1159 | G1099 | A1039 | A979  |
| U1880 | U1820 | A1640 | A1700 | A1640 | A1580 | U1520 | U1460 | U1400 | U1340 | G1280 | G1220 | G1160 | C1100 | A1040 | A980  |
| C1881 | A1821 | C1760 | A1701 | A1641 | G1581 | G1521 | C1461 | G1401 | G1341 | G1281 | C1221 | C1161 | U1101 | G1041 | A981  |
| U1882 | C1822 | U1762 | G1702 | G1642 | C1582 | A1522 | C1462 | U1402 | A1342 | G1282 | U1222 | G1162 | C1102 | G1042 | C982  |
| U1883 | G1823 | G1763 | G1703 | G1643 | A1583 | U1523 | C1463 | A1403 | G1343 | G1283 | G1223 | G1163 | A1103 | C1043 | A983  |
| A1884 | G1824 | C1764 | C1704 | G1644 | U1584 | G1524 | G1464 | A1404 | U1344 | A1284 | U1224 | C1164 | C1104 | C1044 | A984  |
| A1885 | U1825 | U1765 | A1705 | G1645 | C1585 | A1525 | G1465 | U1405 | C1345 | A1285 | G1225 | A1165 | U1105 | G1045 | C985  |
| U1886 | G1826 | C1766 | C1706 | C1646 | A1586 | C1526 | U1466 | U1406 | G1346 | A1286 | A1226 | G1166 | G1106 | A1046 | C986  |
| G1887 | U1827 | U1767 | G1707 | U1647 | G1587 | G1527 | U1467 | G1407 | A1347 | A1287 | G1227 | C1167 | G1107 | G1047 | C987  |
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| G1893 | G1833 | A1773 | A1713 | G1653 | A1593 | C1533 | G1473 | A1413 | A1353 | C1293 | C1233 | C1173 | U1113 | C1053 | G993  |
| C1894 | U1834 | C1774 | U1714 | A1654 | U1594 | U1534 | G1474 | A1414 | A1354 | U1294 | U1234 | U1174 | C1114 | A1054 | C994  |
| G1895 | G1835 | U1775 | G1715 | A1655 | C1595 | A1535 | U1475 | U1415 | G1355 | C1295 | G1235 | A1175 | G1115 | G1055 | C995  |
| G1896 | C1836 | C1776 | U1716 | C1656 | A1596 | C1536 | U1476 | G1416 | G1356 | G1296 | G1236 | U1176 | G1116 | G1056 | A996  |
| G1897 | U1837 | U1777 | A1717 | U1657 | A1597 | G1537 | A1477 | C1417 | C1357 | C1297 | A1237 | G1177 | C1117 | A1057 | G997  |
| A1898 | C1838 | U1778 | G1718 | C1658 | A1598 | G1538 | G1478 | U1418 | G1358 | C1298 | G1238 | C1178 | C1118 | U1058 | C998  |
| A1899 | G1839 | U1779 | G1719 | G1659 | U1599 | U1539 | G1479 | A1419 | A1359 | G1299 | G1239 | G1179 | U1119 | G1059 | U999  |
| A1900 | G1840 | A1780 | U1720 | G1660 | C1600 | G1540 | C1480 | G1420 | G1360 | G1300 | U1240 | U1180 | G1120 | U1060 | A1000 |
| A1901 | U1841 | U1781 | G1721 | G1661 | G1601 | C1541 | U1481 | G1421 | G1361 | A1301 | A1241 | U1181 | C1121 | U1061 | A1001 |
| C1902 | G1842 | U1782 | U1722 | U1662 | U1602 | U1542 | G1482 | G1422 | C1362 | A1302 | U1242 | G1182 | G1122 | G1062 | G1002 |
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| A1904 | C1844 | A1784 | G1724 | A1664 | C1604 | A1544 | U1484 | G1424 | G1364 | A1304 | A1244 | U1184 | G1124 | G1064 | U1004 |
| G1905 | G1845 | A1785 | U1725 | A1665 | C1605 | A1545 | U1485 | G1425 | A1365 | C1305 | G1245 | G1185 | G1125 | U1065 | C1005 |
| G1906 | G1846 | U1786 | G1726 | G1666 | C1606 | G1546 | U1486 | G1426 | A1366 | A1246 | G1246 | G1186 | A1126 | U1066 | C1006 |
| G1907 | A1847 | A1787 | C1727 | G1667 | C1607 | C1547 | U1487 | A1427 | A1367 | A1307 | A1247 | G1187 | A1127 | A1067 | C1007 |
| A1908 | A1848 | C1788 | C1728 | A1668 | A1608 | A1548 | C1488 | C1428 | G1368 | U1308 | G1248 | U1188 | G1128 | G1068 | A1008 |
| C1909 | G1849 | A1789 | U1729 | A1669 | A1609 | A1549 | C1489 | G1429 | G1369 | G1309 | U1249 | A1189 | A1129 | A1069 | A1009 |
| G1910 | G1850 | C1790 | C1730 | C1670 | A1610 | C1550 | A1490 | G1430 | C1370 | G1310 | G1250 | G1190 | U1130 | A1070 | A1010 |
| U1911 | U1851 | A1791 | G1731 | U1671 | C1611 | A1551 | G1491 | A1431 | G1371 | G1311 | C1251 | G1191 | G1131 | G1071 | G1011 |
| A1912 | G1852 | G1792 | C1732 | A1672 | C1612 | A1552 | G1492 | G1432 | U1372 | G1312 | G1252 | G1192 | U1132 | C1072 | U1012 |
| A1913 | A1853 | C1793 | G1733 | G1673 | A1613 | A1553 | C1493 | A1433 | A1373 | U1313 | A1253 | G1193 | A1133 | A1073 | C1013 |
| C1914 | A1854 | A1794 | G1734 | A1674 | A1614 | U1554 | A1494 | A1434 | G1374 | C1314 | A1254 | A1194 | A1134 | G1074 | A1014 |
| U1915 | G1855 | C1795 | A1735 | C1675 | C1615 | G1555 | A1495 | A1435 | U1375 | C1315 | U1255 | G1195 | C1135 | C1075 | U1015 |
| A1916 | U1856 | U1796 | A1736 | A1676 | A1616 | C1556 | A1496 | G1436 | C1376 | U1316 | G1256 | C1196 | G1136 | C1076 | G1016 |
| U1917 | G1857 | U1797 | G1737 | A1677 | C1617 | C1557 | U1497 | C1437 | G1377 | G1317 | C1257 | G1197 | G1137 | A1077 | G1017 |
| A1918 | A1858 | A1798 | G1738 | A1678 | A1618 | C1558 | C1498 | U1438 | A1378 | U1318 | G1258 | U1198 | G1138 | U1078 | U1018 |
| A1919 | U1859 | G1799 | A1739 | A1679 | C1619 | C1559 | C1499 | U1439 | U1379 | G1319 | G1259 | U1199 | G1139 | C1079 | U1019 |
| C1920 | G1860 | C1800 | G1740 | U1680 | G1620 | G1560 | G1500 | U1440 | G1380 | C1320 | A1260 | C1200 | C1140 | A1080 | A1020 |





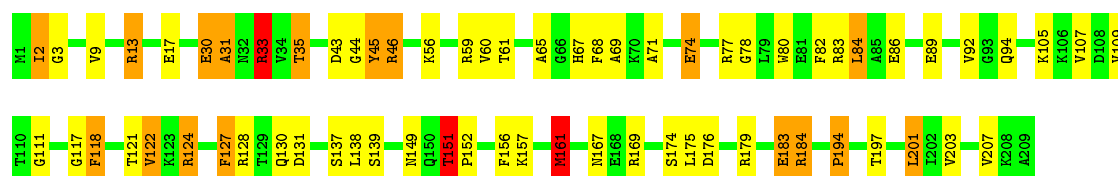
• Molecule 36: 50S RIBOSOMAL PROTEIN L2

Chain BC: 68% 25% 6% .



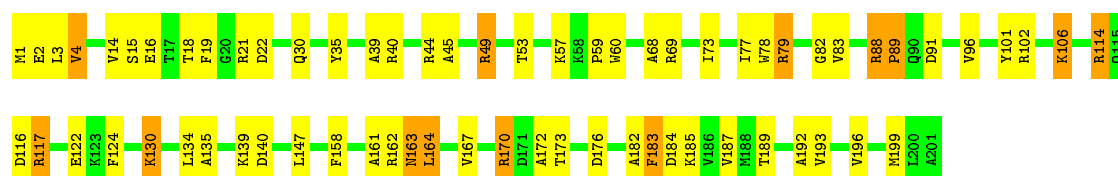
• Molecule 37: 50S RIBOSOMAL PROTEIN L3

Chain BD: 67% 23% 8% .



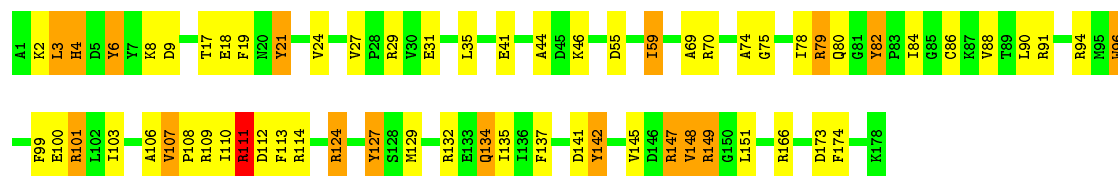
• Molecule 38: 50S RIBOSOMAL PROTEIN L4

Chain BE: 66% 27% 6% .



• Molecule 39: 50S RIBOSOMAL PROTEIN L5

Chain BF: 63% 26% 10% .



• Molecule 40: 50S RIBOSOMAL PROTEIN L6

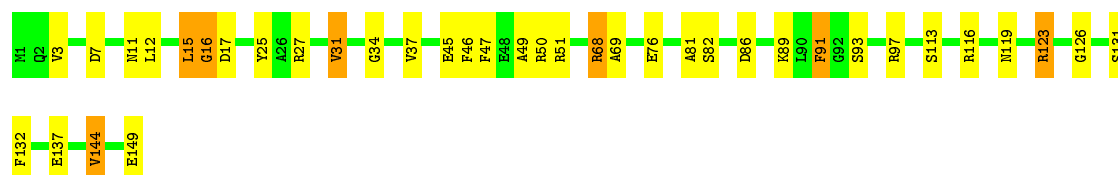
Chain BG: 72% 22% 6% .





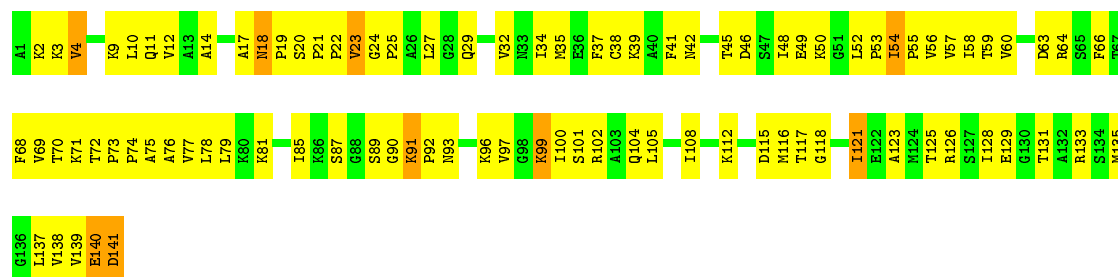
• Molecule 41: 50S RIBOSOMAL PROTEIN L9

Chain BH: 74% 21% 5%



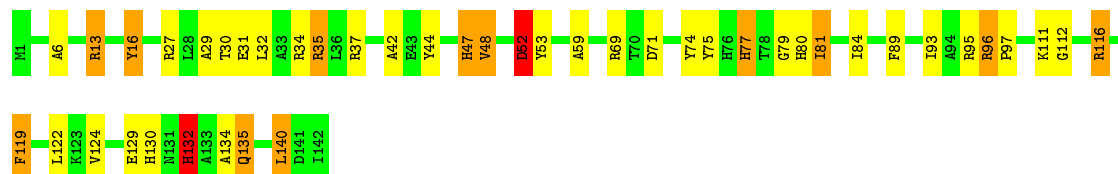
• Molecule 42: 50S RIBOSOMAL PROTEIN L11

Chain BI: 35% 59% 6%



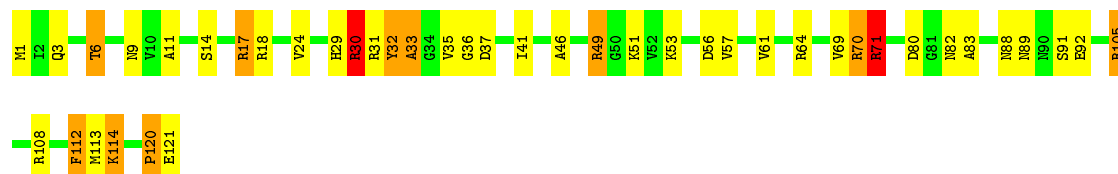
• Molecule 43: 50S RIBOSOMAL PROTEIN L13

Chain BJ: 69% 21% 8%



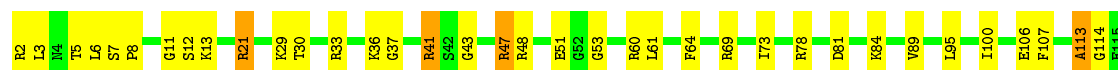
• Molecule 44: 50S RIBOSOMAL PROTEIN L14

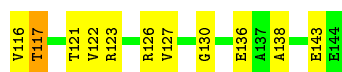
Chain BK: 64% 26% 8%



• Molecule 45: 50S RIBOSOMAL PROTEIN L15

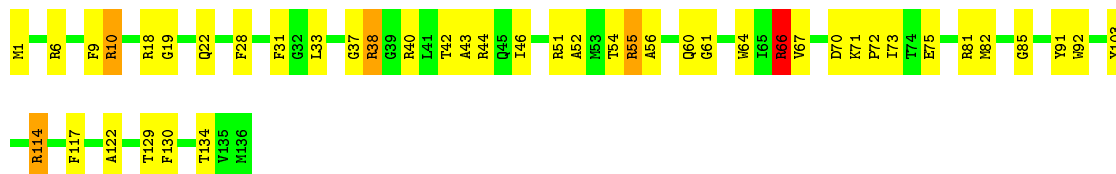
Chain BL: 67% 29%





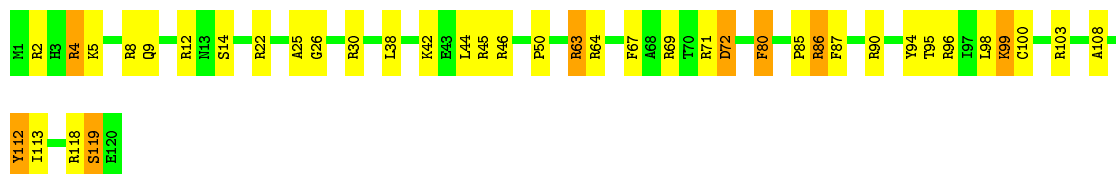
- Molecule 46: 50S RIBOSOMAL PROTEIN L16

Chain BM: 68% 29%



- Molecule 47: 50S RIBOSOMAL PROTEIN L17

Chain BN: 67% 27% 7%



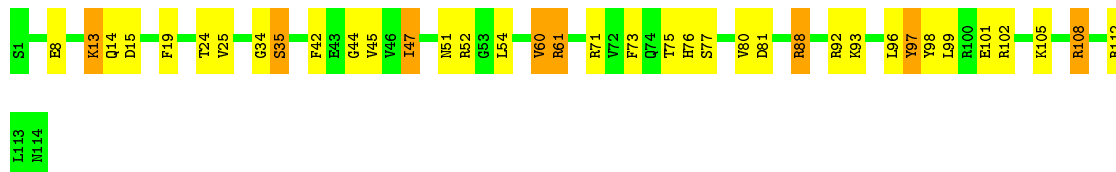
- Molecule 48: 50S RIBOSOMAL PROTEIN L18

Chain BO: 74% 22%



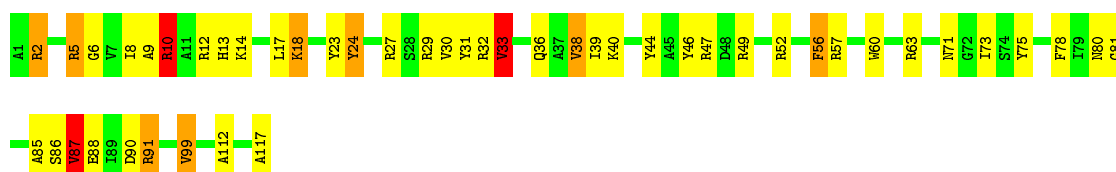
- Molecule 49: 50S RIBOSOMAL PROTEIN L19

Chain BP: 68% 25% 7%

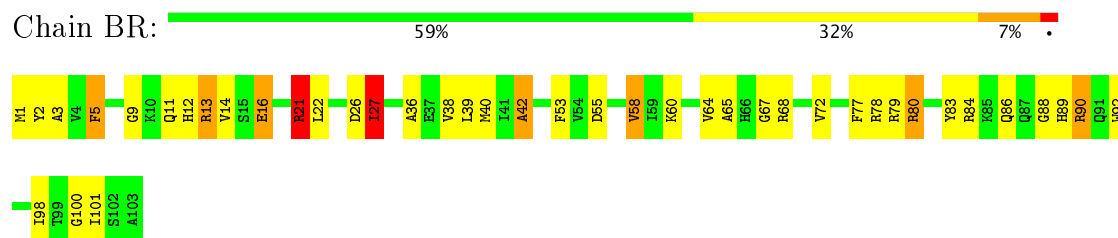


- Molecule 50: 50S RIBOSOMAL PROTEIN L20

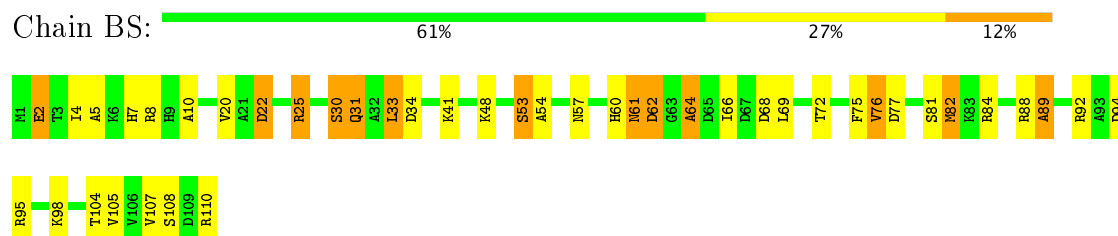
Chain BQ: 60% 31% 7%



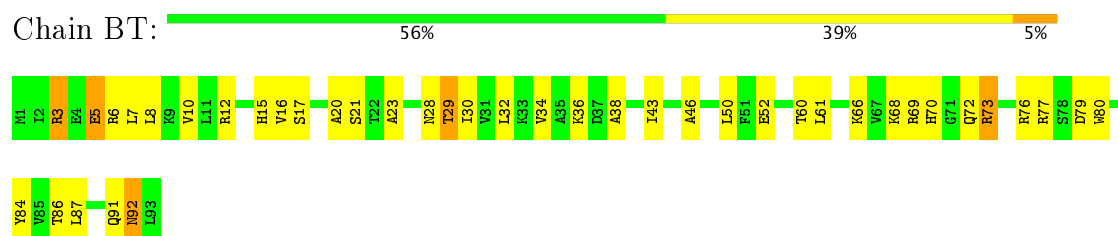
- Molecule 51: 50S RIBOSOMAL PROTEIN L21



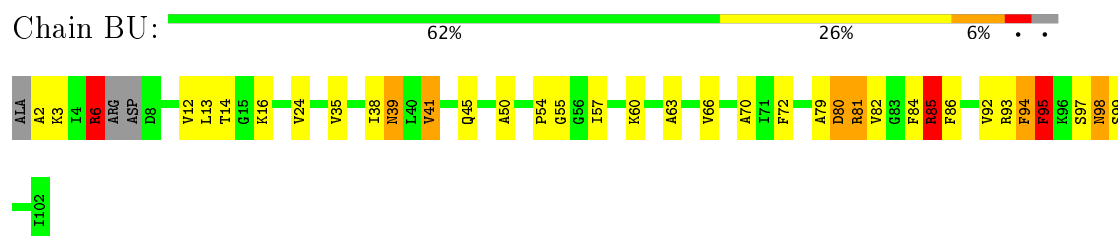
• Molecule 52: 50S RIBOSOMAL PROTEIN L22



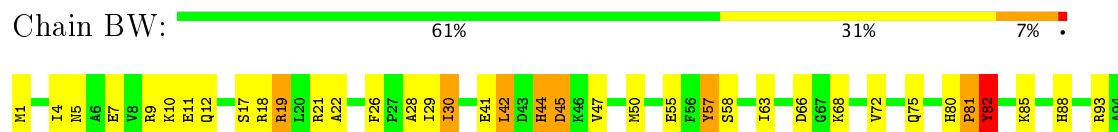
• Molecule 53: 50S RIBOSOMAL PROTEIN L23



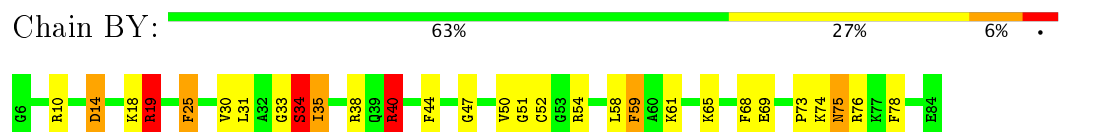
• Molecule 54: 50S RIBOSOMAL PROTEIN L24



• Molecule 55: 50S RIBOSOMAL PROTEIN L25



• Molecule 56: 50S RIBOSOMAL PROTEIN L27



## 4 Experimental information

| Property                             | Value                 | Source    |
|--------------------------------------|-----------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE       | Depositor |
| Imposed symmetry                     | POINT, C1             | Depositor |
| Number of particles used             | 263000                | Depositor |
| Resolution determination method      | Not provided          | Depositor |
| CTF correction method                | DEFOCUS GROUP VOLUMES | Depositor |
| Microscope                           | FEI TECNAI F30        | Depositor |
| Voltage (kV)                         | 300                   | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 20                    | Depositor |
| Minimum defocus (nm)                 | 1000                  | Depositor |
| Maximum defocus (nm)                 | 3000                  | Depositor |
| Magnification                        | 38900                 | Depositor |
| Image detector                       | KODAK SO-163 FILM     | Depositor |



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                    | Bond angles |                      |
|-----|-------|--------------|--------------------|-------------|----------------------|
|     |       | RMSZ         | $\# Z  > 2$        | RMSZ        | $\# Z  > 2$          |
| 1   | AA    | 3.37         | 4837/36762 (13.2%) | 3.72        | 8282/57350 (14.4%)   |
| 10  | AJ    | 1.78         | 11/796 (1.4%)      | 1.89        | 15/1077 (1.4%)       |
| 11  | AK    | 1.75         | 7/893 (0.8%)       | 1.96        | 18/1205 (1.5%)       |
| 12  | AL    | 1.85         | 13/969 (1.3%)      | 1.98        | 28/1300 (2.2%)       |
| 13  | AM    | 1.73         | 12/884 (1.4%)      | 2.02        | 28/1181 (2.4%)       |
| 14  | AN    | 1.80         | 6/785 (0.8%)       | 1.92        | 19/1043 (1.8%)       |
| 15  | AO    | 1.77         | 11/724 (1.5%)      | 1.90        | 24/966 (2.5%)        |
| 16  | AP    | 1.84         | 9/648 (1.4%)       | 2.16        | 26/870 (3.0%)        |
| 17  | AQ    | 1.73         | 4/657 (0.6%)       | 1.93        | 18/881 (2.0%)        |
| 18  | AR    | 1.74         | 6/462 (1.3%)       | 2.28        | 16/621 (2.6%)        |
| 19  | AS    | 1.78         | 8/652 (1.2%)       | 2.15        | 26/877 (3.0%)        |
| 2   | AB    | 1.71         | 14/1735 (0.8%)     | 2.05        | 53/2338 (2.3%)       |
| 20  | AT    | 1.66         | 4/671 (0.6%)       | 1.93        | 17/888 (1.9%)        |
| 21  | AU    | 1.82         | 6/430 (1.4%)       | 2.16        | 13/570 (2.3%)        |
| 22  | AV    | 2.38         | 76/1820 (4.2%)     | 2.84        | 256/2836 (9.0%)      |
| 23  | AX    | 1.81         | 4/264 (1.5%)       | 2.14        | 19/407 (4.7%)        |
| 24  | AZ    | 1.97         | 1/99 (1.0%)        | 1.94        | 5/137 (3.6%)         |
| 25  | B0    | 1.75         | 7/635 (1.1%)       | 2.27        | 19/848 (2.2%)        |
| 26  | B1    | 1.72         | 5/510 (1.0%)       | 1.94        | 14/677 (2.1%)        |
| 27  | B2    | 1.75         | 4/453 (0.9%)       | 1.86        | 10/605 (1.7%)        |
| 28  | B3    | 1.82         | 6/450 (1.3%)       | 2.19        | 16/599 (2.7%)        |
| 29  | B4    | 1.63         | 4/416 (1.0%)       | 2.02        | 13/554 (2.3%)        |
| 3   | AC    | 1.73         | 20/1651 (1.2%)     | 2.05        | 55/2225 (2.5%)       |
| 30  | B5    | 1.56         | 11/1748 (0.6%)     | 1.95        | 40/2355 (1.7%)       |
| 31  | B6    | 1.85         | 4/380 (1.1%)       | 2.31        | 17/498 (3.4%)        |
| 32  | B7    | 1.68         | 4/513 (0.8%)       | 2.03        | 12/676 (1.8%)        |
| 33  | B8    | 1.83         | 4/303 (1.3%)       | 2.01        | 7/397 (1.8%)         |
| 34  | BA    | 3.34         | 356/2753 (12.9%)   | 3.78        | 615/4288 (14.3%)     |
| 35  | BB    | 3.39         | 9308/69800 (13.3%) | 3.73        | 15832/108892 (14.5%) |
| 36  | BC    | 1.81         | 24/2121 (1.1%)     | 2.05        | 60/2852 (2.1%)       |
| 37  | BD    | 1.77         | 16/1586 (1.0%)     | 2.01        | 31/2134 (1.5%)       |
| 38  | BE    | 1.69         | 8/1571 (0.5%)      | 1.97        | 41/2113 (1.9%)       |

| Mol | Chain | Bond lengths |                     | Bond angles |                      |
|-----|-------|--------------|---------------------|-------------|----------------------|
|     |       | RMSZ         | # Z  >2             | RMSZ        | # Z  >2              |
| 39  | BF    | 1.73         | 14/1444 (1.0%)      | 2.17        | 40/1937 (2.1%)       |
| 4   | AD    | 1.80         | 24/1665 (1.4%)      | 2.05        | 48/2227 (2.2%)       |
| 40  | BG    | 1.76         | 13/1335 (1.0%)      | 2.04        | 28/1803 (1.6%)       |
| 41  | BH    | 1.74         | 11/1122 (1.0%)      | 2.05        | 35/1515 (2.3%)       |
| 42  | BI    | 0.62         | 2/1046 (0.2%)       | 0.56        | 1/1410 (0.1%)        |
| 43  | BJ    | 1.77         | 12/1152 (1.0%)      | 2.04        | 30/1551 (1.9%)       |
| 44  | BK    | 1.76         | 13/939 (1.4%)       | 1.99        | 23/1257 (1.8%)       |
| 45  | BL    | 1.78         | 10/1054 (0.9%)      | 1.94        | 28/1403 (2.0%)       |
| 46  | BM    | 1.83         | 9/1093 (0.8%)       | 2.07        | 30/1460 (2.1%)       |
| 47  | BN    | 1.76         | 12/973 (1.2%)       | 2.22        | 32/1301 (2.5%)       |
| 48  | BO    | 1.79         | 15/902 (1.7%)       | 2.02        | 24/1209 (2.0%)       |
| 49  | BP    | 1.68         | 5/929 (0.5%)        | 2.03        | 20/1242 (1.6%)       |
| 5   | AE    | 1.73         | 17/1118 (1.5%)      | 1.97        | 27/1504 (1.8%)       |
| 50  | BQ    | 1.89         | 15/960 (1.6%)       | 2.11        | 29/1278 (2.3%)       |
| 51  | BR    | 1.80         | 11/829 (1.3%)       | 2.03        | 23/1107 (2.1%)       |
| 52  | BS    | 1.71         | 7/864 (0.8%)        | 2.16        | 34/1156 (2.9%)       |
| 53  | BT    | 1.69         | 5/744 (0.7%)        | 1.99        | 18/994 (1.8%)        |
| 54  | BU    | 1.73         | 3/761 (0.4%)        | 2.02        | 25/1013 (2.5%)       |
| 55  | BW    | 1.79         | 13/766 (1.7%)       | 2.05        | 18/1025 (1.8%)       |
| 56  | BY    | 1.73         | 3/603 (0.5%)        | 2.11        | 23/797 (2.9%)        |
| 6   | AF    | 1.77         | 7/835 (0.8%)        | 1.96        | 17/1128 (1.5%)       |
| 7   | AG    | 1.82         | 18/1187 (1.5%)      | 2.01        | 40/1591 (2.5%)       |
| 8   | AH    | 1.79         | 10/989 (1.0%)       | 2.07        | 29/1326 (2.2%)       |
| 9   | AI    | 1.97         | 21/1034 (2.0%)      | 2.09        | 33/1375 (2.4%)       |
| All | All   | 2.98         | 15080/158485 (9.5%) | 3.34        | 26300/236869 (11.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | AA    | 0                   | 740                 |
| 10  | AJ    | 0                   | 6                   |
| 11  | AK    | 0                   | 3                   |
| 12  | AL    | 0                   | 5                   |
| 13  | AM    | 0                   | 9                   |
| 14  | AN    | 0                   | 3                   |
| 15  | AO    | 0                   | 6                   |
| 16  | AP    | 0                   | 4                   |
| 17  | AQ    | 0                   | 1                   |
| 18  | AR    | 0                   | 5                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 19  | AS    | 0                   | 4                   |
| 2   | AB    | 0                   | 5                   |
| 20  | AT    | 0                   | 3                   |
| 22  | AV    | 0                   | 13                  |
| 23  | AX    | 0                   | 4                   |
| 25  | B0    | 0                   | 4                   |
| 26  | B1    | 0                   | 1                   |
| 28  | B3    | 0                   | 2                   |
| 29  | B4    | 0                   | 3                   |
| 3   | AC    | 0                   | 7                   |
| 30  | B5    | 0                   | 6                   |
| 31  | B6    | 0                   | 3                   |
| 32  | B7    | 0                   | 1                   |
| 34  | BA    | 0                   | 50                  |
| 35  | BB    | 0                   | 1343                |
| 36  | BC    | 0                   | 8                   |
| 37  | BD    | 0                   | 6                   |
| 38  | BE    | 0                   | 5                   |
| 39  | BF    | 0                   | 10                  |
| 4   | AD    | 0                   | 11                  |
| 40  | BG    | 0                   | 3                   |
| 41  | BH    | 0                   | 1                   |
| 43  | BJ    | 0                   | 4                   |
| 44  | BK    | 0                   | 5                   |
| 45  | BL    | 0                   | 1                   |
| 46  | BM    | 0                   | 3                   |
| 47  | BN    | 0                   | 5                   |
| 48  | BO    | 0                   | 2                   |
| 49  | BP    | 0                   | 5                   |
| 5   | AE    | 0                   | 5                   |
| 50  | BQ    | 0                   | 5                   |
| 51  | BR    | 0                   | 3                   |
| 52  | BS    | 0                   | 1                   |
| 53  | BT    | 0                   | 1                   |
| 54  | BU    | 0                   | 2                   |
| 55  | BW    | 0                   | 4                   |
| 56  | BY    | 0                   | 5                   |
| 6   | AF    | 0                   | 3                   |
| 7   | AG    | 0                   | 3                   |
| 8   | AH    | 0                   | 3                   |
| 9   | AI    | 0                   | 7                   |
| All | All   | 0                   | 2342                |

All (15080) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 35  | BB    | 1403 | A    | N9-C4 | 21.34  | 1.50        | 1.37     |
| 35  | BB    | 1301 | A    | N7-C5 | -20.38 | 1.27        | 1.39     |
| 1   | AA    | 930  | C    | N1-C6 | 19.80  | 1.49        | 1.37     |
| 1   | AA    | 816  | A    | N7-C5 | -19.29 | 1.27        | 1.39     |
| 35  | BB    | 1821 | A    | N9-C4 | 19.18  | 1.49        | 1.37     |
| 35  | BB    | 2648 | G    | N7-C5 | -18.24 | 1.28        | 1.39     |
| 1   | AA    | 783  | C    | N1-C6 | 17.63  | 1.47        | 1.37     |
| 1   | AA    | 1444 | U    | C2-N3 | 17.34  | 1.49        | 1.37     |
| 35  | BB    | 2831 | G    | N7-C5 | -17.29 | 1.28        | 1.39     |
| 35  | BB    | 1622 | G    | C2-N3 | 17.20  | 1.46        | 1.32     |
| 35  | BB    | 2758 | A    | C8-N7 | -17.19 | 1.19        | 1.31     |
| 35  | BB    | 1435 | G    | N7-C5 | -17.19 | 1.28        | 1.39     |
| 35  | BB    | 36   | G    | N7-C5 | -17.16 | 1.28        | 1.39     |
| 35  | BB    | 457  | A    | N7-C5 | -16.97 | 1.29        | 1.39     |
| 35  | BB    | 505  | A    | N7-C5 | -16.97 | 1.29        | 1.39     |
| 35  | BB    | 1860 | G    | C6-N1 | 16.96  | 1.51        | 1.39     |
| 35  | BB    | 869  | G    | C6-N1 | 16.63  | 1.51        | 1.39     |
| 35  | BB    | 1404 | C    | N1-C6 | -16.52 | 1.27        | 1.37     |
| 1   | AA    | 91   | U    | N3-C4 | 16.48  | 1.53        | 1.38     |
| 35  | BB    | 693  | A    | N7-C5 | -16.41 | 1.29        | 1.39     |
| 35  | BB    | 1721 | G    | N7-C5 | -16.38 | 1.29        | 1.39     |
| 35  | BB    | 1422 | G    | N7-C5 | -16.15 | 1.29        | 1.39     |
| 35  | BB    | 470  | A    | C8-N7 | -16.11 | 1.20        | 1.31     |
| 35  | BB    | 195  | A    | N7-C5 | -16.02 | 1.29        | 1.39     |
| 1   | AA    | 713  | G    | C6-N1 | 15.79  | 1.50        | 1.39     |
| 35  | BB    | 2121 | G    | C6-N1 | 15.74  | 1.50        | 1.39     |
| 35  | BB    | 477  | A    | N3-C4 | -15.66 | 1.25        | 1.34     |
| 35  | BB    | 2048 | G    | C2-N3 | 15.65  | 1.45        | 1.32     |
| 1   | AA    | 979  | C    | N1-C6 | 15.57  | 1.46        | 1.37     |
| 1   | AA    | 572  | A    | N7-C5 | -15.55 | 1.29        | 1.39     |
| 22  | AV    | 39   | G    | N9-C4 | 15.53  | 1.50        | 1.38     |
| 35  | BB    | 1055 | G    | C2-N3 | 15.50  | 1.45        | 1.32     |
| 35  | BB    | 2352 | A    | N7-C5 | -15.50 | 1.29        | 1.39     |
| 35  | BB    | 269  | C    | N1-C6 | -15.41 | 1.27        | 1.37     |
| 35  | BB    | 668  | A    | N7-C5 | 15.39  | 1.48        | 1.39     |
| 1   | AA    | 1218 | C    | N1-C6 | 15.38  | 1.46        | 1.37     |
| 1   | AA    | 888  | G    | N7-C5 | -15.38 | 1.30        | 1.39     |
| 35  | BB    | 2598 | A    | N7-C5 | -15.37 | 1.30        | 1.39     |
| 1   | AA    | 195  | A    | N7-C5 | -15.33 | 1.30        | 1.39     |
| 1   | AA    | 1375 | A    | N9-C4 | 15.33  | 1.47        | 1.37     |
| 35  | BB    | 2509 | G    | C8-N7 | -15.27 | 1.21        | 1.30     |
| 35  | BB    | 1022 | G    | N7-C5 | -15.26 | 1.30        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1   | AA    | 302  | G    | C2-N3 | 15.22  | 1.45        | 1.32     |
| 35  | BB    | 2603 | G    | N7-C5 | -15.21 | 1.30        | 1.39     |
| 35  | BB    | 1828 | G    | N7-C5 | -15.21 | 1.30        | 1.39     |
| 1   | AA    | 421  | U    | C2-N3 | 15.21  | 1.48        | 1.37     |
| 35  | BB    | 570  | G    | N7-C5 | -15.14 | 1.30        | 1.39     |
| 35  | BB    | 294  | A    | N9-C4 | -15.12 | 1.28        | 1.37     |
| 35  | BB    | 238  | C    | N1-C6 | 15.11  | 1.46        | 1.37     |
| 1   | AA    | 1021 | A    | N3-C4 | -15.07 | 1.25        | 1.34     |
| 35  | BB    | 825  | A    | N7-C5 | -15.06 | 1.30        | 1.39     |
| 1   | AA    | 1266 | G    | N7-C5 | -15.04 | 1.30        | 1.39     |
| 35  | BB    | 556  | A    | N7-C5 | -14.98 | 1.30        | 1.39     |
| 35  | BB    | 359  | G    | N7-C5 | -14.92 | 1.30        | 1.39     |
| 35  | BB    | 526  | A    | C6-N6 | 14.92  | 1.45        | 1.33     |
| 1   | AA    | 686  | U    | C2-N3 | 14.91  | 1.48        | 1.37     |
| 35  | BB    | 1532 | A    | N7-C5 | -14.90 | 1.30        | 1.39     |
| 35  | BB    | 49   | A    | N7-C5 | -14.86 | 1.30        | 1.39     |
| 35  | BB    | 411  | G    | N7-C5 | -14.81 | 1.30        | 1.39     |
| 1   | AA    | 1093 | A    | N7-C5 | -14.79 | 1.30        | 1.39     |
| 35  | BB    | 1280 | G    | N7-C5 | -14.77 | 1.30        | 1.39     |
| 35  | BB    | 700  | G    | C6-N1 | 14.73  | 1.49        | 1.39     |
| 1   | AA    | 904  | U    | C2-N3 | 14.72  | 1.48        | 1.37     |
| 35  | BB    | 740  | C    | N1-C6 | 14.64  | 1.46        | 1.37     |
| 1   | AA    | 1455 | G    | N1-C2 | 14.64  | 1.49        | 1.37     |
| 35  | BB    | 669  | G    | N7-C5 | -14.64 | 1.30        | 1.39     |
| 35  | BB    | 1900 | A    | C6-N6 | 14.61  | 1.45        | 1.33     |
| 35  | BB    | 1900 | A    | N7-C5 | -14.58 | 1.30        | 1.39     |
| 35  | BB    | 1775 | U    | C2-N3 | 14.57  | 1.48        | 1.37     |
| 35  | BB    | 425  | G    | C5-C4 | -14.55 | 1.28        | 1.38     |
| 35  | BB    | 1993 | U    | C2-N3 | 14.55  | 1.48        | 1.37     |
| 35  | BB    | 2405 | G    | N7-C5 | -14.54 | 1.30        | 1.39     |
| 1   | AA    | 1502 | A    | N7-C5 | -14.51 | 1.30        | 1.39     |
| 35  | BB    | 1001 | A    | N7-C5 | -14.51 | 1.30        | 1.39     |
| 1   | AA    | 545  | C    | N3-C4 | 14.49  | 1.44        | 1.33     |
| 35  | BB    | 2298 | A    | N7-C5 | -14.47 | 1.30        | 1.39     |
| 35  | BB    | 81   | G    | N7-C5 | -14.46 | 1.30        | 1.39     |
| 1   | AA    | 602  | A    | N7-C5 | -14.42 | 1.30        | 1.39     |
| 1   | AA    | 1468 | A    | N7-C5 | -14.41 | 1.30        | 1.39     |
| 35  | BB    | 2070 | A    | C6-N1 | 14.40  | 1.45        | 1.35     |
| 35  | BB    | 1677 | A    | N7-C5 | -14.39 | 1.30        | 1.39     |
| 35  | BB    | 1690 | A    | N7-C5 | -14.34 | 1.30        | 1.39     |
| 35  | BB    | 2250 | G    | N7-C5 | -14.29 | 1.30        | 1.39     |
| 35  | BB    | 2477 | U    | C4-C5 | 14.21  | 1.56        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 34  | BA    | 61   | G    | C8-N7 | 14.19  | 1.39        | 1.30     |
| 35  | BB    | 2837 | A    | N3-C4 | 14.14  | 1.43        | 1.34     |
| 35  | BB    | 167  | A    | N7-C5 | -14.13 | 1.30        | 1.39     |
| 35  | BB    | 1420 | A    | N7-C5 | -14.11 | 1.30        | 1.39     |
| 35  | BB    | 1240 | U    | C2-N3 | 14.10  | 1.47        | 1.37     |
| 1   | AA    | 1287 | A    | N7-C5 | -14.09 | 1.30        | 1.39     |
| 35  | BB    | 2655 | G    | C2-N3 | 14.08  | 1.44        | 1.32     |
| 35  | BB    | 472  | A    | C6-N6 | 14.06  | 1.45        | 1.33     |
| 35  | BB    | 88   | G    | N7-C5 | -14.04 | 1.30        | 1.39     |
| 1   | AA    | 1455 | G    | N7-C5 | -14.00 | 1.30        | 1.39     |
| 35  | BB    | 77   | G    | C5-C4 | 14.00  | 1.48        | 1.38     |
| 35  | BB    | 1202 | G    | N1-C2 | 13.99  | 1.49        | 1.37     |
| 35  | BB    | 2198 | A    | N9-C4 | 13.99  | 1.46        | 1.37     |
| 1   | AA    | 953  | G    | C2-N3 | 13.99  | 1.44        | 1.32     |
| 35  | BB    | 1302 | A    | N7-C5 | -13.98 | 1.30        | 1.39     |
| 35  | BB    | 603  | A    | N9-C4 | -13.97 | 1.29        | 1.37     |
| 35  | BB    | 761  | A    | C6-N6 | 13.95  | 1.45        | 1.33     |
| 1   | AA    | 1507 | A    | C6-N6 | 13.93  | 1.45        | 1.33     |
| 1   | AA    | 416  | G    | N9-C8 | -13.90 | 1.28        | 1.37     |
| 35  | BB    | 1579 | A    | N7-C5 | -13.89 | 1.30        | 1.39     |
| 35  | BB    | 834  | G    | C6-N1 | 13.87  | 1.49        | 1.39     |
| 35  | BB    | 1603 | A    | N7-C5 | -13.87 | 1.30        | 1.39     |
| 35  | BB    | 1528 | A    | C6-N6 | 13.86  | 1.45        | 1.33     |
| 1   | AA    | 1304 | G    | N3-C4 | 13.86  | 1.45        | 1.35     |
| 35  | BB    | 1410 | G    | N3-C4 | -13.85 | 1.25        | 1.35     |
| 35  | BB    | 2561 | U    | C2-N3 | 13.80  | 1.47        | 1.37     |
| 35  | BB    | 2541 | A    | N7-C5 | -13.80 | 1.30        | 1.39     |
| 35  | BB    | 2101 | A    | N7-C5 | -13.78 | 1.30        | 1.39     |
| 35  | BB    | 2169 | A    | N9-C4 | 13.77  | 1.46        | 1.37     |
| 35  | BB    | 2814 | A    | C6-N6 | 13.76  | 1.45        | 1.33     |
| 35  | BB    | 502  | A    | N7-C5 | -13.76 | 1.30        | 1.39     |
| 1   | AA    | 275  | G    | P-O5' | -13.75 | 1.46        | 1.59     |
| 35  | BB    | 2190 | G    | C8-N7 | -13.75 | 1.22        | 1.30     |
| 1   | AA    | 695  | A    | C6-N1 | 13.75  | 1.45        | 1.35     |
| 1   | AA    | 1204 | A    | N9-C4 | -13.73 | 1.29        | 1.37     |
| 35  | BB    | 2495 | G    | C5-C4 | 13.73  | 1.48        | 1.38     |
| 35  | BB    | 1455 | G    | N7-C5 | -13.73 | 1.31        | 1.39     |
| 35  | BB    | 1989 | G    | N7-C5 | -13.71 | 1.31        | 1.39     |
| 1   | AA    | 812  | G    | C6-N1 | 13.65  | 1.49        | 1.39     |
| 35  | BB    | 2226 | C    | N1-C6 | 13.64  | 1.45        | 1.37     |
| 1   | AA    | 557  | G    | N7-C5 | 13.62  | 1.47        | 1.39     |
| 35  | BB    | 833  | A    | N7-C5 | -13.61 | 1.31        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1   | AA    | 308  | C    | N3-C4 | 13.60  | 1.43        | 1.33     |
| 35  | BB    | 849  | A    | N3-C4 | -13.60 | 1.26        | 1.34     |
| 1   | AA    | 845  | A    | C6-N6 | 13.58  | 1.44        | 1.33     |
| 35  | BB    | 1303 | G    | C6-N1 | 13.58  | 1.49        | 1.39     |
| 35  | BB    | 1017 | G    | N7-C5 | -13.58 | 1.31        | 1.39     |
| 1   | AA    | 663  | A    | N7-C5 | -13.57 | 1.31        | 1.39     |
| 35  | BB    | 1001 | A    | N3-C4 | -13.56 | 1.26        | 1.34     |
| 35  | BB    | 1010 | A    | N7-C5 | -13.55 | 1.31        | 1.39     |
| 1   | AA    | 259  | G    | C8-N7 | -13.54 | 1.22        | 1.30     |
| 35  | BB    | 1254 | A    | N7-C5 | -13.53 | 1.31        | 1.39     |
| 35  | BB    | 802  | A    | N7-C5 | -13.51 | 1.31        | 1.39     |
| 35  | BB    | 1370 | C    | N1-C6 | -13.50 | 1.29        | 1.37     |
| 1   | AA    | 617  | G    | C2-N3 | 13.49  | 1.43        | 1.32     |
| 1   | AA    | 693  | G    | N7-C5 | -13.49 | 1.31        | 1.39     |
| 35  | BB    | 1416 | G    | N9-C4 | 13.47  | 1.48        | 1.38     |
| 35  | BB    | 666  | A    | C6-N6 | 13.47  | 1.44        | 1.33     |
| 35  | BB    | 442  | G    | C6-N1 | 13.43  | 1.49        | 1.39     |
| 35  | BB    | 1919 | A    | N7-C5 | -13.43 | 1.31        | 1.39     |
| 35  | BB    | 2270 | A    | C6-N1 | 13.42  | 1.45        | 1.35     |
| 35  | BB    | 701  | G    | C6-N1 | 13.41  | 1.49        | 1.39     |
| 35  | BB    | 845  | A    | C6-N1 | 13.40  | 1.45        | 1.35     |
| 35  | BB    | 33   | C    | N1-C6 | 13.40  | 1.45        | 1.37     |
| 35  | BB    | 1236 | G    | N7-C5 | -13.39 | 1.31        | 1.39     |
| 1   | AA    | 794  | A    | N7-C5 | -13.38 | 1.31        | 1.39     |
| 35  | BB    | 1899 | A    | N7-C5 | -13.38 | 1.31        | 1.39     |
| 35  | BB    | 690  | G    | N7-C5 | -13.37 | 1.31        | 1.39     |
| 35  | BB    | 83   | A    | N9-C4 | -13.37 | 1.29        | 1.37     |
| 35  | BB    | 54   | G    | C2-N3 | 13.35  | 1.43        | 1.32     |
| 35  | BB    | 2812 | G    | C2-N3 | 13.35  | 1.43        | 1.32     |
| 35  | BB    | 227  | A    | C6-N6 | 13.34  | 1.44        | 1.33     |
| 35  | BB    | 2089 | C    | N1-C6 | -13.33 | 1.29        | 1.37     |
| 1   | AA    | 1072 | G    | N7-C5 | -13.30 | 1.31        | 1.39     |
| 35  | BB    | 1359 | A    | N7-C5 | -13.30 | 1.31        | 1.39     |
| 22  | AV    | 69   | G    | C6-N1 | 13.27  | 1.48        | 1.39     |
| 35  | BB    | 2024 | G    | C2-N3 | 13.24  | 1.43        | 1.32     |
| 35  | BB    | 219  | A    | N7-C5 | -13.23 | 1.31        | 1.39     |
| 35  | BB    | 646  | U    | C2-N3 | 13.23  | 1.47        | 1.37     |
| 35  | BB    | 1659 | G    | P-O5' | -13.23 | 1.46        | 1.59     |
| 35  | BB    | 1696 | G    | N7-C5 | -13.21 | 1.31        | 1.39     |
| 35  | BB    | 497  | A    | N9-C4 | -13.20 | 1.29        | 1.37     |
| 35  | BB    | 2040 | G    | C2-N3 | 13.20  | 1.43        | 1.32     |
| 1   | AA    | 224  | U    | C2-N3 | 13.18  | 1.47        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 35  | BB    | 1926 | U    | C2-N3 | 13.18  | 1.47        | 1.37     |
| 1   | AA    | 546  | A    | N7-C5 | -13.16 | 1.31        | 1.39     |
| 34  | BA    | 58   | A    | N3-C4 | -13.16 | 1.26        | 1.34     |
| 1   | AA    | 845  | A    | N9-C4 | 13.14  | 1.45        | 1.37     |
| 1   | AA    | 83   | C    | C4-N4 | 13.13  | 1.45        | 1.33     |
| 1   | AA    | 1213 | A    | C6-N6 | 13.13  | 1.44        | 1.33     |
| 35  | BB    | 146  | A    | N9-C4 | 13.11  | 1.45        | 1.37     |
| 1   | AA    | 1290 | G    | N7-C5 | -13.11 | 1.31        | 1.39     |
| 35  | BB    | 2870 | C    | N3-C4 | 13.09  | 1.43        | 1.33     |
| 35  | BB    | 733  | G    | N7-C5 | -13.09 | 1.31        | 1.39     |
| 35  | BB    | 186  | G    | C8-N7 | -13.08 | 1.23        | 1.30     |
| 35  | BB    | 2071 | A    | N7-C5 | -13.07 | 1.31        | 1.39     |
| 35  | BB    | 1021 | A    | N3-C4 | -13.06 | 1.27        | 1.34     |
| 35  | BB    | 467  | G    | N7-C5 | -13.04 | 1.31        | 1.39     |
| 35  | BB    | 958  | U    | C2-N3 | 13.03  | 1.46        | 1.37     |
| 35  | BB    | 1750 | G    | C5-C4 | -13.03 | 1.29        | 1.38     |
| 1   | AA    | 807  | A    | N7-C5 | -13.02 | 1.31        | 1.39     |
| 1   | AA    | 1324 | A    | C6-N1 | 13.00  | 1.44        | 1.35     |
| 1   | AA    | 144  | G    | C8-N7 | 12.98  | 1.38        | 1.30     |
| 35  | BB    | 1211 | C    | N3-C4 | 12.97  | 1.43        | 1.33     |
| 34  | BA    | 59   | A    | N7-C5 | -12.96 | 1.31        | 1.39     |
| 22  | AV    | 5    | A    | C6-N1 | 12.96  | 1.44        | 1.35     |
| 1   | AA    | 295  | C    | N1-C6 | 12.96  | 1.45        | 1.37     |
| 35  | BB    | 94   | A    | C8-N7 | -12.95 | 1.22        | 1.31     |
| 1   | AA    | 269  | C    | N1-C6 | 12.94  | 1.45        | 1.37     |
| 34  | BA    | 30   | C    | N3-C4 | 12.94  | 1.43        | 1.33     |
| 35  | BB    | 1530 | G    | N7-C5 | -12.94 | 1.31        | 1.39     |
| 35  | BB    | 2662 | A    | C8-N7 | -12.93 | 1.22        | 1.31     |
| 35  | BB    | 2739 | U    | N3-C4 | 12.92  | 1.50        | 1.38     |
| 35  | BB    | 452  | G    | N7-C5 | -12.91 | 1.31        | 1.39     |
| 35  | BB    | 1153 | C    | N1-C6 | 12.90  | 1.44        | 1.37     |
| 1   | AA    | 592  | G    | C2-N3 | 12.90  | 1.43        | 1.32     |
| 1   | AA    | 1367 | C    | N3-C4 | 12.89  | 1.43        | 1.33     |
| 35  | BB    | 2717 | C    | N1-C6 | 12.88  | 1.44        | 1.37     |
| 35  | BB    | 186  | G    | C6-N1 | 12.87  | 1.48        | 1.39     |
| 1   | AA    | 595  | A    | C6-N6 | 12.87  | 1.44        | 1.33     |
| 35  | BB    | 1288 | G    | N7-C5 | -12.86 | 1.31        | 1.39     |
| 35  | BB    | 199  | A    | N3-C4 | -12.85 | 1.27        | 1.34     |
| 35  | BB    | 2444 | G    | C2-N3 | 12.85  | 1.43        | 1.32     |
| 35  | BB    | 482  | A    | N3-C4 | -12.84 | 1.27        | 1.34     |
| 35  | BB    | 980  | A    | C6-N1 | 12.83  | 1.44        | 1.35     |
| 1   | AA    | 983  | A    | N7-C5 | -12.83 | 1.31        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 35  | BB    | 1935 | G    | C5-C4   | 12.83  | 1.47        | 1.38     |
| 35  | BB    | 1540 | G    | N1-C2   | 12.81  | 1.48        | 1.37     |
| 35  | BB    | 1855 | U    | C2-N3   | 12.81  | 1.46        | 1.37     |
| 35  | BB    | 2663 | G    | N9-C8   | 12.81  | 1.46        | 1.37     |
| 1   | AA    | 325  | A    | C6-N1   | 12.79  | 1.44        | 1.35     |
| 35  | BB    | 1592 | C    | C2-N3   | 12.79  | 1.46        | 1.35     |
| 1   | AA    | 412  | A    | N7-C5   | -12.76 | 1.31        | 1.39     |
| 1   | AA    | 1226 | C    | N3-C4   | 12.76  | 1.42        | 1.33     |
| 1   | AA    | 541  | G    | C6-N1   | 12.75  | 1.48        | 1.39     |
| 35  | BB    | 2225 | A    | N7-C5   | -12.75 | 1.31        | 1.39     |
| 1   | AA    | 475  | C    | N3-C4   | 12.72  | 1.42        | 1.33     |
| 35  | BB    | 2134 | A    | N9-C4   | 12.72  | 1.45        | 1.37     |
| 35  | BB    | 74   | A    | N7-C5   | -12.71 | 1.31        | 1.39     |
| 35  | BB    | 1950 | G    | C6-N1   | 12.70  | 1.48        | 1.39     |
| 35  | BB    | 2802 | G    | C6-N1   | 12.69  | 1.48        | 1.39     |
| 35  | BB    | 1653 | G    | C6-N1   | 12.67  | 1.48        | 1.39     |
| 35  | BB    | 70   | G    | N7-C5   | -12.66 | 1.31        | 1.39     |
| 35  | BB    | 1707 | G    | C2-N3   | 12.62  | 1.42        | 1.32     |
| 35  | BB    | 1703 | G    | C6-N1   | 12.62  | 1.48        | 1.39     |
| 1   | AA    | 31   | G    | N3-C4   | -12.61 | 1.26        | 1.35     |
| 35  | BB    | 1937 | A    | N7-C5   | 12.61  | 1.46        | 1.39     |
| 35  | BB    | 853  | C    | C2'-C1' | -12.61 | 1.39        | 1.53     |
| 1   | AA    | 1005 | A    | N7-C5   | -12.58 | 1.31        | 1.39     |
| 35  | BB    | 751  | A    | N7-C5   | -12.58 | 1.31        | 1.39     |
| 35  | BB    | 2885 | G    | N1-C2   | 12.57  | 1.47        | 1.37     |
| 35  | BB    | 504  | A    | N3-C4   | -12.56 | 1.27        | 1.34     |
| 35  | BB    | 701  | G    | N7-C5   | -12.56 | 1.31        | 1.39     |
| 1   | AA    | 101  | A    | N7-C5   | 12.56  | 1.46        | 1.39     |
| 1   | AA    | 531  | U    | C2-N3   | 12.55  | 1.46        | 1.37     |
| 1   | AA    | 971  | G    | C2-N3   | 12.55  | 1.42        | 1.32     |
| 35  | BB    | 772  | C    | P-O5'   | -12.54 | 1.47        | 1.59     |
| 35  | BB    | 1565 | C    | P-O5'   | -12.54 | 1.47        | 1.59     |
| 1   | AA    | 1036 | A    | C6-N6   | 12.53  | 1.44        | 1.33     |
| 35  | BB    | 1762 | A    | N7-C5   | -12.52 | 1.31        | 1.39     |
| 35  | BB    | 1725 | U    | C2-N3   | 12.52  | 1.46        | 1.37     |
| 35  | BB    | 1115 | G    | C8-N7   | -12.51 | 1.23        | 1.30     |
| 35  | BB    | 2476 | A    | N7-C5   | -12.51 | 1.31        | 1.39     |
| 1   | AA    | 263  | A    | N9-C4   | -12.49 | 1.30        | 1.37     |
| 35  | BB    | 2367 | G    | C6-N1   | 12.49  | 1.48        | 1.39     |
| 35  | BB    | 772  | C    | N1-C6   | -12.48 | 1.29        | 1.37     |
| 35  | BB    | 2742 | G    | C2-N3   | 12.48  | 1.42        | 1.32     |
| 35  | BB    | 1593 | A    | C5-C4   | 12.48  | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 35  | BB    | 939  | G    | C2-N3   | 12.47  | 1.42        | 1.32     |
| 1   | AA    | 1516 | G    | C6-N1   | 12.46  | 1.48        | 1.39     |
| 35  | BB    | 138  | U    | C2-N3   | 12.45  | 1.46        | 1.37     |
| 1   | AA    | 616  | G    | N7-C5   | -12.45 | 1.31        | 1.39     |
| 1   | AA    | 899  | C    | N3-C4   | 12.45  | 1.42        | 1.33     |
| 1   | AA    | 646  | G    | N7-C5   | -12.45 | 1.31        | 1.39     |
| 35  | BB    | 310  | A    | N3-C4   | 12.45  | 1.42        | 1.34     |
| 35  | BB    | 1414 | C    | C4-N4   | 12.44  | 1.45        | 1.33     |
| 1   | AA    | 433  | G    | C2-N3   | 12.44  | 1.42        | 1.32     |
| 1   | AA    | 1014 | A    | N9-C4   | -12.43 | 1.30        | 1.37     |
| 35  | BB    | 263  | G    | N9-C8   | 12.43  | 1.46        | 1.37     |
| 35  | BB    | 2239 | G    | N3-C4   | -12.43 | 1.26        | 1.35     |
| 35  | BB    | 2339 | C    | N3-C4   | 12.41  | 1.42        | 1.33     |
| 35  | BB    | 34   | U    | C4'-C3' | 12.41  | 1.66        | 1.53     |
| 35  | BB    | 2760 | C    | N1-C6   | 12.40  | 1.44        | 1.37     |
| 35  | BB    | 1028 | A    | N9-C4   | -12.38 | 1.30        | 1.37     |
| 35  | BB    | 481  | G    | C2-N3   | 12.35  | 1.42        | 1.32     |
| 1   | AA    | 310  | G    | C8-N7   | -12.35 | 1.23        | 1.30     |
| 35  | BB    | 270  | A    | N7-C5   | -12.34 | 1.31        | 1.39     |
| 1   | AA    | 313  | A    | C6-N6   | 12.34  | 1.43        | 1.33     |
| 1   | AA    | 713  | G    | N7-C5   | -12.33 | 1.31        | 1.39     |
| 35  | BB    | 818  | G    | C2-N3   | 12.32  | 1.42        | 1.32     |
| 35  | BB    | 2777 | G    | C2-N3   | 12.31  | 1.42        | 1.32     |
| 1   | AA    | 475  | C    | N1-C6   | 12.30  | 1.44        | 1.37     |
| 35  | BB    | 497  | A    | N3-C4   | -12.29 | 1.27        | 1.34     |
| 35  | BB    | 327  | G    | N7-C5   | 12.28  | 1.46        | 1.39     |
| 1   | AA    | 576  | C    | N3-C4   | 12.28  | 1.42        | 1.33     |
| 35  | BB    | 633  | A    | C6-N6   | 12.28  | 1.43        | 1.33     |
| 35  | BB    | 1896 | G    | C6-N1   | 12.28  | 1.48        | 1.39     |
| 35  | BB    | 2899 | A    | C6-N6   | 12.28  | 1.43        | 1.33     |
| 35  | BB    | 2198 | A    | N3-C4   | -12.27 | 1.27        | 1.34     |
| 1   | AA    | 1500 | A    | C6-N6   | 12.27  | 1.43        | 1.33     |
| 35  | BB    | 2239 | G    | C6-N1   | 12.26  | 1.48        | 1.39     |
| 35  | BB    | 2532 | G    | C6-N1   | 12.24  | 1.48        | 1.39     |
| 35  | BB    | 864  | G    | N7-C5   | -12.24 | 1.31        | 1.39     |
| 35  | BB    | 338  | G    | N7-C5   | -12.22 | 1.31        | 1.39     |
| 35  | BB    | 1639 | C    | C2-N3   | 12.22  | 1.45        | 1.35     |
| 1   | AA    | 1406 | U    | C2-N3   | 12.21  | 1.46        | 1.37     |
| 1   | AA    | 197  | A    | C6-N1   | 12.21  | 1.44        | 1.35     |
| 35  | BB    | 248  | G    | C6-N1   | 12.21  | 1.48        | 1.39     |
| 35  | BB    | 1760 | C    | N3-C4   | 12.20  | 1.42        | 1.33     |
| 35  | BB    | 2062 | A    | N7-C5   | -12.19 | 1.31        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 35  | BB    | 325  | G    | C2-N3 | 12.19  | 1.42        | 1.32     |
| 1   | AA    | 532  | A    | N9-C4 | 12.19  | 1.45        | 1.37     |
| 1   | AA    | 351  | G    | C6-N1 | 12.18  | 1.48        | 1.39     |
| 1   | AA    | 1361 | G    | N9-C8 | -12.18 | 1.29        | 1.37     |
| 35  | BB    | 2343 | U    | C2-N3 | 12.18  | 1.46        | 1.37     |
| 35  | BB    | 1003 | G    | C2-N3 | 12.18  | 1.42        | 1.32     |
| 35  | BB    | 2125 | G    | N9-C8 | 12.18  | 1.46        | 1.37     |
| 1   | AA    | 1257 | A    | C6-N1 | 12.17  | 1.44        | 1.35     |
| 35  | BB    | 2176 | A    | N9-C4 | 12.17  | 1.45        | 1.37     |
| 1   | AA    | 377  | G    | C2-N3 | 12.17  | 1.42        | 1.32     |
| 22  | AV    | 39   | G    | C2-N3 | 12.17  | 1.42        | 1.32     |
| 35  | BB    | 2144 | G    | C2-N2 | 12.16  | 1.46        | 1.34     |
| 35  | BB    | 10   | A    | C6-N1 | 12.16  | 1.44        | 1.35     |
| 35  | BB    | 1073 | A    | N7-C5 | -12.15 | 1.31        | 1.39     |
| 1   | AA    | 682  | G    | N7-C5 | -12.15 | 1.31        | 1.39     |
| 35  | BB    | 1968 | G    | C8-N7 | -12.14 | 1.23        | 1.30     |
| 35  | BB    | 267  | C    | N1-C6 | 12.14  | 1.44        | 1.37     |
| 35  | BB    | 2326 | C    | P-O5' | -12.14 | 1.47        | 1.59     |
| 35  | BB    | 2612 | C    | N3-C4 | 12.13  | 1.42        | 1.33     |
| 35  | BB    | 2357 | G    | N9-C8 | 12.12  | 1.46        | 1.37     |
| 35  | BB    | 1343 | G    | N7-C5 | -12.11 | 1.31        | 1.39     |
| 1   | AA    | 568  | G    | C6-N1 | 12.11  | 1.48        | 1.39     |
| 1   | AA    | 913  | A    | C5-C4 | 12.10  | 1.47        | 1.38     |
| 35  | BB    | 1863 | G    | N1-C2 | 12.10  | 1.47        | 1.37     |
| 35  | BB    | 2660 | A    | C6-N6 | 12.10  | 1.43        | 1.33     |
| 1   | AA    | 616  | G    | C8-N7 | -12.09 | 1.23        | 1.30     |
| 1   | AA    | 1305 | G    | C2-N3 | 12.09  | 1.42        | 1.32     |
| 1   | AA    | 1077 | G    | C2-N3 | 12.09  | 1.42        | 1.32     |
| 24  | AZ    | 24   | ALA  | C-O   | -12.09 | 1.00        | 1.23     |
| 1   | AA    | 1039 | G    | C8-N7 | -12.08 | 1.23        | 1.30     |
| 35  | BB    | 998  | C    | N3-C4 | 12.08  | 1.42        | 1.33     |
| 35  | BB    | 2749 | A    | N7-C5 | -12.08 | 1.31        | 1.39     |
| 35  | BB    | 684  | G    | N7-C5 | -12.08 | 1.32        | 1.39     |
| 1   | AA    | 510  | A    | N7-C5 | -12.08 | 1.32        | 1.39     |
| 1   | AA    | 1092 | A    | N7-C5 | -12.08 | 1.32        | 1.39     |
| 42  | BI    | 141  | ASP  | C-O   | -12.07 | 1.00        | 1.23     |
| 35  | BB    | 578  | G    | P-O5' | -12.07 | 1.47        | 1.59     |
| 1   | AA    | 76   | G    | N7-C5 | -12.06 | 1.32        | 1.39     |
| 1   | AA    | 1112 | C    | N1-C6 | 12.06  | 1.44        | 1.37     |
| 35  | BB    | 243  | U    | C2-N3 | 12.06  | 1.46        | 1.37     |
| 1   | AA    | 1206 | G    | C6-N1 | 12.06  | 1.48        | 1.39     |
| 35  | BB    | 664  | G    | C8-N7 | -12.06 | 1.23        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 42  | BI    | 141  | ASP  | C-OXT | -12.04 | 1.00        | 1.23     |
| 1   | AA    | 350  | G    | C8-N7 | -12.04 | 1.23        | 1.30     |
| 1   | AA    | 1363 | A    | C8-N7 | -12.04 | 1.23        | 1.31     |
| 34  | BA    | 31   | C    | N3-C4 | 12.03  | 1.42        | 1.33     |
| 35  | BB    | 1589 | U    | C2-N3 | 12.03  | 1.46        | 1.37     |
| 35  | BB    | 2083 | G    | N7-C5 | -12.02 | 1.32        | 1.39     |
| 35  | BB    | 1839 | G    | N3-C4 | 12.02  | 1.43        | 1.35     |
| 35  | BB    | 2888 | C    | N3-C4 | 12.02  | 1.42        | 1.33     |
| 1   | AA    | 857  | C    | N1-C6 | 12.00  | 1.44        | 1.37     |
| 1   | AA    | 906  | A    | N7-C5 | -11.99 | 1.32        | 1.39     |
| 35  | BB    | 880  | G    | C8-N7 | -11.99 | 1.23        | 1.30     |
| 35  | BB    | 1815 | A    | N7-C5 | -11.98 | 1.32        | 1.39     |
| 1   | AA    | 414  | A    | N7-C5 | -11.97 | 1.32        | 1.39     |
| 35  | BB    | 1395 | A    | N7-C5 | -11.97 | 1.32        | 1.39     |
| 35  | BB    | 941  | A    | C8-N7 | -11.96 | 1.23        | 1.31     |
| 1   | AA    | 738  | C    | N1-C6 | 11.96  | 1.44        | 1.37     |
| 35  | BB    | 2385 | C    | C4-N4 | 11.95  | 1.44        | 1.33     |
| 1   | AA    | 833  | G    | N7-C5 | -11.94 | 1.32        | 1.39     |
| 35  | BB    | 1221 | C    | C4-C5 | 11.94  | 1.52        | 1.43     |
| 35  | BB    | 1661 | G    | N1-C2 | 11.94  | 1.47        | 1.37     |
| 35  | BB    | 2281 | A    | C6-N6 | 11.93  | 1.43        | 1.33     |
| 35  | BB    | 1336 | A    | C6-N6 | 11.93  | 1.43        | 1.33     |
| 1   | AA    | 941  | G    | N9-C4 | 11.92  | 1.47        | 1.38     |
| 35  | BB    | 282  | A    | N7-C5 | -11.92 | 1.32        | 1.39     |
| 35  | BB    | 467  | G    | C2-N3 | 11.92  | 1.42        | 1.32     |
| 35  | BB    | 693  | A    | C6-N1 | 11.91  | 1.43        | 1.35     |
| 1   | AA    | 376  | G    | C8-N7 | 11.91  | 1.38        | 1.30     |
| 1   | AA    | 774  | G    | N1-C2 | 11.90  | 1.47        | 1.37     |
| 35  | BB    | 1026 | G    | C8-N7 | -11.90 | 1.23        | 1.30     |
| 35  | BB    | 1952 | A    | N9-C4 | 11.90  | 1.45        | 1.37     |
| 1   | AA    | 445  | G    | N1-C2 | 11.88  | 1.47        | 1.37     |
| 1   | AA    | 1152 | A    | C6-N1 | 11.88  | 1.43        | 1.35     |
| 35  | BB    | 1110 | G    | N1-C2 | -11.88 | 1.28        | 1.37     |
| 1   | AA    | 309  | A    | C6-N6 | 11.87  | 1.43        | 1.33     |
| 1   | AA    | 790  | A    | C6-N1 | 11.87  | 1.43        | 1.35     |
| 1   | AA    | 260  | G    | N7-C5 | -11.86 | 1.32        | 1.39     |
| 35  | BB    | 2632 | A    | N9-C8 | 11.87  | 1.47        | 1.37     |
| 35  | BB    | 583  | G    | C2-N3 | 11.86  | 1.42        | 1.32     |
| 35  | BB    | 2277 | G    | N1-C2 | 11.86  | 1.47        | 1.37     |
| 1   | AA    | 1145 | A    | C6-N6 | 11.86  | 1.43        | 1.33     |
| 35  | BB    | 2682 | A    | N9-C4 | -11.85 | 1.30        | 1.37     |
| 35  | BB    | 2157 | G    | N7-C5 | -11.85 | 1.32        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 35  | BB    | 1618 | A    | N3-C4   | -11.84 | 1.27        | 1.34     |
| 1   | AA    | 1170 | A    | C6-N6   | 11.84  | 1.43        | 1.33     |
| 35  | BB    | 1642 | G    | N7-C5   | -11.83 | 1.32        | 1.39     |
| 35  | BB    | 460  | A    | C6-N1   | 11.83  | 1.43        | 1.35     |
| 35  | BB    | 2802 | G    | C2-N3   | 11.81  | 1.42        | 1.32     |
| 35  | BB    | 1478 | G    | C5-C4   | 11.81  | 1.46        | 1.38     |
| 35  | BB    | 1764 | C    | O3'-P   | -11.81 | 1.47        | 1.61     |
| 35  | BB    | 1510 | G    | C2-N3   | 11.81  | 1.42        | 1.32     |
| 1   | AA    | 186  | C    | N1-C6   | 11.80  | 1.44        | 1.37     |
| 34  | BA    | 19   | C    | P-O5'   | -11.80 | 1.48        | 1.59     |
| 35  | BB    | 1381 | G    | N7-C5   | -11.80 | 1.32        | 1.39     |
| 1   | AA    | 935  | A    | N7-C5   | -11.79 | 1.32        | 1.39     |
| 35  | BB    | 2127 | G    | N9-C4   | 11.79  | 1.47        | 1.38     |
| 35  | BB    | 180  | G    | N7-C5   | -11.79 | 1.32        | 1.39     |
| 1   | AA    | 1024 | G    | N3-C4   | -11.79 | 1.27        | 1.35     |
| 1   | AA    | 245  | U    | C5'-C4' | 11.78  | 1.65        | 1.51     |
| 35  | BB    | 2083 | G    | N1-C2   | 11.78  | 1.47        | 1.37     |
| 35  | BB    | 2469 | A    | N7-C5   | -11.78 | 1.32        | 1.39     |
| 35  | BB    | 2216 | G    | N7-C5   | -11.78 | 1.32        | 1.39     |
| 1   | AA    | 1228 | C    | N1-C6   | -11.77 | 1.30        | 1.37     |
| 35  | BB    | 2035 | G    | C2-N3   | 11.77  | 1.42        | 1.32     |
| 35  | BB    | 2644 | G    | C8-N7   | -11.76 | 1.23        | 1.30     |
| 35  | BB    | 972  | A    | C8-N7   | -11.76 | 1.23        | 1.31     |
| 1   | AA    | 1274 | A    | C5-C4   | 11.76  | 1.47        | 1.38     |
| 35  | BB    | 2570 | G    | C8-N7   | -11.76 | 1.23        | 1.30     |
| 1   | AA    | 1055 | A    | N7-C5   | -11.76 | 1.32        | 1.39     |
| 1   | AA    | 223  | A    | N9-C4   | -11.75 | 1.30        | 1.37     |
| 1   | AA    | 885  | G    | N1-C2   | 11.74  | 1.47        | 1.37     |
| 34  | BA    | 11   | C    | N1-C6   | 11.74  | 1.44        | 1.37     |
| 35  | BB    | 2326 | C    | N1-C6   | 11.74  | 1.44        | 1.37     |
| 35  | BB    | 1531 | C    | N3-C4   | 11.74  | 1.42        | 1.33     |
| 35  | BB    | 1245 | G    | N3-C4   | -11.73 | 1.27        | 1.35     |
| 35  | BB    | 35   | G    | N7-C5   | -11.73 | 1.32        | 1.39     |
| 34  | BA    | 10   | G    | N7-C5   | -11.73 | 1.32        | 1.39     |
| 34  | BA    | 13   | G    | C8-N7   | -11.73 | 1.24        | 1.30     |
| 35  | BB    | 894  | U    | C2-N3   | 11.72  | 1.46        | 1.37     |
| 1   | AA    | 50   | A    | N7-C5   | -11.70 | 1.32        | 1.39     |
| 1   | AA    | 428  | G    | C5-C4   | 11.70  | 1.46        | 1.38     |
| 35  | BB    | 2767 | C    | N1-C6   | 11.70  | 1.44        | 1.37     |
| 35  | BB    | 1062 | G    | N7-C5   | -11.70 | 1.32        | 1.39     |
| 1   | AA    | 1088 | G    | N3-C4   | -11.70 | 1.27        | 1.35     |
| 34  | BA    | 116  | G    | N1-C2   | 11.70  | 1.47        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34  | BA    | 73   | A    | N3-C4   | 11.69  | 1.41        | 1.34     |
| 35  | BB    | 1310 | G    | N3-C4   | -11.69 | 1.27        | 1.35     |
| 1   | AA    | 667  | G    | N1-C2   | 11.68  | 1.47        | 1.37     |
| 1   | AA    | 404  | G    | N1-C2   | 11.67  | 1.47        | 1.37     |
| 35  | BB    | 2231 | U    | C2-N3   | 11.66  | 1.46        | 1.37     |
| 1   | AA    | 698  | G    | N7-C5   | -11.65 | 1.32        | 1.39     |
| 35  | BB    | 2635 | A    | N3-C4   | -11.64 | 1.27        | 1.34     |
| 35  | BB    | 2673 | G    | C6-N1   | 11.64  | 1.47        | 1.39     |
| 35  | BB    | 1524 | G    | C2-N3   | 11.63  | 1.42        | 1.32     |
| 35  | BB    | 2151 | U    | P-O5'   | -11.63 | 1.48        | 1.59     |
| 1   | AA    | 491  | G    | N7-C5   | 11.63  | 1.46        | 1.39     |
| 1   | AA    | 1293 | C    | N1-C6   | -11.62 | 1.30        | 1.37     |
| 35  | BB    | 1509 | A    | C8-N7   | -11.62 | 1.23        | 1.31     |
| 34  | BA    | 85   | G    | C2-N3   | 11.62  | 1.42        | 1.32     |
| 35  | BB    | 2033 | A    | N7-C5   | -11.62 | 1.32        | 1.39     |
| 35  | BB    | 461  | C    | N3-C4   | 11.61  | 1.42        | 1.33     |
| 1   | AA    | 415  | A    | C6-N1   | 11.61  | 1.43        | 1.35     |
| 35  | BB    | 1794 | A    | C6-N6   | 11.61  | 1.43        | 1.33     |
| 1   | AA    | 1161 | C    | C2-N3   | 11.61  | 1.45        | 1.35     |
| 35  | BB    | 1756 | G    | C6-N1   | 11.60  | 1.47        | 1.39     |
| 35  | BB    | 670  | A    | N9-C4   | 11.60  | 1.44        | 1.37     |
| 35  | BB    | 75   | G    | C6-N1   | 11.59  | 1.47        | 1.39     |
| 35  | BB    | 2679 | A    | C6-N6   | 11.59  | 1.43        | 1.33     |
| 1   | AA    | 263  | A    | N3-C4   | -11.59 | 1.27        | 1.34     |
| 35  | BB    | 287  | G    | C6-N1   | 11.59  | 1.47        | 1.39     |
| 35  | BB    | 1350 | C    | C4'-C3' | 11.58  | 1.65        | 1.53     |
| 1   | AA    | 929  | G    | C5-C4   | 11.57  | 1.46        | 1.38     |
| 35  | BB    | 2037 | A    | N3-C4   | -11.57 | 1.27        | 1.34     |
| 35  | BB    | 221  | A    | C8-N7   | -11.55 | 1.23        | 1.31     |
| 35  | BB    | 1223 | G    | N7-C5   | -11.55 | 1.32        | 1.39     |
| 1   | AA    | 266  | G    | N3-C4   | -11.55 | 1.27        | 1.35     |
| 1   | AA    | 1177 | G    | C6-N1   | 11.54  | 1.47        | 1.39     |
| 35  | BB    | 39   | G    | N1-C2   | 11.54  | 1.47        | 1.37     |
| 35  | BB    | 617  | G    | N7-C5   | -11.54 | 1.32        | 1.39     |
| 35  | BB    | 1226 | A    | N7-C5   | -11.53 | 1.32        | 1.39     |
| 1   | AA    | 773  | G    | C2-N3   | 11.52  | 1.42        | 1.32     |
| 35  | BB    | 2045 | C    | P-O5'   | -11.52 | 1.48        | 1.59     |
| 35  | BB    | 2178 | C    | N3-C4   | 11.51  | 1.42        | 1.33     |
| 35  | BB    | 1000 | A    | C6-N6   | 11.51  | 1.43        | 1.33     |
| 1   | AA    | 1022 | A    | C6-N1   | 11.49  | 1.43        | 1.35     |
| 35  | BB    | 2041 | U    | C2-N3   | 11.49  | 1.45        | 1.37     |
| 1   | AA    | 1084 | G    | C8-N7   | -11.48 | 1.24        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | AA    | 1319 | A    | C6-N1   | 11.47  | 1.43        | 1.35     |
| 35  | BB    | 2082 | A    | N7-C5   | -11.47 | 1.32        | 1.39     |
| 35  | BB    | 833  | A    | C6-N1   | 11.46  | 1.43        | 1.35     |
| 35  | BB    | 1045 | C    | N3-C4   | 11.46  | 1.42        | 1.33     |
| 35  | BB    | 1197 | G    | C6-N1   | 11.46  | 1.47        | 1.39     |
| 35  | BB    | 2112 | G    | C2-N3   | 11.46  | 1.42        | 1.32     |
| 35  | BB    | 537  | G    | N7-C5   | -11.46 | 1.32        | 1.39     |
| 35  | BB    | 2389 | G    | N9-C8   | 11.46  | 1.45        | 1.37     |
| 35  | BB    | 2534 | A    | N9-C4   | -11.46 | 1.30        | 1.37     |
| 1   | AA    | 1037 | C    | C4-N4   | 11.46  | 1.44        | 1.33     |
| 35  | BB    | 2093 | G    | C2-N3   | 11.45  | 1.42        | 1.32     |
| 35  | BB    | 2808 | G    | C2-N3   | 11.45  | 1.42        | 1.32     |
| 1   | AA    | 197  | A    | C5-C4   | 11.44  | 1.46        | 1.38     |
| 35  | BB    | 2130 | U    | C2-N3   | 11.44  | 1.45        | 1.37     |
| 35  | BB    | 1160 | G    | N7-C5   | -11.43 | 1.32        | 1.39     |
| 22  | AV    | 39   | G    | N1-C2   | 11.42  | 1.46        | 1.37     |
| 35  | BB    | 473  | G    | C6-N1   | 11.42  | 1.47        | 1.39     |
| 35  | BB    | 1702 | G    | N3-C4   | -11.42 | 1.27        | 1.35     |
| 35  | BB    | 870  | U    | C2-N3   | 11.41  | 1.45        | 1.37     |
| 35  | BB    | 612  | G    | N7-C5   | -11.40 | 1.32        | 1.39     |
| 35  | BB    | 1968 | G    | N7-C5   | -11.40 | 1.32        | 1.39     |
| 35  | BB    | 950  | G    | N7-C5   | -11.40 | 1.32        | 1.39     |
| 35  | BB    | 1459 | G    | N7-C5   | 11.40  | 1.46        | 1.39     |
| 35  | BB    | 380  | G    | N7-C5   | -11.39 | 1.32        | 1.39     |
| 35  | BB    | 820  | A    | N7-C5   | -11.39 | 1.32        | 1.39     |
| 35  | BB    | 1691 | C    | N1-C6   | -11.38 | 1.30        | 1.37     |
| 1   | AA    | 71   | A    | N7-C5   | -11.38 | 1.32        | 1.39     |
| 34  | BA    | 61   | G    | C5-C4   | 11.38  | 1.46        | 1.38     |
| 35  | BB    | 423  | A    | N7-C5   | -11.38 | 1.32        | 1.39     |
| 35  | BB    | 962  | G    | C2'-C1' | -11.38 | 1.40        | 1.53     |
| 35  | BB    | 1875 | G    | N9-C8   | -11.37 | 1.29        | 1.37     |
| 35  | BB    | 718  | A    | N9-C8   | 11.37  | 1.46        | 1.37     |
| 35  | BB    | 2365 | G    | N3-C4   | -11.37 | 1.27        | 1.35     |
| 1   | AA    | 1297 | G    | C8-N7   | 11.37  | 1.37        | 1.30     |
| 35  | BB    | 1162 | G    | C6-N1   | 11.36  | 1.47        | 1.39     |
| 35  | BB    | 1805 | A    | C6-N6   | 11.36  | 1.43        | 1.33     |
| 1   | AA    | 430  | A    | N3-C4   | -11.36 | 1.28        | 1.34     |
| 1   | AA    | 1197 | A    | C8-N7   | -11.36 | 1.23        | 1.31     |
| 35  | BB    | 2663 | G    | N7-C5   | -11.35 | 1.32        | 1.39     |
| 1   | AA    | 1089 | G    | N1-C2   | 11.35  | 1.46        | 1.37     |
| 1   | AA    | 156  | C    | N1-C6   | 11.34  | 1.44        | 1.37     |
| 35  | BB    | 252  | G    | C2-N3   | 11.34  | 1.41        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 35  | BB    | 721  | A    | C6-N6   | 11.34  | 1.43        | 1.33     |
| 1   | AA    | 1212 | U    | C2-N3   | 11.33  | 1.45        | 1.37     |
| 1   | AA    | 731  | G    | N1-C2   | 11.33  | 1.46        | 1.37     |
| 1   | AA    | 689  | C    | P-O5'   | -11.32 | 1.48        | 1.59     |
| 35  | BB    | 2574 | G    | N7-C5   | -11.32 | 1.32        | 1.39     |
| 35  | BB    | 453  | A    | N7-C5   | -11.32 | 1.32        | 1.39     |
| 35  | BB    | 1689 | A    | P-O5'   | -11.32 | 1.48        | 1.59     |
| 35  | BB    | 2746 | U    | C2-N3   | 11.32  | 1.45        | 1.37     |
| 1   | AA    | 432  | A    | N7-C5   | -11.31 | 1.32        | 1.39     |
| 35  | BB    | 2809 | A    | N7-C5   | -11.31 | 1.32        | 1.39     |
| 35  | BB    | 2409 | G    | C8-N7   | -11.29 | 1.24        | 1.30     |
| 35  | BB    | 1397 | U    | C2-N3   | 11.29  | 1.45        | 1.37     |
| 35  | BB    | 1517 | G    | N7-C5   | -11.29 | 1.32        | 1.39     |
| 35  | BB    | 1594 | U    | N1-C6   | 11.29  | 1.48        | 1.38     |
| 35  | BB    | 1710 | G    | C2-N3   | 11.29  | 1.41        | 1.32     |
| 35  | BB    | 1908 | C    | N3-C4   | 11.29  | 1.41        | 1.33     |
| 1   | AA    | 621  | A    | N9-C4   | 11.28  | 1.44        | 1.37     |
| 35  | BB    | 2781 | A    | N7-C5   | -11.28 | 1.32        | 1.39     |
| 35  | BB    | 2455 | G    | N1-C2   | 11.28  | 1.46        | 1.37     |
| 1   | AA    | 130  | A    | C6-N1   | 11.27  | 1.43        | 1.35     |
| 1   | AA    | 360  | G    | N7-C5   | -11.27 | 1.32        | 1.39     |
| 35  | BB    | 27   | G    | C2-N3   | 11.27  | 1.41        | 1.32     |
| 1   | AA    | 1337 | G    | N9-C8   | -11.26 | 1.29        | 1.37     |
| 35  | BB    | 582  | A    | N3-C4   | 11.25  | 1.41        | 1.34     |
| 35  | BB    | 829  | A    | C6-N6   | 11.25  | 1.43        | 1.33     |
| 1   | AA    | 1226 | C    | C4-N4   | 11.25  | 1.44        | 1.33     |
| 35  | BB    | 2361 | G    | C2-N3   | 11.24  | 1.41        | 1.32     |
| 35  | BB    | 205  | G    | C4'-C3' | 11.24  | 1.65        | 1.53     |
| 35  | BB    | 775  | G    | C8-N7   | 11.24  | 1.37        | 1.30     |
| 35  | BB    | 2416 | C    | C2-N3   | 11.24  | 1.44        | 1.35     |
| 35  | BB    | 1022 | G    | N1-C2   | 11.24  | 1.46        | 1.37     |
| 1   | AA    | 785  | G    | C6-N1   | 11.23  | 1.47        | 1.39     |
| 1   | AA    | 1279 | G    | C6-N1   | 11.22  | 1.47        | 1.39     |
| 35  | BB    | 1236 | G    | N3-C4   | -11.22 | 1.27        | 1.35     |
| 35  | BB    | 375  | G    | N1-C2   | 11.21  | 1.46        | 1.37     |
| 35  | BB    | 1266 | G    | N1-C2   | 11.21  | 1.46        | 1.37     |
| 34  | BA    | 52   | A    | C6-N1   | 11.21  | 1.43        | 1.35     |
| 35  | BB    | 2742 | G    | N9-C8   | -11.21 | 1.30        | 1.37     |
| 35  | BB    | 2515 | C    | N3-C4   | 11.21  | 1.41        | 1.33     |
| 1   | AA    | 799  | G    | C6-N1   | 11.20  | 1.47        | 1.39     |
| 1   | AA    | 844  | G    | N7-C5   | -11.20 | 1.32        | 1.39     |
| 35  | BB    | 625  | G    | C2-N3   | 11.20  | 1.41        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | AA    | 1497 | G    | N7-C5   | -11.20 | 1.32        | 1.39     |
| 1   | AA    | 885  | G    | C2'-C1' | -11.20 | 1.41        | 1.53     |
| 35  | BB    | 1705 | A    | C6-N6   | 11.20  | 1.43        | 1.33     |
| 35  | BB    | 1000 | A    | N7-C5   | -11.19 | 1.32        | 1.39     |
| 1   | AA    | 347  | G    | N1-C2   | 11.19  | 1.46        | 1.37     |
| 35  | BB    | 2005 | A    | N7-C5   | -11.19 | 1.32        | 1.39     |
| 35  | BB    | 181  | A    | N7-C5   | -11.19 | 1.32        | 1.39     |
| 1   | AA    | 33   | A    | N9-C4   | 11.18  | 1.44        | 1.37     |
| 1   | AA    | 817  | C    | C2'-C1' | -11.18 | 1.41        | 1.53     |
| 35  | BB    | 1811 | G    | C6-N1   | 11.17  | 1.47        | 1.39     |
| 1   | AA    | 1200 | C    | C2'-C1' | -11.17 | 1.41        | 1.53     |
| 35  | BB    | 1824 | G    | N7-C5   | -11.17 | 1.32        | 1.39     |
| 1   | AA    | 1389 | C    | C4-N4   | 11.17  | 1.44        | 1.33     |
| 1   | AA    | 459  | A    | C6-N6   | 11.16  | 1.42        | 1.33     |
| 35  | BB    | 2544 | G    | N7-C5   | -11.16 | 1.32        | 1.39     |
| 35  | BB    | 295  | G    | C6-N1   | 11.15  | 1.47        | 1.39     |
| 1   | AA    | 435  | A    | C6-N6   | 11.15  | 1.42        | 1.33     |
| 35  | BB    | 1492 | G    | N1-C2   | 11.15  | 1.46        | 1.37     |
| 1   | AA    | 1132 | C    | N3-C4   | 11.14  | 1.41        | 1.33     |
| 35  | BB    | 2214 | C    | N3-C4   | 11.14  | 1.41        | 1.33     |
| 1   | AA    | 1190 | G    | C2-N3   | 11.13  | 1.41        | 1.32     |
| 35  | BB    | 873  | C    | N1-C6   | 11.13  | 1.43        | 1.37     |
| 1   | AA    | 518  | C    | N1-C6   | 11.13  | 1.43        | 1.37     |
| 1   | AA    | 629  | A    | N3-C4   | -11.13 | 1.28        | 1.34     |
| 35  | BB    | 1128 | G    | N7-C5   | -11.13 | 1.32        | 1.39     |
| 35  | BB    | 2849 | U    | C2-N3   | 11.13  | 1.45        | 1.37     |
| 35  | BB    | 2208 | C    | C2'-C1' | -11.13 | 1.41        | 1.53     |
| 35  | BB    | 2429 | G    | N3-C4   | 11.12  | 1.43        | 1.35     |
| 35  | BB    | 859  | G    | N9-C8   | -11.12 | 1.30        | 1.37     |
| 35  | BB    | 899  | A    | C6-N6   | 11.12  | 1.42        | 1.33     |
| 35  | BB    | 394  | C    | N3-C4   | 11.11  | 1.41        | 1.33     |
| 1   | AA    | 351  | G    | P-O5'   | -11.11 | 1.48        | 1.59     |
| 1   | AA    | 692  | U    | P-O5'   | -11.11 | 1.48        | 1.59     |
| 35  | BB    | 177  | G    | C6-N1   | 11.11  | 1.47        | 1.39     |
| 35  | BB    | 2844 | G    | N7-C5   | -11.10 | 1.32        | 1.39     |
| 34  | BA    | 47   | C    | N1-C6   | 11.10  | 1.43        | 1.37     |
| 1   | AA    | 514  | C    | N3-C4   | 11.10  | 1.41        | 1.33     |
| 35  | BB    | 1419 | A    | N3-C4   | -11.10 | 1.28        | 1.34     |
| 35  | BB    | 70   | G    | N9-C8   | -11.09 | 1.30        | 1.37     |
| 35  | BB    | 1296 | G    | C5-C4   | 11.09  | 1.46        | 1.38     |
| 35  | BB    | 1503 | A    | N9-C4   | 11.09  | 1.44        | 1.37     |
| 1   | AA    | 1255 | G    | C2-N3   | 11.08  | 1.41        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 35  | BB    | 430  | A    | N7-C5   | -11.08 | 1.32        | 1.39     |
| 35  | BB    | 1277 | G    | C2-N3   | 11.08  | 1.41        | 1.32     |
| 1   | AA    | 200  | G    | N9-C8   | 11.08  | 1.45        | 1.37     |
| 1   | AA    | 1214 | C    | N1-C6   | 11.08  | 1.43        | 1.37     |
| 35  | BB    | 172  | A    | C6-N1   | 11.08  | 1.43        | 1.35     |
| 35  | BB    | 1038 | G    | C2-N3   | 11.07  | 1.41        | 1.32     |
| 35  | BB    | 1566 | A    | N7-C5   | -11.07 | 1.32        | 1.39     |
| 35  | BB    | 2872 | A    | N7-C5   | -11.07 | 1.32        | 1.39     |
| 1   | AA    | 1435 | G    | N7-C5   | -11.07 | 1.32        | 1.39     |
| 1   | AA    | 768  | A    | N7-C5   | -11.06 | 1.32        | 1.39     |
| 1   | AA    | 68   | G    | C8-N7   | -11.06 | 1.24        | 1.30     |
| 35  | BB    | 1101 | U    | N3-C4   | 11.05  | 1.48        | 1.38     |
| 1   | AA    | 982  | U    | O3'-P   | -11.05 | 1.47        | 1.61     |
| 35  | BB    | 2830 | C    | N1-C6   | 11.05  | 1.43        | 1.37     |
| 1   | AA    | 1042 | A    | N7-C5   | -11.04 | 1.32        | 1.39     |
| 35  | BB    | 1295 | C    | N1-C6   | 11.04  | 1.43        | 1.37     |
| 35  | BB    | 1897 | G    | N3-C4   | -11.04 | 1.27        | 1.35     |
| 35  | BB    | 491  | G    | N7-C5   | -11.04 | 1.32        | 1.39     |
| 35  | BB    | 902  | C    | N1-C6   | 11.03  | 1.43        | 1.37     |
| 35  | BB    | 121  | G    | C2-N3   | 11.03  | 1.41        | 1.32     |
| 35  | BB    | 419  | U    | C2-N3   | 11.03  | 1.45        | 1.37     |
| 1   | AA    | 867  | G    | C6-N1   | 11.03  | 1.47        | 1.39     |
| 1   | AA    | 923  | A    | N7-C5   | -11.03 | 1.32        | 1.39     |
| 35  | BB    | 572  | A    | C8-N7   | -11.02 | 1.23        | 1.31     |
| 34  | BA    | 66   | A    | N7-C5   | -11.02 | 1.32        | 1.39     |
| 1   | AA    | 353  | A    | C8-N7   | -11.02 | 1.23        | 1.31     |
| 35  | BB    | 1317 | G    | C2-N3   | 11.01  | 1.41        | 1.32     |
| 1   | AA    | 1228 | C    | C4-N4   | 11.01  | 1.43        | 1.33     |
| 1   | AA    | 1486 | G    | C2-N3   | 11.01  | 1.41        | 1.32     |
| 35  | BB    | 1710 | G    | C8-N7   | -10.99 | 1.24        | 1.30     |
| 35  | BB    | 156  | A    | C4'-O4' | 10.99  | 1.59        | 1.45     |
| 35  | BB    | 715  | A    | N7-C5   | -10.99 | 1.32        | 1.39     |
| 34  | BA    | 75   | G    | C2-N3   | 10.99  | 1.41        | 1.32     |
| 35  | BB    | 1127 | A    | N9-C4   | -10.99 | 1.31        | 1.37     |
| 35  | BB    | 2872 | A    | C5-C4   | 10.99  | 1.46        | 1.38     |
| 1   | AA    | 1291 | U    | C2-N3   | 10.99  | 1.45        | 1.37     |
| 34  | BA    | 81   | G    | N7-C5   | -10.99 | 1.32        | 1.39     |
| 35  | BB    | 177  | G    | C5-C4   | 10.99  | 1.46        | 1.38     |
| 35  | BB    | 2470 | G    | N7-C5   | -10.99 | 1.32        | 1.39     |
| 1   | AA    | 29   | U    | C2-N3   | 10.98  | 1.45        | 1.37     |
| 35  | BB    | 954  | G    | C5-C4   | 10.97  | 1.46        | 1.38     |
| 1   | AA    | 582  | C    | C4-N4   | 10.97  | 1.43        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 35  | BB    | 1527 | G    | C2-N3 | 10.97  | 1.41        | 1.32     |
| 35  | BB    | 2566 | A    | N7-C5 | -10.96 | 1.32        | 1.39     |
| 35  | BB    | 443  | A    | N3-C4 | -10.96 | 1.28        | 1.34     |
| 35  | BB    | 2389 | G    | N7-C5 | -10.95 | 1.32        | 1.39     |
| 35  | BB    | 788  | A    | C6-N6 | 10.95  | 1.42        | 1.33     |
| 1   | AA    | 330  | C    | N1-C6 | -10.95 | 1.30        | 1.37     |
| 35  | BB    | 1988 | G    | C6-N1 | 10.95  | 1.47        | 1.39     |
| 35  | BB    | 1543 | G    | C8-N7 | 10.94  | 1.37        | 1.30     |
| 1   | AA    | 1360 | A    | N9-C4 | -10.94 | 1.31        | 1.37     |
| 35  | BB    | 95   | A    | N7-C5 | -10.94 | 1.32        | 1.39     |
| 35  | BB    | 2638 | G    | N7-C5 | -10.94 | 1.32        | 1.39     |
| 34  | BA    | 64   | G    | N7-C5 | -10.94 | 1.32        | 1.39     |
| 35  | BB    | 668  | A    | C6-N6 | 10.93  | 1.42        | 1.33     |
| 35  | BB    | 1466 | U    | P-O5' | -10.93 | 1.48        | 1.59     |
| 35  | BB    | 1317 | G    | N7-C5 | -10.93 | 1.32        | 1.39     |
| 1   | AA    | 967  | C    | N1-C6 | -10.93 | 1.30        | 1.37     |
| 1   | AA    | 821  | G    | C6-N1 | 10.93  | 1.47        | 1.39     |
| 1   | AA    | 1108 | G    | C8-N7 | -10.92 | 1.24        | 1.30     |
| 1   | AA    | 567  | G    | N9-C4 | -10.92 | 1.29        | 1.38     |
| 35  | BB    | 560  | C    | N1-C6 | 10.92  | 1.43        | 1.37     |
| 35  | BB    | 1221 | C    | C4-N4 | 10.92  | 1.43        | 1.33     |
| 35  | BB    | 1895 | C    | C2-N3 | 10.92  | 1.44        | 1.35     |
| 1   | AA    | 1446 | A    | N7-C5 | -10.91 | 1.32        | 1.39     |
| 1   | AA    | 725  | G    | C6-N1 | 10.91  | 1.47        | 1.39     |
| 1   | AA    | 944  | G    | O3'-P | -10.90 | 1.48        | 1.61     |
| 35  | BB    | 1462 | C    | N1-C6 | -10.90 | 1.30        | 1.37     |
| 35  | BB    | 1212 | G    | C6-N1 | 10.90  | 1.47        | 1.39     |
| 1   | AA    | 551  | U    | C2-N3 | 10.90  | 1.45        | 1.37     |
| 35  | BB    | 422  | A    | C6-N6 | 10.90  | 1.42        | 1.33     |
| 35  | BB    | 223  | A    | C6-N6 | 10.89  | 1.42        | 1.33     |
| 35  | BB    | 2241 | A    | N9-C8 | -10.89 | 1.29        | 1.37     |
| 35  | BB    | 382  | A    | N7-C5 | -10.88 | 1.32        | 1.39     |
| 35  | BB    | 1089 | A    | N9-C4 | -10.88 | 1.31        | 1.37     |
| 35  | BB    | 1283 | G    | C5-C4 | 10.88  | 1.46        | 1.38     |
| 35  | BB    | 1802 | A    | N7-C5 | -10.88 | 1.32        | 1.39     |
| 1   | AA    | 1197 | A    | C6-N6 | 10.87  | 1.42        | 1.33     |
| 35  | BB    | 382  | A    | N3-C4 | -10.87 | 1.28        | 1.34     |
| 35  | BB    | 1884 | G    | C5-C4 | -10.86 | 1.30        | 1.38     |
| 1   | AA    | 939  | G    | N7-C5 | -10.86 | 1.32        | 1.39     |
| 35  | BB    | 2642 | G    | N3-C4 | -10.86 | 1.27        | 1.35     |
| 35  | BB    | 2488 | G    | C2-N3 | 10.85  | 1.41        | 1.32     |
| 35  | BB    | 2766 | A    | N7-C5 | -10.85 | 1.32        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | AA    | 652  | U    | C2-N3   | 10.84  | 1.45        | 1.37     |
| 35  | BB    | 1663 | G    | O3'-P   | -10.84 | 1.48        | 1.61     |
| 35  | BB    | 1296 | G    | N7-C5   | -10.84 | 1.32        | 1.39     |
| 35  | BB    | 348  | A    | N3-C4   | -10.84 | 1.28        | 1.34     |
| 35  | BB    | 2327 | A    | N7-C5   | -10.83 | 1.32        | 1.39     |
| 35  | BB    | 2446 | G    | N9-C4   | 10.83  | 1.46        | 1.38     |
| 1   | AA    | 422  | C    | C2-N3   | 10.83  | 1.44        | 1.35     |
| 35  | BB    | 1264 | A    | C6-N6   | 10.83  | 1.42        | 1.33     |
| 35  | BB    | 2030 | A    | C6-N1   | 10.83  | 1.43        | 1.35     |
| 1   | AA    | 717  | U    | C2-N3   | 10.83  | 1.45        | 1.37     |
| 35  | BB    | 939  | G    | N1-C2   | 10.83  | 1.46        | 1.37     |
| 35  | BB    | 1057 | A    | N7-C5   | -10.83 | 1.32        | 1.39     |
| 1   | AA    | 444  | G    | C6-N1   | 10.82  | 1.47        | 1.39     |
| 35  | BB    | 2168 | G    | N9-C4   | -10.82 | 1.29        | 1.38     |
| 1   | AA    | 673  | A    | N7-C5   | -10.82 | 1.32        | 1.39     |
| 35  | BB    | 1129 | A    | P-O5'   | -10.82 | 1.49        | 1.59     |
| 1   | AA    | 1079 | G    | P-O5'   | -10.81 | 1.49        | 1.59     |
| 35  | BB    | 23   | G    | P-O5'   | -10.81 | 1.49        | 1.59     |
| 1   | AA    | 755  | G    | N7-C5   | -10.81 | 1.32        | 1.39     |
| 35  | BB    | 375  | G    | C8-N7   | -10.81 | 1.24        | 1.30     |
| 35  | BB    | 1501 | G    | C2-N3   | 10.81  | 1.41        | 1.32     |
| 35  | BB    | 1772 | A    | N3-C4   | -10.81 | 1.28        | 1.34     |
| 35  | BB    | 953  | G    | C6-N1   | 10.80  | 1.47        | 1.39     |
| 35  | BB    | 62   | U    | C2-N3   | 10.80  | 1.45        | 1.37     |
| 1   | AA    | 637  | C    | N3-C4   | 10.80  | 1.41        | 1.33     |
| 1   | AA    | 458  | U    | C2-N3   | 10.79  | 1.45        | 1.37     |
| 35  | BB    | 1127 | A    | N7-C5   | -10.80 | 1.32        | 1.39     |
| 35  | BB    | 1823 | G    | C2-N2   | 10.80  | 1.45        | 1.34     |
| 35  | BB    | 2835 | A    | N9-C4   | 10.79  | 1.44        | 1.37     |
| 1   | AA    | 1097 | C    | C4-C5   | 10.79  | 1.51        | 1.43     |
| 34  | BA    | 27   | C    | P-O5'   | -10.79 | 1.49        | 1.59     |
| 35  | BB    | 1440 | U    | C2-N3   | 10.79  | 1.45        | 1.37     |
| 1   | AA    | 700  | G    | C6-N1   | 10.79  | 1.47        | 1.39     |
| 1   | AA    | 1251 | A    | C6-N1   | 10.78  | 1.43        | 1.35     |
| 35  | BB    | 216  | A    | C5-C4   | 10.78  | 1.46        | 1.38     |
| 35  | BB    | 697  | G    | N3-C4   | -10.78 | 1.27        | 1.35     |
| 35  | BB    | 1198 | U    | C2-N3   | 10.78  | 1.45        | 1.37     |
| 35  | BB    | 1786 | A    | O3'-P   | -10.78 | 1.48        | 1.61     |
| 35  | BB    | 1799 | G    | P-O5'   | -10.78 | 1.49        | 1.59     |
| 35  | BB    | 1828 | G    | C8-N7   | -10.78 | 1.24        | 1.30     |
| 1   | AA    | 729  | A    | N7-C5   | -10.77 | 1.32        | 1.39     |
| 35  | BB    | 2119 | A    | C5'-C4' | 10.77  | 1.64        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | AA    | 769  | G    | C2-N3   | 10.76  | 1.41        | 1.32     |
| 35  | BB    | 2748 | A    | N9-C4   | -10.76 | 1.31        | 1.37     |
| 35  | BB    | 1912 | A    | C6-N1   | 10.76  | 1.43        | 1.35     |
| 35  | BB    | 2903 | U    | C2-N3   | 10.76  | 1.45        | 1.37     |
| 1   | AA    | 821  | G    | N7-C5   | -10.75 | 1.32        | 1.39     |
| 35  | BB    | 1907 | G    | N7-C5   | -10.75 | 1.32        | 1.39     |
| 35  | BB    | 2719 | G    | N7-C5   | -10.75 | 1.32        | 1.39     |
| 35  | BB    | 1989 | G    | O3'-P   | -10.74 | 1.48        | 1.61     |
| 35  | BB    | 858  | G    | N7-C5   | -10.74 | 1.32        | 1.39     |
| 35  | BB    | 131  | A    | N7-C5   | -10.74 | 1.32        | 1.39     |
| 35  | BB    | 1011 | G    | C6-N1   | 10.73  | 1.47        | 1.39     |
| 35  | BB    | 2706 | A    | C6-N6   | 10.73  | 1.42        | 1.33     |
| 1   | AA    | 1036 | A    | N9-C4   | -10.73 | 1.31        | 1.37     |
| 35  | BB    | 2172 | U    | N3-C4   | 10.73  | 1.48        | 1.38     |
| 1   | AA    | 462  | G    | C6-N1   | 10.72  | 1.47        | 1.39     |
| 34  | BA    | 102  | G    | C2-N3   | 10.72  | 1.41        | 1.32     |
| 35  | BB    | 2741 | A    | C6-N1   | 10.72  | 1.43        | 1.35     |
| 35  | BB    | 2380 | C    | C4-N4   | 10.72  | 1.43        | 1.33     |
| 35  | BB    | 282  | A    | C6-N6   | 10.72  | 1.42        | 1.33     |
| 1   | AA    | 1120 | C    | C2-N3   | 10.71  | 1.44        | 1.35     |
| 35  | BB    | 1653 | G    | P-O5'   | -10.71 | 1.49        | 1.59     |
| 35  | BB    | 559  | G    | C2-N3   | 10.71  | 1.41        | 1.32     |
| 35  | BB    | 2811 | G    | N9-C8   | -10.71 | 1.30        | 1.37     |
| 1   | AA    | 345  | C    | N1-C6   | -10.69 | 1.30        | 1.37     |
| 1   | AA    | 1417 | G    | N7-C5   | -10.69 | 1.32        | 1.39     |
| 35  | BB    | 2216 | G    | C6-N1   | 10.69  | 1.47        | 1.39     |
| 1   | AA    | 1274 | A    | N9-C4   | -10.68 | 1.31        | 1.37     |
| 1   | AA    | 1312 | G    | N1-C2   | 10.68  | 1.46        | 1.37     |
| 1   | AA    | 491  | G    | C6-N1   | 10.67  | 1.47        | 1.39     |
| 35  | BB    | 597  | G    | C8-N7   | 10.67  | 1.37        | 1.30     |
| 35  | BB    | 1126 | A    | N9-C4   | 10.67  | 1.44        | 1.37     |
| 35  | BB    | 1336 | A    | N7-C5   | -10.67 | 1.32        | 1.39     |
| 35  | BB    | 2218 | G    | N1-C2   | 10.67  | 1.46        | 1.37     |
| 35  | BB    | 768  | G    | N7-C5   | -10.67 | 1.32        | 1.39     |
| 35  | BB    | 1408 | G    | C2-N3   | 10.67  | 1.41        | 1.32     |
| 35  | BB    | 2455 | G    | C2-N3   | 10.67  | 1.41        | 1.32     |
| 1   | AA    | 1005 | A    | C2'-C1' | -10.67 | 1.41        | 1.53     |
| 35  | BB    | 1191 | G    | N7-C5   | -10.67 | 1.32        | 1.39     |
| 1   | AA    | 1245 | C    | C2-N3   | 10.67  | 1.44        | 1.35     |
| 35  | BB    | 2623 | G    | N9-C8   | -10.66 | 1.30        | 1.37     |
| 1   | AA    | 341  | C    | C4-N4   | 10.66  | 1.43        | 1.33     |
| 1   | AA    | 691  | G    | N9-C8   | -10.66 | 1.30        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | AA    | 468  | A    | C6-N6   | 10.66  | 1.42        | 1.33     |
| 1   | AA    | 605  | U    | C2-N3   | 10.66  | 1.45        | 1.37     |
| 35  | BB    | 749  | A    | N7-C5   | -10.65 | 1.32        | 1.39     |
| 35  | BB    | 294  | A    | N7-C5   | -10.65 | 1.32        | 1.39     |
| 35  | BB    | 1885 | A    | C8-N7   | -10.65 | 1.24        | 1.31     |
| 1   | AA    | 463  | U    | C2-N3   | 10.64  | 1.45        | 1.37     |
| 1   | AA    | 869  | G    | C6-N1   | 10.64  | 1.47        | 1.39     |
| 35  | BB    | 912  | C    | N3-C4   | 10.64  | 1.41        | 1.33     |
| 1   | AA    | 120  | A    | N7-C5   | -10.64 | 1.32        | 1.39     |
| 1   | AA    | 574  | A    | O3'-P   | -10.64 | 1.48        | 1.61     |
| 22  | AV    | 5    | A    | C6-N6   | 10.63  | 1.42        | 1.33     |
| 35  | BB    | 1867 | G    | C2'-C1' | -10.63 | 1.41        | 1.53     |
| 35  | BB    | 2873 | A    | P-O5'   | -10.63 | 1.49        | 1.59     |
| 35  | BB    | 2881 | U    | C2-N3   | 10.63  | 1.45        | 1.37     |
| 35  | BB    | 611  | C    | N3-C4   | 10.63  | 1.41        | 1.33     |
| 35  | BB    | 189  | G    | N3-C4   | -10.63 | 1.28        | 1.35     |
| 35  | BB    | 899  | A    | N3-C4   | 10.63  | 1.41        | 1.34     |
| 35  | BB    | 2759 | G    | N1-C2   | 10.63  | 1.46        | 1.37     |
| 35  | BB    | 1167 | C    | N3-C4   | 10.62  | 1.41        | 1.33     |
| 35  | BB    | 2733 | A    | C2'-C1' | -10.62 | 1.41        | 1.53     |
| 35  | BB    | 2665 | A    | N7-C5   | -10.62 | 1.32        | 1.39     |
| 35  | BB    | 2825 | G    | C6-N1   | 10.62  | 1.47        | 1.39     |
| 35  | BB    | 2193 | G    | N9-C8   | -10.61 | 1.30        | 1.37     |
| 35  | BB    | 2720 | U    | C2-N3   | 10.61  | 1.45        | 1.37     |
| 1   | AA    | 420  | U    | C2-N3   | 10.61  | 1.45        | 1.37     |
| 1   | AA    | 907  | A    | C6-N6   | 10.61  | 1.42        | 1.33     |
| 35  | BB    | 254  | G    | C8-N7   | -10.61 | 1.24        | 1.30     |
| 35  | BB    | 2109 | U    | C2-N3   | 10.61  | 1.45        | 1.37     |
| 35  | BB    | 1988 | G    | N7-C5   | -10.60 | 1.32        | 1.39     |
| 1   | AA    | 1018 | G    | N3-C4   | -10.60 | 1.28        | 1.35     |
| 35  | BB    | 1803 | A    | N9-C4   | -10.60 | 1.31        | 1.37     |
| 1   | AA    | 833  | G    | C2'-C1' | -10.59 | 1.41        | 1.53     |
| 35  | BB    | 1432 | G    | N7-C5   | -10.59 | 1.32        | 1.39     |
| 35  | BB    | 72   | U    | C2-N3   | 10.59  | 1.45        | 1.37     |
| 35  | BB    | 1519 | G    | N9-C8   | -10.59 | 1.30        | 1.37     |
| 35  | BB    | 317  | G    | N3-C4   | -10.59 | 1.28        | 1.35     |
| 1   | AA    | 1285 | A    | C6-N6   | 10.59  | 1.42        | 1.33     |
| 1   | AA    | 941  | G    | N7-C5   | -10.59 | 1.32        | 1.39     |
| 35  | BB    | 2353 | G    | N7-C5   | -10.59 | 1.32        | 1.39     |
| 35  | BB    | 2430 | A    | C6-N6   | 10.59  | 1.42        | 1.33     |
| 35  | BB    | 2546 | U    | C2-N3   | 10.59  | 1.45        | 1.37     |
| 35  | BB    | 1380 | G    | C8-N7   | 10.58  | 1.37        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | AA    | 922  | G    | N9-C8   | 10.58  | 1.45        | 1.37     |
| 1   | AA    | 1216 | A    | C4'-C3' | -10.58 | 1.41        | 1.53     |
| 35  | BB    | 1136 | G    | C2-N3   | 10.58  | 1.41        | 1.32     |
| 35  | BB    | 1876 | A    | P-O5'   | -10.58 | 1.49        | 1.59     |
| 35  | BB    | 1966 | A    | N7-C5   | -10.58 | 1.32        | 1.39     |
| 35  | BB    | 2838 | G    | N7-C5   | -10.58 | 1.32        | 1.39     |
| 1   | AA    | 953  | G    | P-O5'   | -10.57 | 1.49        | 1.59     |
| 1   | AA    | 467  | U    | N3-C4   | 10.56  | 1.48        | 1.38     |
| 35  | BB    | 1769 | U    | C5'-C4' | 10.56  | 1.64        | 1.51     |
| 35  | BB    | 2665 | A    | C6-N6   | 10.56  | 1.42        | 1.33     |
| 35  | BB    | 2799 | A    | N9-C4   | 10.56  | 1.44        | 1.37     |
| 35  | BB    | 2820 | A    | N3-C4   | 10.56  | 1.41        | 1.34     |
| 35  | BB    | 1361 | G    | C2-N3   | 10.56  | 1.41        | 1.32     |
| 1   | AA    | 1353 | G    | C2-N3   | 10.56  | 1.41        | 1.32     |
| 22  | AV    | 67   | G    | N9-C4   | 10.55  | 1.46        | 1.38     |
| 35  | BB    | 195  | A    | N9-C4   | -10.55 | 1.31        | 1.37     |
| 1   | AA    | 455  | G    | N7-C5   | -10.55 | 1.32        | 1.39     |
| 1   | AA    | 557  | G    | C2-N3   | 10.55  | 1.41        | 1.32     |
| 35  | BB    | 2198 | A    | C8-N7   | -10.55 | 1.24        | 1.31     |
| 1   | AA    | 854  | U    | C2-N3   | 10.55  | 1.45        | 1.37     |
| 35  | BB    | 505  | A    | N9-C4   | -10.54 | 1.31        | 1.37     |
| 35  | BB    | 2311 | A    | C8-N7   | -10.54 | 1.24        | 1.31     |
| 35  | BB    | 1535 | A    | P-O5'   | -10.54 | 1.49        | 1.59     |
| 1   | AA    | 276  | G    | N7-C5   | -10.54 | 1.32        | 1.39     |
| 35  | BB    | 141  | G    | C2-N2   | 10.54  | 1.45        | 1.34     |
| 35  | BB    | 1521 | G    | N7-C5   | -10.54 | 1.32        | 1.39     |
| 1   | AA    | 1272 | G    | N1-C2   | 10.54  | 1.46        | 1.37     |
| 35  | BB    | 259  | G    | N7-C5   | -10.53 | 1.32        | 1.39     |
| 1   | AA    | 309  | A    | N3-C4   | -10.53 | 1.28        | 1.34     |
| 1   | AA    | 276  | G    | P-O5'   | -10.53 | 1.49        | 1.59     |
| 1   | AA    | 1275 | A    | N7-C5   | -10.52 | 1.32        | 1.39     |
| 35  | BB    | 1380 | G    | N7-C5   | -10.52 | 1.32        | 1.39     |
| 1   | AA    | 816  | A    | C5-C4   | 10.52  | 1.46        | 1.38     |
| 35  | BB    | 1382 | G    | N1-C2   | 10.52  | 1.46        | 1.37     |
| 35  | BB    | 1792 | G    | N3-C4   | -10.52 | 1.28        | 1.35     |
| 35  | BB    | 883  | G    | N7-C5   | -10.51 | 1.32        | 1.39     |
| 1   | AA    | 978  | A    | C5-C4   | 10.51  | 1.46        | 1.38     |
| 35  | BB    | 912  | C    | O3'-P   | -10.51 | 1.48        | 1.61     |
| 1   | AA    | 937  | A    | C6-N1   | 10.50  | 1.43        | 1.35     |
| 1   | AA    | 1138 | G    | N3-C4   | 10.50  | 1.42        | 1.35     |
| 35  | BB    | 1551 | A    | O3'-P   | -10.50 | 1.48        | 1.61     |
| 34  | BA    | 12   | C    | O3'-P   | -10.49 | 1.48        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | AA    | 1026 | G    | C2-N3   | 10.49  | 1.41        | 1.32     |
| 35  | BB    | 1686 | C    | N1-C6   | -10.49 | 1.30        | 1.37     |
| 1   | AA    | 74   | A    | C6-N6   | 10.48  | 1.42        | 1.33     |
| 1   | AA    | 705  | G    | C4'-C3' | 10.48  | 1.64        | 1.53     |
| 35  | BB    | 2770 | G    | N1-C2   | 10.48  | 1.46        | 1.37     |
| 35  | BB    | 2332 | C    | N3-C4   | 10.48  | 1.41        | 1.33     |
| 1   | AA    | 1109 | C    | N1-C6   | 10.47  | 1.43        | 1.37     |
| 35  | BB    | 827  | U    | C2-N3   | 10.47  | 1.45        | 1.37     |
| 1   | AA    | 1146 | A    | C5-C4   | -10.47 | 1.31        | 1.38     |
| 35  | BB    | 908  | C    | P-O5'   | -10.47 | 1.49        | 1.59     |
| 35  | BB    | 1401 | G    | N1-C2   | 10.47  | 1.46        | 1.37     |
| 1   | AA    | 1349 | A    | N7-C5   | -10.47 | 1.32        | 1.39     |
| 1   | AA    | 1319 | A    | C6-N6   | 10.46  | 1.42        | 1.33     |
| 35  | BB    | 95   | A    | N3-C4   | 10.46  | 1.41        | 1.34     |
| 35  | BB    | 2068 | U    | C4-C5   | 10.46  | 1.52        | 1.43     |
| 1   | AA    | 210  | C    | C4-N4   | 10.45  | 1.43        | 1.33     |
| 1   | AA    | 724  | G    | C2-N3   | 10.45  | 1.41        | 1.32     |
| 1   | AA    | 1418 | A    | N3-C4   | -10.45 | 1.28        | 1.34     |
| 35  | BB    | 1679 | A    | C8-N7   | -10.45 | 1.24        | 1.31     |
| 35  | BB    | 2037 | A    | C6-N1   | 10.45  | 1.42        | 1.35     |
| 35  | BB    | 1903 | G    | C5-C4   | -10.45 | 1.31        | 1.38     |
| 1   | AA    | 802  | A    | C5-C4   | -10.44 | 1.31        | 1.38     |
| 35  | BB    | 2542 | A    | N7-C5   | -10.44 | 1.32        | 1.39     |
| 35  | BB    | 2842 | G    | N7-C5   | 10.44  | 1.45        | 1.39     |
| 35  | BB    | 2581 | G    | N1-C2   | 10.44  | 1.46        | 1.37     |
| 35  | BB    | 401  | A    | N7-C5   | -10.43 | 1.32        | 1.39     |
| 35  | BB    | 1631 | G    | N1-C2   | 10.43  | 1.46        | 1.37     |
| 35  | BB    | 1850 | G    | C8-N7   | 10.43  | 1.37        | 1.30     |
| 35  | BB    | 491  | G    | C2-N3   | 10.43  | 1.41        | 1.32     |
| 34  | BA    | 118  | C    | N1-C6   | 10.42  | 1.43        | 1.37     |
| 35  | BB    | 2028 | U    | C3'-C2' | -10.42 | 1.41        | 1.52     |
| 1   | AA    | 876  | C    | N3-C4   | 10.42  | 1.41        | 1.33     |
| 35  | BB    | 1204 | A    | N7-C5   | -10.42 | 1.32        | 1.39     |
| 35  | BB    | 1901 | A    | C6-N1   | 10.42  | 1.42        | 1.35     |
| 35  | BB    | 2710 | C    | N1-C6   | -10.42 | 1.30        | 1.37     |
| 1   | AA    | 1007 | U    | N3-C4   | 10.42  | 1.47        | 1.38     |
| 1   | AA    | 1110 | A    | N3-C4   | -10.42 | 1.28        | 1.34     |
| 35  | BB    | 748  | G    | C2-N3   | 10.41  | 1.41        | 1.32     |
| 34  | BA    | 28   | C    | N1-C6   | 10.41  | 1.43        | 1.37     |
| 35  | BB    | 927  | A    | N3-C4   | -10.41 | 1.28        | 1.34     |
| 35  | BB    | 1246 | A    | C6-N6   | 10.41  | 1.42        | 1.33     |
| 1   | AA    | 1267 | C    | N3-C4   | 10.40  | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | AA    | 397  | A    | N3-C4   | -10.40 | 1.28        | 1.34     |
| 35  | BB    | 1373 | A    | C8-N7   | -10.40 | 1.24        | 1.31     |
| 35  | BB    | 1803 | A    | N7-C5   | -10.40 | 1.33        | 1.39     |
| 35  | BB    | 982  | C    | C2-N3   | 10.39  | 1.44        | 1.35     |
| 1   | AA    | 1055 | A    | C8-N7   | -10.39 | 1.24        | 1.31     |
| 1   | AA    | 1429 | A    | N7-C5   | -10.39 | 1.33        | 1.39     |
| 1   | AA    | 335  | C    | O3'-P   | -10.38 | 1.48        | 1.61     |
| 35  | BB    | 1868 | C    | O3'-P   | -10.38 | 1.48        | 1.61     |
| 1   | AA    | 31   | G    | N7-C5   | -10.38 | 1.33        | 1.39     |
| 35  | BB    | 1464 | G    | C2-N3   | 10.38  | 1.41        | 1.32     |
| 1   | AA    | 569  | C    | C2'-C1' | -10.38 | 1.42        | 1.53     |
| 35  | BB    | 1532 | A    | C5-C4   | 10.38  | 1.46        | 1.38     |
| 35  | BB    | 104  | A    | N3-C4   | -10.38 | 1.28        | 1.34     |
| 35  | BB    | 141  | G    | C8-N7   | 10.38  | 1.37        | 1.30     |
| 35  | BB    | 2396 | G    | C2-N3   | 10.38  | 1.41        | 1.32     |
| 35  | BB    | 1694 | C    | N3-C4   | 10.38  | 1.41        | 1.33     |
| 35  | BB    | 799  | G    | N7-C5   | -10.37 | 1.33        | 1.39     |
| 35  | BB    | 1702 | G    | C2-N3   | 10.38  | 1.41        | 1.32     |
| 35  | BB    | 1215 | G    | C5'-C4' | 10.37  | 1.63        | 1.51     |
| 35  | BB    | 600  | G    | C6-N1   | -10.37 | 1.32        | 1.39     |
| 35  | BB    | 51   | G    | C5-C6   | -10.36 | 1.31        | 1.42     |
| 1   | AA    | 1171 | A    | C5-C4   | 10.36  | 1.46        | 1.38     |
| 35  | BB    | 2445 | G    | N1-C2   | 10.36  | 1.46        | 1.37     |
| 35  | BB    | 1763 | G    | N7-C5   | -10.36 | 1.33        | 1.39     |
| 35  | BB    | 75   | G    | N7-C5   | -10.36 | 1.33        | 1.39     |
| 35  | BB    | 2061 | G    | C2-N3   | 10.36  | 1.41        | 1.32     |
| 1   | AA    | 849  | G    | C8-N7   | 10.35  | 1.37        | 1.30     |
| 34  | BA    | 17   | C    | C4-N4   | 10.35  | 1.43        | 1.33     |
| 35  | BB    | 1110 | G    | N7-C5   | -10.34 | 1.33        | 1.39     |
| 35  | BB    | 2432 | A    | N9-C4   | 10.34  | 1.44        | 1.37     |
| 35  | BB    | 1024 | G    | P-O5'   | 10.33  | 1.70        | 1.59     |
| 35  | BB    | 836  | G    | C6-N1   | 10.33  | 1.46        | 1.39     |
| 35  | BB    | 2152 | G    | C6-N1   | 10.33  | 1.46        | 1.39     |
| 35  | BB    | 2322 | A    | C6-N6   | 10.32  | 1.42        | 1.33     |
| 1   | AA    | 138  | G    | C2-N3   | 10.31  | 1.41        | 1.32     |
| 35  | BB    | 106  | C    | C4-C5   | 10.31  | 1.51        | 1.43     |
| 1   | AA    | 119  | A    | C6-N1   | 10.31  | 1.42        | 1.35     |
| 35  | BB    | 2409 | G    | C2-N3   | 10.31  | 1.41        | 1.32     |
| 1   | AA    | 1279 | G    | N7-C5   | -10.30 | 1.33        | 1.39     |
| 35  | BB    | 877  | A    | N7-C5   | -10.30 | 1.33        | 1.39     |
| 35  | BB    | 1653 | G    | N7-C5   | -10.30 | 1.33        | 1.39     |
| 35  | BB    | 2869 | G    | N7-C5   | -10.30 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | AA    | 1437 | A    | C6-N6   | 10.29  | 1.42        | 1.33     |
| 34  | BA    | 58   | A    | C2'-C1' | -10.29 | 1.42        | 1.53     |
| 35  | BB    | 41   | C    | C2-N3   | 10.29  | 1.44        | 1.35     |
| 35  | BB    | 2019 | A    | C5-C4   | 10.29  | 1.46        | 1.38     |
| 35  | BB    | 1803 | A    | C6-N6   | 10.29  | 1.42        | 1.33     |
| 35  | BB    | 2027 | G    | C6-N1   | 10.29  | 1.46        | 1.39     |
| 35  | BB    | 2218 | G    | N9-C8   | 10.29  | 1.45        | 1.37     |
| 1   | AA    | 855  | U    | P-O5'   | -10.29 | 1.49        | 1.59     |
| 35  | BB    | 1362 | C    | P-O5'   | -10.29 | 1.49        | 1.59     |
| 1   | AA    | 111  | G    | N7-C5   | -10.28 | 1.33        | 1.39     |
| 1   | AA    | 1398 | A    | C6-N1   | 10.28  | 1.42        | 1.35     |
| 1   | AA    | 416  | G    | N7-C5   | -10.28 | 1.33        | 1.39     |
| 1   | AA    | 148  | G    | C6-N1   | -10.28 | 1.32        | 1.39     |
| 1   | AA    | 650  | G    | C2-N3   | 10.28  | 1.41        | 1.32     |
| 1   | AA    | 378  | G    | C2-N3   | 10.28  | 1.41        | 1.32     |
| 35  | BB    | 538  | A    | N7-C5   | -10.28 | 1.33        | 1.39     |
| 1   | AA    | 1026 | G    | C4'-C3' | -10.27 | 1.41        | 1.53     |
| 34  | BA    | 54   | G    | N9-C8   | 10.27  | 1.45        | 1.37     |
| 35  | BB    | 2366 | A    | N7-C5   | -10.27 | 1.33        | 1.39     |
| 35  | BB    | 966  | G    | C2-N3   | 10.27  | 1.41        | 1.32     |
| 35  | BB    | 2340 | A    | N7-C5   | -10.26 | 1.33        | 1.39     |
| 35  | BB    | 2    | G    | C2-N3   | 10.26  | 1.41        | 1.32     |
| 35  | BB    | 2060 | A    | N9-C4   | -10.26 | 1.31        | 1.37     |
| 35  | BB    | 761  | A    | C8-N7   | -10.25 | 1.24        | 1.31     |
| 1   | AA    | 65   | A    | C6-N1   | 10.25  | 1.42        | 1.35     |
| 1   | AA    | 1206 | G    | C2-N3   | 10.25  | 1.41        | 1.32     |
| 1   | AA    | 96   | U    | O3'-P   | -10.25 | 1.48        | 1.61     |
| 35  | BB    | 198  | C    | O3'-P   | -10.25 | 1.48        | 1.61     |
| 35  | BB    | 4    | U    | N3-C4   | 10.25  | 1.47        | 1.38     |
| 35  | BB    | 300  | A    | N7-C5   | -10.24 | 1.33        | 1.39     |
| 35  | BB    | 344  | A    | N7-C5   | -10.24 | 1.33        | 1.39     |
| 35  | BB    | 462  | C    | N3-C4   | 10.24  | 1.41        | 1.33     |
| 35  | BB    | 186  | G    | N7-C5   | -10.23 | 1.33        | 1.39     |
| 35  | BB    | 1334 | G    | N9-C8   | -10.23 | 1.30        | 1.37     |
| 35  | BB    | 2371 | G    | C8-N7   | 10.23  | 1.37        | 1.30     |
| 35  | BB    | 2867 | G    | C2-N2   | 10.23  | 1.44        | 1.34     |
| 35  | BB    | 837  | C    | N3-C4   | 10.22  | 1.41        | 1.33     |
| 35  | BB    | 577  | G    | N7-C5   | -10.22 | 1.33        | 1.39     |
| 35  | BB    | 1970 | A    | N3-C4   | -10.22 | 1.28        | 1.34     |
| 34  | BA    | 117  | G    | N7-C5   | -10.21 | 1.33        | 1.39     |
| 35  | BB    | 2397 | G    | N1-C2   | 10.21  | 1.46        | 1.37     |
| 1   | AA    | 1418 | A    | N9-C4   | -10.20 | 1.31        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 35  | BB    | 49   | A    | N9-C4   | 10.21  | 1.44        | 1.37     |
| 35  | BB    | 716  | A    | C6-N6   | 10.20  | 1.42        | 1.33     |
| 35  | BB    | 2448 | A    | N3-C4   | -10.20 | 1.28        | 1.34     |
| 1   | AA    | 406  | G    | N1-C2   | 10.20  | 1.46        | 1.37     |
| 35  | BB    | 830  | G    | N1-C2   | 10.20  | 1.46        | 1.37     |
| 35  | BB    | 2407 | A    | N7-C5   | -10.20 | 1.33        | 1.39     |
| 35  | BB    | 620  | G    | C8-N7   | 10.20  | 1.37        | 1.30     |
| 35  | BB    | 1214 | A    | N7-C5   | -10.20 | 1.33        | 1.39     |
| 1   | AA    | 1375 | A    | P-O5'   | -10.19 | 1.49        | 1.59     |
| 35  | BB    | 1470 | A    | N9-C4   | -10.19 | 1.31        | 1.37     |
| 35  | BB    | 1029 | A    | C6-N6   | 10.18  | 1.42        | 1.33     |
| 35  | BB    | 1129 | A    | C6-N6   | 10.18  | 1.42        | 1.33     |
| 1   | AA    | 417  | G    | N7-C5   | -10.18 | 1.33        | 1.39     |
| 1   | AA    | 666  | G    | N1-C2   | 10.18  | 1.45        | 1.37     |
| 35  | BB    | 1866 | A    | C2'-C1' | -10.18 | 1.42        | 1.53     |
| 1   | AA    | 1533 | C    | N3-C4   | 10.17  | 1.41        | 1.33     |
| 35  | BB    | 730  | A    | C6-N6   | 10.17  | 1.42        | 1.33     |
| 35  | BB    | 2749 | A    | N9-C4   | -10.17 | 1.31        | 1.37     |
| 35  | BB    | 2781 | A    | N3-C4   | -10.17 | 1.28        | 1.34     |
| 1   | AA    | 1167 | A    | C5-C4   | 10.16  | 1.45        | 1.38     |
| 35  | BB    | 17   | G    | C2-N3   | 10.16  | 1.40        | 1.32     |
| 35  | BB    | 281  | C    | N3-C4   | 10.16  | 1.41        | 1.33     |
| 35  | BB    | 1651 | G    | C5-C4   | -10.16 | 1.31        | 1.38     |
| 35  | BB    | 2713 | U    | P-O5'   | 10.16  | 1.70        | 1.59     |
| 1   | AA    | 1220 | G    | N7-C5   | -10.16 | 1.33        | 1.39     |
| 1   | AA    | 1386 | G    | C2'-C1' | -10.16 | 1.42        | 1.53     |
| 35  | BB    | 401  | A    | N3-C4   | 10.16  | 1.41        | 1.34     |
| 35  | BB    | 633  | A    | N7-C5   | -10.16 | 1.33        | 1.39     |
| 35  | BB    | 2566 | A    | N9-C4   | -10.16 | 1.31        | 1.37     |
| 35  | BB    | 2107 | G    | C5-C4   | 10.15  | 1.45        | 1.38     |
| 35  | BB    | 1151 | A    | N9-C4   | 10.15  | 1.44        | 1.37     |
| 35  | BB    | 2097 | A    | N7-C5   | -10.15 | 1.33        | 1.39     |
| 35  | BB    | 2123 | G    | C6-N1   | 10.15  | 1.46        | 1.39     |
| 1   | AA    | 53   | A    | N7-C5   | -10.15 | 1.33        | 1.39     |
| 1   | AA    | 286  | C    | N3-C4   | 10.15  | 1.41        | 1.33     |
| 35  | BB    | 950  | G    | C2-N3   | 10.15  | 1.40        | 1.32     |
| 34  | BA    | 83   | G    | C5-C6   | -10.14 | 1.32        | 1.42     |
| 35  | BB    | 579  | G    | N1-C2   | 10.14  | 1.45        | 1.37     |
| 35  | BB    | 2550 | G    | C2-N3   | 10.14  | 1.40        | 1.32     |
| 1   | AA    | 161  | A    | C6-N1   | 10.14  | 1.42        | 1.35     |
| 35  | BB    | 144  | A    | N9-C4   | 10.14  | 1.44        | 1.37     |
| 35  | BB    | 311  | A    | C6-N1   | 10.14  | 1.42        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 35  | BB    | 186  | G    | C2-N3   | 10.14  | 1.40        | 1.32     |
| 35  | BB    | 466  | A    | N7-C5   | -10.14 | 1.33        | 1.39     |
| 35  | BB    | 2685 | G    | C8-N7   | 10.14  | 1.37        | 1.30     |
| 35  | BB    | 14   | A    | N7-C5   | -10.13 | 1.33        | 1.39     |
| 1   | AA    | 316  | C    | C2-N3   | 10.12  | 1.43        | 1.35     |
| 35  | BB    | 2466 | C    | N3-C4   | 10.12  | 1.41        | 1.33     |
| 35  | BB    | 1237 | A    | N9-C4   | 10.12  | 1.44        | 1.37     |
| 35  | BB    | 2134 | A    | C2'-C1' | -10.12 | 1.42        | 1.53     |
| 1   | AA    | 873  | A    | C6-N6   | 10.12  | 1.42        | 1.33     |
| 35  | BB    | 1902 | C    | C4-N4   | 10.12  | 1.43        | 1.33     |
| 35  | BB    | 2370 | G    | C6-N1   | 10.12  | 1.46        | 1.39     |
| 35  | BB    | 808  | G    | N3-C4   | 10.12  | 1.42        | 1.35     |
| 1   | AA    | 199  | A    | C6-N1   | 10.11  | 1.42        | 1.35     |
| 35  | BB    | 1660 | G    | C2-N3   | 10.11  | 1.40        | 1.32     |
| 1   | AA    | 1139 | G    | N7-C5   | -10.11 | 1.33        | 1.39     |
| 35  | BB    | 989  | G    | C2-N2   | 10.11  | 1.44        | 1.34     |
| 35  | BB    | 784  | G    | C2-N3   | 10.11  | 1.40        | 1.32     |
| 35  | BB    | 315  | G    | N1-C2   | 10.10  | 1.45        | 1.37     |
| 1   | AA    | 1504 | G    | C6-N1   | 10.10  | 1.46        | 1.39     |
| 35  | BB    | 671  | C    | N3-C4   | 10.10  | 1.41        | 1.33     |
| 35  | BB    | 1453 | A    | C6-N6   | 10.10  | 1.42        | 1.33     |
| 35  | BB    | 2341 | G    | C6-N1   | 10.10  | 1.46        | 1.39     |
| 35  | BB    | 2461 | A    | N3-C4   | -10.10 | 1.28        | 1.34     |
| 35  | BB    | 1553 | A    | C6-N6   | 10.10  | 1.42        | 1.33     |
| 35  | BB    | 625  | G    | N9-C8   | -10.09 | 1.30        | 1.37     |
| 35  | BB    | 1995 | U    | N3-C4   | 10.09  | 1.47        | 1.38     |
| 1   | AA    | 1377 | A    | C6-N6   | 10.09  | 1.42        | 1.33     |
| 35  | BB    | 1569 | A    | C6-N6   | 10.09  | 1.42        | 1.33     |
| 35  | BB    | 505  | A    | C6-N6   | 10.09  | 1.42        | 1.33     |
| 35  | BB    | 2535 | G    | C8-N7   | -10.08 | 1.24        | 1.30     |
| 1   | AA    | 786  | G    | C6-N1   | 10.08  | 1.46        | 1.39     |
| 35  | BB    | 808  | G    | N7-C5   | -10.08 | 1.33        | 1.39     |
| 1   | AA    | 1469 | C    | N1-C6   | 10.07  | 1.43        | 1.37     |
| 35  | BB    | 8    | C    | C2-N3   | 10.07  | 1.43        | 1.35     |
| 35  | BB    | 1228 | G    | N3-C4   | -10.07 | 1.28        | 1.35     |
| 1   | AA    | 1094 | G    | N1-C2   | 10.06  | 1.45        | 1.37     |
| 35  | BB    | 403  | U    | C5'-C4' | 10.06  | 1.63        | 1.51     |
| 35  | BB    | 1000 | A    | C6-N1   | 10.06  | 1.42        | 1.35     |
| 35  | BB    | 2088 | A    | N9-C4   | 10.06  | 1.43        | 1.37     |
| 1   | AA    | 10   | A    | N7-C5   | -10.06 | 1.33        | 1.39     |
| 35  | BB    | 861  | A    | C6-N6   | 10.06  | 1.42        | 1.33     |
| 35  | BB    | 1499 | C    | N3-C4   | 10.06  | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 35  | BB    | 934  | U    | C2'-C1' | -10.06 | 1.42        | 1.53     |
| 1   | AA    | 164  | G    | N7-C5   | 10.05  | 1.45        | 1.39     |
| 1   | AA    | 315  | A    | O3'-P   | -10.05 | 1.49        | 1.61     |
| 1   | AA    | 517  | G    | N1-C2   | 10.05  | 1.45        | 1.37     |
| 35  | BB    | 2688 | G    | C2-N3   | 10.05  | 1.40        | 1.32     |
| 1   | AA    | 1077 | G    | N9-C8   | 10.05  | 1.44        | 1.37     |
| 1   | AA    | 1108 | G    | N3-C4   | 10.05  | 1.42        | 1.35     |
| 1   | AA    | 1242 | G    | N1-C2   | 10.05  | 1.45        | 1.37     |
| 35  | BB    | 1526 | C    | N3-C4   | 10.05  | 1.41        | 1.33     |
| 1   | AA    | 701  | U    | C2-N3   | 10.04  | 1.44        | 1.37     |
| 1   | AA    | 1036 | A    | N7-C5   | -10.05 | 1.33        | 1.39     |
| 1   | AA    | 751  | U    | C2-N3   | 10.04  | 1.44        | 1.37     |
| 1   | AA    | 747  | A    | C6-N6   | 10.04  | 1.42        | 1.33     |
| 35  | BB    | 1168 | G    | C3'-C2' | -10.04 | 1.41        | 1.52     |
| 35  | BB    | 1641 | A    | N7-C5   | -10.04 | 1.33        | 1.39     |
| 35  | BB    | 2738 | A    | C6-N6   | 10.03  | 1.42        | 1.33     |
| 1   | AA    | 985  | C    | N1-C6   | 10.03  | 1.43        | 1.37     |
| 35  | BB    | 675  | A    | N7-C5   | -10.03 | 1.33        | 1.39     |
| 35  | BB    | 2013 | A    | N7-C5   | -10.03 | 1.33        | 1.39     |
| 35  | BB    | 2737 | G    | C6-N1   | 10.03  | 1.46        | 1.39     |
| 35  | BB    | 1235 | G    | N7-C5   | -10.02 | 1.33        | 1.39     |
| 1   | AA    | 64   | G    | N9-C8   | 10.02  | 1.44        | 1.37     |
| 1   | AA    | 72   | A    | N7-C5   | -10.02 | 1.33        | 1.39     |
| 35  | BB    | 1737 | G    | N7-C5   | -10.02 | 1.33        | 1.39     |
| 1   | AA    | 762  | U    | N3-C4   | 10.02  | 1.47        | 1.38     |
| 1   | AA    | 852  | G    | C8-N7   | 10.02  | 1.36        | 1.30     |
| 35  | BB    | 1490 | A    | N7-C5   | -10.02 | 1.33        | 1.39     |
| 35  | BB    | 2733 | A    | C6-N6   | 10.01  | 1.42        | 1.33     |
| 1   | AA    | 183  | C    | N1-C6   | 10.01  | 1.43        | 1.37     |
| 1   | AA    | 893  | C    | N3-C4   | 10.01  | 1.41        | 1.33     |
| 35  | BB    | 352  | A    | N3-C4   | -10.01 | 1.28        | 1.34     |
| 35  | BB    | 1025 | G    | C8-N7   | -10.01 | 1.25        | 1.30     |
| 35  | BB    | 1567 | G    | C8-N7   | -10.01 | 1.25        | 1.30     |
| 1   | AA    | 38   | G    | C8-N7   | -10.01 | 1.25        | 1.30     |
| 1   | AA    | 980  | C    | N3-C4   | 10.01  | 1.41        | 1.33     |
| 34  | BA    | 86   | G    | N7-C5   | -10.01 | 1.33        | 1.39     |
| 35  | BB    | 515  | A    | C6-N6   | 10.01  | 1.42        | 1.33     |
| 35  | BB    | 1387 | A    | N3-C4   | -10.01 | 1.28        | 1.34     |
| 35  | BB    | 1792 | G    | C6-N1   | 10.01  | 1.46        | 1.39     |
| 35  | BB    | 1040 | A    | N3-C4   | 10.00  | 1.40        | 1.34     |
| 1   | AA    | 818  | G    | N9-C4   | -10.00 | 1.29        | 1.38     |
| 1   | AA    | 77   | A    | N7-C5   | 10.00  | 1.45        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 35  | BB    | 1276 | A    | C6-N6   | 10.00  | 1.42        | 1.33     |
| 35  | BB    | 2180 | U    | C5-C6   | -10.00 | 1.25        | 1.34     |
| 35  | BB    | 2553 | G    | C2-N3   | 10.00  | 1.40        | 1.32     |
| 1   | AA    | 1260 | G    | C5-C4   | 9.99   | 1.45        | 1.38     |
| 22  | AV    | 37   | G    | C2-N3   | 9.99   | 1.40        | 1.32     |
| 35  | BB    | 423  | A    | C2'-C1' | -9.99  | 1.42        | 1.53     |
| 35  | BB    | 1601 | G    | N7-C5   | -9.99  | 1.33        | 1.39     |
| 35  | BB    | 1794 | A    | C2'-C1' | -9.99  | 1.42        | 1.53     |
| 1   | AA    | 1128 | C    | N1-C6   | 9.98   | 1.43        | 1.37     |
| 35  | BB    | 983  | A    | C6-N6   | 9.98   | 1.42        | 1.33     |
| 22  | AV    | 67   | G    | N7-C5   | 9.98   | 1.45        | 1.39     |
| 35  | BB    | 2466 | C    | N1-C6   | 9.98   | 1.43        | 1.37     |
| 35  | BB    | 2325 | G    | N7-C5   | -9.97  | 1.33        | 1.39     |
| 1   | AA    | 146  | G    | N7-C5   | -9.97  | 1.33        | 1.39     |
| 1   | AA    | 162  | A    | N7-C5   | -9.97  | 1.33        | 1.39     |
| 35  | BB    | 638  | G    | N7-C5   | -9.97  | 1.33        | 1.39     |
| 1   | AA    | 1294 | G    | N7-C5   | -9.97  | 1.33        | 1.39     |
| 1   | AA    | 1065 | U    | O3'-P   | -9.97  | 1.49        | 1.61     |
| 35  | BB    | 2289 | G    | C8-N7   | -9.97  | 1.25        | 1.30     |
| 35  | BB    | 2705 | A    | P-O5'   | -9.96  | 1.49        | 1.59     |
| 35  | BB    | 1534 | U    | N3-C4   | 9.95   | 1.47        | 1.38     |
| 35  | BB    | 1765 | U    | N3-C4   | 9.95   | 1.47        | 1.38     |
| 35  | BB    | 196  | A    | C6-N6   | 9.95   | 1.42        | 1.33     |
| 35  | BB    | 517  | C    | O3'-P   | -9.95  | 1.49        | 1.61     |
| 35  | BB    | 1370 | C    | N3-C4   | 9.95   | 1.41        | 1.33     |
| 35  | BB    | 2523 | G    | N7-C5   | -9.95  | 1.33        | 1.39     |
| 35  | BB    | 2087 | G    | C5-C4   | -9.94  | 1.31        | 1.38     |
| 1   | AA    | 80   | A    | C8-N7   | -9.94  | 1.24        | 1.31     |
| 35  | BB    | 2727 | A    | N7-C5   | -9.94  | 1.33        | 1.39     |
| 1   | AA    | 1421 | G    | C6-N1   | 9.93   | 1.46        | 1.39     |
| 35  | BB    | 2530 | A    | C6-N6   | 9.93   | 1.41        | 1.33     |
| 35  | BB    | 2789 | C    | C4-N4   | 9.93   | 1.42        | 1.33     |
| 1   | AA    | 340  | U    | C2-N3   | 9.93   | 1.44        | 1.37     |
| 34  | BA    | 70   | C    | C4-N4   | 9.93   | 1.42        | 1.33     |
| 35  | BB    | 1861 | G    | C8-N7   | -9.93  | 1.25        | 1.30     |
| 1   | AA    | 1347 | G    | P-O5'   | -9.93  | 1.49        | 1.59     |
| 35  | BB    | 1444 | G    | N1-C2   | 9.93   | 1.45        | 1.37     |
| 1   | AA    | 371  | A    | O3'-P   | -9.93  | 1.49        | 1.61     |
| 35  | BB    | 1348 | C    | N3-C4   | 9.93   | 1.40        | 1.33     |
| 35  | BB    | 1140 | C    | N1-C6   | 9.92   | 1.43        | 1.37     |
| 35  | BB    | 1549 | A    | N9-C4   | -9.92  | 1.31        | 1.37     |
| 35  | BB    | 1580 | A    | N1-C2   | 9.92   | 1.43        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1050 | A    | C6-N1   | 9.92  | 1.42        | 1.35     |
| 34  | BA    | 20   | G    | N3-C4   | -9.92 | 1.28        | 1.35     |
| 34  | BA    | 61   | G    | C2-N3   | 9.92  | 1.40        | 1.32     |
| 35  | BB    | 1983 | G    | C2-N3   | 9.91  | 1.40        | 1.32     |
| 35  | BB    | 2525 | G    | C2-N3   | 9.91  | 1.40        | 1.32     |
| 1   | AA    | 1088 | G    | P-O5'   | -9.91 | 1.49        | 1.59     |
| 35  | BB    | 926  | G    | C2'-C1' | -9.91 | 1.42        | 1.53     |
| 34  | BA    | 16   | G    | C2-N3   | 9.91  | 1.40        | 1.32     |
| 35  | BB    | 2886 | A    | C6-N6   | 9.91  | 1.41        | 1.33     |
| 1   | AA    | 1104 | G    | C6-N1   | 9.91  | 1.46        | 1.39     |
| 35  | BB    | 1794 | A    | N7-C5   | -9.91 | 1.33        | 1.39     |
| 35  | BB    | 611  | C    | C2'-C1' | -9.90 | 1.42        | 1.53     |
| 35  | BB    | 1372 | U    | C2'-C1' | -9.90 | 1.42        | 1.53     |
| 35  | BB    | 2379 | G    | N7-C5   | 9.90  | 1.45        | 1.39     |
| 35  | BB    | 1864 | U    | O3'-P   | -9.90 | 1.49        | 1.61     |
| 35  | BB    | 2004 | G    | C6-N1   | 9.90  | 1.46        | 1.39     |
| 35  | BB    | 250  | G    | C2-N3   | 9.90  | 1.40        | 1.32     |
| 35  | BB    | 2468 | A    | N9-C4   | -9.89 | 1.31        | 1.37     |
| 35  | BB    | 2459 | A    | N9-C4   | 9.89  | 1.43        | 1.37     |
| 35  | BB    | 2718 | G    | N7-C5   | -9.89 | 1.33        | 1.39     |
| 35  | BB    | 2510 | C    | P-O5'   | -9.89 | 1.49        | 1.59     |
| 35  | BB    | 2662 | A    | N7-C5   | -9.89 | 1.33        | 1.39     |
| 1   | AA    | 745  | G    | P-O5'   | -9.88 | 1.49        | 1.59     |
| 1   | AA    | 749  | A    | C6-N1   | 9.88  | 1.42        | 1.35     |
| 1   | AA    | 1061 | G    | N1-C2   | 9.88  | 1.45        | 1.37     |
| 1   | AA    | 1466 | C    | C4-N4   | 9.88  | 1.42        | 1.33     |
| 34  | BA    | 95   | U    | C2-N3   | 9.88  | 1.44        | 1.37     |
| 35  | BB    | 2186 | G    | N1-C2   | 9.88  | 1.45        | 1.37     |
| 35  | BB    | 2808 | G    | C2'-C1' | -9.88 | 1.42        | 1.53     |
| 35  | BB    | 1181 | U    | C2'-C1' | -9.88 | 1.42        | 1.53     |
| 35  | BB    | 1460 | U    | C4-C5   | 9.87  | 1.52        | 1.43     |
| 35  | BB    | 268  | C    | C2-N3   | 9.87  | 1.43        | 1.35     |
| 35  | BB    | 1853 | A    | N7-C5   | -9.87 | 1.33        | 1.39     |
| 35  | BB    | 1326 | U    | O3'-P   | -9.87 | 1.49        | 1.61     |
| 35  | BB    | 971  | G    | N1-C2   | 9.87  | 1.45        | 1.37     |
| 1   | AA    | 128  | G    | N7-C5   | -9.87 | 1.33        | 1.39     |
| 35  | BB    | 829  | A    | C6-N1   | 9.86  | 1.42        | 1.35     |
| 35  | BB    | 1310 | G    | O3'-P   | -9.87 | 1.49        | 1.61     |
| 35  | BB    | 1441 | G    | C8-N7   | 9.87  | 1.36        | 1.30     |
| 35  | BB    | 2447 | G    | C2-N3   | 9.87  | 1.40        | 1.32     |
| 35  | BB    | 2453 | A    | C6-N6   | 9.87  | 1.41        | 1.33     |
| 35  | BB    | 1086 | A    | N9-C4   | -9.86 | 1.31        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1959 | G    | N7-C5   | -9.86 | 1.33        | 1.39     |
| 1   | AA    | 1526 | G    | C2-N3   | 9.86  | 1.40        | 1.32     |
| 1   | AA    | 760  | G    | C2-N3   | 9.85  | 1.40        | 1.32     |
| 1   | AA    | 1297 | G    | C6-N1   | 9.85  | 1.46        | 1.39     |
| 1   | AA    | 1333 | A    | N7-C5   | -9.85 | 1.33        | 1.39     |
| 35  | BB    | 1318 | U    | N3-C4   | 9.85  | 1.47        | 1.38     |
| 35  | BB    | 1376 | C    | P-O5'   | -9.85 | 1.50        | 1.59     |
| 35  | BB    | 1821 | A    | N7-C5   | 9.85  | 1.45        | 1.39     |
| 35  | BB    | 2329 | U    | C3'-C2' | -9.85 | 1.42        | 1.52     |
| 35  | BB    | 666  | A    | C6-N1   | 9.84  | 1.42        | 1.35     |
| 35  | BB    | 957  | C    | N1-C6   | 9.84  | 1.43        | 1.37     |
| 1   | AA    | 697  | U    | C2-N3   | 9.84  | 1.44        | 1.37     |
| 35  | BB    | 218  | A    | N9-C8   | 9.84  | 1.45        | 1.37     |
| 35  | BB    | 335  | C    | N3-C4   | 9.84  | 1.40        | 1.33     |
| 35  | BB    | 711  | G    | N7-C5   | -9.83 | 1.33        | 1.39     |
| 1   | AA    | 1252 | A    | C2-N3   | 9.83  | 1.42        | 1.33     |
| 35  | BB    | 1390 | U    | N3-C4   | 9.83  | 1.47        | 1.38     |
| 35  | BB    | 1205 | A    | C6-N1   | 9.83  | 1.42        | 1.35     |
| 35  | BB    | 1452 | G    | P-O5'   | -9.83 | 1.50        | 1.59     |
| 35  | BB    | 1434 | A    | C6-N1   | 9.83  | 1.42        | 1.35     |
| 1   | AA    | 538  | G    | C6-N1   | 9.82  | 1.46        | 1.39     |
| 35  | BB    | 1341 | G    | C6-N1   | 9.82  | 1.46        | 1.39     |
| 35  | BB    | 2614 | A    | O3'-P   | -9.82 | 1.49        | 1.61     |
| 1   | AA    | 1079 | G    | C2-N3   | 9.82  | 1.40        | 1.32     |
| 35  | BB    | 396  | G    | C2'-C1' | -9.82 | 1.42        | 1.53     |
| 35  | BB    | 2635 | A    | C6-N6   | 9.82  | 1.41        | 1.33     |
| 1   | AA    | 1187 | G    | N7-C5   | -9.81 | 1.33        | 1.39     |
| 35  | BB    | 2086 | U    | N1-C2   | -9.81 | 1.29        | 1.38     |
| 1   | AA    | 521  | G    | N3-C4   | -9.81 | 1.28        | 1.35     |
| 35  | BB    | 119  | A    | N9-C4   | -9.81 | 1.31        | 1.37     |
| 1   | AA    | 739  | C    | C4-N4   | 9.80  | 1.42        | 1.33     |
| 35  | BB    | 632  | A    | N3-C4   | 9.80  | 1.40        | 1.34     |
| 35  | BB    | 1620 | G    | N1-C2   | 9.81  | 1.45        | 1.37     |
| 1   | AA    | 554  | A    | N3-C4   | -9.80 | 1.28        | 1.34     |
| 1   | AA    | 299  | G    | N3-C4   | -9.80 | 1.28        | 1.35     |
| 1   | AA    | 1216 | A    | C5-C6   | -9.80 | 1.32        | 1.41     |
| 35  | BB    | 913  | U    | C2-N3   | 9.80  | 1.44        | 1.37     |
| 35  | BB    | 2555 | U    | C2-N3   | 9.80  | 1.44        | 1.37     |
| 35  | BB    | 2625 | G    | C6-N1   | 9.80  | 1.46        | 1.39     |
| 1   | AA    | 1494 | G    | N9-C8   | 9.80  | 1.44        | 1.37     |
| 1   | AA    | 251  | G    | N9-C8   | 9.79  | 1.44        | 1.37     |
| 35  | BB    | 474  | G    | N7-C5   | -9.79 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 262  | A    | N9-C4   | -9.79 | 1.31        | 1.37     |
| 35  | BB    | 2043 | C    | P-O5'   | -9.79 | 1.50        | 1.59     |
| 35  | BB    | 2404 | U    | C3'-C2' | -9.79 | 1.42        | 1.52     |
| 35  | BB    | 2544 | G    | N1-C2   | 9.78  | 1.45        | 1.37     |
| 35  | BB    | 691  | C    | P-O5'   | -9.78 | 1.50        | 1.59     |
| 35  | BB    | 1889 | A    | N7-C5   | -9.78 | 1.33        | 1.39     |
| 1   | AA    | 1408 | A    | C5-C4   | -9.78 | 1.31        | 1.38     |
| 35  | BB    | 2536 | G    | C6-N1   | 9.78  | 1.46        | 1.39     |
| 1   | AA    | 965  | U    | N3-C4   | 9.77  | 1.47        | 1.38     |
| 35  | BB    | 322  | A    | C6-N1   | 9.77  | 1.42        | 1.35     |
| 35  | BB    | 2196 | C    | N1-C6   | 9.77  | 1.43        | 1.37     |
| 35  | BB    | 2699 | C    | C4-N4   | 9.77  | 1.42        | 1.33     |
| 35  | BB    | 2283 | C    | N3-C4   | 9.77  | 1.40        | 1.33     |
| 35  | BB    | 2887 | A    | C6-N6   | 9.77  | 1.41        | 1.33     |
| 1   | AA    | 300  | A    | N7-C5   | -9.76 | 1.33        | 1.39     |
| 35  | BB    | 753  | A    | N9-C8   | -9.76 | 1.29        | 1.37     |
| 35  | BB    | 879  | G    | N9-C8   | 9.76  | 1.44        | 1.37     |
| 35  | BB    | 1853 | A    | C5-C4   | 9.76  | 1.45        | 1.38     |
| 1   | AA    | 312  | C    | N3-C4   | 9.76  | 1.40        | 1.33     |
| 1   | AA    | 1289 | A    | N7-C5   | -9.76 | 1.33        | 1.39     |
| 35  | BB    | 1047 | G    | N3-C4   | -9.76 | 1.28        | 1.35     |
| 35  | BB    | 1697 | G    | C5-C4   | 9.76  | 1.45        | 1.38     |
| 35  | BB    | 2570 | G    | N9-C8   | 9.76  | 1.44        | 1.37     |
| 1   | AA    | 181  | A    | N3-C4   | -9.76 | 1.28        | 1.34     |
| 35  | BB    | 2140 | G    | N7-C5   | -9.76 | 1.33        | 1.39     |
| 35  | BB    | 2721 | A    | C6-N1   | 9.75  | 1.42        | 1.35     |
| 1   | AA    | 911  | U    | C4'-C3' | 9.75  | 1.63        | 1.53     |
| 34  | BA    | 105  | G    | C6-N1   | 9.75  | 1.46        | 1.39     |
| 35  | BB    | 2085 | U    | C2-N3   | 9.75  | 1.44        | 1.37     |
| 22  | AV    | 70   | C    | N1-C6   | 9.75  | 1.43        | 1.37     |
| 35  | BB    | 256  | A    | C5-C4   | 9.75  | 1.45        | 1.38     |
| 35  | BB    | 283  | G    | N7-C5   | -9.75 | 1.33        | 1.39     |
| 35  | BB    | 2753 | A    | C6-N6   | 9.75  | 1.41        | 1.33     |
| 35  | BB    | 1935 | G    | N7-C5   | -9.75 | 1.33        | 1.39     |
| 35  | BB    | 180  | G    | C6-N1   | 9.74  | 1.46        | 1.39     |
| 35  | BB    | 2585 | U    | O3'-P   | -9.74 | 1.49        | 1.61     |
| 1   | AA    | 1150 | A    | C8-N7   | -9.74 | 1.24        | 1.31     |
| 35  | BB    | 1115 | G    | C5-C4   | -9.74 | 1.31        | 1.38     |
| 35  | BB    | 647  | G    | C8-N7   | 9.74  | 1.36        | 1.30     |
| 35  | BB    | 1356 | G    | C6-N1   | 9.74  | 1.46        | 1.39     |
| 35  | BB    | 1519 | G    | C6-N1   | 9.74  | 1.46        | 1.39     |
| 22  | AV    | 5    | A    | N7-C5   | -9.73 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 523  | C    | N1-C6   | 9.73  | 1.43        | 1.37     |
| 1   | AA    | 362  | G    | C2-N3   | 9.73  | 1.40        | 1.32     |
| 1   | AA    | 1137 | C    | C2-N3   | 9.73  | 1.43        | 1.35     |
| 35  | BB    | 2245 | U    | C4-O4   | 9.73  | 1.31        | 1.23     |
| 35  | BB    | 2663 | G    | N1-C2   | 9.73  | 1.45        | 1.37     |
| 35  | BB    | 1814 | G    | C6-N1   | 9.72  | 1.46        | 1.39     |
| 35  | BB    | 1858 | A    | C5-C6   | -9.72 | 1.32        | 1.41     |
| 35  | BB    | 302  | C    | C3'-C2' | -9.72 | 1.42        | 1.52     |
| 35  | BB    | 1298 | C    | P-O5'   | -9.72 | 1.50        | 1.59     |
| 35  | BB    | 2761 | A    | N7-C5   | -9.72 | 1.33        | 1.39     |
| 1   | AA    | 108  | G    | N7-C5   | -9.72 | 1.33        | 1.39     |
| 1   | AA    | 1044 | A    | N3-C4   | 9.72  | 1.40        | 1.34     |
| 35  | BB    | 1369 | G    | C2-N3   | 9.72  | 1.40        | 1.32     |
| 35  | BB    | 570  | G    | C2-N3   | 9.72  | 1.40        | 1.32     |
| 35  | BB    | 1293 | C    | C2'-C1' | -9.71 | 1.42        | 1.53     |
| 35  | BB    | 845  | A    | C6-N6   | 9.71  | 1.41        | 1.33     |
| 35  | BB    | 1410 | G    | C2-N3   | 9.71  | 1.40        | 1.32     |
| 35  | BB    | 1103 | A    | N7-C5   | -9.71 | 1.33        | 1.39     |
| 1   | AA    | 450  | G    | C6-N1   | 9.71  | 1.46        | 1.39     |
| 35  | BB    | 2670 | A    | C6-N6   | 9.71  | 1.41        | 1.33     |
| 35  | BB    | 2382 | G    | C8-N7   | 9.71  | 1.36        | 1.30     |
| 35  | BB    | 1529 | G    | C2-N3   | 9.70  | 1.40        | 1.32     |
| 35  | BB    | 1344 | U    | N3-C4   | 9.70  | 1.47        | 1.38     |
| 1   | AA    | 1024 | G    | C2-N2   | 9.70  | 1.44        | 1.34     |
| 35  | BB    | 1445 | G    | C2'-C1' | -9.70 | 1.42        | 1.53     |
| 35  | BB    | 2659 | G    | C2-N3   | 9.70  | 1.40        | 1.32     |
| 1   | AA    | 753  | A    | C6-N1   | 9.69  | 1.42        | 1.35     |
| 35  | BB    | 2066 | C    | N3-C4   | 9.69  | 1.40        | 1.33     |
| 1   | AA    | 608  | A    | N7-C5   | -9.69 | 1.33        | 1.39     |
| 35  | BB    | 1373 | A    | N3-C4   | -9.69 | 1.29        | 1.34     |
| 35  | BB    | 288  | U    | C5'-C4' | 9.69  | 1.62        | 1.51     |
| 35  | BB    | 1251 | C    | N3-C4   | 9.69  | 1.40        | 1.33     |
| 35  | BB    | 2693 | G    | N1-C2   | 9.69  | 1.45        | 1.37     |
| 35  | BB    | 414  | C    | C2'-C1' | -9.69 | 1.42        | 1.53     |
| 35  | BB    | 2890 | G    | N1-C2   | 9.68  | 1.45        | 1.37     |
| 35  | BB    | 480  | A    | N7-C5   | -9.68 | 1.33        | 1.39     |
| 35  | BB    | 506  | G    | N7-C5   | 9.68  | 1.45        | 1.39     |
| 35  | BB    | 1210 | G    | P-O5'   | 9.68  | 1.69        | 1.59     |
| 35  | BB    | 1550 | C    | P-O5'   | -9.68 | 1.50        | 1.59     |
| 35  | BB    | 415  | A    | N9-C4   | 9.68  | 1.43        | 1.37     |
| 35  | BB    | 1157 | G    | N9-C4   | 9.68  | 1.45        | 1.38     |
| 1   | AA    | 487  | A    | N9-C4   | -9.67 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34  | BA    | 110  | C    | C4-C5   | 9.67  | 1.50        | 1.43     |
| 35  | BB    | 2076 | U    | O3'-P   | -9.67 | 1.49        | 1.61     |
| 35  | BB    | 2484 | G    | C8-N7   | 9.67  | 1.36        | 1.30     |
| 35  | BB    | 2490 | G    | N3-C4   | -9.67 | 1.28        | 1.35     |
| 1   | AA    | 1476 | A    | C6-N6   | 9.67  | 1.41        | 1.33     |
| 1   | AA    | 1482 | G    | C2-N3   | 9.67  | 1.40        | 1.32     |
| 34  | BA    | 27   | C    | N1-C6   | 9.67  | 1.43        | 1.37     |
| 35  | BB    | 2557 | G    | N9-C8   | 9.67  | 1.44        | 1.37     |
| 1   | AA    | 1414 | U    | C2-N3   | 9.66  | 1.44        | 1.37     |
| 35  | BB    | 2242 | G    | N1-C2   | 9.66  | 1.45        | 1.37     |
| 35  | BB    | 2470 | G    | N1-C2   | 9.66  | 1.45        | 1.37     |
| 1   | AA    | 768  | A    | C6-N6   | 9.66  | 1.41        | 1.33     |
| 35  | BB    | 514  | A    | N7-C5   | -9.66 | 1.33        | 1.39     |
| 1   | AA    | 476  | U    | C2-N3   | 9.66  | 1.44        | 1.37     |
| 1   | AA    | 983  | A    | N3-C4   | -9.66 | 1.29        | 1.34     |
| 1   | AA    | 1141 | C    | N3-C4   | 9.66  | 1.40        | 1.33     |
| 35  | BB    | 2228 | G    | N7-C5   | -9.66 | 1.33        | 1.39     |
| 35  | BB    | 2708 | G    | C6-N1   | 9.66  | 1.46        | 1.39     |
| 1   | AA    | 346  | G    | N3-C4   | 9.65  | 1.42        | 1.35     |
| 35  | BB    | 1427 | A    | N7-C5   | -9.65 | 1.33        | 1.39     |
| 35  | BB    | 972  | A    | C6-N6   | 9.65  | 1.41        | 1.33     |
| 35  | BB    | 1127 | A    | C5-C4   | 9.65  | 1.45        | 1.38     |
| 35  | BB    | 1722 | A    | C8-N7   | -9.65 | 1.24        | 1.31     |
| 1   | AA    | 1474 | U    | C2-O2   | 9.65  | 1.31        | 1.22     |
| 35  | BB    | 2734 | A    | C6-N6   | 9.65  | 1.41        | 1.33     |
| 1   | AA    | 83   | C    | N3-C4   | 9.65  | 1.40        | 1.33     |
| 1   | AA    | 1504 | G    | N3-C4   | -9.65 | 1.28        | 1.35     |
| 35  | BB    | 2692 | G    | N7-C5   | -9.64 | 1.33        | 1.39     |
| 1   | AA    | 157  | U    | C2-N3   | 9.64  | 1.44        | 1.37     |
| 1   | AA    | 1271 | A    | N9-C4   | 9.64  | 1.43        | 1.37     |
| 35  | BB    | 504  | A    | C6-N1   | 9.64  | 1.42        | 1.35     |
| 35  | BB    | 671  | C    | C2-N3   | 9.64  | 1.43        | 1.35     |
| 35  | BB    | 1445 | G    | N1-C2   | 9.64  | 1.45        | 1.37     |
| 1   | AA    | 1441 | A    | O4'-C1' | 9.64  | 1.54        | 1.41     |
| 35  | BB    | 271  | G    | C2'-C1' | -9.64 | 1.42        | 1.53     |
| 35  | BB    | 1823 | G    | N1-C2   | 9.64  | 1.45        | 1.37     |
| 35  | BB    | 53   | A    | N9-C4   | 9.63  | 1.43        | 1.37     |
| 35  | BB    | 2829 | A    | C5-C4   | -9.63 | 1.32        | 1.38     |
| 1   | AA    | 1111 | A    | N7-C5   | -9.63 | 1.33        | 1.39     |
| 1   | AA    | 1077 | G    | N1-C2   | 9.63  | 1.45        | 1.37     |
| 1   | AA    | 1504 | G    | C2-N3   | 9.62  | 1.40        | 1.32     |
| 35  | BB    | 391  | A    | N9-C4   | 9.62  | 1.43        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2352 | A    | C6-N6   | 9.62  | 1.41        | 1.33     |
| 35  | BB    | 319  | G    | C6-N1   | 9.62  | 1.46        | 1.39     |
| 1   | AA    | 888  | G    | C6-N1   | 9.61  | 1.46        | 1.39     |
| 35  | BB    | 274  | C    | C4-N4   | 9.61  | 1.42        | 1.33     |
| 1   | AA    | 444  | G    | C4'-C3' | 9.60  | 1.63        | 1.53     |
| 1   | AA    | 1111 | A    | N3-C4   | -9.60 | 1.29        | 1.34     |
| 1   | AA    | 741  | G    | N3-C4   | 9.60  | 1.42        | 1.35     |
| 35  | BB    | 1873 | G    | N7-C5   | -9.60 | 1.33        | 1.39     |
| 35  | BB    | 1077 | A    | N3-C4   | -9.60 | 1.29        | 1.34     |
| 1   | AA    | 167  | A    | N9-C4   | 9.60  | 1.43        | 1.37     |
| 1   | AA    | 596  | A    | C8-N7   | -9.60 | 1.24        | 1.31     |
| 35  | BB    | 995  | C    | N3-C4   | 9.60  | 1.40        | 1.33     |
| 35  | BB    | 1269 | A    | N7-C5   | -9.60 | 1.33        | 1.39     |
| 35  | BB    | 1587 | G    | N7-C5   | -9.60 | 1.33        | 1.39     |
| 1   | AA    | 832  | G    | C5'-C4' | 9.59  | 1.62        | 1.51     |
| 35  | BB    | 1757 | A    | C5-C4   | 9.59  | 1.45        | 1.38     |
| 1   | AA    | 949  | A    | N7-C5   | -9.59 | 1.33        | 1.39     |
| 35  | BB    | 1475 | G    | N1-C2   | 9.59  | 1.45        | 1.37     |
| 35  | BB    | 2327 | A    | N3-C4   | -9.59 | 1.29        | 1.34     |
| 35  | BB    | 1350 | C    | C2-N3   | -9.59 | 1.28        | 1.35     |
| 1   | AA    | 997  | U    | C5'-C4' | 9.59  | 1.62        | 1.51     |
| 35  | BB    | 2389 | G    | N1-C2   | 9.59  | 1.45        | 1.37     |
| 1   | AA    | 1188 | A    | C6-N6   | 9.58  | 1.41        | 1.33     |
| 35  | BB    | 690  | G    | C2'-C1' | -9.58 | 1.42        | 1.53     |
| 35  | BB    | 2434 | A    | C5'-C4' | 9.58  | 1.62        | 1.51     |
| 1   | AA    | 275  | G    | N7-C5   | -9.58 | 1.33        | 1.39     |
| 35  | BB    | 73   | A    | N3-C4   | -9.58 | 1.29        | 1.34     |
| 35  | BB    | 896  | A    | N7-C5   | 9.58  | 1.45        | 1.39     |
| 35  | BB    | 32   | C    | C3'-C2' | 9.57  | 1.63        | 1.52     |
| 35  | BB    | 852  | U    | P-O5'   | -9.57 | 1.50        | 1.59     |
| 35  | BB    | 855  | G    | N1-C2   | 9.57  | 1.45        | 1.37     |
| 35  | BB    | 1254 | A    | C6-N1   | 9.57  | 1.42        | 1.35     |
| 35  | BB    | 447  | A    | N7-C5   | -9.57 | 1.33        | 1.39     |
| 35  | BB    | 718  | A    | C6-N1   | 9.57  | 1.42        | 1.35     |
| 35  | BB    | 1684 | G    | N9-C8   | 9.57  | 1.44        | 1.37     |
| 1   | AA    | 800  | G    | C2'-C1' | -9.57 | 1.42        | 1.53     |
| 35  | BB    | 138  | U    | P-O5'   | 9.57  | 1.69        | 1.59     |
| 35  | BB    | 638  | G    | N3-C4   | -9.57 | 1.28        | 1.35     |
| 35  | BB    | 2077 | A    | N9-C4   | -9.56 | 1.32        | 1.37     |
| 35  | BB    | 2867 | G    | C2-N3   | 9.56  | 1.40        | 1.32     |
| 1   | AA    | 751  | U    | C3'-C2' | -9.56 | 1.42        | 1.52     |
| 1   | AA    | 317  | U    | C2'-C1' | -9.56 | 1.42        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 916  | G    | N9-C4   | 9.56  | 1.45        | 1.38     |
| 35  | BB    | 6    | A    | C5-C4   | -9.56 | 1.32        | 1.38     |
| 35  | BB    | 1056 | G    | C5-C6   | -9.56 | 1.32        | 1.42     |
| 1   | AA    | 1492 | A    | N7-C5   | -9.55 | 1.33        | 1.39     |
| 35  | BB    | 2810 | A    | P-O5'   | -9.55 | 1.50        | 1.59     |
| 1   | AA    | 16   | A    | C6-N6   | 9.55  | 1.41        | 1.33     |
| 35  | BB    | 393  | C    | C5'-C4' | 9.55  | 1.62        | 1.51     |
| 35  | BB    | 733  | G    | C6-N1   | 9.55  | 1.46        | 1.39     |
| 35  | BB    | 2209 | G    | C5-C4   | -9.55 | 1.31        | 1.38     |
| 35  | BB    | 824  | U    | P-O5'   | -9.55 | 1.50        | 1.59     |
| 35  | BB    | 633  | A    | N3-C4   | -9.55 | 1.29        | 1.34     |
| 1   | AA    | 1200 | C    | N3-C4   | 9.55  | 1.40        | 1.33     |
| 35  | BB    | 1229 | C    | N3-C4   | 9.55  | 1.40        | 1.33     |
| 35  | BB    | 992  | C    | N3-C4   | 9.54  | 1.40        | 1.33     |
| 1   | AA    | 97   | G    | N7-C5   | -9.54 | 1.33        | 1.39     |
| 1   | AA    | 203  | G    | N7-C5   | -9.54 | 1.33        | 1.39     |
| 1   | AA    | 1439 | G    | C8-N7   | -9.54 | 1.25        | 1.30     |
| 34  | BA    | 81   | G    | N1-C2   | 9.54  | 1.45        | 1.37     |
| 35  | BB    | 99   | U    | C2-N3   | 9.54  | 1.44        | 1.37     |
| 35  | BB    | 1216 | G    | C2'-C1' | -9.54 | 1.42        | 1.53     |
| 35  | BB    | 555  | G    | N7-C5   | -9.54 | 1.33        | 1.39     |
| 1   | AA    | 908  | A    | C3'-C2' | 9.54  | 1.63        | 1.52     |
| 35  | BB    | 805  | G    | C2'-C1' | -9.53 | 1.42        | 1.53     |
| 35  | BB    | 1098 | A    | N7-C5   | -9.54 | 1.33        | 1.39     |
| 1   | AA    | 835  | U    | P-O5'   | -9.53 | 1.50        | 1.59     |
| 35  | BB    | 2151 | U    | N3-C4   | 9.53  | 1.47        | 1.38     |
| 1   | AA    | 64   | G    | C2-N3   | 9.53  | 1.40        | 1.32     |
| 1   | AA    | 1381 | U    | N1-C2   | 9.53  | 1.47        | 1.38     |
| 35  | BB    | 1178 | C    | N1-C6   | 9.53  | 1.42        | 1.37     |
| 35  | BB    | 1273 | U    | P-O5'   | 9.53  | 1.69        | 1.59     |
| 35  | BB    | 1665 | A    | C6-N1   | 9.53  | 1.42        | 1.35     |
| 35  | BB    | 1686 | C    | O3'-P   | -9.53 | 1.49        | 1.61     |
| 35  | BB    | 2675 | A    | N7-C5   | -9.52 | 1.33        | 1.39     |
| 1   | AA    | 990  | C    | N3-C4   | 9.52  | 1.40        | 1.33     |
| 1   | AA    | 1154 | G    | N7-C5   | -9.52 | 1.33        | 1.39     |
| 34  | BA    | 106  | G    | N1-C2   | 9.52  | 1.45        | 1.37     |
| 35  | BB    | 2585 | U    | C2-N3   | 9.52  | 1.44        | 1.37     |
| 35  | BB    | 1784 | A    | N7-C5   | -9.52 | 1.33        | 1.39     |
| 35  | BB    | 2394 | C    | C4-C5   | 9.52  | 1.50        | 1.43     |
| 1   | AA    | 1054 | C    | C4-C5   | 9.51  | 1.50        | 1.43     |
| 1   | AA    | 1459 | G    | N3-C4   | 9.51  | 1.42        | 1.35     |
| 1   | AA    | 1313 | U    | C2'-C1' | -9.51 | 1.42        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 364  | A    | C6-N1   | 9.51  | 1.42        | 1.35     |
| 1   | AA    | 474  | G    | N3-C4   | -9.51 | 1.28        | 1.35     |
| 35  | BB    | 1750 | G    | C8-N7   | -9.51 | 1.25        | 1.30     |
| 35  | BB    | 2455 | G    | P-O5'   | -9.51 | 1.50        | 1.59     |
| 1   | AA    | 658  | C    | P-O5'   | -9.50 | 1.50        | 1.59     |
| 1   | AA    | 1034 | G    | C2-N3   | 9.50  | 1.40        | 1.32     |
| 35  | BB    | 909  | A    | N9-C8   | 9.50  | 1.45        | 1.37     |
| 35  | BB    | 1776 | G    | C2-N3   | 9.50  | 1.40        | 1.32     |
| 35  | BB    | 327  | G    | C2-N2   | 9.50  | 1.44        | 1.34     |
| 35  | BB    | 2290 | G    | C2-N3   | 9.50  | 1.40        | 1.32     |
| 1   | AA    | 338  | A    | C2'-C1' | -9.50 | 1.43        | 1.53     |
| 35  | BB    | 1144 | A    | C6-N1   | 9.50  | 1.42        | 1.35     |
| 1   | AA    | 434  | U    | N1-C2   | 9.49  | 1.47        | 1.38     |
| 1   | AA    | 1522 | U    | N3-C4   | 9.49  | 1.47        | 1.38     |
| 35  | BB    | 1670 | C    | N1-C6   | 9.49  | 1.42        | 1.37     |
| 35  | BB    | 2636 | C    | N1-C6   | 9.49  | 1.42        | 1.37     |
| 35  | BB    | 621  | A    | P-O5'   | -9.49 | 1.50        | 1.59     |
| 35  | BB    | 1308 | A    | N3-C4   | 9.49  | 1.40        | 1.34     |
| 35  | BB    | 1069 | A    | N7-C5   | -9.49 | 1.33        | 1.39     |
| 1   | AA    | 149  | A    | N9-C4   | 9.49  | 1.43        | 1.37     |
| 1   | AA    | 490  | C    | C4'-O4' | 9.49  | 1.57        | 1.45     |
| 1   | AA    | 1026 | G    | C5-C6   | 9.49  | 1.51        | 1.42     |
| 1   | AA    | 1253 | G    | N1-C2   | 9.48  | 1.45        | 1.37     |
| 35  | BB    | 763  | G    | N9-C8   | -9.48 | 1.31        | 1.37     |
| 35  | BB    | 1603 | A    | C6-N1   | 9.48  | 1.42        | 1.35     |
| 1   | AA    | 1250 | A    | N7-C5   | -9.48 | 1.33        | 1.39     |
| 35  | BB    | 1945 | G    | N7-C5   | -9.48 | 1.33        | 1.39     |
| 1   | AA    | 1187 | G    | C5-C4   | 9.48  | 1.45        | 1.38     |
| 35  | BB    | 1218 | G    | C8-N7   | 9.48  | 1.36        | 1.30     |
| 1   | AA    | 148  | G    | C8-N7   | 9.47  | 1.36        | 1.30     |
| 35  | BB    | 407  | G    | N9-C4   | -9.47 | 1.30        | 1.38     |
| 35  | BB    | 2788 | C    | C4-N4   | 9.47  | 1.42        | 1.33     |
| 22  | AV    | 73   | A    | N7-C5   | -9.47 | 1.33        | 1.39     |
| 35  | BB    | 1861 | G    | C6-N1   | 9.47  | 1.46        | 1.39     |
| 35  | BB    | 394  | C    | P-O5'   | -9.47 | 1.50        | 1.59     |
| 35  | BB    | 627  | A    | C6-N6   | 9.46  | 1.41        | 1.33     |
| 35  | BB    | 2733 | A    | P-O5'   | -9.46 | 1.50        | 1.59     |
| 35  | BB    | 319  | G    | C2-N3   | 9.46  | 1.40        | 1.32     |
| 35  | BB    | 470  | A    | N7-C5   | -9.46 | 1.33        | 1.39     |
| 1   | AA    | 1047 | G    | N9-C8   | -9.46 | 1.31        | 1.37     |
| 1   | AA    | 1236 | A    | C4'-C3' | 9.46  | 1.63        | 1.53     |
| 35  | BB    | 1322 | A    | N9-C4   | -9.46 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1341 | U    | C2-N3   | 9.45  | 1.44        | 1.37     |
| 35  | BB    | 2010 | G    | C6-N1   | 9.46  | 1.46        | 1.39     |
| 35  | BB    | 2481 | G    | C2-N2   | 9.46  | 1.44        | 1.34     |
| 35  | BB    | 220  | G    | C2-N3   | 9.45  | 1.40        | 1.32     |
| 35  | BB    | 1556 | C    | N1-C6   | 9.45  | 1.42        | 1.37     |
| 34  | BA    | 4    | C    | C2-N3   | 9.45  | 1.43        | 1.35     |
| 35  | BB    | 729  | G    | N1-C2   | 9.45  | 1.45        | 1.37     |
| 35  | BB    | 1110 | G    | C6-N1   | 9.45  | 1.46        | 1.39     |
| 1   | AA    | 1346 | A    | C8-N7   | 9.45  | 1.38        | 1.31     |
| 35  | BB    | 990  | A    | C6-N1   | 9.45  | 1.42        | 1.35     |
| 35  | BB    | 2778 | A    | N9-C4   | 9.45  | 1.43        | 1.37     |
| 1   | AA    | 7    | A    | N7-C5   | -9.45 | 1.33        | 1.39     |
| 1   | AA    | 1300 | G    | C5'-C4' | 9.45  | 1.62        | 1.51     |
| 34  | BA    | 5    | U    | C2-N3   | 9.45  | 1.44        | 1.37     |
| 35  | BB    | 1755 | A    | N3-C4   | 9.45  | 1.40        | 1.34     |
| 35  | BB    | 1028 | A    | N7-C5   | -9.44 | 1.33        | 1.39     |
| 35  | BB    | 706  | A    | N7-C5   | -9.44 | 1.33        | 1.39     |
| 35  | BB    | 1743 | G    | C2-N3   | 9.44  | 1.40        | 1.32     |
| 1   | AA    | 722  | G    | N7-C5   | -9.44 | 1.33        | 1.39     |
| 35  | BB    | 2613 | U    | C2-N3   | 9.44  | 1.44        | 1.37     |
| 1   | AA    | 220  | G    | N3-C4   | -9.44 | 1.28        | 1.35     |
| 1   | AA    | 1331 | G    | P-O5'   | -9.44 | 1.50        | 1.59     |
| 34  | BA    | 53   | A    | N3-C4   | -9.44 | 1.29        | 1.34     |
| 35  | BB    | 317  | G    | N7-C5   | -9.44 | 1.33        | 1.39     |
| 1   | AA    | 696  | A    | C8-N7   | -9.43 | 1.25        | 1.31     |
| 1   | AA    | 780  | A    | C6-N1   | 9.43  | 1.42        | 1.35     |
| 35  | BB    | 308  | G    | N7-C5   | -9.43 | 1.33        | 1.39     |
| 35  | BB    | 2722 | G    | C2-N3   | 9.43  | 1.40        | 1.32     |
| 35  | BB    | 2025 | C    | N1-C6   | -9.43 | 1.31        | 1.37     |
| 1   | AA    | 236  | A    | N7-C5   | -9.43 | 1.33        | 1.39     |
| 1   | AA    | 614  | C    | N3-C4   | 9.43  | 1.40        | 1.33     |
| 35  | BB    | 1829 | A    | N7-C5   | -9.43 | 1.33        | 1.39     |
| 1   | AA    | 443  | C    | C4-N4   | 9.43  | 1.42        | 1.33     |
| 35  | BB    | 259  | G    | C3'-C2' | 9.43  | 1.63        | 1.52     |
| 35  | BB    | 377  | G    | N1-C2   | 9.43  | 1.45        | 1.37     |
| 35  | BB    | 1497 | U    | N3-C4   | 9.43  | 1.47        | 1.38     |
| 35  | BB    | 1436 | G    | N7-C5   | -9.42 | 1.33        | 1.39     |
| 1   | AA    | 793  | U    | P-O5'   | -9.42 | 1.50        | 1.59     |
| 35  | BB    | 288  | U    | N3-C4   | 9.42  | 1.47        | 1.38     |
| 35  | BB    | 947  | A    | N3-C4   | 9.42  | 1.40        | 1.34     |
| 35  | BB    | 1755 | A    | N7-C5   | -9.42 | 1.33        | 1.39     |
| 35  | BB    | 1823 | G    | C5-C6   | -9.42 | 1.32        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1948 | G    | O3'-P   | -9.42 | 1.49        | 1.61     |
| 35  | BB    | 2589 | A    | N7-C5   | -9.42 | 1.33        | 1.39     |
| 35  | BB    | 2764 | A    | C5-C4   | 9.42  | 1.45        | 1.38     |
| 1   | AA    | 447  | G    | N9-C8   | 9.42  | 1.44        | 1.37     |
| 35  | BB    | 214  | G    | N7-C5   | -9.42 | 1.33        | 1.39     |
| 1   | AA    | 621  | A    | C6-N1   | 9.42  | 1.42        | 1.35     |
| 35  | BB    | 1693 | U    | C4'-C3' | 9.41  | 1.63        | 1.53     |
| 1   | AA    | 710  | G    | N9-C4   | -9.41 | 1.30        | 1.38     |
| 35  | BB    | 1974 | C    | C4-C5   | 9.41  | 1.50        | 1.43     |
| 35  | BB    | 2091 | C    | O3'-P   | -9.41 | 1.49        | 1.61     |
| 1   | AA    | 757  | U    | C2-N3   | 9.41  | 1.44        | 1.37     |
| 35  | BB    | 598  | U    | C2-N3   | 9.41  | 1.44        | 1.37     |
| 35  | BB    | 779  | U    | C4-C5   | 9.41  | 1.52        | 1.43     |
| 35  | BB    | 1187 | G    | N7-C5   | -9.41 | 1.33        | 1.39     |
| 35  | BB    | 1470 | A    | N7-C5   | -9.41 | 1.33        | 1.39     |
| 35  | BB    | 2273 | A    | N7-C5   | -9.41 | 1.33        | 1.39     |
| 1   | AA    | 60   | A    | N3-C4   | -9.41 | 1.29        | 1.34     |
| 1   | AA    | 1251 | A    | N3-C4   | -9.41 | 1.29        | 1.34     |
| 1   | AA    | 409  | U    | C2-N3   | 9.40  | 1.44        | 1.37     |
| 35  | BB    | 188  | G    | C8-N7   | -9.40 | 1.25        | 1.30     |
| 1   | AA    | 780  | A    | N9-C4   | 9.40  | 1.43        | 1.37     |
| 35  | BB    | 1213 | A    | N7-C5   | -9.40 | 1.33        | 1.39     |
| 1   | AA    | 1310 | G    | C2'-C1' | -9.40 | 1.43        | 1.53     |
| 1   | AA    | 329  | A    | N7-C5   | -9.40 | 1.33        | 1.39     |
| 1   | AA    | 951  | G    | N7-C5   | 9.40  | 1.44        | 1.39     |
| 1   | AA    | 993  | G    | C5-C4   | 9.40  | 1.45        | 1.38     |
| 35  | BB    | 1826 | G    | N9-C4   | -9.40 | 1.30        | 1.38     |
| 35  | BB    | 2031 | A    | N3-C4   | -9.40 | 1.29        | 1.34     |
| 35  | BB    | 1505 | A    | C6-N1   | 9.40  | 1.42        | 1.35     |
| 35  | BB    | 1960 | A    | C6-N6   | 9.40  | 1.41        | 1.33     |
| 35  | BB    | 2388 | A    | C4'-C3' | -9.39 | 1.42        | 1.53     |
| 1   | AA    | 416  | G    | N3-C4   | -9.39 | 1.28        | 1.35     |
| 34  | BA    | 74   | U    | O3'-P   | -9.39 | 1.49        | 1.61     |
| 35  | BB    | 659  | G    | N9-C8   | 9.39  | 1.44        | 1.37     |
| 1   | AA    | 322  | C    | C2-N3   | 9.39  | 1.43        | 1.35     |
| 35  | BB    | 23   | G    | C5-C6   | -9.39 | 1.32        | 1.42     |
| 35  | BB    | 471  | A    | N7-C5   | -9.39 | 1.33        | 1.39     |
| 1   | AA    | 560  | A    | C8-N7   | -9.38 | 1.25        | 1.31     |
| 34  | BA    | 29   | A    | N7-C5   | -9.38 | 1.33        | 1.39     |
| 35  | BB    | 460  | A    | N7-C5   | -9.38 | 1.33        | 1.39     |
| 1   | AA    | 1119 | C    | N3-C4   | 9.38  | 1.40        | 1.33     |
| 35  | BB    | 801  | G    | C2-N3   | 9.38  | 1.40        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2781 | A    | C6-N6   | 9.37  | 1.41        | 1.33     |
| 35  | BB    | 959  | A    | C6-N1   | 9.37  | 1.42        | 1.35     |
| 35  | BB    | 2047 | C    | N3-C4   | 9.37  | 1.40        | 1.33     |
| 35  | BB    | 36   | G    | C2'-C1' | -9.37 | 1.43        | 1.53     |
| 35  | BB    | 1668 | A    | N9-C4   | -9.37 | 1.32        | 1.37     |
| 1   | AA    | 112  | G    | N7-C5   | -9.37 | 1.33        | 1.39     |
| 1   | AA    | 974  | A    | C5-C4   | -9.37 | 1.32        | 1.38     |
| 34  | BA    | 43   | C    | C4-C5   | 9.37  | 1.50        | 1.43     |
| 35  | BB    | 7    | G    | C6-N1   | 9.36  | 1.46        | 1.39     |
| 35  | BB    | 1566 | A    | N1-C2   | 9.37  | 1.42        | 1.34     |
| 1   | AA    | 311  | C    | C4-N4   | 9.36  | 1.42        | 1.33     |
| 35  | BB    | 2110 | G    | N1-C2   | 9.36  | 1.45        | 1.37     |
| 1   | AA    | 11   | G    | N9-C8   | 9.36  | 1.44        | 1.37     |
| 35  | BB    | 429  | A    | C6-N1   | 9.36  | 1.42        | 1.35     |
| 1   | AA    | 297  | G    | N7-C5   | -9.36 | 1.33        | 1.39     |
| 1   | AA    | 1213 | A    | C5'-C4' | 9.36  | 1.62        | 1.51     |
| 35  | BB    | 367  | G    | C2-N3   | 9.36  | 1.40        | 1.32     |
| 35  | BB    | 474  | G    | C2'-C1' | -9.36 | 1.43        | 1.53     |
| 35  | BB    | 1856 | U    | C4'-C3' | 9.36  | 1.63        | 1.53     |
| 1   | AA    | 1252 | A    | N3-C4   | -9.35 | 1.29        | 1.34     |
| 1   | AA    | 1391 | U    | C3'-C2' | 9.35  | 1.63        | 1.52     |
| 35  | BB    | 2023 | C    | C2-N3   | -9.35 | 1.28        | 1.35     |
| 1   | AA    | 1175 | G    | C5-C4   | 9.35  | 1.44        | 1.38     |
| 35  | BB    | 216  | A    | N3-C4   | -9.35 | 1.29        | 1.34     |
| 34  | BA    | 29   | A    | C8-N7   | -9.35 | 1.25        | 1.31     |
| 35  | BB    | 1930 | G    | N7-C5   | -9.35 | 1.33        | 1.39     |
| 35  | BB    | 2480 | C    | C4-C5   | 9.35  | 1.50        | 1.43     |
| 1   | AA    | 479  | U    | P-O5'   | -9.35 | 1.50        | 1.59     |
| 35  | BB    | 2680 | U    | N3-C4   | 9.35  | 1.46        | 1.38     |
| 1   | AA    | 1081 | A    | C6-N1   | 9.34  | 1.42        | 1.35     |
| 1   | AA    | 1453 | G    | N1-C2   | 9.34  | 1.45        | 1.37     |
| 35  | BB    | 2740 | A    | N3-C4   | -9.34 | 1.29        | 1.34     |
| 35  | BB    | 343  | C    | N1-C6   | 9.34  | 1.42        | 1.37     |
| 35  | BB    | 391  | A    | C8-N7   | -9.34 | 1.25        | 1.31     |
| 1   | AA    | 917  | G    | C8-N7   | 9.34  | 1.36        | 1.30     |
| 1   | AA    | 1365 | G    | C5-C4   | -9.34 | 1.31        | 1.38     |
| 22  | AV    | 1    | C    | C2-N3   | 9.34  | 1.43        | 1.35     |
| 35  | BB    | 507  | A    | C8-N7   | 9.34  | 1.38        | 1.31     |
| 35  | BB    | 1120 | G    | C2-N3   | 9.34  | 1.40        | 1.32     |
| 1   | AA    | 566  | G    | N1-C2   | 9.34  | 1.45        | 1.37     |
| 35  | BB    | 1186 | G    | C8-N7   | -9.34 | 1.25        | 1.30     |
| 1   | AA    | 654  | G    | C2-N3   | 9.33  | 1.40        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2350 | C    | C4-C5   | 9.33  | 1.50        | 1.43     |
| 1   | AA    | 298  | A    | N3-C4   | 9.33  | 1.40        | 1.34     |
| 35  | BB    | 2401 | U    | P-O5'   | -9.33 | 1.50        | 1.59     |
| 35  | BB    | 478  | A    | N7-C5   | -9.33 | 1.33        | 1.39     |
| 35  | BB    | 2657 | A    | N7-C5   | -9.33 | 1.33        | 1.39     |
| 35  | BB    | 1037 | G    | C2-N3   | 9.32  | 1.40        | 1.32     |
| 35  | BB    | 1968 | G    | C6-N1   | 9.32  | 1.46        | 1.39     |
| 35  | BB    | 2020 | A    | C6-N6   | 9.32  | 1.41        | 1.33     |
| 1   | AA    | 122  | G    | N9-C8   | -9.32 | 1.31        | 1.37     |
| 1   | AA    | 896  | C    | N1-C6   | 9.32  | 1.42        | 1.37     |
| 35  | BB    | 1042 | G    | N3-C4   | -9.31 | 1.28        | 1.35     |
| 35  | BB    | 1443 | U    | N3-C4   | 9.31  | 1.46        | 1.38     |
| 1   | AA    | 1011 | C    | C2-N3   | 9.31  | 1.43        | 1.35     |
| 35  | BB    | 1030 | C    | N3-C4   | 9.31  | 1.40        | 1.33     |
| 35  | BB    | 979  | A    | P-O5'   | -9.31 | 1.50        | 1.59     |
| 35  | BB    | 1964 | G    | N7-C5   | -9.31 | 1.33        | 1.39     |
| 35  | BB    | 2406 | A    | N7-C5   | -9.31 | 1.33        | 1.39     |
| 35  | BB    | 2574 | G    | N1-C2   | 9.31  | 1.45        | 1.37     |
| 1   | AA    | 863  | U    | C2-N3   | 9.31  | 1.44        | 1.37     |
| 35  | BB    | 1418 | G    | C2-N2   | 9.31  | 1.43        | 1.34     |
| 1   | AA    | 382  | A    | O3'-P   | -9.30 | 1.50        | 1.61     |
| 1   | AA    | 645  | G    | C2-N3   | 9.30  | 1.40        | 1.32     |
| 35  | BB    | 696  | G    | C2-N3   | 9.30  | 1.40        | 1.32     |
| 35  | BB    | 1618 | A    | C2'-C1' | -9.30 | 1.43        | 1.53     |
| 35  | BB    | 2253 | G    | N1-C2   | 9.30  | 1.45        | 1.37     |
| 35  | BB    | 1292 | G    | C2-N3   | 9.30  | 1.40        | 1.32     |
| 35  | BB    | 2532 | G    | N3-C4   | -9.30 | 1.28        | 1.35     |
| 35  | BB    | 2547 | A    | N7-C5   | -9.30 | 1.33        | 1.39     |
| 35  | BB    | 144  | A    | P-O5'   | -9.30 | 1.50        | 1.59     |
| 1   | AA    | 683  | G    | N3-C4   | -9.30 | 1.28        | 1.35     |
| 35  | BB    | 1298 | C    | C5'-C4' | 9.30  | 1.62        | 1.51     |
| 1   | AA    | 649  | A    | N3-C4   | -9.30 | 1.29        | 1.34     |
| 35  | BB    | 476  | G    | P-O5'   | -9.29 | 1.50        | 1.59     |
| 35  | BB    | 1969 | A    | C8-N7   | -9.29 | 1.25        | 1.31     |
| 35  | BB    | 2846 | G    | N1-C2   | 9.29  | 1.45        | 1.37     |
| 35  | BB    | 2127 | G    | C2-N3   | 9.29  | 1.40        | 1.32     |
| 1   | AA    | 204  | G    | C2-N3   | 9.29  | 1.40        | 1.32     |
| 1   | AA    | 216  | U    | O4'-C1' | 9.29  | 1.53        | 1.41     |
| 1   | AA    | 521  | G    | N1-C2   | 9.29  | 1.45        | 1.37     |
| 35  | BB    | 523  | C    | N3-C4   | 9.29  | 1.40        | 1.33     |
| 35  | BB    | 2479 | U    | C2-N3   | 9.29  | 1.44        | 1.37     |
| 1   | AA    | 987  | G    | C6-N1   | 9.28  | 1.46        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1528 | A    | N3-C4   | -9.29 | 1.29        | 1.34     |
| 1   | AA    | 868  | C    | C4-C5   | -9.28 | 1.35        | 1.43     |
| 1   | AA    | 1421 | G    | C8-N7   | 9.28  | 1.36        | 1.30     |
| 1   | AA    | 460  | A    | N3-C4   | -9.28 | 1.29        | 1.34     |
| 35  | BB    | 425  | G    | C2'-C1' | -9.28 | 1.43        | 1.53     |
| 35  | BB    | 1650 | A    | C6-N6   | 9.28  | 1.41        | 1.33     |
| 35  | BB    | 1720 | U    | C2-N3   | 9.28  | 1.44        | 1.37     |
| 1   | AA    | 489  | C    | C4-N4   | 9.27  | 1.42        | 1.33     |
| 1   | AA    | 813  | U    | C4-C5   | 9.27  | 1.51        | 1.43     |
| 1   | AA    | 581  | G    | C2-N3   | 9.27  | 1.40        | 1.32     |
| 1   | AA    | 1287 | A    | P-O5'   | 9.27  | 1.69        | 1.59     |
| 34  | BA    | 100  | G    | C2-N3   | 9.27  | 1.40        | 1.32     |
| 35  | BB    | 1122 | G    | O3'-P   | -9.27 | 1.50        | 1.61     |
| 35  | BB    | 1781 | U    | C2'-C1' | -9.27 | 1.43        | 1.53     |
| 35  | BB    | 1797 | G    | N1-C2   | 9.27  | 1.45        | 1.37     |
| 35  | BB    | 1961 | C    | C5-C6   | -9.27 | 1.26        | 1.34     |
| 35  | BB    | 2371 | G    | C4'-C3' | -9.27 | 1.43        | 1.53     |
| 35  | BB    | 2542 | A    | N9-C8   | -9.27 | 1.30        | 1.37     |
| 1   | AA    | 1152 | A    | N9-C4   | -9.27 | 1.32        | 1.37     |
| 35  | BB    | 1825 | U    | C2-N3   | 9.27  | 1.44        | 1.37     |
| 1   | AA    | 79   | G    | O4'-C1' | 9.27  | 1.53        | 1.41     |
| 1   | AA    | 382  | A    | N9-C8   | -9.27 | 1.30        | 1.37     |
| 1   | AA    | 1197 | A    | N9-C4   | 9.27  | 1.43        | 1.37     |
| 1   | AA    | 1366 | C    | N1-C6   | 9.27  | 1.42        | 1.37     |
| 35  | BB    | 1530 | G    | C5-C4   | 9.27  | 1.44        | 1.38     |
| 35  | BB    | 2791 | G    | N7-C5   | -9.27 | 1.33        | 1.39     |
| 1   | AA    | 509  | A    | P-O5'   | -9.26 | 1.50        | 1.59     |
| 35  | BB    | 122  | G    | P-O5'   | -9.26 | 1.50        | 1.59     |
| 35  | BB    | 178  | G    | N7-C5   | -9.26 | 1.33        | 1.39     |
| 35  | BB    | 412  | A    | N7-C5   | -9.26 | 1.33        | 1.39     |
| 35  | BB    | 2274 | A    | N7-C5   | -9.26 | 1.33        | 1.39     |
| 1   | AA    | 816  | A    | P-O5'   | -9.26 | 1.50        | 1.59     |
| 1   | AA    | 1290 | G    | N1-C2   | 9.26  | 1.45        | 1.37     |
| 35  | BB    | 2234 | G    | C2-N3   | 9.26  | 1.40        | 1.32     |
| 35  | BB    | 1938 | A    | N9-C4   | -9.26 | 1.32        | 1.37     |
| 1   | AA    | 1194 | U    | C2-N3   | 9.26  | 1.44        | 1.37     |
| 1   | AA    | 1292 | G    | C8-N7   | -9.26 | 1.25        | 1.30     |
| 1   | AA    | 499  | A    | C2-N3   | 9.25  | 1.41        | 1.33     |
| 1   | AA    | 1386 | G    | C5-C6   | -9.25 | 1.33        | 1.42     |
| 35  | BB    | 2613 | U    | C4'-C3' | 9.25  | 1.63        | 1.53     |
| 1   | AA    | 236  | A    | N1-C2   | 9.25  | 1.42        | 1.34     |
| 35  | BB    | 2564 | A    | O3'-P   | -9.25 | 1.50        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 801  | U    | C5-C6   | -9.25 | 1.25        | 1.34     |
| 1   | AA    | 1516 | G    | N7-C5   | -9.25 | 1.33        | 1.39     |
| 35  | BB    | 2497 | A    | C6-N6   | 9.25  | 1.41        | 1.33     |
| 35  | BB    | 938  | G    | N7-C5   | -9.24 | 1.33        | 1.39     |
| 35  | BB    | 1177 | G    | N7-C5   | -9.24 | 1.33        | 1.39     |
| 35  | BB    | 2363 | G    | C6-N1   | 9.24  | 1.46        | 1.39     |
| 1   | AA    | 1249 | C    | C4-C5   | 9.24  | 1.50        | 1.43     |
| 35  | BB    | 15   | G    | N7-C5   | -9.24 | 1.33        | 1.39     |
| 35  | BB    | 2882 | A    | N7-C5   | -9.24 | 1.33        | 1.39     |
| 34  | BA    | 51   | G    | N9-C8   | 9.23  | 1.44        | 1.37     |
| 35  | BB    | 753  | A    | C8-N7   | -9.23 | 1.25        | 1.31     |
| 35  | BB    | 1429 | G    | N1-C2   | 9.23  | 1.45        | 1.37     |
| 35  | BB    | 1224 | U    | C2'-C1' | -9.23 | 1.43        | 1.53     |
| 1   | AA    | 444  | G    | N3-C4   | 9.23  | 1.42        | 1.35     |
| 35  | BB    | 1301 | A    | C6-N1   | 9.23  | 1.42        | 1.35     |
| 1   | AA    | 544  | G    | C8-N7   | 9.22  | 1.36        | 1.30     |
| 35  | BB    | 183  | C    | P-O5'   | 9.22  | 1.69        | 1.59     |
| 1   | AA    | 1140 | C    | C4-C5   | -9.22 | 1.35        | 1.43     |
| 1   | AA    | 1343 | G    | N7-C5   | 9.22  | 1.44        | 1.39     |
| 35  | BB    | 333  | G    | C2-N3   | 9.22  | 1.40        | 1.32     |
| 35  | BB    | 1749 | A    | C2'-C1' | -9.22 | 1.43        | 1.53     |
| 35  | BB    | 2112 | G    | C8-N7   | 9.22  | 1.36        | 1.30     |
| 35  | BB    | 463  | G    | C6-N1   | 9.22  | 1.46        | 1.39     |
| 35  | BB    | 1389 | G    | C2'-C1' | -9.22 | 1.43        | 1.53     |
| 1   | AA    | 657  | U    | C2-N3   | 9.22  | 1.44        | 1.37     |
| 35  | BB    | 72   | U    | N3-C4   | 9.22  | 1.46        | 1.38     |
| 35  | BB    | 618  | G    | C8-N7   | -9.22 | 1.25        | 1.30     |
| 35  | BB    | 690  | G    | C8-N7   | 9.22  | 1.36        | 1.30     |
| 35  | BB    | 1664 | A    | P-O5'   | -9.22 | 1.50        | 1.59     |
| 35  | BB    | 2047 | C    | C2'-C1' | -9.22 | 1.43        | 1.53     |
| 35  | BB    | 299  | A    | N7-C5   | -9.22 | 1.33        | 1.39     |
| 35  | BB    | 2310 | C    | C5'-C4' | 9.22  | 1.62        | 1.51     |
| 35  | BB    | 2406 | A    | C2'-C1' | -9.22 | 1.43        | 1.53     |
| 35  | BB    | 2712 | C    | C2-N3   | 9.21  | 1.43        | 1.35     |
| 1   | AA    | 248  | C    | N3-C4   | 9.21  | 1.40        | 1.33     |
| 1   | AA    | 179  | A    | C6-N1   | 9.21  | 1.42        | 1.35     |
| 1   | AA    | 1255 | G    | N7-C5   | -9.21 | 1.33        | 1.39     |
| 35  | BB    | 590  | A    | N7-C5   | 9.21  | 1.44        | 1.39     |
| 1   | AA    | 1292 | G    | C2-N3   | 9.21  | 1.40        | 1.32     |
| 1   | AA    | 1108 | G    | N9-C4   | -9.21 | 1.30        | 1.38     |
| 1   | AA    | 1226 | C    | C3'-C2' | -9.21 | 1.42        | 1.52     |
| 1   | AA    | 1344 | C    | N3-C4   | 9.21  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1032 | G    | C6-N1   | 9.21  | 1.46        | 1.39     |
| 1   | AA    | 1422 | G    | N1-C2   | 9.21  | 1.45        | 1.37     |
| 35  | BB    | 460  | A    | C2'-C1' | -9.21 | 1.43        | 1.53     |
| 35  | BB    | 2430 | A    | N7-C5   | -9.21 | 1.33        | 1.39     |
| 35  | BB    | 1288 | G    | N9-C4   | 9.20  | 1.45        | 1.38     |
| 35  | BB    | 1310 | G    | N7-C5   | -9.20 | 1.33        | 1.39     |
| 35  | BB    | 1682 | G    | N3-C4   | 9.20  | 1.41        | 1.35     |
| 35  | BB    | 259  | G    | C5-C6   | -9.19 | 1.33        | 1.42     |
| 35  | BB    | 2860 | A    | C8-N7   | -9.19 | 1.25        | 1.31     |
| 1   | AA    | 311  | C    | N3-C4   | 9.19  | 1.40        | 1.33     |
| 1   | AA    | 1241 | G    | N3-C4   | -9.19 | 1.29        | 1.35     |
| 35  | BB    | 1907 | G    | N9-C8   | 9.19  | 1.44        | 1.37     |
| 1   | AA    | 211  | G    | N1-C2   | 9.19  | 1.45        | 1.37     |
| 1   | AA    | 352  | C    | C4-C5   | 9.19  | 1.50        | 1.43     |
| 35  | BB    | 2311 | A    | O3'-P   | -9.19 | 1.50        | 1.61     |
| 35  | BB    | 1635 | A    | C2'-C1' | -9.18 | 1.43        | 1.53     |
| 1   | AA    | 30   | U    | C2-N3   | 9.18  | 1.44        | 1.37     |
| 35  | BB    | 1264 | A    | N7-C5   | -9.18 | 1.33        | 1.39     |
| 1   | AA    | 1404 | C    | C4-N4   | 9.18  | 1.42        | 1.33     |
| 35  | BB    | 1567 | G    | C6-N1   | 9.18  | 1.46        | 1.39     |
| 35  | BB    | 1958 | C    | C4-C5   | 9.18  | 1.50        | 1.43     |
| 35  | BB    | 703  | U    | C2-N3   | 9.17  | 1.44        | 1.37     |
| 35  | BB    | 2618 | G    | C2-N3   | 9.17  | 1.40        | 1.32     |
| 1   | AA    | 1057 | G    | N1-C2   | 9.17  | 1.45        | 1.37     |
| 35  | BB    | 798  | G    | C2-N3   | 9.17  | 1.40        | 1.32     |
| 35  | BB    | 1879 | C    | N3-C4   | 9.17  | 1.40        | 1.33     |
| 35  | BB    | 2790 | U    | N1-C6   | 9.17  | 1.46        | 1.38     |
| 1   | AA    | 974  | A    | N9-C4   | 9.17  | 1.43        | 1.37     |
| 35  | BB    | 149  | A    | N7-C5   | -9.16 | 1.33        | 1.39     |
| 35  | BB    | 1770 | G    | N9-C8   | 9.16  | 1.44        | 1.37     |
| 35  | BB    | 400  | G    | N7-C5   | -9.16 | 1.33        | 1.39     |
| 35  | BB    | 1355 | G    | N7-C5   | -9.16 | 1.33        | 1.39     |
| 35  | BB    | 2646 | C    | N1-C6   | 9.16  | 1.42        | 1.37     |
| 35  | BB    | 2740 | A    | C5-C6   | 9.16  | 1.49        | 1.41     |
| 1   | AA    | 1442 | G    | C2-N3   | 9.16  | 1.40        | 1.32     |
| 35  | BB    | 1508 | A    | P-O5'   | -9.16 | 1.50        | 1.59     |
| 35  | BB    | 2217 | G    | N7-C5   | -9.16 | 1.33        | 1.39     |
| 35  | BB    | 2388 | A    | N7-C5   | -9.16 | 1.33        | 1.39     |
| 1   | AA    | 435  | A    | N7-C5   | -9.15 | 1.33        | 1.39     |
| 35  | BB    | 1533 | C    | C2-N3   | 9.15  | 1.43        | 1.35     |
| 1   | AA    | 463  | U    | C4-C5   | 9.15  | 1.51        | 1.43     |
| 1   | AA    | 973  | G    | N7-C5   | 9.15  | 1.44        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1062 | U    | P-O5'   | -9.15 | 1.50        | 1.59     |
| 35  | BB    | 2523 | G    | N1-C2   | 9.15  | 1.45        | 1.37     |
| 35  | BB    | 1156 | A    | N7-C5   | -9.15 | 1.33        | 1.39     |
| 35  | BB    | 1233 | C    | C2'-C1' | -9.15 | 1.43        | 1.53     |
| 1   | AA    | 184  | G    | C2-N3   | 9.15  | 1.40        | 1.32     |
| 35  | BB    | 849  | A    | C6-N6   | 9.15  | 1.41        | 1.33     |
| 35  | BB    | 1424 | G    | N9-C8   | 9.15  | 1.44        | 1.37     |
| 35  | BB    | 2736 | A    | N7-C5   | -9.15 | 1.33        | 1.39     |
| 35  | BB    | 179  | C    | N3-C4   | 9.14  | 1.40        | 1.33     |
| 35  | BB    | 359  | G    | P-O5'   | -9.14 | 1.50        | 1.59     |
| 35  | BB    | 445  | C    | O3'-P   | -9.14 | 1.50        | 1.61     |
| 1   | AA    | 363  | A    | N7-C5   | -9.14 | 1.33        | 1.39     |
| 35  | BB    | 220  | G    | N7-C5   | -9.14 | 1.33        | 1.39     |
| 35  | BB    | 513  | A    | N7-C5   | -9.14 | 1.33        | 1.39     |
| 35  | BB    | 2531 | A    | N7-C5   | -9.14 | 1.33        | 1.39     |
| 35  | BB    | 2626 | C    | N1-C6   | -9.14 | 1.31        | 1.37     |
| 1   | AA    | 938  | A    | N7-C5   | -9.13 | 1.33        | 1.39     |
| 35  | BB    | 484  | C    | C2-N3   | 9.13  | 1.43        | 1.35     |
| 35  | BB    | 1760 | C    | C5'-C4' | 9.13  | 1.62        | 1.51     |
| 35  | BB    | 2369 | A    | P-O5'   | -9.13 | 1.50        | 1.59     |
| 1   | AA    | 575  | G    | C2-N2   | 9.13  | 1.43        | 1.34     |
| 1   | AA    | 111  | G    | N1-C2   | 9.13  | 1.45        | 1.37     |
| 35  | BB    | 2092 | U    | P-O5'   | -9.13 | 1.50        | 1.59     |
| 35  | BB    | 2713 | U    | N3-C4   | 9.13  | 1.46        | 1.38     |
| 1   | AA    | 328  | C    | O3'-P   | -9.12 | 1.50        | 1.61     |
| 35  | BB    | 773  | U    | P-O5'   | -9.13 | 1.50        | 1.59     |
| 1   | AA    | 1334 | G    | N1-C2   | 9.12  | 1.45        | 1.37     |
| 35  | BB    | 996  | A    | C4'-C3' | 9.12  | 1.63        | 1.53     |
| 35  | BB    | 2006 | C    | P-O5'   | -9.12 | 1.50        | 1.59     |
| 1   | AA    | 1417 | G    | C2-N3   | 9.12  | 1.40        | 1.32     |
| 35  | BB    | 583  | G    | N9-C8   | 9.12  | 1.44        | 1.37     |
| 35  | BB    | 729  | G    | N3-C4   | -9.12 | 1.29        | 1.35     |
| 35  | BB    | 2059 | A    | C6-N6   | 9.12  | 1.41        | 1.33     |
| 1   | AA    | 654  | G    | N3-C4   | -9.12 | 1.29        | 1.35     |
| 1   | AA    | 1131 | G    | N7-C5   | -9.12 | 1.33        | 1.39     |
| 1   | AA    | 1385 | G    | C2-N3   | 9.12  | 1.40        | 1.32     |
| 1   | AA    | 424  | G    | N7-C5   | -9.12 | 1.33        | 1.39     |
| 35  | BB    | 244  | A    | C6-N6   | 9.12  | 1.41        | 1.33     |
| 35  | BB    | 259  | G    | N9-C8   | -9.12 | 1.31        | 1.37     |
| 1   | AA    | 629  | A    | P-O5'   | 9.11  | 1.68        | 1.59     |
| 35  | BB    | 937  | C    | C2'-C1' | -9.11 | 1.43        | 1.53     |
| 1   | AA    | 1145 | A    | C6-N1   | 9.11  | 1.42        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1957 | C    | P-O5'   | -9.11 | 1.50        | 1.59     |
| 35  | BB    | 712  | G    | N9-C8   | 9.11  | 1.44        | 1.37     |
| 1   | AA    | 1096 | C    | N1-C6   | 9.11  | 1.42        | 1.37     |
| 35  | BB    | 699  | A    | C6-N1   | 9.11  | 1.42        | 1.35     |
| 1   | AA    | 1304 | G    | N7-C5   | -9.11 | 1.33        | 1.39     |
| 35  | BB    | 694  | U    | C2'-C1' | -9.11 | 1.43        | 1.53     |
| 35  | BB    | 2758 | A    | C5-C6   | -9.11 | 1.32        | 1.41     |
| 35  | BB    | 1238 | G    | N7-C5   | -9.11 | 1.33        | 1.39     |
| 35  | BB    | 325  | G    | N1-C2   | 9.10  | 1.45        | 1.37     |
| 35  | BB    | 1515 | A    | N9-C4   | -9.10 | 1.32        | 1.37     |
| 35  | BB    | 2614 | A    | N7-C5   | -9.10 | 1.33        | 1.39     |
| 1   | AA    | 723  | U    | C2-N3   | 9.10  | 1.44        | 1.37     |
| 1   | AA    | 927  | G    | C2-N3   | 9.10  | 1.40        | 1.32     |
| 35  | BB    | 963  | U    | C5'-C4' | 9.10  | 1.62        | 1.51     |
| 35  | BB    | 1560 | G    | N7-C5   | -9.10 | 1.33        | 1.39     |
| 1   | AA    | 572  | A    | N9-C4   | -9.10 | 1.32        | 1.37     |
| 1   | AA    | 838  | G    | N1-C2   | 9.10  | 1.45        | 1.37     |
| 35  | BB    | 1059 | G    | P-O5'   | -9.10 | 1.50        | 1.59     |
| 1   | AA    | 1513 | A    | C6-N6   | 9.10  | 1.41        | 1.33     |
| 35  | BB    | 1080 | A    | N7-C5   | -9.10 | 1.33        | 1.39     |
| 35  | BB    | 2028 | U    | C2'-C1' | -9.10 | 1.43        | 1.53     |
| 34  | BA    | 61   | G    | O3'-P   | -9.09 | 1.50        | 1.61     |
| 1   | AA    | 148  | G    | N7-C5   | -9.09 | 1.33        | 1.39     |
| 1   | AA    | 654  | G    | C8-N7   | -9.09 | 1.25        | 1.30     |
| 1   | AA    | 1253 | G    | C2-N3   | 9.09  | 1.40        | 1.32     |
| 1   | AA    | 1011 | C    | C4'-C3' | -9.09 | 1.43        | 1.53     |
| 1   | AA    | 803  | G    | N7-C5   | -9.09 | 1.33        | 1.39     |
| 35  | BB    | 733  | G    | N9-C8   | 9.09  | 1.44        | 1.37     |
| 35  | BB    | 1710 | G    | C2'-C1' | -9.09 | 1.43        | 1.53     |
| 35  | BB    | 503  | A    | N3-C4   | -9.08 | 1.29        | 1.34     |
| 1   | AA    | 1054 | C    | C4-N4   | 9.08  | 1.42        | 1.33     |
| 34  | BA    | 37   | C    | N1-C6   | 9.08  | 1.42        | 1.37     |
| 1   | AA    | 207  | C    | C4-N4   | 9.08  | 1.42        | 1.33     |
| 1   | AA    | 717  | U    | C4-C5   | 9.08  | 1.51        | 1.43     |
| 35  | BB    | 172  | A    | N7-C5   | -9.08 | 1.33        | 1.39     |
| 1   | AA    | 1256 | A    | C6-N6   | 9.08  | 1.41        | 1.33     |
| 1   | AA    | 1441 | A    | N9-C4   | -9.08 | 1.32        | 1.37     |
| 35  | BB    | 173  | A    | C8-N7   | 9.08  | 1.38        | 1.31     |
| 35  | BB    | 1099 | G    | N1-C2   | 9.08  | 1.45        | 1.37     |
| 35  | BB    | 1196 | C    | N3-C4   | 9.08  | 1.40        | 1.33     |
| 35  | BB    | 2191 | A    | C4'-O4' | -9.08 | 1.33        | 1.45     |
| 35  | BB    | 2623 | G    | C2-N3   | 9.08  | 1.40        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 80   | A    | C6-N6   | 9.07  | 1.41        | 1.33     |
| 1   | AA    | 1204 | A    | C5-C4   | 9.07  | 1.45        | 1.38     |
| 35  | BB    | 2693 | G    | P-O5'   | -9.07 | 1.50        | 1.59     |
| 35  | BB    | 237  | C    | N3-C4   | 9.07  | 1.40        | 1.33     |
| 35  | BB    | 530  | G    | C8-N7   | -9.07 | 1.25        | 1.30     |
| 35  | BB    | 1215 | G    | N1-C2   | 9.07  | 1.45        | 1.37     |
| 35  | BB    | 1481 | U    | C4'-C3' | -9.07 | 1.43        | 1.53     |
| 35  | BB    | 216  | A    | C6-N1   | 9.07  | 1.41        | 1.35     |
| 35  | BB    | 1551 | A    | N3-C4   | -9.07 | 1.29        | 1.34     |
| 1   | AA    | 418  | C    | N1-C6   | 9.07  | 1.42        | 1.37     |
| 35  | BB    | 1159 | U    | C2-N3   | 9.07  | 1.44        | 1.37     |
| 35  | BB    | 841  | G    | C5'-C4' | 9.07  | 1.62        | 1.51     |
| 35  | BB    | 2385 | C    | C2-N3   | 9.06  | 1.43        | 1.35     |
| 35  | BB    | 2860 | A    | C6-N1   | 9.06  | 1.41        | 1.35     |
| 35  | BB    | 635  | C    | N3-C4   | 9.06  | 1.40        | 1.33     |
| 35  | BB    | 1702 | G    | N7-C5   | -9.06 | 1.33        | 1.39     |
| 35  | BB    | 2766 | A    | C8-N7   | -9.06 | 1.25        | 1.31     |
| 1   | AA    | 442  | G    | N7-C5   | 9.06  | 1.44        | 1.39     |
| 35  | BB    | 879  | G    | N1-C2   | 9.06  | 1.45        | 1.37     |
| 35  | BB    | 1137 | G    | C5-C4   | 9.06  | 1.44        | 1.38     |
| 35  | BB    | 1551 | A    | C8-N7   | -9.06 | 1.25        | 1.31     |
| 35  | BB    | 2304 | G    | C2-N3   | 9.06  | 1.40        | 1.32     |
| 35  | BB    | 2349 | G    | C8-N7   | -9.06 | 1.25        | 1.30     |
| 1   | AA    | 1137 | C    | N1-C6   | -9.06 | 1.31        | 1.37     |
| 35  | BB    | 389  | G    | C2-N3   | 9.06  | 1.40        | 1.32     |
| 1   | AA    | 743  | A    | C6-N6   | 9.05  | 1.41        | 1.33     |
| 35  | BB    | 613  | A    | C6-N6   | 9.05  | 1.41        | 1.33     |
| 1   | AA    | 758  | C    | C2'-C1' | -9.05 | 1.43        | 1.53     |
| 35  | BB    | 1766 | G    | N9-C4   | -9.05 | 1.30        | 1.38     |
| 1   | AA    | 933  | G    | C6-N1   | 9.05  | 1.45        | 1.39     |
| 35  | BB    | 113  | U    | C4-C5   | 9.05  | 1.51        | 1.43     |
| 35  | BB    | 2265 | U    | O3'-P   | -9.05 | 1.50        | 1.61     |
| 35  | BB    | 2838 | G    | O3'-P   | -9.05 | 1.50        | 1.61     |
| 35  | BB    | 1182 | G    | O3'-P   | -9.04 | 1.50        | 1.61     |
| 35  | BB    | 1749 | A    | C6-N6   | 9.04  | 1.41        | 1.33     |
| 1   | AA    | 1322 | C    | O3'-P   | -9.04 | 1.50        | 1.61     |
| 35  | BB    | 370  | G    | N1-C2   | 9.04  | 1.45        | 1.37     |
| 35  | BB    | 1761 | C    | C4'-C3' | 9.04  | 1.63        | 1.53     |
| 35  | BB    | 1217 | U    | N3-C4   | 9.04  | 1.46        | 1.38     |
| 35  | BB    | 1944 | U    | C2-N3   | 9.04  | 1.44        | 1.37     |
| 1   | AA    | 95   | C    | N1-C6   | 9.04  | 1.42        | 1.37     |
| 1   | AA    | 408  | A    | N9-C8   | 9.04  | 1.45        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 795  | C    | C4-C5   | -9.04 | 1.35        | 1.43     |
| 1   | AA    | 1362 | A    | C6-N1   | 9.04  | 1.41        | 1.35     |
| 35  | BB    | 1847 | A    | C2'-C1' | -9.04 | 1.43        | 1.53     |
| 1   | AA    | 1093 | A    | C6-N1   | 9.04  | 1.41        | 1.35     |
| 35  | BB    | 13   | A    | N9-C8   | 9.04  | 1.45        | 1.37     |
| 35  | BB    | 601  | C    | C5-C6   | 9.03  | 1.41        | 1.34     |
| 35  | BB    | 860  | U    | C2'-C1' | -9.04 | 1.43        | 1.53     |
| 35  | BB    | 1213 | A    | C8-N7   | -9.03 | 1.25        | 1.31     |
| 1   | AA    | 785  | G    | N3-C4   | -9.03 | 1.29        | 1.35     |
| 35  | BB    | 1056 | G    | C2'-C1' | -9.03 | 1.43        | 1.53     |
| 35  | BB    | 1068 | G    | C5-C4   | 9.03  | 1.44        | 1.38     |
| 35  | BB    | 1380 | G    | N3-C4   | -9.03 | 1.29        | 1.35     |
| 35  | BB    | 787  | C    | C2-N3   | 9.03  | 1.43        | 1.35     |
| 35  | BB    | 1557 | C    | N3-C4   | 9.03  | 1.40        | 1.33     |
| 35  | BB    | 1826 | G    | N1-C2   | 9.03  | 1.45        | 1.37     |
| 1   | AA    | 953  | G    | N7-C5   | -9.03 | 1.33        | 1.39     |
| 35  | BB    | 504  | A    | C2-N3   | 9.03  | 1.41        | 1.33     |
| 35  | BB    | 1354 | A    | P-O5'   | -9.03 | 1.50        | 1.59     |
| 35  | BB    | 2361 | G    | N7-C5   | 9.03  | 1.44        | 1.39     |
| 35  | BB    | 2587 | A    | N7-C5   | -9.03 | 1.33        | 1.39     |
| 1   | AA    | 119  | A    | N7-C5   | -9.02 | 1.33        | 1.39     |
| 1   | AA    | 1362 | A    | C5-C4   | 9.02  | 1.45        | 1.38     |
| 35  | BB    | 2531 | A    | C6-N1   | 9.02  | 1.41        | 1.35     |
| 35  | BB    | 2854 | G    | C8-N7   | -9.02 | 1.25        | 1.30     |
| 35  | BB    | 145  | C    | C4-N4   | 9.02  | 1.42        | 1.33     |
| 35  | BB    | 2443 | C    | C2'-C1' | -9.02 | 1.43        | 1.53     |
| 35  | BB    | 289  | G    | C8-N7   | 9.02  | 1.36        | 1.30     |
| 1   | AA    | 708  | C    | N1-C6   | 9.02  | 1.42        | 1.37     |
| 35  | BB    | 91   | A    | C2'-C1' | -9.02 | 1.43        | 1.53     |
| 35  | BB    | 2825 | G    | N9-C8   | -9.02 | 1.31        | 1.37     |
| 35  | BB    | 562  | U    | N1-C2   | 9.01  | 1.46        | 1.38     |
| 35  | BB    | 1016 | G    | N9-C8   | 9.01  | 1.44        | 1.37     |
| 1   | AA    | 394  | G    | N3-C4   | -9.01 | 1.29        | 1.35     |
| 1   | AA    | 889  | A    | P-O5'   | -9.01 | 1.50        | 1.59     |
| 35  | BB    | 95   | A    | C3'-C2' | 9.01  | 1.62        | 1.52     |
| 1   | AA    | 296  | U    | C4-C5   | -9.01 | 1.35        | 1.43     |
| 1   | AA    | 573  | A    | C6-N1   | 9.01  | 1.41        | 1.35     |
| 1   | AA    | 716  | A    | C6-N6   | 9.01  | 1.41        | 1.33     |
| 1   | AA    | 782  | A    | N3-C4   | 9.01  | 1.40        | 1.34     |
| 35  | BB    | 507  | A    | N7-C5   | -9.01 | 1.33        | 1.39     |
| 1   | AA    | 303  | A    | C8-N7   | -9.00 | 1.25        | 1.31     |
| 34  | BA    | 2    | G    | C2'-C1' | -9.00 | 1.43        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1488 | G    | C6-N1   | 9.00  | 1.45        | 1.39     |
| 35  | BB    | 1195 | G    | C2-N3   | 9.00  | 1.40        | 1.32     |
| 35  | BB    | 2527 | C    | P-O5'   | -9.00 | 1.50        | 1.59     |
| 35  | BB    | 2721 | A    | N7-C5   | -9.00 | 1.33        | 1.39     |
| 35  | BB    | 998  | C    | N1-C6   | -9.00 | 1.31        | 1.37     |
| 1   | AA    | 267  | C    | C2-N3   | 8.99  | 1.43        | 1.35     |
| 1   | AA    | 1274 | A    | C5'-C4' | 8.99  | 1.62        | 1.51     |
| 35  | BB    | 681  | G    | C6-N1   | 8.99  | 1.45        | 1.39     |
| 35  | BB    | 960  | A    | C6-N1   | 8.99  | 1.41        | 1.35     |
| 1   | AA    | 1361 | G    | N7-C5   | -8.99 | 1.33        | 1.39     |
| 35  | BB    | 2278 | A    | N7-C5   | -8.99 | 1.33        | 1.39     |
| 35  | BB    | 739  | A    | N9-C4   | 8.99  | 1.43        | 1.37     |
| 1   | AA    | 115  | G    | C5-C4   | -8.98 | 1.32        | 1.38     |
| 35  | BB    | 63   | A    | C6-N6   | 8.98  | 1.41        | 1.33     |
| 35  | BB    | 465  | G    | N3-C4   | -8.98 | 1.29        | 1.35     |
| 35  | BB    | 886  | A    | N7-C5   | -8.98 | 1.33        | 1.39     |
| 35  | BB    | 2697 | G    | C6-N1   | 8.98  | 1.45        | 1.39     |
| 35  | BB    | 1014 | A    | N9-C4   | -8.98 | 1.32        | 1.37     |
| 1   | AA    | 508  | U    | P-O5'   | 8.98  | 1.68        | 1.59     |
| 35  | BB    | 1889 | A    | C4'-C3' | -8.98 | 1.43        | 1.53     |
| 35  | BB    | 733  | G    | C5-C6   | -8.98 | 1.33        | 1.42     |
| 1   | AA    | 68   | G    | C5-C6   | -8.97 | 1.33        | 1.42     |
| 35  | BB    | 819  | A    | N7-C5   | -8.97 | 1.33        | 1.39     |
| 35  | BB    | 2363 | G    | N1-C2   | 8.97  | 1.45        | 1.37     |
| 1   | AA    | 1124 | G    | C4'-C3' | -8.97 | 1.43        | 1.53     |
| 35  | BB    | 495  | G    | C8-N7   | -8.97 | 1.25        | 1.30     |
| 35  | BB    | 748  | G    | C6-N1   | 8.97  | 1.45        | 1.39     |
| 35  | BB    | 1252 | G    | P-O5'   | -8.97 | 1.50        | 1.59     |
| 35  | BB    | 2022 | U    | N1-C6   | -8.97 | 1.29        | 1.38     |
| 1   | AA    | 567  | G    | N7-C5   | -8.97 | 1.33        | 1.39     |
| 1   | AA    | 753  | A    | C4'-C3' | 8.97  | 1.63        | 1.53     |
| 35  | BB    | 383  | C    | N1-C6   | 8.97  | 1.42        | 1.37     |
| 1   | AA    | 977  | A    | C5-C4   | 8.96  | 1.45        | 1.38     |
| 35  | BB    | 1808 | A    | N7-C5   | -8.96 | 1.33        | 1.39     |
| 35  | BB    | 2007 | U    | N3-C4   | 8.96  | 1.46        | 1.38     |
| 35  | BB    | 2582 | G    | C2-N3   | 8.96  | 1.40        | 1.32     |
| 35  | BB    | 221  | A    | C6-N1   | 8.96  | 1.41        | 1.35     |
| 35  | BB    | 950  | G    | N9-C8   | -8.96 | 1.31        | 1.37     |
| 35  | BB    | 969  | G    | C2-N3   | 8.96  | 1.40        | 1.32     |
| 35  | BB    | 1138 | G    | N9-C8   | 8.96  | 1.44        | 1.37     |
| 35  | BB    | 1542 | U    | C4'-C3' | -8.96 | 1.43        | 1.53     |
| 35  | BB    | 2065 | C    | N1-C6   | 8.96  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 482  | A    | N3-C4   | 8.96  | 1.40        | 1.34     |
| 35  | BB    | 528  | A    | C6-N1   | 8.96  | 1.41        | 1.35     |
| 1   | AA    | 1332 | A    | N7-C5   | -8.96 | 1.33        | 1.39     |
| 35  | BB    | 850  | U    | N3-C4   | 8.95  | 1.46        | 1.38     |
| 35  | BB    | 1502 | A    | C6-N6   | 8.95  | 1.41        | 1.33     |
| 35  | BB    | 2879 | A    | N7-C5   | -8.95 | 1.33        | 1.39     |
| 1   | AA    | 538  | G    | C8-N7   | -8.95 | 1.25        | 1.30     |
| 1   | AA    | 1097 | C    | C2'-C1' | -8.95 | 1.43        | 1.53     |
| 1   | AA    | 89   | U    | C2-N3   | 8.94  | 1.44        | 1.37     |
| 35  | BB    | 1023 | U    | C2'-C1' | -8.95 | 1.43        | 1.53     |
| 35  | BB    | 117  | G    | C8-N7   | -8.94 | 1.25        | 1.30     |
| 35  | BB    | 1277 | G    | C5-C4   | -8.94 | 1.32        | 1.38     |
| 35  | BB    | 1785 | A    | N3-C4   | 8.94  | 1.40        | 1.34     |
| 1   | AA    | 181  | A    | N7-C5   | -8.94 | 1.33        | 1.39     |
| 35  | BB    | 924  | G    | P-O5'   | -8.94 | 1.50        | 1.59     |
| 35  | BB    | 479  | A    | C5'-C4' | 8.94  | 1.62        | 1.51     |
| 35  | BB    | 1281 | G    | N3-C4   | -8.94 | 1.29        | 1.35     |
| 1   | AA    | 974  | A    | N9-C8   | -8.94 | 1.30        | 1.37     |
| 34  | BA    | 116  | G    | C2-N3   | 8.94  | 1.39        | 1.32     |
| 35  | BB    | 2774 | C    | N3-C4   | 8.94  | 1.40        | 1.33     |
| 35  | BB    | 262  | A    | N7-C5   | -8.94 | 1.33        | 1.39     |
| 35  | BB    | 2152 | G    | N1-C2   | 8.94  | 1.44        | 1.37     |
| 1   | AA    | 49   | U    | C5'-C4' | 8.93  | 1.62        | 1.51     |
| 1   | AA    | 752  | G    | C6-N1   | 8.93  | 1.45        | 1.39     |
| 1   | AA    | 1057 | G    | C2-N3   | 8.93  | 1.39        | 1.32     |
| 35  | BB    | 629  | G    | N9-C4   | -8.93 | 1.30        | 1.38     |
| 35  | BB    | 701  | G    | N9-C4   | -8.93 | 1.30        | 1.38     |
| 35  | BB    | 893  | C    | N3-C4   | 8.93  | 1.40        | 1.33     |
| 1   | AA    | 351  | G    | C2-N3   | 8.93  | 1.39        | 1.32     |
| 1   | AA    | 406  | G    | C6-N1   | 8.93  | 1.45        | 1.39     |
| 35  | BB    | 562  | U    | C2-N3   | 8.93  | 1.44        | 1.37     |
| 35  | BB    | 1697 | G    | N1-C2   | 8.92  | 1.44        | 1.37     |
| 35  | BB    | 225  | C    | N1-C6   | 8.92  | 1.42        | 1.37     |
| 1   | AA    | 702  | A    | C6-N6   | 8.92  | 1.41        | 1.33     |
| 22  | AV    | 7    | G    | C8-N7   | -8.92 | 1.25        | 1.30     |
| 35  | BB    | 574  | A    | C2'-C1' | -8.92 | 1.43        | 1.53     |
| 35  | BB    | 1799 | G    | C2-N3   | 8.92  | 1.39        | 1.32     |
| 1   | AA    | 771  | G    | C8-N7   | 8.92  | 1.36        | 1.30     |
| 1   | AA    | 942  | G    | N9-C4   | 8.92  | 1.45        | 1.38     |
| 35  | BB    | 1388 | G    | C2-N3   | 8.92  | 1.39        | 1.32     |
| 35  | BB    | 1828 | G    | N9-C8   | -8.92 | 1.31        | 1.37     |
| 34  | BA    | 59   | A    | N9-C8   | -8.92 | 1.30        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1483 | G    | C2-N3   | 8.92  | 1.39        | 1.32     |
| 35  | BB    | 2246 | G    | N3-C4   | 8.92  | 1.41        | 1.35     |
| 1   | AA    | 778  | G    | N3-C4   | 8.91  | 1.41        | 1.35     |
| 35  | BB    | 1124 | G    | P-O5'   | -8.91 | 1.50        | 1.59     |
| 35  | BB    | 2284 | A    | N7-C5   | -8.91 | 1.33        | 1.39     |
| 35  | BB    | 1283 | G    | N1-C2   | 8.91  | 1.44        | 1.37     |
| 35  | BB    | 1544 | A    | N9-C4   | 8.91  | 1.43        | 1.37     |
| 35  | BB    | 2060 | A    | N3-C4   | 8.91  | 1.40        | 1.34     |
| 35  | BB    | 2428 | G    | N7-C5   | 8.91  | 1.44        | 1.39     |
| 35  | BB    | 87   | U    | P-O5'   | -8.91 | 1.50        | 1.59     |
| 35  | BB    | 345  | A    | C6-N1   | 8.91  | 1.41        | 1.35     |
| 1   | AA    | 609  | A    | C8-N7   | -8.90 | 1.25        | 1.31     |
| 1   | AA    | 825  | A    | P-O5'   | -8.90 | 1.50        | 1.59     |
| 35  | BB    | 422  | A    | N9-C4   | 8.90  | 1.43        | 1.37     |
| 1   | AA    | 472  | U    | C2-N3   | 8.90  | 1.44        | 1.37     |
| 1   | AA    | 1426 | G    | N1-C2   | 8.90  | 1.44        | 1.37     |
| 35  | BB    | 2738 | A    | C3'-C2' | -8.90 | 1.43        | 1.52     |
| 1   | AA    | 1021 | A    | C6-N6   | 8.90  | 1.41        | 1.33     |
| 35  | BB    | 326  | G    | N9-C8   | 8.90  | 1.44        | 1.37     |
| 35  | BB    | 2156 | G    | C6-N1   | 8.90  | 1.45        | 1.39     |
| 35  | BB    | 822  | G    | N1-C2   | 8.90  | 1.44        | 1.37     |
| 1   | AA    | 787  | A    | C6-N1   | 8.89  | 1.41        | 1.35     |
| 1   | AA    | 1260 | G    | C2-N3   | 8.89  | 1.39        | 1.32     |
| 1   | AA    | 485  | U    | P-O5'   | -8.89 | 1.50        | 1.59     |
| 35  | BB    | 428  | A    | N7-C5   | -8.89 | 1.33        | 1.39     |
| 35  | BB    | 123  | G    | C5-C4   | -8.89 | 1.32        | 1.38     |
| 35  | BB    | 2144 | G    | N1-C2   | 8.89  | 1.44        | 1.37     |
| 1   | AA    | 789  | U    | O3'-P   | -8.89 | 1.50        | 1.61     |
| 35  | BB    | 101  | A    | N7-C5   | -8.89 | 1.33        | 1.39     |
| 35  | BB    | 1178 | C    | C2-N3   | 8.89  | 1.42        | 1.35     |
| 1   | AA    | 270  | A    | N7-C5   | -8.89 | 1.33        | 1.39     |
| 35  | BB    | 1600 | C    | N3-C4   | 8.88  | 1.40        | 1.33     |
| 35  | BB    | 1990 | C    | N3-C4   | 8.88  | 1.40        | 1.33     |
| 35  | BB    | 2457 | U    | N3-C4   | 8.88  | 1.46        | 1.38     |
| 35  | BB    | 2788 | C    | C5'-C4' | 8.88  | 1.62        | 1.51     |
| 1   | AA    | 659  | U    | N3-C4   | 8.88  | 1.46        | 1.38     |
| 35  | BB    | 2718 | G    | N9-C8   | 8.88  | 1.44        | 1.37     |
| 1   | AA    | 694  | A    | C6-N1   | 8.88  | 1.41        | 1.35     |
| 1   | AA    | 1292 | G    | N1-C2   | 8.88  | 1.44        | 1.37     |
| 35  | BB    | 395  | U    | N3-C4   | 8.88  | 1.46        | 1.38     |
| 35  | BB    | 585  | G    | N7-C5   | -8.88 | 1.33        | 1.39     |
| 35  | BB    | 1333 | G    | C2-N3   | 8.88  | 1.39        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2572 | A    | N9-C4   | -8.88 | 1.32        | 1.37     |
| 1   | AA    | 44   | A    | N7-C5   | -8.87 | 1.33        | 1.39     |
| 1   | AA    | 467  | U    | C2-N3   | 8.87  | 1.44        | 1.37     |
| 1   | AA    | 1382 | C    | N3-C4   | 8.87  | 1.40        | 1.33     |
| 22  | AV    | 69   | G    | N1-C2   | 8.87  | 1.44        | 1.37     |
| 35  | BB    | 1050 | A    | N9-C8   | 8.87  | 1.44        | 1.37     |
| 35  | BB    | 2172 | U    | C5'-C4' | 8.87  | 1.61        | 1.51     |
| 1   | AA    | 841  | C    | C2-N3   | 8.87  | 1.42        | 1.35     |
| 1   | AA    | 1217 | C    | N3-C4   | 8.87  | 1.40        | 1.33     |
| 1   | AA    | 912  | C    | N1-C6   | -8.87 | 1.31        | 1.37     |
| 35  | BB    | 239  | C    | N1-C6   | 8.87  | 1.42        | 1.37     |
| 35  | BB    | 696  | G    | C5-C4   | -8.87 | 1.32        | 1.38     |
| 1   | AA    | 108  | G    | C6-N1   | 8.86  | 1.45        | 1.39     |
| 35  | BB    | 908  | C    | N1-C6   | -8.86 | 1.31        | 1.37     |
| 35  | BB    | 2532 | G    | C8-N7   | -8.86 | 1.25        | 1.30     |
| 35  | BB    | 2664 | G    | C6-N1   | 8.86  | 1.45        | 1.39     |
| 35  | BB    | 240  | C    | N1-C6   | 8.86  | 1.42        | 1.37     |
| 35  | BB    | 497  | A    | N7-C5   | -8.86 | 1.33        | 1.39     |
| 35  | BB    | 771  | G    | N7-C5   | -8.86 | 1.33        | 1.39     |
| 35  | BB    | 1275 | A    | N3-C4   | 8.86  | 1.40        | 1.34     |
| 1   | AA    | 1198 | G    | N7-C5   | -8.86 | 1.33        | 1.39     |
| 1   | AA    | 91   | U    | C4'-C3' | -8.85 | 1.43        | 1.53     |
| 1   | AA    | 1483 | A    | C8-N7   | -8.85 | 1.25        | 1.31     |
| 35  | BB    | 1190 | G    | N1-C2   | 8.85  | 1.44        | 1.37     |
| 35  | BB    | 661  | A    | N7-C5   | -8.85 | 1.33        | 1.39     |
| 35  | BB    | 825  | A    | C6-N6   | 8.85  | 1.41        | 1.33     |
| 35  | BB    | 1879 | C    | C2'-C1' | -8.85 | 1.43        | 1.53     |
| 35  | BB    | 1505 | A    | C8-N7   | -8.85 | 1.25        | 1.31     |
| 35  | BB    | 1033 | U    | N3-C4   | 8.85  | 1.46        | 1.38     |
| 35  | BB    | 795  | C    | C2-N3   | 8.85  | 1.42        | 1.35     |
| 35  | BB    | 2661 | G    | C5-C4   | 8.85  | 1.44        | 1.38     |
| 1   | AA    | 951  | G    | C6-N1   | 8.85  | 1.45        | 1.39     |
| 35  | BB    | 1344 | U    | C2-N3   | 8.85  | 1.44        | 1.37     |
| 35  | BB    | 68   | G    | C6-N1   | 8.85  | 1.45        | 1.39     |
| 35  | BB    | 905  | A    | N9-C8   | 8.85  | 1.44        | 1.37     |
| 35  | BB    | 2643 | G    | N7-C5   | -8.85 | 1.33        | 1.39     |
| 35  | BB    | 2686 | G    | N1-C2   | 8.85  | 1.44        | 1.37     |
| 35  | BB    | 1485 | U    | N3-C4   | 8.84  | 1.46        | 1.38     |
| 1   | AA    | 1177 | G    | C2'-C1' | -8.84 | 1.43        | 1.53     |
| 1   | AA    | 674  | G    | P-O5'   | -8.84 | 1.50        | 1.59     |
| 1   | AA    | 1472 | U    | C4-C5   | 8.84  | 1.51        | 1.43     |
| 35  | BB    | 1705 | A    | N7-C5   | -8.84 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2032 | G    | C2-N3   | 8.84  | 1.39        | 1.32     |
| 1   | AA    | 335  | C    | N3-C4   | 8.83  | 1.40        | 1.33     |
| 1   | AA    | 1306 | A    | O3'-P   | -8.83 | 1.50        | 1.61     |
| 35  | BB    | 2234 | G    | C2'-C1' | -8.83 | 1.43        | 1.53     |
| 35  | BB    | 601  | C    | N1-C6   | -8.83 | 1.31        | 1.37     |
| 35  | BB    | 339  | U    | C2-N3   | 8.83  | 1.44        | 1.37     |
| 35  | BB    | 1545 | A    | C2'-C1' | -8.83 | 1.43        | 1.53     |
| 1   | AA    | 1445 | U    | O3'-P   | -8.82 | 1.50        | 1.61     |
| 34  | BA    | 24   | G    | C2-N2   | 8.82  | 1.43        | 1.34     |
| 35  | BB    | 1081 | U    | C2-N3   | 8.82  | 1.44        | 1.37     |
| 35  | BB    | 1192 | G    | N7-C5   | -8.82 | 1.33        | 1.39     |
| 35  | BB    | 1241 | A    | N9-C4   | 8.82  | 1.43        | 1.37     |
| 35  | BB    | 1886 | U    | C5-C6   | -8.82 | 1.26        | 1.34     |
| 35  | BB    | 2771 | C    | C4-N4   | 8.82  | 1.41        | 1.33     |
| 1   | AA    | 194  | C    | N1-C6   | -8.82 | 1.31        | 1.37     |
| 1   | AA    | 422  | C    | N1-C6   | 8.82  | 1.42        | 1.37     |
| 1   | AA    | 1274 | A    | C2'-C1' | -8.82 | 1.43        | 1.53     |
| 35  | BB    | 63   | A    | O3'-P   | -8.82 | 1.50        | 1.61     |
| 35  | BB    | 1898 | U    | P-O5'   | -8.82 | 1.50        | 1.59     |
| 1   | AA    | 472  | U    | O3'-P   | -8.82 | 1.50        | 1.61     |
| 1   | AA    | 1371 | G    | C2-N3   | 8.82  | 1.39        | 1.32     |
| 35  | BB    | 266  | G    | C2-N3   | 8.82  | 1.39        | 1.32     |
| 1   | AA    | 548  | G    | O3'-P   | -8.81 | 1.50        | 1.61     |
| 35  | BB    | 499  | U    | C2-N3   | 8.81  | 1.44        | 1.37     |
| 1   | AA    | 548  | G    | N7-C5   | -8.81 | 1.33        | 1.39     |
| 35  | BB    | 299  | A    | N9-C4   | -8.81 | 1.32        | 1.37     |
| 35  | BB    | 883  | G    | O3'-P   | -8.81 | 1.50        | 1.61     |
| 35  | BB    | 1149 | G    | N1-C2   | 8.81  | 1.44        | 1.37     |
| 35  | BB    | 1232 | G    | N7-C5   | -8.81 | 1.33        | 1.39     |
| 1   | AA    | 1021 | A    | N9-C4   | 8.80  | 1.43        | 1.37     |
| 35  | BB    | 1304 | A    | C6-N6   | 8.80  | 1.41        | 1.33     |
| 35  | BB    | 2231 | U    | C4-C5   | 8.80  | 1.51        | 1.43     |
| 35  | BB    | 1406 | U    | P-O5'   | -8.80 | 1.50        | 1.59     |
| 35  | BB    | 2370 | G    | N9-C4   | 8.80  | 1.45        | 1.38     |
| 35  | BB    | 111  | A    | N7-C5   | -8.80 | 1.33        | 1.39     |
| 35  | BB    | 1734 | G    | N7-C5   | -8.80 | 1.33        | 1.39     |
| 35  | BB    | 1322 | A    | N7-C5   | -8.80 | 1.33        | 1.39     |
| 35  | BB    | 1660 | G    | C5-C4   | 8.80  | 1.44        | 1.38     |
| 35  | BB    | 2369 | A    | C5'-C4' | 8.80  | 1.61        | 1.51     |
| 35  | BB    | 2542 | A    | N3-C4   | -8.80 | 1.29        | 1.34     |
| 35  | BB    | 207  | A    | C6-N1   | 8.80  | 1.41        | 1.35     |
| 35  | BB    | 888  | C    | C2-N3   | 8.80  | 1.42        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1377 | G    | C2-N3   | 8.80  | 1.39        | 1.32     |
| 35  | BB    | 2171 | A    | C3'-C2' | 8.80  | 1.62        | 1.52     |
| 1   | AA    | 42   | G    | C6-N1   | 8.79  | 1.45        | 1.39     |
| 1   | AA    | 115  | G    | C5'-C4' | 8.79  | 1.61        | 1.51     |
| 1   | AA    | 729  | A    | C5-C4   | 8.80  | 1.45        | 1.38     |
| 1   | AA    | 1178 | G    | C2-N3   | 8.79  | 1.39        | 1.32     |
| 35  | BB    | 1450 | G    | C8-N7   | -8.80 | 1.25        | 1.30     |
| 35  | BB    | 1294 | U    | P-O5'   | -8.79 | 1.50        | 1.59     |
| 35  | BB    | 2645 | G    | N7-C5   | -8.79 | 1.33        | 1.39     |
| 1   | AA    | 484  | G    | C2-N3   | 8.79  | 1.39        | 1.32     |
| 1   | AA    | 654  | G    | N1-C2   | 8.79  | 1.44        | 1.37     |
| 1   | AA    | 804  | U    | P-O5'   | -8.79 | 1.50        | 1.59     |
| 1   | AA    | 983  | A    | N9-C4   | 8.79  | 1.43        | 1.37     |
| 35  | BB    | 1328 | A    | C6-N1   | 8.79  | 1.41        | 1.35     |
| 35  | BB    | 2871 | U    | N1-C6   | -8.79 | 1.30        | 1.38     |
| 1   | AA    | 941  | G    | C3'-C2' | -8.79 | 1.43        | 1.52     |
| 1   | AA    | 1309 | G    | C5-C4   | 8.79  | 1.44        | 1.38     |
| 1   | AA    | 1394 | A    | C6-N6   | 8.79  | 1.41        | 1.33     |
| 35  | BB    | 105  | C    | N3-C4   | 8.79  | 1.40        | 1.33     |
| 35  | BB    | 2437 | G    | C8-N7   | 8.79  | 1.36        | 1.30     |
| 35  | BB    | 170  | U    | C5'-C4' | 8.79  | 1.61        | 1.51     |
| 35  | BB    | 1206 | G    | C2-N3   | 8.79  | 1.39        | 1.32     |
| 35  | BB    | 2494 | G    | C2-N3   | 8.79  | 1.39        | 1.32     |
| 1   | AA    | 361  | G    | C3'-C2' | -8.79 | 1.43        | 1.52     |
| 35  | BB    | 1766 | G    | C2-N3   | 8.79  | 1.39        | 1.32     |
| 1   | AA    | 216  | U    | N1-C2   | 8.78  | 1.46        | 1.38     |
| 1   | AA    | 240  | G    | P-O5'   | 8.78  | 1.68        | 1.59     |
| 34  | BA    | 88   | C    | C4'-C3' | -8.78 | 1.43        | 1.53     |
| 35  | BB    | 2210 | U    | N1-C6   | 8.78  | 1.45        | 1.38     |
| 35  | BB    | 2502 | G    | P-O5'   | -8.78 | 1.50        | 1.59     |
| 35  | BB    | 2488 | G    | N7-C5   | 8.78  | 1.44        | 1.39     |
| 1   | AA    | 1326 | U    | P-O5'   | -8.78 | 1.50        | 1.59     |
| 1   | AA    | 1412 | C    | C4-C5   | -8.78 | 1.35        | 1.43     |
| 35  | BB    | 89   | A    | P-O5'   | -8.77 | 1.50        | 1.59     |
| 35  | BB    | 335  | C    | N1-C6   | 8.77  | 1.42        | 1.37     |
| 1   | AA    | 773  | G    | C6-N1   | 8.77  | 1.45        | 1.39     |
| 35  | BB    | 993  | G    | C2-N2   | 8.77  | 1.43        | 1.34     |
| 1   | AA    | 962  | C    | N1-C6   | 8.77  | 1.42        | 1.37     |
| 35  | BB    | 1392 | A    | C6-N6   | 8.77  | 1.41        | 1.33     |
| 35  | BB    | 1436 | G    | N1-C2   | 8.77  | 1.44        | 1.37     |
| 35  | BB    | 211  | C    | C2-N3   | 8.77  | 1.42        | 1.35     |
| 1   | AA    | 92   | U    | N1-C6   | 8.77  | 1.45        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 712  | G    | N3-C4   | -8.77 | 1.29        | 1.35     |
| 35  | BB    | 1654 | A    | C6-N1   | 8.77  | 1.41        | 1.35     |
| 35  | BB    | 1478 | G    | N7-C5   | 8.76  | 1.44        | 1.39     |
| 35  | BB    | 194  | G    | N3-C4   | -8.76 | 1.29        | 1.35     |
| 35  | BB    | 1934 | C    | N1-C6   | 8.76  | 1.42        | 1.37     |
| 35  | BB    | 1445 | G    | N3-C4   | -8.76 | 1.29        | 1.35     |
| 1   | AA    | 46   | G    | N1-C2   | 8.76  | 1.44        | 1.37     |
| 35  | BB    | 2471 | A    | N7-C5   | -8.76 | 1.33        | 1.39     |
| 35  | BB    | 1429 | G    | C2-N3   | 8.76  | 1.39        | 1.32     |
| 35  | BB    | 1475 | G    | C2'-C1' | -8.76 | 1.43        | 1.53     |
| 1   | AA    | 700  | G    | C2-N2   | 8.75  | 1.43        | 1.34     |
| 35  | BB    | 1034 | G    | N7-C5   | -8.75 | 1.33        | 1.39     |
| 35  | BB    | 74   | A    | C5'-C4' | 8.75  | 1.61        | 1.51     |
| 35  | BB    | 409  | G    | N9-C4   | -8.75 | 1.30        | 1.38     |
| 35  | BB    | 2169 | A    | C5'-C4' | 8.75  | 1.61        | 1.51     |
| 34  | BA    | 42   | C    | C4-N4   | 8.74  | 1.41        | 1.33     |
| 1   | AA    | 674  | G    | C5-C6   | -8.74 | 1.33        | 1.42     |
| 35  | BB    | 2021 | C    | C4-N4   | 8.74  | 1.41        | 1.33     |
| 34  | BA    | 15   | A    | N7-C5   | -8.74 | 1.34        | 1.39     |
| 34  | BA    | 59   | A    | C6-N6   | 8.74  | 1.41        | 1.33     |
| 35  | BB    | 741  | U    | C2'-C1' | -8.74 | 1.43        | 1.53     |
| 1   | AA    | 831  | A    | N7-C5   | -8.74 | 1.34        | 1.39     |
| 35  | BB    | 2603 | G    | N1-C2   | 8.74  | 1.44        | 1.37     |
| 35  | BB    | 49   | A    | C6-N6   | 8.73  | 1.41        | 1.33     |
| 35  | BB    | 480  | A    | C6-N1   | 8.73  | 1.41        | 1.35     |
| 1   | AA    | 24   | U    | C4'-C3' | 8.73  | 1.62        | 1.53     |
| 35  | BB    | 1532 | A    | P-O5'   | -8.73 | 1.51        | 1.59     |
| 35  | BB    | 2031 | A    | N9-C4   | 8.73  | 1.43        | 1.37     |
| 1   | AA    | 1227 | A    | C6-N1   | 8.72  | 1.41        | 1.35     |
| 35  | BB    | 1205 | A    | C8-N7   | -8.72 | 1.25        | 1.31     |
| 35  | BB    | 1286 | A    | C5-C4   | 8.72  | 1.44        | 1.38     |
| 35  | BB    | 1332 | G    | N7-C5   | -8.72 | 1.34        | 1.39     |
| 1   | AA    | 213  | G    | C2'-C1' | -8.72 | 1.43        | 1.53     |
| 35  | BB    | 2170 | A    | N3-C4   | 8.72  | 1.40        | 1.34     |
| 1   | AA    | 600  | A    | C6-N6   | 8.72  | 1.41        | 1.33     |
| 1   | AA    | 761  | G    | N9-C8   | 8.72  | 1.44        | 1.37     |
| 35  | BB    | 1475 | G    | C5-C4   | 8.72  | 1.44        | 1.38     |
| 35  | BB    | 1475 | G    | N9-C8   | 8.72  | 1.44        | 1.37     |
| 35  | BB    | 1784 | A    | N9-C4   | -8.72 | 1.32        | 1.37     |
| 1   | AA    | 1142 | G    | C5'-C4' | 8.72  | 1.61        | 1.51     |
| 1   | AA    | 495  | A    | N3-C4   | 8.71  | 1.40        | 1.34     |
| 1   | AA    | 579  | A    | N9-C8   | -8.71 | 1.30        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1395 | A    | N9-C8   | -8.71 | 1.30        | 1.37     |
| 35  | BB    | 2491 | U    | C2-N3   | 8.72  | 1.43        | 1.37     |
| 1   | AA    | 1426 | G    | C2-N2   | 8.71  | 1.43        | 1.34     |
| 1   | AA    | 1480 | A    | C6-N1   | -8.71 | 1.29        | 1.35     |
| 35  | BB    | 32   | C    | N1-C6   | 8.71  | 1.42        | 1.37     |
| 35  | BB    | 1195 | G    | C6-N1   | 8.71  | 1.45        | 1.39     |
| 1   | AA    | 841  | C    | N3-C4   | 8.71  | 1.40        | 1.33     |
| 1   | AA    | 1518 | A    | C6-N6   | 8.71  | 1.41        | 1.33     |
| 1   | AA    | 1127 | G    | C2-N3   | 8.71  | 1.39        | 1.32     |
| 1   | AA    | 1061 | G    | P-O5'   | -8.70 | 1.51        | 1.59     |
| 1   | AA    | 1152 | A    | N3-C4   | 8.70  | 1.40        | 1.34     |
| 35  | BB    | 86   | G    | C6-N1   | 8.70  | 1.45        | 1.39     |
| 1   | AA    | 1218 | C    | N3-C4   | 8.70  | 1.40        | 1.33     |
| 35  | BB    | 1027 | A    | N3-C4   | -8.70 | 1.29        | 1.34     |
| 1   | AA    | 161  | A    | N7-C5   | -8.70 | 1.34        | 1.39     |
| 1   | AA    | 570  | G    | C2-N3   | 8.70  | 1.39        | 1.32     |
| 35  | BB    | 1162 | G    | N1-C2   | 8.70  | 1.44        | 1.37     |
| 35  | BB    | 2529 | G    | N9-C4   | -8.70 | 1.30        | 1.38     |
| 35  | BB    | 8    | C    | N1-C6   | 8.70  | 1.42        | 1.37     |
| 35  | BB    | 2759 | G    | N3-C4   | -8.70 | 1.29        | 1.35     |
| 1   | AA    | 1274 | A    | N7-C5   | -8.69 | 1.34        | 1.39     |
| 35  | BB    | 73   | A    | N7-C5   | -8.70 | 1.34        | 1.39     |
| 35  | BB    | 252  | G    | N3-C4   | -8.70 | 1.29        | 1.35     |
| 35  | BB    | 1088 | A    | C6-N6   | 8.69  | 1.41        | 1.33     |
| 35  | BB    | 2750 | A    | N7-C5   | -8.69 | 1.34        | 1.39     |
| 35  | BB    | 95   | A    | C2'-C1' | -8.69 | 1.43        | 1.53     |
| 1   | AA    | 877  | G    | N9-C8   | -8.69 | 1.31        | 1.37     |
| 1   | AA    | 883  | C    | C4-N4   | 8.69  | 1.41        | 1.33     |
| 1   | AA    | 1262 | C    | C2-N3   | 8.69  | 1.42        | 1.35     |
| 1   | AA    | 536  | C    | N3-C4   | 8.69  | 1.40        | 1.33     |
| 35  | BB    | 1900 | A    | N9-C4   | -8.69 | 1.32        | 1.37     |
| 35  | BB    | 2648 | G    | C6-N1   | 8.69  | 1.45        | 1.39     |
| 1   | AA    | 238  | A    | C6-N6   | 8.68  | 1.40        | 1.33     |
| 34  | BA    | 47   | C    | O3'-P   | -8.68 | 1.50        | 1.61     |
| 1   | AA    | 844  | G    | C8-N7   | -8.68 | 1.25        | 1.30     |
| 35  | BB    | 941  | A    | P-O5'   | -8.68 | 1.51        | 1.59     |
| 35  | BB    | 979  | A    | C6-N6   | 8.68  | 1.40        | 1.33     |
| 35  | BB    | 1871 | A    | N7-C5   | -8.68 | 1.34        | 1.39     |
| 35  | BB    | 572  | A    | C2'-C1' | -8.68 | 1.43        | 1.53     |
| 1   | AA    | 609  | A    | N9-C4   | -8.67 | 1.32        | 1.37     |
| 1   | AA    | 201  | G    | N1-C2   | 8.67  | 1.44        | 1.37     |
| 35  | BB    | 561  | G    | N1-C2   | 8.67  | 1.44        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 776  | G    | C5-C4   | 8.67  | 1.44        | 1.38     |
| 35  | BB    | 2160 | C    | C4'-C3' | 8.67  | 1.62        | 1.53     |
| 35  | BB    | 996  | A    | N9-C4   | 8.67  | 1.43        | 1.37     |
| 35  | BB    | 149  | A    | C6-N1   | 8.66  | 1.41        | 1.35     |
| 35  | BB    | 1230 | A    | C6-N1   | 8.66  | 1.41        | 1.35     |
| 1   | AA    | 667  | G    | N7-C5   | -8.66 | 1.34        | 1.39     |
| 35  | BB    | 1684 | G    | C2-N3   | 8.66  | 1.39        | 1.32     |
| 35  | BB    | 1814 | G    | N7-C5   | -8.66 | 1.34        | 1.39     |
| 35  | BB    | 2719 | G    | C2-N3   | 8.66  | 1.39        | 1.32     |
| 35  | BB    | 2893 | A    | C6-N1   | 8.66  | 1.41        | 1.35     |
| 1   | AA    | 193  | C    | N3-C4   | 8.66  | 1.40        | 1.33     |
| 35  | BB    | 291  | G    | N9-C8   | 8.66  | 1.44        | 1.37     |
| 35  | BB    | 1191 | G    | C5-C4   | 8.66  | 1.44        | 1.38     |
| 1   | AA    | 25   | C    | C4-N4   | 8.65  | 1.41        | 1.33     |
| 1   | AA    | 320  | A    | C8-N7   | -8.65 | 1.25        | 1.31     |
| 1   | AA    | 453  | G    | C2-N3   | 8.65  | 1.39        | 1.32     |
| 35  | BB    | 2535 | G    | N7-C5   | -8.65 | 1.34        | 1.39     |
| 35  | BB    | 2647 | U    | C2-N3   | 8.65  | 1.43        | 1.37     |
| 1   | AA    | 778  | G    | C8-N7   | 8.65  | 1.36        | 1.30     |
| 35  | BB    | 2653 | U    | C4-C5   | 8.65  | 1.51        | 1.43     |
| 1   | AA    | 118  | U    | C2-N3   | 8.65  | 1.43        | 1.37     |
| 35  | BB    | 1131 | G    | C2-N2   | 8.65  | 1.43        | 1.34     |
| 35  | BB    | 1450 | G    | N1-C2   | 8.65  | 1.44        | 1.37     |
| 1   | AA    | 311  | C    | C2'-C1' | -8.65 | 1.43        | 1.53     |
| 1   | AA    | 921  | U    | P-O5'   | -8.65 | 1.51        | 1.59     |
| 1   | AA    | 1456 | A    | C8-N7   | 8.65  | 1.37        | 1.31     |
| 22  | AV    | 75   | C    | N1-C6   | 8.65  | 1.42        | 1.37     |
| 35  | BB    | 212  | G    | N9-C8   | -8.65 | 1.31        | 1.37     |
| 35  | BB    | 579  | G    | C2-N3   | 8.65  | 1.39        | 1.32     |
| 1   | AA    | 833  | G    | N9-C8   | 8.65  | 1.44        | 1.37     |
| 35  | BB    | 1085 | A    | C6-N1   | 8.65  | 1.41        | 1.35     |
| 35  | BB    | 1385 | A    | P-O5'   | -8.65 | 1.51        | 1.59     |
| 1   | AA    | 246  | A    | N1-C2   | -8.64 | 1.26        | 1.34     |
| 1   | AA    | 1484 | C    | N1-C6   | -8.64 | 1.31        | 1.37     |
| 1   | AA    | 1505 | G    | C2'-C1' | -8.64 | 1.43        | 1.53     |
| 35  | BB    | 464  | U    | C2'-C1' | -8.64 | 1.43        | 1.53     |
| 35  | BB    | 1214 | A    | C6-N6   | 8.64  | 1.40        | 1.33     |
| 35  | BB    | 1293 | C    | C4'-C3' | -8.64 | 1.43        | 1.53     |
| 35  | BB    | 1533 | C    | N3-C4   | 8.64  | 1.40        | 1.33     |
| 35  | BB    | 2569 | G    | N9-C8   | 8.64  | 1.44        | 1.37     |
| 1   | AA    | 808  | C    | N3-C4   | 8.64  | 1.40        | 1.33     |
| 35  | BB    | 274  | C    | C5'-C4' | 8.64  | 1.61        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 892  | A    | C6-N6   | 8.64  | 1.40        | 1.33     |
| 35  | BB    | 1180 | U    | N1-C6   | -8.64 | 1.30        | 1.38     |
| 35  | BB    | 2314 | A    | N9-C4   | -8.64 | 1.32        | 1.37     |
| 1   | AA    | 332  | G    | N9-C4   | 8.64  | 1.44        | 1.38     |
| 1   | AA    | 937  | A    | N9-C4   | 8.64  | 1.43        | 1.37     |
| 35  | BB    | 504  | A    | C8-N7   | -8.64 | 1.25        | 1.31     |
| 35  | BB    | 1639 | C    | N3-C4   | 8.64  | 1.40        | 1.33     |
| 1   | AA    | 386  | C    | N1-C6   | 8.63  | 1.42        | 1.37     |
| 35  | BB    | 1948 | G    | N7-C5   | -8.64 | 1.34        | 1.39     |
| 35  | BB    | 127  | A    | C6-N1   | 8.63  | 1.41        | 1.35     |
| 1   | AA    | 704  | A    | P-O5'   | -8.63 | 1.51        | 1.59     |
| 1   | AA    | 1419 | G    | C2-N3   | 8.63  | 1.39        | 1.32     |
| 35  | BB    | 2692 | G    | N9-C4   | -8.63 | 1.31        | 1.38     |
| 35  | BB    | 2859 | G    | C6-N1   | 8.63  | 1.45        | 1.39     |
| 1   | AA    | 39   | G    | N7-C5   | -8.63 | 1.34        | 1.39     |
| 1   | AA    | 929  | G    | N1-C2   | 8.63  | 1.44        | 1.37     |
| 34  | BA    | 114  | C    | N1-C6   | 8.63  | 1.42        | 1.37     |
| 35  | BB    | 2242 | G    | C5-C4   | 8.63  | 1.44        | 1.38     |
| 1   | AA    | 399  | G    | N1-C2   | 8.63  | 1.44        | 1.37     |
| 34  | BA    | 116  | G    | C6-O6   | -8.63 | 1.16        | 1.24     |
| 35  | BB    | 1910 | G    | N9-C8   | 8.62  | 1.43        | 1.37     |
| 35  | BB    | 2869 | G    | C5-C6   | -8.63 | 1.33        | 1.42     |
| 35  | BB    | 1442 | U    | C2'-C1' | -8.62 | 1.43        | 1.53     |
| 35  | BB    | 1537 | G    | C6-N1   | 8.62  | 1.45        | 1.39     |
| 1   | AA    | 149  | A    | C2'-C1' | -8.62 | 1.43        | 1.53     |
| 35  | BB    | 778  | G    | C6-N1   | 8.62  | 1.45        | 1.39     |
| 35  | BB    | 1291 | C    | C2-N3   | 8.62  | 1.42        | 1.35     |
| 35  | BB    | 2058 | A    | N3-C4   | 8.62  | 1.40        | 1.34     |
| 1   | AA    | 346  | G    | C6-N1   | 8.62  | 1.45        | 1.39     |
| 1   | AA    | 351  | G    | N7-C5   | -8.62 | 1.34        | 1.39     |
| 1   | AA    | 1391 | U    | C4'-O4' | 8.62  | 1.56        | 1.45     |
| 35  | BB    | 22   | C    | C4-C5   | 8.62  | 1.49        | 1.43     |
| 35  | BB    | 2015 | A    | N9-C4   | -8.62 | 1.32        | 1.37     |
| 1   | AA    | 1176 | A    | N7-C5   | -8.61 | 1.34        | 1.39     |
| 35  | BB    | 2891 | U    | O3'-P   | -8.61 | 1.50        | 1.61     |
| 35  | BB    | 777  | G    | N7-C5   | -8.61 | 1.34        | 1.39     |
| 35  | BB    | 811  | U    | P-O5'   | -8.61 | 1.51        | 1.59     |
| 35  | BB    | 976  | G    | C8-N7   | -8.61 | 1.25        | 1.30     |
| 35  | BB    | 2858 | C    | C4-C5   | 8.61  | 1.49        | 1.43     |
| 35  | BB    | 579  | G    | C8-N7   | 8.61  | 1.36        | 1.30     |
| 35  | BB    | 2292 | U    | N3-C4   | 8.61  | 1.46        | 1.38     |
| 35  | BB    | 70   | G    | C2-N3   | 8.61  | 1.39        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34  | BA    | 88   | C    | C4'-O4' | 8.61  | 1.56        | 1.45     |
| 1   | AA    | 382  | A    | C2'-C1' | -8.60 | 1.43        | 1.53     |
| 35  | BB    | 1274 | A    | N1-C2   | 8.60  | 1.42        | 1.34     |
| 35  | BB    | 1639 | C    | C5'-C4' | 8.60  | 1.61        | 1.51     |
| 35  | BB    | 1718 | G    | C2-N2   | 8.60  | 1.43        | 1.34     |
| 35  | BB    | 2250 | G    | C8-N7   | 8.60  | 1.36        | 1.30     |
| 1   | AA    | 1149 | C    | N1-C6   | -8.60 | 1.31        | 1.37     |
| 35  | BB    | 426  | C    | N1-C6   | 8.60  | 1.42        | 1.37     |
| 1   | AA    | 1493 | A    | N9-C4   | -8.60 | 1.32        | 1.37     |
| 35  | BB    | 480  | A    | C1'-N9  | 8.60  | 1.61        | 1.48     |
| 35  | BB    | 1154 | G    | C2-N2   | -8.60 | 1.25        | 1.34     |
| 34  | BA    | 62   | C    | C2'-C1' | -8.60 | 1.43        | 1.53     |
| 35  | BB    | 586  | A    | N9-C4   | 8.60  | 1.43        | 1.37     |
| 35  | BB    | 835  | C    | C4-C5   | 8.60  | 1.49        | 1.43     |
| 1   | AA    | 66   | A    | C6-N6   | 8.59  | 1.40        | 1.33     |
| 1   | AA    | 1136 | C    | C5-C6   | 8.59  | 1.41        | 1.34     |
| 1   | AA    | 1166 | G    | C6-N1   | 8.59  | 1.45        | 1.39     |
| 35  | BB    | 1423 | G    | N7-C5   | -8.59 | 1.34        | 1.39     |
| 35  | BB    | 1948 | G    | C6-N1   | 8.59  | 1.45        | 1.39     |
| 35  | BB    | 2095 | A    | C6-N6   | 8.59  | 1.40        | 1.33     |
| 35  | BB    | 1778 | U    | C2-N3   | 8.59  | 1.43        | 1.37     |
| 1   | AA    | 182  | A    | N7-C5   | -8.59 | 1.34        | 1.39     |
| 35  | BB    | 682  | G    | N9-C4   | -8.59 | 1.31        | 1.38     |
| 35  | BB    | 1285 | A    | C6-N1   | 8.59  | 1.41        | 1.35     |
| 35  | BB    | 1441 | G    | C6-N1   | 8.59  | 1.45        | 1.39     |
| 35  | BB    | 2178 | C    | N1-C6   | 8.59  | 1.42        | 1.37     |
| 35  | BB    | 2881 | U    | P-O5'   | -8.59 | 1.51        | 1.59     |
| 1   | AA    | 1276 | G    | C2'-C1' | -8.58 | 1.44        | 1.53     |
| 35  | BB    | 1738 | G    | C3'-C2' | 8.58  | 1.62        | 1.52     |
| 1   | AA    | 829  | G    | C4'-O4' | 8.58  | 1.56        | 1.45     |
| 35  | BB    | 502  | A    | N9-C4   | -8.58 | 1.32        | 1.37     |
| 1   | AA    | 684  | U    | N1-C6   | 8.58  | 1.45        | 1.38     |
| 1   | AA    | 1421 | G    | C5-C4   | 8.58  | 1.44        | 1.38     |
| 35  | BB    | 123  | G    | N1-C2   | 8.58  | 1.44        | 1.37     |
| 1   | AA    | 791  | G    | C2-N3   | 8.58  | 1.39        | 1.32     |
| 1   | AA    | 1146 | A    | C8-N7   | -8.58 | 1.25        | 1.31     |
| 35  | BB    | 167  | A    | C6-N1   | 8.58  | 1.41        | 1.35     |
| 35  | BB    | 1077 | A    | N7-C5   | -8.58 | 1.34        | 1.39     |
| 35  | BB    | 1473 | G    | C2'-C1' | -8.58 | 1.44        | 1.53     |
| 35  | BB    | 2618 | G    | N7-C5   | -8.58 | 1.34        | 1.39     |
| 35  | BB    | 1537 | G    | N3-C4   | 8.58  | 1.41        | 1.35     |
| 1   | AA    | 1263 | C    | C5'-C4' | 8.57  | 1.61        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 89   | A    | N7-C5   | -8.57 | 1.34        | 1.39     |
| 1   | AA    | 87   | C    | N3-C4   | 8.57  | 1.40        | 1.33     |
| 35  | BB    | 697  | G    | C8-N7   | -8.57 | 1.25        | 1.30     |
| 35  | BB    | 1248 | G    | N1-C2   | 8.57  | 1.44        | 1.37     |
| 1   | AA    | 1225 | A    | P-O5'   | -8.57 | 1.51        | 1.59     |
| 35  | BB    | 608  | A    | C6-N6   | 8.57  | 1.40        | 1.33     |
| 35  | BB    | 1220 | G    | N7-C5   | -8.57 | 1.34        | 1.39     |
| 35  | BB    | 1421 | G    | N7-C5   | -8.57 | 1.34        | 1.39     |
| 35  | BB    | 970  | U    | C5'-C4' | 8.56  | 1.61        | 1.51     |
| 35  | BB    | 966  | G    | O4'-C1' | 8.56  | 1.52        | 1.41     |
| 35  | BB    | 1570 | A    | C6-N6   | 8.56  | 1.40        | 1.33     |
| 1   | AA    | 919  | A    | C6-N6   | 8.56  | 1.40        | 1.33     |
| 1   | AA    | 1004 | A    | N7-C5   | -8.56 | 1.34        | 1.39     |
| 35  | BB    | 1031 | G    | C6-N1   | 8.56  | 1.45        | 1.39     |
| 35  | BB    | 1100 | C    | N1-C6   | -8.56 | 1.32        | 1.37     |
| 1   | AA    | 1063 | C    | N3-C4   | 8.56  | 1.40        | 1.33     |
| 35  | BB    | 1086 | A    | C6-N6   | 8.56  | 1.40        | 1.33     |
| 35  | BB    | 1263 | U    | C4-C5   | -8.56 | 1.35        | 1.43     |
| 1   | AA    | 66   | A    | N3-C4   | 8.56  | 1.40        | 1.34     |
| 35  | BB    | 2153 | C    | N3-C4   | 8.56  | 1.40        | 1.33     |
| 35  | BB    | 302  | C    | N3-C4   | 8.55  | 1.40        | 1.33     |
| 35  | BB    | 2051 | A    | C4'-C3' | -8.55 | 1.43        | 1.53     |
| 1   | AA    | 750  | C    | N3-C4   | 8.55  | 1.40        | 1.33     |
| 1   | AA    | 877  | G    | C2-N3   | 8.55  | 1.39        | 1.32     |
| 35  | BB    | 1954 | G    | C5'-C4' | 8.55  | 1.61        | 1.51     |
| 35  | BB    | 2469 | A    | N3-C4   | -8.55 | 1.29        | 1.34     |
| 35  | BB    | 1713 | A    | N3-C4   | -8.55 | 1.29        | 1.34     |
| 1   | AA    | 449  | G    | C6-N1   | 8.54  | 1.45        | 1.39     |
| 35  | BB    | 280  | U    | C2'-C1' | -8.55 | 1.44        | 1.53     |
| 35  | BB    | 852  | U    | C2-N3   | 8.55  | 1.43        | 1.37     |
| 1   | AA    | 1509 | C    | N1-C6   | 8.54  | 1.42        | 1.37     |
| 34  | BA    | 51   | G    | C6-N1   | 8.54  | 1.45        | 1.39     |
| 35  | BB    | 722  | A    | C6-N1   | 8.54  | 1.41        | 1.35     |
| 35  | BB    | 58   | G    | C2-N3   | 8.54  | 1.39        | 1.32     |
| 35  | BB    | 2879 | A    | C2'-C1' | -8.54 | 1.44        | 1.53     |
| 35  | BB    | 2396 | G    | N1-C2   | 8.54  | 1.44        | 1.37     |
| 35  | BB    | 2775 | G    | C5-C4   | 8.54  | 1.44        | 1.38     |
| 1   | AA    | 143  | A    | C6-N6   | 8.54  | 1.40        | 1.33     |
| 35  | BB    | 2663 | G    | C2'-C1' | -8.54 | 1.44        | 1.53     |
| 1   | AA    | 1164 | G    | C8-N7   | -8.54 | 1.25        | 1.30     |
| 35  | BB    | 2283 | C    | C4-N4   | 8.53  | 1.41        | 1.33     |
| 1   | AA    | 902  | G    | N1-C2   | 8.53  | 1.44        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 586  | A    | N3-C4   | -8.53 | 1.29        | 1.34     |
| 35  | BB    | 119  | A    | C4'-C3' | 8.53  | 1.62        | 1.53     |
| 35  | BB    | 423  | A    | P-O5'   | -8.53 | 1.51        | 1.59     |
| 35  | BB    | 1067 | A    | N9-C4   | 8.53  | 1.43        | 1.37     |
| 35  | BB    | 2797 | U    | C5'-C4' | 8.53  | 1.61        | 1.51     |
| 35  | BB    | 1807 | G    | C6-N1   | 8.52  | 1.45        | 1.39     |
| 35  | BB    | 2561 | U    | C5'-C4' | 8.52  | 1.61        | 1.51     |
| 35  | BB    | 2837 | A    | C8-N7   | -8.52 | 1.25        | 1.31     |
| 1   | AA    | 168  | G    | C5-C4   | 8.52  | 1.44        | 1.38     |
| 1   | AA    | 349  | A    | C5'-C4' | 8.52  | 1.61        | 1.51     |
| 1   | AA    | 887  | G    | C6-N1   | 8.52  | 1.45        | 1.39     |
| 35  | BB    | 1650 | A    | C6-N1   | 8.52  | 1.41        | 1.35     |
| 1   | AA    | 1143 | G    | N9-C8   | 8.52  | 1.43        | 1.37     |
| 35  | BB    | 1822 | C    | N3-C4   | 8.52  | 1.40        | 1.33     |
| 35  | BB    | 2225 | A    | N3-C4   | -8.52 | 1.29        | 1.34     |
| 1   | AA    | 1346 | A    | N7-C5   | -8.52 | 1.34        | 1.39     |
| 35  | BB    | 649  | G    | N9-C4   | -8.52 | 1.31        | 1.38     |
| 35  | BB    | 2322 | A    | N3-C4   | -8.52 | 1.29        | 1.34     |
| 1   | AA    | 1113 | C    | N3-C4   | 8.52  | 1.40        | 1.33     |
| 1   | AA    | 1130 | A    | N7-C5   | -8.52 | 1.34        | 1.39     |
| 35  | BB    | 1464 | G    | C4'-C3' | 8.52  | 1.62        | 1.53     |
| 35  | BB    | 2240 | U    | C4-C5   | 8.52  | 1.51        | 1.43     |
| 1   | AA    | 1332 | A    | C6-N1   | 8.51  | 1.41        | 1.35     |
| 34  | BA    | 36   | C    | C5-C6   | -8.51 | 1.27        | 1.34     |
| 35  | BB    | 2255 | G    | C6-N1   | 8.51  | 1.45        | 1.39     |
| 35  | BB    | 1607 | C    | C2-N3   | 8.51  | 1.42        | 1.35     |
| 35  | BB    | 1408 | G    | C5'-C4' | 8.51  | 1.61        | 1.51     |
| 35  | BB    | 1809 | A    | N9-C4   | 8.51  | 1.43        | 1.37     |
| 1   | AA    | 1005 | A    | C8-N7   | -8.51 | 1.25        | 1.31     |
| 1   | AA    | 1382 | C    | P-O5'   | -8.51 | 1.51        | 1.59     |
| 35  | BB    | 1403 | A    | N7-C5   | -8.51 | 1.34        | 1.39     |
| 35  | BB    | 2683 | C    | N1-C2   | 8.51  | 1.48        | 1.40     |
| 35  | BB    | 2802 | G    | C8-N7   | -8.51 | 1.25        | 1.30     |
| 35  | BB    | 728  | G    | N1-C2   | 8.51  | 1.44        | 1.37     |
| 1   | AA    | 181  | A    | N9-C4   | -8.50 | 1.32        | 1.37     |
| 1   | AA    | 183  | C    | C4-N4   | 8.50  | 1.41        | 1.33     |
| 1   | AA    | 584  | G    | C8-N7   | -8.50 | 1.25        | 1.30     |
| 35  | BB    | 258  | G    | N1-C2   | 8.50  | 1.44        | 1.37     |
| 35  | BB    | 1716 | U    | O3'-P   | -8.50 | 1.50        | 1.61     |
| 1   | AA    | 38   | G    | C5-C4   | 8.50  | 1.44        | 1.38     |
| 1   | AA    | 490  | C    | C4-C5   | -8.50 | 1.36        | 1.43     |
| 1   | AA    | 1223 | C    | C4-N4   | 8.50  | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1482 | G    | C2'-C1' | -8.50 | 1.44        | 1.53     |
| 1   | AA    | 1483 | A    | C6-N6   | 8.50  | 1.40        | 1.33     |
| 35  | BB    | 288  | U    | C2'-C1' | -8.50 | 1.44        | 1.53     |
| 35  | BB    | 1367 | A    | N3-C4   | -8.50 | 1.29        | 1.34     |
| 1   | AA    | 107  | G    | N7-C5   | -8.49 | 1.34        | 1.39     |
| 1   | AA    | 1127 | G    | N7-C5   | -8.49 | 1.34        | 1.39     |
| 35  | BB    | 844  | A    | P-O5'   | -8.49 | 1.51        | 1.59     |
| 35  | BB    | 1891 | G    | N9-C4   | -8.49 | 1.31        | 1.38     |
| 1   | AA    | 25   | C    | C3'-C2' | 8.49  | 1.62        | 1.52     |
| 1   | AA    | 1081 | A    | N7-C5   | -8.49 | 1.34        | 1.39     |
| 35  | BB    | 1175 | A    | N3-C4   | -8.49 | 1.29        | 1.34     |
| 35  | BB    | 2657 | A    | N9-C8   | -8.49 | 1.30        | 1.37     |
| 1   | AA    | 945  | G    | N7-C5   | -8.49 | 1.34        | 1.39     |
| 1   | AA    | 464  | U    | C2-N3   | 8.49  | 1.43        | 1.37     |
| 1   | AA    | 470  | C    | C4-N4   | 8.49  | 1.41        | 1.33     |
| 1   | AA    | 835  | U    | C4'-C3' | 8.49  | 1.62        | 1.53     |
| 35  | BB    | 276  | U    | N1-C6   | -8.49 | 1.30        | 1.38     |
| 35  | BB    | 684  | G    | C2-N2   | 8.49  | 1.43        | 1.34     |
| 35  | BB    | 2103 | C    | N3-C4   | 8.49  | 1.39        | 1.33     |
| 35  | BB    | 2238 | G    | N1-C2   | 8.49  | 1.44        | 1.37     |
| 1   | AA    | 1518 | A    | N7-C5   | -8.49 | 1.34        | 1.39     |
| 35  | BB    | 723  | C    | C2'-C1' | -8.49 | 1.44        | 1.53     |
| 1   | AA    | 159  | G    | P-O5'   | -8.48 | 1.51        | 1.59     |
| 1   | AA    | 1382 | C    | C4-N4   | 8.48  | 1.41        | 1.33     |
| 1   | AA    | 620  | C    | P-O5'   | -8.48 | 1.51        | 1.59     |
| 1   | AA    | 1056 | U    | C5-C6   | 8.48  | 1.41        | 1.34     |
| 1   | AA    | 1371 | G    | C6-N1   | -8.48 | 1.33        | 1.39     |
| 35  | BB    | 457  | A    | C2'-C1' | -8.48 | 1.44        | 1.53     |
| 35  | BB    | 1027 | A    | C8-N7   | -8.48 | 1.25        | 1.31     |
| 35  | BB    | 1965 | C    | C4-C5   | 8.48  | 1.49        | 1.43     |
| 35  | BB    | 2162 | G    | C8-N7   | 8.48  | 1.36        | 1.30     |
| 35  | BB    | 1898 | U    | C5'-C4' | 8.48  | 1.61        | 1.51     |
| 1   | AA    | 132  | C    | N3-C4   | 8.48  | 1.39        | 1.33     |
| 35  | BB    | 1650 | A    | N9-C4   | 8.48  | 1.43        | 1.37     |
| 35  | BB    | 2661 | G    | C6-N1   | 8.48  | 1.45        | 1.39     |
| 35  | BB    | 2747 | G    | P-O5'   | -8.48 | 1.51        | 1.59     |
| 1   | AA    | 1035 | A    | N7-C5   | -8.48 | 1.34        | 1.39     |
| 1   | AA    | 1404 | C    | N1-C6   | 8.48  | 1.42        | 1.37     |
| 35  | BB    | 2877 | G    | N3-C4   | -8.48 | 1.29        | 1.35     |
| 1   | AA    | 124  | C    | N1-C6   | 8.48  | 1.42        | 1.37     |
| 1   | AA    | 1459 | G    | C5-C4   | -8.48 | 1.32        | 1.38     |
| 35  | BB    | 312  | G    | C8-N7   | -8.48 | 1.25        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 437  | U    | C2-N3   | 8.48  | 1.43        | 1.37     |
| 35  | BB    | 649  | G    | P-O5'   | -8.48 | 1.51        | 1.59     |
| 35  | BB    | 750  | A    | N7-C5   | -8.48 | 1.34        | 1.39     |
| 35  | BB    | 1557 | C    | O3'-P   | -8.48 | 1.50        | 1.61     |
| 35  | BB    | 2143 | C    | O3'-P   | -8.48 | 1.50        | 1.61     |
| 1   | AA    | 1297 | G    | C2-N3   | 8.48  | 1.39        | 1.32     |
| 35  | BB    | 1003 | G    | C6-N1   | 8.48  | 1.45        | 1.39     |
| 35  | BB    | 1138 | G    | C2-N3   | 8.48  | 1.39        | 1.32     |
| 1   | AA    | 718  | A    | C6-N6   | 8.47  | 1.40        | 1.33     |
| 35  | BB    | 1547 | C    | N3-C4   | 8.47  | 1.39        | 1.33     |
| 35  | BB    | 2411 | A    | C2'-C1' | -8.47 | 1.44        | 1.53     |
| 1   | AA    | 251  | G    | C6-N1   | 8.47  | 1.45        | 1.39     |
| 1   | AA    | 1392 | G    | N1-C2   | 8.47  | 1.44        | 1.37     |
| 1   | AA    | 1491 | G    | C4'-O4' | -8.47 | 1.34        | 1.45     |
| 1   | AA    | 824  | G    | N1-C2   | 8.47  | 1.44        | 1.37     |
| 35  | BB    | 926  | G    | C6-N1   | 8.47  | 1.45        | 1.39     |
| 35  | BB    | 1066 | U    | O3'-P   | -8.47 | 1.50        | 1.61     |
| 35  | BB    | 1619 | G    | N9-C8   | 8.47  | 1.43        | 1.37     |
| 35  | BB    | 1747 | U    | P-O5'   | -8.47 | 1.51        | 1.59     |
| 35  | BB    | 1937 | A    | C6-N6   | 8.47  | 1.40        | 1.33     |
| 35  | BB    | 2001 | C    | P-O5'   | -8.47 | 1.51        | 1.59     |
| 35  | BB    | 2058 | A    | C6-N1   | 8.47  | 1.41        | 1.35     |
| 1   | AA    | 1173 | U    | C2-N3   | 8.47  | 1.43        | 1.37     |
| 35  | BB    | 147  | C    | N3-C4   | 8.47  | 1.39        | 1.33     |
| 35  | BB    | 764  | A    | N9-C4   | -8.47 | 1.32        | 1.37     |
| 35  | BB    | 1934 | C    | N3-C4   | 8.47  | 1.39        | 1.33     |
| 1   | AA    | 946  | A    | N9-C4   | -8.47 | 1.32        | 1.37     |
| 35  | BB    | 2242 | G    | N9-C8   | 8.47  | 1.43        | 1.37     |
| 1   | AA    | 58   | C    | N3-C4   | 8.46  | 1.39        | 1.33     |
| 1   | AA    | 327  | A    | N9-C4   | -8.46 | 1.32        | 1.37     |
| 1   | AA    | 718  | A    | C2'-C1' | -8.46 | 1.44        | 1.53     |
| 1   | AA    | 1464 | U    | C4'-C3' | 8.46  | 1.62        | 1.53     |
| 35  | BB    | 1397 | U    | C4-C5   | -8.46 | 1.35        | 1.43     |
| 1   | AA    | 728  | A    | C6-N6   | 8.46  | 1.40        | 1.33     |
| 35  | BB    | 425  | G    | C6-N1   | 8.46  | 1.45        | 1.39     |
| 35  | BB    | 478  | A    | C6-N6   | 8.46  | 1.40        | 1.33     |
| 1   | AA    | 710  | G    | N7-C5   | -8.46 | 1.34        | 1.39     |
| 1   | AA    | 549  | C    | N3-C4   | 8.46  | 1.39        | 1.33     |
| 1   | AA    | 871  | U    | C3'-O3' | 8.46  | 1.53        | 1.42     |
| 34  | BA    | 117  | G    | O3'-P   | -8.46 | 1.51        | 1.61     |
| 35  | BB    | 309  | A    | C8-N7   | 8.46  | 1.37        | 1.31     |
| 35  | BB    | 400  | G    | C2-N3   | 8.46  | 1.39        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 628  | G    | N7-C5   | -8.46 | 1.34        | 1.39     |
| 35  | BB    | 1084 | A    | C6-N6   | 8.46  | 1.40        | 1.33     |
| 35  | BB    | 1756 | G    | C5-C4   | -8.45 | 1.32        | 1.38     |
| 35  | BB    | 1888 | G    | C6-N1   | -8.45 | 1.33        | 1.39     |
| 1   | AA    | 61   | G    | C8-N7   | -8.45 | 1.25        | 1.30     |
| 1   | AA    | 937  | A    | C6-N6   | 8.45  | 1.40        | 1.33     |
| 23  | AX    | 19   | A    | C6-N1   | 8.45  | 1.41        | 1.35     |
| 1   | AA    | 315  | A    | C6-N1   | 8.45  | 1.41        | 1.35     |
| 35  | BB    | 204  | A    | N9-C4   | -8.45 | 1.32        | 1.37     |
| 1   | AA    | 208  | U    | C2-N3   | 8.44  | 1.43        | 1.37     |
| 1   | AA    | 1117 | A    | N9-C4   | 8.45  | 1.43        | 1.37     |
| 35  | BB    | 1930 | G    | C6-N1   | 8.45  | 1.45        | 1.39     |
| 35  | BB    | 891  | G    | C2-N3   | 8.44  | 1.39        | 1.32     |
| 1   | AA    | 289  | G    | N7-C5   | 8.44  | 1.44        | 1.39     |
| 1   | AA    | 293  | G    | C8-N7   | -8.44 | 1.25        | 1.30     |
| 1   | AA    | 363  | A    | C6-N1   | 8.44  | 1.41        | 1.35     |
| 1   | AA    | 604  | G    | C8-N7   | 8.44  | 1.36        | 1.30     |
| 1   | AA    | 733  | G    | C6-N1   | 8.44  | 1.45        | 1.39     |
| 35  | BB    | 213  | A    | C6-N1   | 8.44  | 1.41        | 1.35     |
| 35  | BB    | 855  | G    | N9-C8   | -8.44 | 1.31        | 1.37     |
| 35  | BB    | 1245 | G    | N7-C5   | -8.44 | 1.34        | 1.39     |
| 35  | BB    | 1478 | G    | N9-C8   | 8.44  | 1.43        | 1.37     |
| 35  | BB    | 2098 | U    | N1-C2   | 8.44  | 1.46        | 1.38     |
| 1   | AA    | 530  | G    | C5-C4   | 8.43  | 1.44        | 1.38     |
| 35  | BB    | 1071 | G    | C6-N1   | 8.43  | 1.45        | 1.39     |
| 35  | BB    | 2239 | G    | N7-C5   | -8.43 | 1.34        | 1.39     |
| 1   | AA    | 250  | A    | N9-C4   | 8.43  | 1.43        | 1.37     |
| 35  | BB    | 1084 | A    | C4'-C3' | 8.43  | 1.62        | 1.53     |
| 1   | AA    | 328  | C    | N1-C2   | 8.43  | 1.48        | 1.40     |
| 1   | AA    | 778  | G    | N7-C5   | -8.43 | 1.34        | 1.39     |
| 1   | AA    | 1254 | A    | N3-C4   | -8.43 | 1.29        | 1.34     |
| 35  | BB    | 260  | G    | C8-N7   | -8.43 | 1.25        | 1.30     |
| 35  | BB    | 1008 | A    | O3'-P   | -8.43 | 1.51        | 1.61     |
| 35  | BB    | 1812 | U    | P-O5'   | -8.43 | 1.51        | 1.59     |
| 1   | AA    | 1181 | G    | C2'-C1' | -8.43 | 1.44        | 1.53     |
| 34  | BA    | 89   | U    | C2-N3   | 8.43  | 1.43        | 1.37     |
| 34  | BA    | 115  | A    | N3-C4   | -8.43 | 1.29        | 1.34     |
| 35  | BB    | 728  | G    | N9-C4   | -8.43 | 1.31        | 1.38     |
| 35  | BB    | 2171 | A    | C4'-C3' | 8.43  | 1.62        | 1.53     |
| 35  | BB    | 1246 | A    | N7-C5   | -8.42 | 1.34        | 1.39     |
| 1   | AA    | 859  | G    | C6-N1   | 8.42  | 1.45        | 1.39     |
| 35  | BB    | 1731 | G    | O3'-P   | -8.42 | 1.51        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 144  | G    | C5-C4   | 8.42  | 1.44        | 1.38     |
| 35  | BB    | 1423 | G    | C5-C4   | 8.42  | 1.44        | 1.38     |
| 1   | AA    | 110  | C    | C2-N3   | 8.41  | 1.42        | 1.35     |
| 9   | AI    | 40   | ARG  | CZ-NH2  | 8.41  | 1.44        | 1.33     |
| 35  | BB    | 122  | G    | N3-C4   | -8.41 | 1.29        | 1.35     |
| 35  | BB    | 1008 | A    | N1-C2   | 8.41  | 1.42        | 1.34     |
| 35  | BB    | 2252 | G    | N3-C4   | -8.41 | 1.29        | 1.35     |
| 35  | BB    | 2434 | A    | C6-N1   | 8.41  | 1.41        | 1.35     |
| 35  | BB    | 2749 | A    | C6-N6   | 8.41  | 1.40        | 1.33     |
| 1   | AA    | 829  | G    | O3'-P   | -8.41 | 1.51        | 1.61     |
| 1   | AA    | 1204 | A    | C4'-C3' | -8.41 | 1.44        | 1.53     |
| 35  | BB    | 327  | G    | N1-C2   | 8.41  | 1.44        | 1.37     |
| 35  | BB    | 611  | C    | C5-C6   | 8.41  | 1.41        | 1.34     |
| 35  | BB    | 1749 | A    | C5-C4   | 8.41  | 1.44        | 1.38     |
| 35  | BB    | 2703 | C    | N1-C6   | 8.41  | 1.42        | 1.37     |
| 1   | AA    | 902  | G    | N9-C8   | 8.41  | 1.43        | 1.37     |
| 35  | BB    | 1552 | A    | N7-C5   | -8.41 | 1.34        | 1.39     |
| 1   | AA    | 226  | G    | C8-N7   | -8.41 | 1.25        | 1.30     |
| 1   | AA    | 1353 | G    | N3-C4   | 8.41  | 1.41        | 1.35     |
| 1   | AA    | 1434 | A    | N3-C4   | 8.41  | 1.39        | 1.34     |
| 1   | AA    | 1278 | G    | C8-N7   | -8.40 | 1.25        | 1.30     |
| 35  | BB    | 2824 | C    | C2-O2   | 8.40  | 1.32        | 1.24     |
| 1   | AA    | 608  | A    | C8-N7   | -8.40 | 1.25        | 1.31     |
| 35  | BB    | 1654 | A    | C6-N6   | 8.40  | 1.40        | 1.33     |
| 1   | AA    | 168  | G    | N1-C2   | 8.40  | 1.44        | 1.37     |
| 1   | AA    | 1427 | C    | C2-N3   | 8.40  | 1.42        | 1.35     |
| 35  | BB    | 806  | C    | C2-N3   | 8.40  | 1.42        | 1.35     |
| 51  | BR    | 79   | ARG  | NE-CZ   | 8.40  | 1.44        | 1.33     |
| 35  | BB    | 1227 | G    | C2-N2   | 8.40  | 1.43        | 1.34     |
| 35  | BB    | 2567 | G    | N7-C5   | -8.40 | 1.34        | 1.39     |
| 35  | BB    | 2657 | A    | C6-N1   | 8.39  | 1.41        | 1.35     |
| 1   | AA    | 1177 | G    | C5-C4   | 8.39  | 1.44        | 1.38     |
| 35  | BB    | 775  | G    | C2-N3   | 8.39  | 1.39        | 1.32     |
| 35  | BB    | 1464 | G    | N7-C5   | -8.39 | 1.34        | 1.39     |
| 35  | BB    | 1266 | G    | C6-N1   | 8.39  | 1.45        | 1.39     |
| 1   | AA    | 242  | G    | C5-C4   | 8.39  | 1.44        | 1.38     |
| 1   | AA    | 1299 | A    | N7-C5   | -8.39 | 1.34        | 1.39     |
| 35  | BB    | 1431 | A    | C2'-C1' | -8.39 | 1.44        | 1.53     |
| 35  | BB    | 2850 | A    | N7-C5   | 8.39  | 1.44        | 1.39     |
| 35  | BB    | 954  | G    | N7-C5   | -8.38 | 1.34        | 1.39     |
| 35  | BB    | 966  | G    | C3'-O3' | -8.39 | 1.30        | 1.42     |
| 35  | BB    | 1464 | G    | C8-N7   | -8.38 | 1.25        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1535 | A    | N3-C4   | -8.38 | 1.29        | 1.34     |
| 35  | BB    | 1636 | U    | C2'-C1' | -8.39 | 1.44        | 1.53     |
| 50  | BQ    | 27   | ARG  | CD-NE   | 8.38  | 1.60        | 1.46     |
| 35  | BB    | 1013 | C    | C2-N3   | 8.38  | 1.42        | 1.35     |
| 1   | AA    | 32   | A    | N3-C4   | 8.38  | 1.39        | 1.34     |
| 35  | BB    | 2701 | U    | C4-C5   | 8.38  | 1.51        | 1.43     |
| 1   | AA    | 838  | G    | P-O5'   | -8.38 | 1.51        | 1.59     |
| 35  | BB    | 580  | U    | C2-N3   | 8.38  | 1.43        | 1.37     |
| 35  | BB    | 1360 | G    | N1-C2   | 8.38  | 1.44        | 1.37     |
| 35  | BB    | 1764 | C    | P-O5'   | 8.38  | 1.68        | 1.59     |
| 35  | BB    | 2109 | U    | O3'-P   | -8.38 | 1.51        | 1.61     |
| 1   | AA    | 1329 | A    | C2'-C1' | -8.38 | 1.44        | 1.53     |
| 35  | BB    | 50   | U    | O3'-P   | -8.38 | 1.51        | 1.61     |
| 35  | BB    | 523  | C    | C4-N4   | 8.38  | 1.41        | 1.33     |
| 35  | BB    | 2221 | G    | C2-N3   | 8.38  | 1.39        | 1.32     |
| 35  | BB    | 639  | U    | C2-N3   | 8.38  | 1.43        | 1.37     |
| 35  | BB    | 2800 | A    | N7-C5   | -8.38 | 1.34        | 1.39     |
| 35  | BB    | 210  | C    | N3-C4   | 8.38  | 1.39        | 1.33     |
| 1   | AA    | 48   | C    | C3'-C2' | -8.37 | 1.43        | 1.52     |
| 1   | AA    | 501  | C    | C2-N3   | 8.38  | 1.42        | 1.35     |
| 35  | BB    | 348  | A    | C5'-C4' | 8.38  | 1.61        | 1.51     |
| 35  | BB    | 1247 | A    | C6-N1   | 8.38  | 1.41        | 1.35     |
| 35  | BB    | 2224 | G    | N7-C5   | -8.38 | 1.34        | 1.39     |
| 1   | AA    | 500  | G    | C6-N1   | 8.37  | 1.45        | 1.39     |
| 1   | AA    | 860  | A    | C6-N1   | 8.37  | 1.41        | 1.35     |
| 35  | BB    | 201  | C    | C4-N4   | 8.37  | 1.41        | 1.33     |
| 35  | BB    | 561  | G    | O3'-P   | -8.37 | 1.51        | 1.61     |
| 35  | BB    | 980  | A    | C2-N3   | 8.37  | 1.41        | 1.33     |
| 35  | BB    | 1187 | G    | C2-N2   | 8.37  | 1.43        | 1.34     |
| 35  | BB    | 1260 | A    | O3'-P   | -8.37 | 1.51        | 1.61     |
| 35  | BB    | 1854 | A    | N7-C5   | -8.37 | 1.34        | 1.39     |
| 35  | BB    | 681  | G    | O3'-P   | -8.37 | 1.51        | 1.61     |
| 8   | AH    | 12   | ARG  | CZ-NH1  | 8.37  | 1.44        | 1.33     |
| 35  | BB    | 169  | G    | N1-C2   | 8.37  | 1.44        | 1.37     |
| 35  | BB    | 1033 | U    | C5'-C4' | 8.37  | 1.61        | 1.51     |
| 1   | AA    | 66   | A    | N7-C5   | -8.37 | 1.34        | 1.39     |
| 1   | AA    | 251  | G    | N7-C5   | -8.37 | 1.34        | 1.39     |
| 1   | AA    | 1173 | U    | N3-C4   | 8.37  | 1.46        | 1.38     |
| 35  | BB    | 528  | A    | N7-C5   | -8.37 | 1.34        | 1.39     |
| 1   | AA    | 1512 | U    | C2-N3   | 8.36  | 1.43        | 1.37     |
| 35  | BB    | 1565 | C    | C4-N4   | 8.36  | 1.41        | 1.33     |
| 35  | BB    | 2142 | A    | C5-C4   | 8.36  | 1.44        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 229  | C    | P-O5'   | -8.36 | 1.51        | 1.59     |
| 35  | BB    | 1133 | A    | O3'-P   | -8.36 | 1.51        | 1.61     |
| 35  | BB    | 1329 | U    | C2-N3   | 8.36  | 1.43        | 1.37     |
| 35  | BB    | 2882 | A    | C6-N6   | 8.36  | 1.40        | 1.33     |
| 35  | BB    | 866  | A    | N3-C4   | -8.36 | 1.29        | 1.34     |
| 1   | AA    | 122  | G    | C8-N7   | -8.36 | 1.25        | 1.30     |
| 1   | AA    | 582  | C    | P-O5'   | -8.36 | 1.51        | 1.59     |
| 35  | BB    | 17   | G    | C5-C4   | -8.36 | 1.32        | 1.38     |
| 1   | AA    | 1110 | A    | C6-N1   | 8.35  | 1.41        | 1.35     |
| 35  | BB    | 974  | G    | N3-C4   | -8.35 | 1.29        | 1.35     |
| 1   | AA    | 582  | C    | N1-C6   | -8.35 | 1.32        | 1.37     |
| 35  | BB    | 2709 | G    | N1-C2   | 8.35  | 1.44        | 1.37     |
| 35  | BB    | 626  | A    | N9-C4   | -8.35 | 1.32        | 1.37     |
| 35  | BB    | 2246 | G    | N7-C5   | -8.35 | 1.34        | 1.39     |
| 1   | AA    | 1117 | A    | N9-C8   | -8.35 | 1.31        | 1.37     |
| 35  | BB    | 892  | A    | C5-C4   | 8.35  | 1.44        | 1.38     |
| 35  | BB    | 1754 | A    | O3'-P   | -8.35 | 1.51        | 1.61     |
| 35  | BB    | 2507 | C    | P-O5'   | -8.35 | 1.51        | 1.59     |
| 1   | AA    | 1251 | A    | N9-C4   | 8.35  | 1.42        | 1.37     |
| 34  | BA    | 105  | G    | O3'-P   | -8.35 | 1.51        | 1.61     |
| 35  | BB    | 905  | A    | C6-N1   | 8.35  | 1.41        | 1.35     |
| 35  | BB    | 449  | A    | N9-C4   | -8.35 | 1.32        | 1.37     |
| 35  | BB    | 951  | C    | O4'-C1' | 8.35  | 1.52        | 1.41     |
| 35  | BB    | 2377 | A    | P-O5'   | -8.35 | 1.51        | 1.59     |
| 35  | BB    | 1504 | A    | N3-C4   | -8.34 | 1.29        | 1.34     |
| 35  | BB    | 2347 | C    | N1-C6   | 8.34  | 1.42        | 1.37     |
| 35  | BB    | 2026 | U    | C2-N3   | 8.34  | 1.43        | 1.37     |
| 35  | BB    | 2497 | A    | N1-C2   | 8.34  | 1.41        | 1.34     |
| 35  | BB    | 2831 | G    | C6-N1   | 8.34  | 1.45        | 1.39     |
| 35  | BB    | 1658 | C    | C4-C5   | 8.34  | 1.49        | 1.43     |
| 1   | AA    | 72   | A    | C6-N6   | 8.34  | 1.40        | 1.33     |
| 1   | AA    | 196  | A    | C6-N1   | 8.34  | 1.41        | 1.35     |
| 1   | AA    | 1513 | A    | C5-C4   | 8.34  | 1.44        | 1.38     |
| 35  | BB    | 68   | G    | C2-N3   | 8.34  | 1.39        | 1.32     |
| 35  | BB    | 629  | G    | C2-N3   | 8.34  | 1.39        | 1.32     |
| 35  | BB    | 993  | G    | N7-C5   | -8.34 | 1.34        | 1.39     |
| 1   | AA    | 117  | G    | N9-C8   | -8.33 | 1.32        | 1.37     |
| 1   | AA    | 822  | U    | C2'-C1' | -8.33 | 1.44        | 1.53     |
| 1   | AA    | 1258 | G    | N9-C8   | 8.33  | 1.43        | 1.37     |
| 1   | AA    | 716  | A    | N7-C5   | -8.33 | 1.34        | 1.39     |
| 35  | BB    | 2669 | G    | N9-C8   | 8.33  | 1.43        | 1.37     |
| 35  | BB    | 1825 | U    | N1-C2   | 8.33  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2685 | G    | C5-C4   | 8.33  | 1.44        | 1.38     |
| 35  | BB    | 812  | C    | C4-C5   | 8.33  | 1.49        | 1.43     |
| 1   | AA    | 497  | G    | N7-C5   | -8.33 | 1.34        | 1.39     |
| 35  | BB    | 956  | G    | N7-C5   | -8.33 | 1.34        | 1.39     |
| 35  | BB    | 1175 | A    | P-O5'   | 8.33  | 1.68        | 1.59     |
| 35  | BB    | 1248 | G    | N9-C8   | -8.33 | 1.32        | 1.37     |
| 35  | BB    | 1604 | C    | N3-C4   | 8.32  | 1.39        | 1.33     |
| 1   | AA    | 993  | G    | N7-C5   | -8.32 | 1.34        | 1.39     |
| 35  | BB    | 718  | A    | C2'-C1' | -8.32 | 1.44        | 1.53     |
| 35  | BB    | 1732 | C    | C4-N4   | 8.32  | 1.41        | 1.33     |
| 35  | BB    | 1543 | G    | C2-N3   | 8.32  | 1.39        | 1.32     |
| 35  | BB    | 517  | C    | N3-C4   | 8.32  | 1.39        | 1.33     |
| 35  | BB    | 1408 | G    | N1-C2   | 8.32  | 1.44        | 1.37     |
| 35  | BB    | 1758 | U    | C3'-O3' | 8.32  | 1.53        | 1.42     |
| 35  | BB    | 2173 | A    | N7-C5   | -8.32 | 1.34        | 1.39     |
| 35  | BB    | 2759 | G    | C6-N1   | 8.32  | 1.45        | 1.39     |
| 1   | AA    | 1251 | A    | C6-N6   | 8.32  | 1.40        | 1.33     |
| 35  | BB    | 2482 | A    | N7-C5   | -8.32 | 1.34        | 1.39     |
| 1   | AA    | 574  | A    | N7-C5   | -8.31 | 1.34        | 1.39     |
| 35  | BB    | 124  | G    | N1-C2   | 8.31  | 1.44        | 1.37     |
| 35  | BB    | 1272 | A    | C6-N1   | 8.31  | 1.41        | 1.35     |
| 35  | BB    | 2230 | G    | N7-C5   | 8.31  | 1.44        | 1.39     |
| 35  | BB    | 1770 | G    | N9-C4   | -8.31 | 1.31        | 1.38     |
| 35  | BB    | 1838 | C    | P-O5'   | -8.31 | 1.51        | 1.59     |
| 1   | AA    | 104  | G    | N3-C4   | 8.31  | 1.41        | 1.35     |
| 1   | AA    | 259  | G    | N9-C4   | -8.31 | 1.31        | 1.38     |
| 1   | AA    | 487  | A    | N7-C5   | -8.31 | 1.34        | 1.39     |
| 1   | AA    | 1355 | G    | P-O5'   | -8.31 | 1.51        | 1.59     |
| 35  | BB    | 1566 | A    | C4'-C3' | 8.31  | 1.62        | 1.53     |
| 35  | BB    | 2303 | G    | N9-C4   | -8.31 | 1.31        | 1.38     |
| 1   | AA    | 1150 | A    | N9-C8   | 8.31  | 1.44        | 1.37     |
| 1   | AA    | 1099 | G    | C2-N3   | 8.31  | 1.39        | 1.32     |
| 1   | AA    | 1204 | A    | C2'-C1' | -8.31 | 1.44        | 1.53     |
| 1   | AA    | 238  | A    | N7-C5   | -8.30 | 1.34        | 1.39     |
| 1   | AA    | 832  | G    | C5-C4   | -8.31 | 1.32        | 1.38     |
| 1   | AA    | 1508 | A    | N3-C4   | -8.31 | 1.29        | 1.34     |
| 35  | BB    | 468  | G    | N1-C2   | 8.31  | 1.44        | 1.37     |
| 35  | BB    | 2328 | A    | N7-C5   | -8.31 | 1.34        | 1.39     |
| 1   | AA    | 359  | G    | N7-C5   | -8.30 | 1.34        | 1.39     |
| 35  | BB    | 789  | A    | N7-C5   | -8.30 | 1.34        | 1.39     |
| 35  | BB    | 1907 | G    | C2-N3   | 8.30  | 1.39        | 1.32     |
| 35  | BB    | 1966 | A    | P-O5'   | -8.30 | 1.51        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2154 | A    | O3'-P   | -8.30 | 1.51        | 1.61     |
| 35  | BB    | 2732 | G    | N7-C5   | 8.30  | 1.44        | 1.39     |
| 35  | BB    | 1253 | A    | N7-C5   | -8.30 | 1.34        | 1.39     |
| 35  | BB    | 1641 | A    | N9-C4   | -8.30 | 1.32        | 1.37     |
| 1   | AA    | 79   | G    | C3'-C2' | 8.30  | 1.62        | 1.52     |
| 1   | AA    | 668  | G    | N9-C8   | 8.30  | 1.43        | 1.37     |
| 1   | AA    | 721  | G    | C5'-C4' | 8.30  | 1.61        | 1.51     |
| 1   | AA    | 886  | G    | C5-C4   | 8.30  | 1.44        | 1.38     |
| 35  | BB    | 217  | A    | C8-N7   | -8.30 | 1.25        | 1.31     |
| 34  | BA    | 63   | C    | C4-N4   | 8.30  | 1.41        | 1.33     |
| 1   | AA    | 1425 | U    | C2'-C1' | -8.30 | 1.44        | 1.53     |
| 35  | BB    | 1089 | A    | C6-N6   | 8.30  | 1.40        | 1.33     |
| 1   | AA    | 702  | A    | P-O5'   | -8.30 | 1.51        | 1.59     |
| 34  | BA    | 20   | G    | C8-N7   | 8.30  | 1.35        | 1.30     |
| 35  | BB    | 55   | G    | N1-C2   | 8.30  | 1.44        | 1.37     |
| 35  | BB    | 847  | U    | C2'-C1' | -8.30 | 1.44        | 1.53     |
| 35  | BB    | 932  | U    | P-O5'   | -8.30 | 1.51        | 1.59     |
| 35  | BB    | 2445 | G    | C6-N1   | 8.30  | 1.45        | 1.39     |
| 46  | BM    | 10   | ARG  | CZ-NH2  | 8.30  | 1.43        | 1.33     |
| 35  | BB    | 2155 | U    | C5-C6   | 8.30  | 1.41        | 1.34     |
| 1   | AA    | 1385 | G    | N3-C4   | -8.29 | 1.29        | 1.35     |
| 35  | BB    | 100  | U    | N1-C6   | 8.29  | 1.45        | 1.38     |
| 35  | BB    | 954  | G    | C8-N7   | -8.29 | 1.25        | 1.30     |
| 35  | BB    | 1476 | U    | C2-N3   | 8.29  | 1.43        | 1.37     |
| 1   | AA    | 929  | G    | N9-C8   | 8.29  | 1.43        | 1.37     |
| 35  | BB    | 2133 | G    | C2-N3   | 8.29  | 1.39        | 1.32     |
| 1   | AA    | 1034 | G    | N1-C2   | 8.29  | 1.44        | 1.37     |
| 35  | BB    | 118  | A    | N7-C5   | -8.29 | 1.34        | 1.39     |
| 35  | BB    | 142  | A    | N3-C4   | -8.29 | 1.29        | 1.34     |
| 35  | BB    | 980  | A    | N3-C4   | -8.29 | 1.29        | 1.34     |
| 35  | BB    | 2134 | A    | N3-C4   | -8.28 | 1.29        | 1.34     |
| 1   | AA    | 517  | G    | C6-N1   | 8.28  | 1.45        | 1.39     |
| 35  | BB    | 899  | A    | N7-C5   | -8.28 | 1.34        | 1.39     |
| 35  | BB    | 461  | C    | O3'-P   | -8.28 | 1.51        | 1.61     |
| 1   | AA    | 1277 | C    | N1-C6   | 8.28  | 1.42        | 1.37     |
| 35  | BB    | 341  | C    | N1-C6   | -8.28 | 1.32        | 1.37     |
| 35  | BB    | 799  | G    | C5'-C4' | 8.28  | 1.61        | 1.51     |
| 1   | AA    | 105  | G    | C2-N2   | 8.27  | 1.42        | 1.34     |
| 1   | AA    | 481  | G    | C2-N3   | 8.27  | 1.39        | 1.32     |
| 1   | AA    | 1185 | G    | N7-C5   | -8.27 | 1.34        | 1.39     |
| 35  | BB    | 36   | G    | N3-C4   | 8.27  | 1.41        | 1.35     |
| 35  | BB    | 471  | A    | N3-C4   | -8.27 | 1.29        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 358  | U    | N3-C4   | 8.27  | 1.45        | 1.38     |
| 35  | BB    | 2167 | U    | N3-C4   | 8.27  | 1.45        | 1.38     |
| 35  | BB    | 2632 | A    | C1'-N9  | -8.27 | 1.35        | 1.46     |
| 36  | BC    | 261  | ARG  | CZ-NH1  | 8.27  | 1.43        | 1.33     |
| 35  | BB    | 2842 | G    | C4'-C3' | 8.27  | 1.62        | 1.53     |
| 35  | BB    | 2900 | A    | N9-C4   | -8.27 | 1.32        | 1.37     |
| 1   | AA    | 858  | G    | C5-C6   | -8.27 | 1.34        | 1.42     |
| 1   | AA    | 1518 | A    | C8-N7   | -8.27 | 1.25        | 1.31     |
| 35  | BB    | 574  | A    | C6-N6   | 8.27  | 1.40        | 1.33     |
| 35  | BB    | 371  | A    | C5-C4   | 8.27  | 1.44        | 1.38     |
| 35  | BB    | 1542 | U    | O4'-C1' | -8.27 | 1.30        | 1.41     |
| 35  | BB    | 2828 | G    | N1-C2   | 8.27  | 1.44        | 1.37     |
| 1   | AA    | 413  | G    | N7-C5   | -8.27 | 1.34        | 1.39     |
| 1   | AA    | 709  | U    | C2-N3   | 8.27  | 1.43        | 1.37     |
| 1   | AA    | 1387 | G    | C5-C4   | -8.27 | 1.32        | 1.38     |
| 34  | BA    | 10   | G    | N9-C8   | 8.27  | 1.43        | 1.37     |
| 35  | BB    | 223  | A    | O3'-P   | -8.27 | 1.51        | 1.61     |
| 35  | BB    | 969  | G    | N9-C4   | 8.27  | 1.44        | 1.38     |
| 1   | AA    | 1206 | G    | N9-C4   | 8.26  | 1.44        | 1.38     |
| 35  | BB    | 57   | C    | N1-C2   | 8.26  | 1.48        | 1.40     |
| 35  | BB    | 494  | G    | C2-N3   | 8.26  | 1.39        | 1.32     |
| 35  | BB    | 831  | G    | P-O5'   | -8.26 | 1.51        | 1.59     |
| 35  | BB    | 1515 | A    | C3'-C2' | -8.26 | 1.43        | 1.52     |
| 1   | AA    | 96   | U    | N3-C4   | 8.26  | 1.45        | 1.38     |
| 35  | BB    | 690  | G    | P-O5'   | -8.26 | 1.51        | 1.59     |
| 36  | BC    | 257  | ARG  | NE-CZ   | 8.26  | 1.43        | 1.33     |
| 1   | AA    | 629  | A    | C2'-C1' | -8.26 | 1.44        | 1.53     |
| 1   | AA    | 1410 | A    | N9-C4   | -8.26 | 1.32        | 1.37     |
| 35  | BB    | 2542 | A    | P-O5'   | -8.26 | 1.51        | 1.59     |
| 35  | BB    | 2624 | G    | C6-N1   | 8.26  | 1.45        | 1.39     |
| 1   | AA    | 110  | C    | N1-C6   | -8.26 | 1.32        | 1.37     |
| 1   | AA    | 1400 | C    | C2'-C1' | -8.26 | 1.44        | 1.53     |
| 1   | AA    | 187  | G    | C2'-C1' | -8.26 | 1.44        | 1.53     |
| 1   | AA    | 1504 | G    | N7-C5   | -8.26 | 1.34        | 1.39     |
| 35  | BB    | 194  | G    | N7-C5   | -8.26 | 1.34        | 1.39     |
| 35  | BB    | 1516 | G    | C6-N1   | 8.26  | 1.45        | 1.39     |
| 35  | BB    | 2270 | A    | C2'-C1' | -8.26 | 1.44        | 1.53     |
| 1   | AA    | 819  | A    | N9-C4   | 8.26  | 1.42        | 1.37     |
| 35  | BB    | 1118 | C    | C4-C5   | 8.26  | 1.49        | 1.43     |
| 1   | AA    | 126  | G    | C2-N3   | 8.25  | 1.39        | 1.32     |
| 1   | AA    | 1009 | U    | N1-C2   | -8.25 | 1.31        | 1.38     |
| 1   | AA    | 1385 | G    | N7-C5   | -8.25 | 1.34        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2230 | G    | C6-N1   | 8.25  | 1.45        | 1.39     |
| 35  | BB    | 2501 | C    | N3-C4   | 8.25  | 1.39        | 1.33     |
| 1   | AA    | 861  | G    | N7-C5   | -8.25 | 1.34        | 1.39     |
| 1   | AA    | 1021 | A    | C6-N1   | -8.25 | 1.29        | 1.35     |
| 35  | BB    | 532  | A    | N9-C8   | -8.25 | 1.31        | 1.37     |
| 1   | AA    | 1410 | A    | N9-C8   | 8.25  | 1.44        | 1.37     |
| 35  | BB    | 1008 | A    | N9-C8   | -8.25 | 1.31        | 1.37     |
| 35  | BB    | 2581 | G    | N7-C5   | -8.25 | 1.34        | 1.39     |
| 35  | BB    | 2625 | G    | C2-N3   | 8.25  | 1.39        | 1.32     |
| 35  | BB    | 1919 | A    | C6-N6   | 8.25  | 1.40        | 1.33     |
| 1   | AA    | 731  | G    | N7-C5   | 8.25  | 1.44        | 1.39     |
| 35  | BB    | 753  | A    | C4'-C3' | -8.25 | 1.44        | 1.53     |
| 1   | AA    | 262  | A    | C6-N1   | 8.24  | 1.41        | 1.35     |
| 1   | AA    | 1117 | A    | C6-N1   | 8.24  | 1.41        | 1.35     |
| 35  | BB    | 1297 | C    | O3'-P   | -8.24 | 1.51        | 1.61     |
| 1   | AA    | 774  | G    | P-O5'   | -8.24 | 1.51        | 1.59     |
| 1   | AA    | 1423 | G    | C5-C4   | 8.24  | 1.44        | 1.38     |
| 35  | BB    | 917  | A    | N3-C4   | -8.24 | 1.29        | 1.34     |
| 35  | BB    | 756  | A    | N3-C4   | -8.24 | 1.29        | 1.34     |
| 1   | AA    | 797  | C    | C3'-C2' | 8.24  | 1.62        | 1.52     |
| 1   | AA    | 1150 | A    | N3-C4   | 8.24  | 1.39        | 1.34     |
| 1   | AA    | 1296 | C    | P-O5'   | -8.24 | 1.51        | 1.59     |
| 35  | BB    | 930  | G    | C6-N1   | 8.24  | 1.45        | 1.39     |
| 35  | BB    | 1568 | G    | C6-N1   | 8.24  | 1.45        | 1.39     |
| 35  | BB    | 2131 | U    | N3-C4   | 8.24  | 1.45        | 1.38     |
| 35  | BB    | 2627 | G    | C5'-C4' | 8.24  | 1.61        | 1.51     |
| 35  | BB    | 525  | U    | N1-C6   | 8.23  | 1.45        | 1.38     |
| 1   | AA    | 999  | C    | N1-C6   | 8.23  | 1.42        | 1.37     |
| 35  | BB    | 726  | G    | N7-C5   | -8.23 | 1.34        | 1.39     |
| 1   | AA    | 278  | G    | C5-C6   | 8.23  | 1.50        | 1.42     |
| 35  | BB    | 196  | A    | N9-C8   | 8.23  | 1.44        | 1.37     |
| 35  | BB    | 1087 | G    | C6-N1   | 8.23  | 1.45        | 1.39     |
| 35  | BB    | 1377 | G    | N7-C5   | -8.23 | 1.34        | 1.39     |
| 35  | BB    | 1    | G    | C2-N3   | 8.23  | 1.39        | 1.32     |
| 35  | BB    | 1065 | U    | C2-N3   | 8.23  | 1.43        | 1.37     |
| 35  | BB    | 1961 | C    | C2-N3   | 8.23  | 1.42        | 1.35     |
| 1   | AA    | 1269 | A    | N9-C8   | 8.23  | 1.44        | 1.37     |
| 35  | BB    | 549  | G    | P-O5'   | -8.23 | 1.51        | 1.59     |
| 35  | BB    | 1398 | C    | C3'-O3' | 8.23  | 1.53        | 1.42     |
| 1   | AA    | 60   | A    | C8-N7   | -8.23 | 1.25        | 1.31     |
| 35  | BB    | 1961 | C    | N3-C4   | 8.22  | 1.39        | 1.33     |
| 35  | BB    | 2309 | A    | C6-N1   | 8.22  | 1.41        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2440 | C    | C2'-C1' | -8.22 | 1.44        | 1.53     |
| 1   | AA    | 528  | C    | N1-C6   | 8.22  | 1.42        | 1.37     |
| 1   | AA    | 1117 | A    | N3-C4   | 8.22  | 1.39        | 1.34     |
| 1   | AA    | 1454 | G    | N3-C4   | -8.22 | 1.29        | 1.35     |
| 35  | BB    | 1709 | U    | N3-C4   | -8.22 | 1.31        | 1.38     |
| 1   | AA    | 1392 | G    | C6-N1   | 8.22  | 1.45        | 1.39     |
| 35  | BB    | 1607 | C    | C4-C5   | 8.22  | 1.49        | 1.43     |
| 35  | BB    | 2753 | A    | N9-C4   | -8.22 | 1.32        | 1.37     |
| 1   | AA    | 424  | G    | N9-C8   | -8.22 | 1.32        | 1.37     |
| 35  | BB    | 1516 | G    | C2-N3   | 8.22  | 1.39        | 1.32     |
| 1   | AA    | 487  | A    | C5-C4   | 8.22  | 1.44        | 1.38     |
| 1   | AA    | 1379 | G    | N7-C5   | -8.21 | 1.34        | 1.39     |
| 34  | BA    | 26   | C    | N3-C4   | 8.21  | 1.39        | 1.33     |
| 35  | BB    | 1532 | A    | N3-C4   | -8.21 | 1.29        | 1.34     |
| 1   | AA    | 52   | C    | N3-C4   | 8.21  | 1.39        | 1.33     |
| 1   | AA    | 206  | C    | N3-C4   | 8.21  | 1.39        | 1.33     |
| 1   | AA    | 1320 | C    | N3-C4   | -8.21 | 1.28        | 1.33     |
| 1   | AA    | 1445 | U    | C2'-C1' | -8.21 | 1.44        | 1.53     |
| 35  | BB    | 53   | A    | C2-N3   | 8.21  | 1.41        | 1.33     |
| 35  | BB    | 806  | C    | N1-C6   | 8.21  | 1.42        | 1.37     |
| 35  | BB    | 954  | G    | N9-C4   | -8.21 | 1.31        | 1.38     |
| 35  | BB    | 1489 | C    | C5'-C4' | 8.21  | 1.61        | 1.51     |
| 35  | BB    | 1821 | A    | C8-N7   | 8.21  | 1.37        | 1.31     |
| 35  | BB    | 2351 | G    | N7-C5   | -8.21 | 1.34        | 1.39     |
| 1   | AA    | 433  | G    | N9-C8   | 8.21  | 1.43        | 1.37     |
| 1   | AA    | 568  | G    | C2'-C1' | -8.21 | 1.44        | 1.53     |
| 1   | AA    | 777  | A    | N1-C2   | 8.21  | 1.41        | 1.34     |
| 35  | BB    | 2421 | G    | N7-C5   | -8.21 | 1.34        | 1.39     |
| 1   | AA    | 982  | U    | C2'-C1' | -8.21 | 1.44        | 1.53     |
| 35  | BB    | 706  | A    | N1-C2   | 8.21  | 1.41        | 1.34     |
| 35  | BB    | 1183 | U    | C4'-O4' | -8.21 | 1.34        | 1.45     |
| 35  | BB    | 1331 | G    | C2-N2   | 8.21  | 1.42        | 1.34     |
| 35  | BB    | 261  | G    | P-O5'   | -8.21 | 1.51        | 1.59     |
| 35  | BB    | 884  | U    | C2-N3   | 8.21  | 1.43        | 1.37     |
| 1   | AA    | 1462 | C    | C4'-C3' | 8.20  | 1.62        | 1.53     |
| 35  | BB    | 194  | G    | N1-C2   | 8.20  | 1.44        | 1.37     |
| 35  | BB    | 340  | A    | C6-N1   | 8.20  | 1.41        | 1.35     |
| 35  | BB    | 674  | G    | N7-C5   | -8.20 | 1.34        | 1.39     |
| 35  | BB    | 920  | A    | C8-N7   | -8.20 | 1.25        | 1.31     |
| 35  | BB    | 956  | G    | C2-N3   | 8.20  | 1.39        | 1.32     |
| 35  | BB    | 965  | C    | C4-C5   | 8.20  | 1.49        | 1.43     |
| 35  | BB    | 1901 | A    | N7-C5   | 8.20  | 1.44        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2497 | A    | P-O5'   | -8.20 | 1.51        | 1.59     |
| 35  | BB    | 266  | G    | N1-C2   | 8.20  | 1.44        | 1.37     |
| 35  | BB    | 1437 | C    | N1-C6   | -8.20 | 1.32        | 1.37     |
| 35  | BB    | 1571 | A    | C8-N7   | -8.20 | 1.25        | 1.31     |
| 1   | AA    | 146  | G    | N9-C8   | 8.20  | 1.43        | 1.37     |
| 35  | BB    | 514  | A    | C6-N1   | 8.20  | 1.41        | 1.35     |
| 35  | BB    | 519  | U    | C4-C5   | 8.20  | 1.50        | 1.43     |
| 35  | BB    | 2670 | A    | C4'-O4' | 8.20  | 1.56        | 1.45     |
| 1   | AA    | 968  | A    | C5'-C4' | 8.20  | 1.61        | 1.51     |
| 1   | AA    | 1518 | A    | N9-C4   | -8.20 | 1.32        | 1.37     |
| 34  | BA    | 5    | U    | N3-C4   | 8.20  | 1.45        | 1.38     |
| 35  | BB    | 570  | G    | C5'-C4' | 8.20  | 1.61        | 1.51     |
| 35  | BB    | 1235 | G    | C6-N1   | 8.20  | 1.45        | 1.39     |
| 35  | BB    | 1283 | G    | C2-N3   | 8.20  | 1.39        | 1.32     |
| 35  | BB    | 368  | A    | C8-N7   | -8.19 | 1.25        | 1.31     |
| 1   | AA    | 131  | A    | C6-N6   | 8.19  | 1.40        | 1.33     |
| 1   | AA    | 136  | C    | C3'-C2' | -8.19 | 1.43        | 1.52     |
| 1   | AA    | 919  | A    | N3-C4   | -8.19 | 1.29        | 1.34     |
| 35  | BB    | 1469 | A    | C6-N6   | 8.19  | 1.40        | 1.33     |
| 1   | AA    | 985  | C    | C4-N4   | 8.19  | 1.41        | 1.33     |
| 1   | AA    | 1349 | A    | N1-C2   | -8.19 | 1.26        | 1.34     |
| 1   | AA    | 1365 | G    | N1-C2   | 8.19  | 1.44        | 1.37     |
| 35  | BB    | 13   | A    | C6-N6   | 8.19  | 1.40        | 1.33     |
| 1   | AA    | 638  | U    | C2-N3   | 8.19  | 1.43        | 1.37     |
| 35  | BB    | 677  | A    | N9-C4   | -8.19 | 1.32        | 1.37     |
| 35  | BB    | 2444 | G    | N7-C5   | 8.19  | 1.44        | 1.39     |
| 1   | AA    | 1234 | C    | N3-C4   | 8.19  | 1.39        | 1.33     |
| 35  | BB    | 998  | C    | C2'-C1' | -8.19 | 1.44        | 1.53     |
| 1   | AA    | 530  | G    | C6-N1   | 8.19  | 1.45        | 1.39     |
| 1   | AA    | 1174 | G    | C6-N1   | 8.19  | 1.45        | 1.39     |
| 35  | BB    | 1308 | A    | C6-N1   | 8.19  | 1.41        | 1.35     |
| 35  | BB    | 1699 | G    | N1-C2   | 8.19  | 1.44        | 1.37     |
| 35  | BB    | 1678 | A    | C6-N6   | 8.19  | 1.40        | 1.33     |
| 35  | BB    | 2035 | G    | N7-C5   | -8.19 | 1.34        | 1.39     |
| 1   | AA    | 703  | G    | N7-C5   | -8.18 | 1.34        | 1.39     |
| 1   | AA    | 1300 | G    | C2'-C1' | -8.18 | 1.44        | 1.53     |
| 1   | AA    | 821  | G    | C2-N3   | 8.18  | 1.39        | 1.32     |
| 34  | BA    | 75   | G    | N9-C8   | 8.18  | 1.43        | 1.37     |
| 35  | BB    | 1702 | G    | C5-C4   | 8.18  | 1.44        | 1.38     |
| 35  | BB    | 2169 | A    | N7-C5   | -8.18 | 1.34        | 1.39     |
| 35  | BB    | 868  | U    | C4-C5   | 8.18  | 1.50        | 1.43     |
| 1   | AA    | 688  | G    | C5-C4   | -8.18 | 1.32        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1114 | C    | C2'-C1' | -8.18 | 1.44        | 1.53     |
| 35  | BB    | 1808 | A    | C4'-C3' | 8.18  | 1.62        | 1.53     |
| 1   | AA    | 1493 | A    | N7-C5   | -8.18 | 1.34        | 1.39     |
| 1   | AA    | 920  | U    | C5'-C4' | 8.18  | 1.61        | 1.51     |
| 1   | AA    | 1035 | A    | N9-C4   | -8.18 | 1.32        | 1.37     |
| 1   | AA    | 1378 | C    | P-O5'   | -8.18 | 1.51        | 1.59     |
| 35  | BB    | 608  | A    | N7-C5   | -8.18 | 1.34        | 1.39     |
| 35  | BB    | 622  | G    | O3'-P   | -8.18 | 1.51        | 1.61     |
| 35  | BB    | 2035 | G    | C1'-N9  | -8.18 | 1.35        | 1.46     |
| 1   | AA    | 158  | G    | N7-C5   | -8.17 | 1.34        | 1.39     |
| 1   | AA    | 780  | A    | N7-C5   | -8.17 | 1.34        | 1.39     |
| 35  | BB    | 1443 | U    | C2-N3   | 8.17  | 1.43        | 1.37     |
| 1   | AA    | 1013 | G    | N9-C8   | -8.17 | 1.32        | 1.37     |
| 35  | BB    | 2803 | G    | N7-C5   | -8.17 | 1.34        | 1.39     |
| 1   | AA    | 453  | G    | N1-C2   | 8.17  | 1.44        | 1.37     |
| 1   | AA    | 475  | C    | C4-N4   | 8.17  | 1.41        | 1.33     |
| 35  | BB    | 556  | A    | P-O5'   | -8.17 | 1.51        | 1.59     |
| 1   | AA    | 392  | C    | C4'-C3' | 8.17  | 1.62        | 1.53     |
| 35  | BB    | 121  | G    | N9-C4   | 8.17  | 1.44        | 1.38     |
| 1   | AA    | 1362 | A    | C2'-C1' | -8.17 | 1.44        | 1.53     |
| 35  | BB    | 695  | G    | N7-C5   | -8.17 | 1.34        | 1.39     |
| 35  | BB    | 864  | G    | C2-N3   | 8.17  | 1.39        | 1.32     |
| 35  | BB    | 1324 | G    | N9-C4   | 8.17  | 1.44        | 1.38     |
| 1   | AA    | 410  | G    | C5-C4   | -8.16 | 1.32        | 1.38     |
| 1   | AA    | 772  | U    | C4-C5   | 8.16  | 1.50        | 1.43     |
| 1   | AA    | 944  | G    | N1-C2   | 8.16  | 1.44        | 1.37     |
| 35  | BB    | 2184 | A    | C6-N6   | 8.16  | 1.40        | 1.33     |
| 35  | BB    | 2597 | G    | C2-N3   | 8.16  | 1.39        | 1.32     |
| 1   | AA    | 682  | G    | N9-C8   | 8.16  | 1.43        | 1.37     |
| 35  | BB    | 713  | G    | C2-N3   | 8.16  | 1.39        | 1.32     |
| 35  | BB    | 1862 | G    | C2-N3   | 8.16  | 1.39        | 1.32     |
| 35  | BB    | 2725 | A    | P-O5'   | -8.16 | 1.51        | 1.59     |
| 1   | AA    | 274  | A    | N9-C4   | 8.16  | 1.42        | 1.37     |
| 1   | AA    | 1140 | C    | O4'-C1' | 8.16  | 1.52        | 1.41     |
| 1   | AA    | 1511 | G    | C2-N3   | 8.16  | 1.39        | 1.32     |
| 35  | BB    | 37   | C    | N1-C6   | 8.16  | 1.42        | 1.37     |
| 35  | BB    | 2147 | A    | N9-C4   | -8.16 | 1.32        | 1.37     |
| 35  | BB    | 387  | U    | C2-N3   | 8.16  | 1.43        | 1.37     |
| 35  | BB    | 2759 | G    | C2-N2   | 8.16  | 1.42        | 1.34     |
| 1   | AA    | 968  | A    | C6-N1   | 8.16  | 1.41        | 1.35     |
| 1   | AA    | 998  | C    | P-O5'   | -8.16 | 1.51        | 1.59     |
| 34  | BA    | 107  | G    | N3-C4   | 8.16  | 1.41        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1382 | G    | N9-C4   | -8.16 | 1.31        | 1.38     |
| 35  | BB    | 1491 | G    | N1-C2   | 8.16  | 1.44        | 1.37     |
| 35  | BB    | 1689 | A    | N7-C5   | -8.16 | 1.34        | 1.39     |
| 35  | BB    | 1817 | G    | N9-C4   | -8.16 | 1.31        | 1.38     |
| 35  | BB    | 1935 | G    | C8-N7   | 8.16  | 1.35        | 1.30     |
| 35  | BB    | 2126 | A    | C6-N6   | 8.16  | 1.40        | 1.33     |
| 1   | AA    | 950  | U    | C2-N3   | 8.15  | 1.43        | 1.37     |
| 35  | BB    | 84   | A    | C4'-C3' | 8.15  | 1.62        | 1.53     |
| 35  | BB    | 887  | U    | N3-C4   | 8.15  | 1.45        | 1.38     |
| 35  | BB    | 1325 | U    | C1'-N1  | 8.15  | 1.60        | 1.48     |
| 35  | BB    | 801  | G    | N7-C5   | -8.15 | 1.34        | 1.39     |
| 35  | BB    | 1200 | C    | N3-C4   | 8.15  | 1.39        | 1.33     |
| 1   | AA    | 400  | C    | O3'-P   | -8.15 | 1.51        | 1.61     |
| 35  | BB    | 1129 | A    | C5-C4   | 8.15  | 1.44        | 1.38     |
| 35  | BB    | 1659 | G    | C2-N3   | 8.15  | 1.39        | 1.32     |
| 1   | AA    | 988  | G    | C2-N3   | 8.15  | 1.39        | 1.32     |
| 1   | AA    | 1375 | A    | N3-C4   | -8.15 | 1.29        | 1.34     |
| 35  | BB    | 459  | U    | N3-C4   | 8.15  | 1.45        | 1.38     |
| 35  | BB    | 2637 | U    | C4'-C3' | -8.15 | 1.44        | 1.53     |
| 35  | BB    | 1458 | U    | N1-C2   | 8.15  | 1.45        | 1.38     |
| 35  | BB    | 1576 | U    | N3-C4   | 8.15  | 1.45        | 1.38     |
| 1   | AA    | 654  | G    | N7-C5   | -8.14 | 1.34        | 1.39     |
| 35  | BB    | 1737 | G    | C6-N1   | 8.14  | 1.45        | 1.39     |
| 35  | BB    | 2079 | U    | C2-N3   | 8.14  | 1.43        | 1.37     |
| 35  | BB    | 2415 | G    | P-O5'   | -8.14 | 1.51        | 1.59     |
| 1   | AA    | 149  | A    | C6-N6   | 8.14  | 1.40        | 1.33     |
| 35  | BB    | 473  | G    | C5-C4   | 8.14  | 1.44        | 1.38     |
| 35  | BB    | 617  | G    | C5'-C4' | 8.14  | 1.61        | 1.51     |
| 35  | BB    | 2257 | U    | C2-N3   | 8.14  | 1.43        | 1.37     |
| 1   | AA    | 131  | A    | C6-N1   | 8.14  | 1.41        | 1.35     |
| 1   | AA    | 1017 | U    | C2'-C1' | -8.14 | 1.44        | 1.53     |
| 35  | BB    | 712  | G    | N7-C5   | -8.14 | 1.34        | 1.39     |
| 35  | BB    | 2505 | G    | N9-C8   | 8.14  | 1.43        | 1.37     |
| 35  | BB    | 2894 | G    | P-O5'   | -8.14 | 1.51        | 1.59     |
| 1   | AA    | 168  | G    | C8-N7   | -8.13 | 1.26        | 1.30     |
| 1   | AA    | 746  | A    | C8-N7   | 8.14  | 1.37        | 1.31     |
| 35  | BB    | 2409 | G    | C6-N1   | 8.13  | 1.45        | 1.39     |
| 35  | BB    | 2495 | G    | P-O5'   | -8.13 | 1.51        | 1.59     |
| 35  | BB    | 2534 | A    | N9-C8   | -8.14 | 1.31        | 1.37     |
| 1   | AA    | 821  | G    | C8-N7   | -8.13 | 1.26        | 1.30     |
| 22  | AV    | 38   | U    | C2'-C1' | -8.13 | 1.44        | 1.53     |
| 34  | BA    | 99   | A    | C6-N1   | -8.13 | 1.29        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 362  | A    | P-O5'   | 8.13  | 1.67        | 1.59     |
| 35  | BB    | 1290 | C    | C2'-C1' | -8.13 | 1.44        | 1.53     |
| 35  | BB    | 1365 | A    | C5-C4   | 8.13  | 1.44        | 1.38     |
| 35  | BB    | 1772 | A    | N9-C4   | 8.13  | 1.42        | 1.37     |
| 35  | BB    | 2701 | U    | C2-N3   | 8.13  | 1.43        | 1.37     |
| 35  | BB    | 2775 | G    | C5'-C4' | 8.13  | 1.61        | 1.51     |
| 35  | BB    | 13   | A    | N7-C5   | -8.13 | 1.34        | 1.39     |
| 35  | BB    | 13   | A    | N3-C4   | -8.13 | 1.29        | 1.34     |
| 35  | BB    | 784  | G    | N7-C5   | -8.13 | 1.34        | 1.39     |
| 35  | BB    | 2654 | A    | C6-N6   | 8.13  | 1.40        | 1.33     |
| 1   | AA    | 115  | G    | N1-C2   | 8.13  | 1.44        | 1.37     |
| 1   | AA    | 1263 | C    | N3-C4   | 8.12  | 1.39        | 1.33     |
| 35  | BB    | 491  | G    | C2-N2   | 8.12  | 1.42        | 1.34     |
| 1   | AA    | 298  | A    | N9-C4   | -8.12 | 1.32        | 1.37     |
| 34  | BA    | 88   | C    | N1-C6   | 8.12  | 1.42        | 1.37     |
| 35  | BB    | 798  | G    | N9-C8   | 8.12  | 1.43        | 1.37     |
| 35  | BB    | 917  | A    | C6-N6   | 8.12  | 1.40        | 1.33     |
| 35  | BB    | 1131 | G    | P-O5'   | -8.12 | 1.51        | 1.59     |
| 35  | BB    | 2300 | C    | C2-N3   | -8.12 | 1.29        | 1.35     |
| 35  | BB    | 482  | A    | O3'-P   | -8.12 | 1.51        | 1.61     |
| 35  | BB    | 672  | C    | C4-N4   | 8.12  | 1.41        | 1.33     |
| 1   | AA    | 1273 | C    | C4-N4   | 8.12  | 1.41        | 1.33     |
| 35  | BB    | 2694 | G    | C5-C4   | 8.12  | 1.44        | 1.38     |
| 35  | BB    | 2357 | G    | C6-N1   | 8.11  | 1.45        | 1.39     |
| 35  | BB    | 2832 | U    | C2'-C1' | -8.12 | 1.44        | 1.53     |
| 35  | BB    | 2893 | A    | C6-N6   | 8.12  | 1.40        | 1.33     |
| 35  | BB    | 718  | A    | C6-N6   | 8.11  | 1.40        | 1.33     |
| 35  | BB    | 978  | G    | N9-C8   | -8.11 | 1.32        | 1.37     |
| 35  | BB    | 1640 | A    | N7-C5   | -8.11 | 1.34        | 1.39     |
| 35  | BB    | 455  | C    | C2'-C1' | -8.11 | 1.44        | 1.53     |
| 35  | BB    | 1332 | G    | C2'-C1' | -8.11 | 1.44        | 1.53     |
| 35  | BB    | 1605 | C    | C2-N3   | 8.11  | 1.42        | 1.35     |
| 35  | BB    | 1351 | C    | C3'-C2' | -8.11 | 1.43        | 1.52     |
| 1   | AA    | 140  | U    | N3-C4   | 8.11  | 1.45        | 1.38     |
| 35  | BB    | 469  | G    | C5'-C4' | 8.11  | 1.61        | 1.51     |
| 35  | BB    | 1018 | U    | C2-N3   | 8.11  | 1.43        | 1.37     |
| 35  | BB    | 1427 | A    | C5-C6   | -8.11 | 1.33        | 1.41     |
| 35  | BB    | 2674 | G    | N9-C8   | -8.11 | 1.32        | 1.37     |
| 1   | AA    | 1343 | G    | C6-O6   | -8.10 | 1.16        | 1.24     |
| 35  | BB    | 1511 | G    | O3'-P   | -8.10 | 1.51        | 1.61     |
| 1   | AA    | 154  | U    | P-O5'   | -8.10 | 1.51        | 1.59     |
| 35  | BB    | 530  | G    | N3-C4   | -8.10 | 1.29        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1918 | A    | N7-C5   | -8.10 | 1.34        | 1.39     |
| 1   | AA    | 32   | A    | N9-C4   | 8.10  | 1.42        | 1.37     |
| 35  | BB    | 1342 | A    | N7-C5   | -8.10 | 1.34        | 1.39     |
| 35  | BB    | 1764 | C    | N3-C4   | 8.10  | 1.39        | 1.33     |
| 35  | BB    | 2418 | A    | C6-N6   | 8.10  | 1.40        | 1.33     |
| 22  | AV    | 4    | C    | C2-N3   | 8.10  | 1.42        | 1.35     |
| 35  | BB    | 1599 | U    | N3-C4   | 8.10  | 1.45        | 1.38     |
| 1   | AA    | 741  | G    | C2-N2   | 8.10  | 1.42        | 1.34     |
| 35  | BB    | 541  | A    | O3'-P   | -8.10 | 1.51        | 1.61     |
| 35  | BB    | 1871 | A    | C4'-C3' | 8.10  | 1.62        | 1.53     |
| 35  | BB    | 108  | G    | C2-N2   | 8.09  | 1.42        | 1.34     |
| 35  | BB    | 1982 | U    | P-O5'   | -8.09 | 1.51        | 1.59     |
| 1   | AA    | 288  | A    | C2'-C1' | -8.09 | 1.44        | 1.53     |
| 1   | AA    | 1279 | G    | N3-C4   | -8.09 | 1.29        | 1.35     |
| 1   | AA    | 1429 | A    | C3'-C2' | -8.09 | 1.43        | 1.52     |
| 1   | AA    | 887  | G    | N9-C4   | -8.09 | 1.31        | 1.38     |
| 1   | AA    | 996  | A    | C6-N1   | 8.09  | 1.41        | 1.35     |
| 34  | BA    | 46   | A    | N9-C4   | 8.09  | 1.42        | 1.37     |
| 35  | BB    | 482  | A    | N7-C5   | -8.09 | 1.34        | 1.39     |
| 35  | BB    | 1099 | G    | C2'-C1' | -8.09 | 1.44        | 1.53     |
| 35  | BB    | 1767 | G    | C2-N3   | 8.09  | 1.39        | 1.32     |
| 35  | BB    | 2470 | G    | N9-C8   | 8.09  | 1.43        | 1.37     |
| 35  | BB    | 1972 | G    | N9-C4   | -8.09 | 1.31        | 1.38     |
| 35  | BB    | 401  | A    | C2'-C1' | -8.09 | 1.44        | 1.53     |
| 35  | BB    | 2052 | A    | C2'-C1' | -8.09 | 1.44        | 1.53     |
| 35  | BB    | 2190 | G    | C2'-C1' | -8.09 | 1.44        | 1.53     |
| 1   | AA    | 103  | U    | N3-C4   | 8.09  | 1.45        | 1.38     |
| 1   | AA    | 733  | G    | O4'-C1' | -8.08 | 1.31        | 1.41     |
| 35  | BB    | 482  | A    | C2'-C1' | -8.08 | 1.44        | 1.53     |
| 35  | BB    | 1551 | A    | C2'-C1' | -8.08 | 1.44        | 1.53     |
| 35  | BB    | 2429 | G    | O3'-P   | -8.08 | 1.51        | 1.61     |
| 1   | AA    | 47   | C    | C2-N3   | 8.08  | 1.42        | 1.35     |
| 1   | AA    | 702  | A    | C8-N7   | -8.08 | 1.25        | 1.31     |
| 1   | AA    | 880  | C    | O3'-P   | -8.08 | 1.51        | 1.61     |
| 1   | AA    | 1398 | A    | N7-C5   | -8.08 | 1.34        | 1.39     |
| 35  | BB    | 931  | U    | C2-N3   | 8.08  | 1.43        | 1.37     |
| 1   | AA    | 1282 | C    | C4-N4   | 8.08  | 1.41        | 1.33     |
| 35  | BB    | 632  | A    | N7-C5   | -8.08 | 1.34        | 1.39     |
| 35  | BB    | 1450 | G    | N9-C8   | 8.08  | 1.43        | 1.37     |
| 35  | BB    | 2751 | G    | N7-C5   | -8.08 | 1.34        | 1.39     |
| 1   | AA    | 913  | A    | C6-N6   | 8.08  | 1.40        | 1.33     |
| 35  | BB    | 166  | U    | O3'-P   | -8.08 | 1.51        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2339 | C    | C2'-C1' | -8.08 | 1.44        | 1.53     |
| 1   | AA    | 69   | G    | C2-N3   | 8.07  | 1.39        | 1.32     |
| 1   | AA    | 155  | A    | N9-C4   | 8.07  | 1.42        | 1.37     |
| 35  | BB    | 1000 | A    | P-O5'   | -8.07 | 1.51        | 1.59     |
| 35  | BB    | 1074 | G    | C2-N3   | 8.07  | 1.39        | 1.32     |
| 1   | AA    | 145  | G    | C6-N1   | 8.07  | 1.45        | 1.39     |
| 1   | AA    | 993  | G    | C6-N1   | 8.07  | 1.45        | 1.39     |
| 35  | BB    | 166  | U    | C5'-C4' | 8.07  | 1.61        | 1.51     |
| 35  | BB    | 2557 | G    | C5'-C4' | 8.07  | 1.61        | 1.51     |
| 1   | AA    | 363  | A    | N9-C4   | -8.07 | 1.33        | 1.37     |
| 1   | AA    | 658  | C    | N1-C6   | 8.07  | 1.42        | 1.37     |
| 35  | BB    | 160  | A    | N7-C5   | -8.07 | 1.34        | 1.39     |
| 35  | BB    | 622  | G    | C5'-C4' | 8.07  | 1.61        | 1.51     |
| 35  | BB    | 1624 | U    | C2-N3   | 8.07  | 1.43        | 1.37     |
| 35  | BB    | 2013 | A    | N9-C4   | 8.07  | 1.42        | 1.37     |
| 1   | AA    | 332  | G    | C2'-C1' | -8.06 | 1.44        | 1.53     |
| 35  | BB    | 2588 | G    | N1-C2   | 8.06  | 1.44        | 1.37     |
| 1   | AA    | 160  | A    | N9-C4   | -8.06 | 1.33        | 1.37     |
| 1   | AA    | 809  | G    | N1-C2   | 8.06  | 1.44        | 1.37     |
| 35  | BB    | 1553 | A    | C6-N1   | 8.06  | 1.41        | 1.35     |
| 35  | BB    | 2199 | A    | C8-N7   | -8.06 | 1.25        | 1.31     |
| 35  | BB    | 2845 | U    | C1'-N1  | 8.06  | 1.60        | 1.48     |
| 1   | AA    | 90   | C    | C2-N3   | 8.06  | 1.42        | 1.35     |
| 1   | AA    | 646  | G    | N9-C8   | 8.06  | 1.43        | 1.37     |
| 35  | BB    | 1667 | G    | P-O5'   | -8.06 | 1.51        | 1.59     |
| 1   | AA    | 211  | G    | N7-C5   | -8.06 | 1.34        | 1.39     |
| 35  | BB    | 876  | C    | N1-C6   | 8.06  | 1.42        | 1.37     |
| 35  | BB    | 2088 | A    | N7-C5   | 8.06  | 1.44        | 1.39     |
| 35  | BB    | 2623 | G    | N7-C5   | -8.06 | 1.34        | 1.39     |
| 34  | BA    | 117  | G    | C6-N1   | 8.05  | 1.45        | 1.39     |
| 35  | BB    | 2125 | G    | C4'-O4' | -8.05 | 1.35        | 1.45     |
| 35  | BB    | 2459 | A    | N7-C5   | -8.05 | 1.34        | 1.39     |
| 22  | AV    | 70   | C    | P-O5'   | -8.05 | 1.51        | 1.59     |
| 1   | AA    | 1053 | G    | N1-C2   | 8.05  | 1.44        | 1.37     |
| 35  | BB    | 62   | U    | N1-C6   | 8.05  | 1.45        | 1.38     |
| 35  | BB    | 2594 | C    | C2-N3   | 8.05  | 1.42        | 1.35     |
| 35  | BB    | 2807 | U    | C2-N3   | 8.05  | 1.43        | 1.37     |
| 1   | AA    | 1255 | G    | N9-C4   | 8.05  | 1.44        | 1.38     |
| 35  | BB    | 2357 | G    | C5-C6   | -8.05 | 1.34        | 1.42     |
| 1   | AA    | 623  | C    | C2'-C1' | -8.04 | 1.44        | 1.53     |
| 1   | AA    | 1254 | A    | N7-C5   | -8.04 | 1.34        | 1.39     |
| 35  | BB    | 366  | C    | O4'-C1' | -8.04 | 1.31        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1247 | A    | C6-N6   | 8.04  | 1.40        | 1.33     |
| 35  | BB    | 2590 | A    | C6-N1   | 8.04  | 1.41        | 1.35     |
| 35  | BB    | 119  | A    | N7-C5   | -8.04 | 1.34        | 1.39     |
| 35  | BB    | 266  | G    | N9-C8   | 8.04  | 1.43        | 1.37     |
| 35  | BB    | 1281 | G    | C5'-C4' | 8.04  | 1.61        | 1.51     |
| 35  | BB    | 1707 | G    | N7-C5   | -8.04 | 1.34        | 1.39     |
| 35  | BB    | 2850 | A    | N9-C4   | -8.04 | 1.33        | 1.37     |
| 1   | AA    | 874  | G    | N7-C5   | -8.04 | 1.34        | 1.39     |
| 1   | AA    | 962  | C    | N3-C4   | 8.04  | 1.39        | 1.33     |
| 35  | BB    | 402  | A    | N7-C5   | -8.04 | 1.34        | 1.39     |
| 35  | BB    | 2219 | U    | C2-N3   | 8.04  | 1.43        | 1.37     |
| 35  | BB    | 2416 | C    | C4-N4   | 8.04  | 1.41        | 1.33     |
| 35  | BB    | 852  | U    | C3'-C2' | -8.04 | 1.44        | 1.52     |
| 35  | BB    | 2474 | U    | N1-C6   | -8.04 | 1.30        | 1.38     |
| 1   | AA    | 524  | G    | C8-N7   | 8.04  | 1.35        | 1.30     |
| 35  | BB    | 665  | U    | N1-C6   | 8.04  | 1.45        | 1.38     |
| 35  | BB    | 1010 | A    | C5-C4   | 8.04  | 1.44        | 1.38     |
| 1   | AA    | 21   | G    | N3-C4   | -8.03 | 1.29        | 1.35     |
| 1   | AA    | 727  | G    | N1-C2   | 8.03  | 1.44        | 1.37     |
| 1   | AA    | 127  | G    | N7-C5   | -8.03 | 1.34        | 1.39     |
| 1   | AA    | 667  | G    | O3'-P   | -8.03 | 1.51        | 1.61     |
| 35  | BB    | 2294 | G    | N7-C5   | -8.03 | 1.34        | 1.39     |
| 35  | BB    | 1189 | A    | N7-C5   | -8.03 | 1.34        | 1.39     |
| 35  | BB    | 2758 | A    | C5-C4   | -8.03 | 1.33        | 1.38     |
| 35  | BB    | 283  | G    | C2-N3   | 8.03  | 1.39        | 1.32     |
| 35  | BB    | 356  | G    | C8-N7   | -8.03 | 1.26        | 1.30     |
| 35  | BB    | 1503 | A    | C5'-C4' | 8.03  | 1.60        | 1.51     |
| 35  | BB    | 1649 | G    | C6-N1   | 8.03  | 1.45        | 1.39     |
| 35  | BB    | 1943 | U    | C2-N3   | 8.03  | 1.43        | 1.37     |
| 1   | AA    | 182  | A    | C2'-C1' | -8.02 | 1.44        | 1.53     |
| 35  | BB    | 2722 | G    | N7-C5   | -8.02 | 1.34        | 1.39     |
| 1   | AA    | 391  | G    | N9-C8   | 8.02  | 1.43        | 1.37     |
| 1   | AA    | 1515 | G    | N9-C4   | 8.02  | 1.44        | 1.38     |
| 1   | AA    | 852  | G    | C4'-O4' | -8.02 | 1.35        | 1.45     |
| 1   | AA    | 1096 | C    | C2'-C1' | -8.02 | 1.44        | 1.53     |
| 34  | BA    | 36   | C    | N1-C6   | 8.02  | 1.42        | 1.37     |
| 35  | BB    | 517  | C    | C4-C5   | 8.02  | 1.49        | 1.43     |
| 35  | BB    | 844  | A    | N7-C5   | -8.02 | 1.34        | 1.39     |
| 35  | BB    | 1793 | C    | O3'-P   | -8.02 | 1.51        | 1.61     |
| 35  | BB    | 2428 | G    | C2-N3   | 8.02  | 1.39        | 1.32     |
| 1   | AA    | 1523 | G    | N3-C4   | 8.02  | 1.41        | 1.35     |
| 35  | BB    | 643  | A    | C6-N6   | 8.02  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1682 | G    | N1-C2   | 8.02  | 1.44        | 1.37     |
| 1   | AA    | 760  | G    | N3-C4   | -8.02 | 1.29        | 1.35     |
| 1   | AA    | 1126 | U    | P-O5'   | -8.02 | 1.51        | 1.59     |
| 35  | BB    | 661  | A    | N9-C4   | -8.02 | 1.33        | 1.37     |
| 35  | BB    | 1952 | A    | C5-C4   | 8.02  | 1.44        | 1.38     |
| 35  | BB    | 1788 | C    | P-O5'   | -8.01 | 1.51        | 1.59     |
| 1   | AA    | 487  | A    | C4'-C3' | 8.01  | 1.61        | 1.53     |
| 1   | AA    | 1215 | G    | C2-N3   | 8.01  | 1.39        | 1.32     |
| 35  | BB    | 363  | G    | C8-N7   | -8.01 | 1.26        | 1.30     |
| 35  | BB    | 1538 | G    | C5-C4   | -8.01 | 1.32        | 1.38     |
| 35  | BB    | 2140 | G    | C8-N7   | 8.01  | 1.35        | 1.30     |
| 35  | BB    | 2799 | A    | C6-N6   | 8.01  | 1.40        | 1.33     |
| 1   | AA    | 816  | A    | N9-C8   | 8.01  | 1.44        | 1.37     |
| 35  | BB    | 1784 | A    | C8-N7   | -8.01 | 1.25        | 1.31     |
| 1   | AA    | 1058 | G    | C3'-C2' | -8.01 | 1.44        | 1.52     |
| 1   | AA    | 256  | U    | N3-C4   | 8.01  | 1.45        | 1.38     |
| 1   | AA    | 1092 | A    | O3'-P   | -8.01 | 1.51        | 1.61     |
| 35  | BB    | 194  | G    | C5-C4   | 8.01  | 1.44        | 1.38     |
| 35  | BB    | 2274 | A    | C2'-C1' | -8.01 | 1.44        | 1.53     |
| 35  | BB    | 2366 | A    | C8-N7   | -8.01 | 1.25        | 1.31     |
| 35  | BB    | 2282 | G    | N1-C2   | 8.01  | 1.44        | 1.37     |
| 1   | AA    | 471  | U    | O4'-C1' | 8.00  | 1.52        | 1.41     |
| 1   | AA    | 933  | G    | C4'-C3' | 8.00  | 1.61        | 1.53     |
| 34  | BA    | 20   | G    | C5-C4   | 8.00  | 1.44        | 1.38     |
| 35  | BB    | 51   | G    | C6-N1   | 8.00  | 1.45        | 1.39     |
| 35  | BB    | 1094 | U    | N3-C4   | 8.00  | 1.45        | 1.38     |
| 1   | AA    | 19   | A    | N7-C5   | -8.00 | 1.34        | 1.39     |
| 1   | AA    | 837  | U    | P-O5'   | -8.00 | 1.51        | 1.59     |
| 1   | AA    | 1064 | G    | C2'-C1' | -8.00 | 1.44        | 1.53     |
| 1   | AA    | 1409 | C    | C4-N4   | 8.00  | 1.41        | 1.33     |
| 1   | AA    | 50   | A    | P-O5'   | -8.00 | 1.51        | 1.59     |
| 35  | BB    | 776  | G    | C6-N1   | 8.00  | 1.45        | 1.39     |
| 35  | BB    | 1215 | G    | C5-C6   | -8.00 | 1.34        | 1.42     |
| 35  | BB    | 843  | G    | C8-N7   | -7.99 | 1.26        | 1.30     |
| 35  | BB    | 2092 | U    | C2-N3   | 7.99  | 1.43        | 1.37     |
| 35  | BB    | 2100 | G    | N7-C5   | -7.99 | 1.34        | 1.39     |
| 35  | BB    | 2776 | A    | C2'-C1' | -7.99 | 1.44        | 1.53     |
| 1   | AA    | 819  | A    | N3-C4   | -7.99 | 1.30        | 1.34     |
| 35  | BB    | 1617 | C    | N1-C6   | 7.99  | 1.42        | 1.37     |
| 35  | BB    | 2627 | G    | N9-C4   | -7.99 | 1.31        | 1.38     |
| 1   | AA    | 750  | C    | P-O5'   | -7.99 | 1.51        | 1.59     |
| 1   | AA    | 868  | C    | C4-N4   | 7.99  | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1801 | A    | N9-C4   | 7.99  | 1.42        | 1.37     |
| 1   | AA    | 379  | C    | C2'-C1' | -7.99 | 1.44        | 1.53     |
| 35  | BB    | 2354 | C    | C4'-C3' | -7.99 | 1.44        | 1.53     |
| 35  | BB    | 789  | A    | C6-N1   | 7.99  | 1.41        | 1.35     |
| 35  | BB    | 2259 | U    | C4-C5   | 7.99  | 1.50        | 1.43     |
| 35  | BB    | 2508 | G    | C6-N1   | 7.99  | 1.45        | 1.39     |
| 35  | BB    | 2759 | G    | N7-C5   | -7.99 | 1.34        | 1.39     |
| 35  | BB    | 2883 | A    | C6-N1   | 7.99  | 1.41        | 1.35     |
| 1   | AA    | 830  | G    | C6-N1   | 7.98  | 1.45        | 1.39     |
| 1   | AA    | 1284 | C    | N1-C6   | 7.98  | 1.42        | 1.37     |
| 35  | BB    | 294  | A    | C6-N6   | 7.98  | 1.40        | 1.33     |
| 1   | AA    | 907  | A    | C4'-C3' | -7.98 | 1.44        | 1.53     |
| 1   | AA    | 1503 | A    | C5'-C4' | 7.98  | 1.60        | 1.51     |
| 34  | BA    | 108  | A    | C6-N1   | 7.98  | 1.41        | 1.35     |
| 35  | BB    | 34   | U    | C2-N3   | 7.98  | 1.43        | 1.37     |
| 35  | BB    | 834  | G    | C2-N3   | 7.98  | 1.39        | 1.32     |
| 1   | AA    | 236  | A    | C8-N7   | -7.98 | 1.25        | 1.31     |
| 1   | AA    | 336  | A    | N9-C4   | -7.98 | 1.33        | 1.37     |
| 1   | AA    | 1061 | G    | N3-C4   | 7.98  | 1.41        | 1.35     |
| 35  | BB    | 1536 | C    | N1-C2   | 7.98  | 1.48        | 1.40     |
| 35  | BB    | 1643 | G    | N9-C8   | -7.98 | 1.32        | 1.37     |
| 35  | BB    | 1951 | U    | C5-C6   | 7.98  | 1.41        | 1.34     |
| 35  | BB    | 1266 | G    | N7-C5   | 7.98  | 1.44        | 1.39     |
| 1   | AA    | 728  | A    | N3-C4   | 7.98  | 1.39        | 1.34     |
| 35  | BB    | 1171 | G    | N9-C8   | 7.98  | 1.43        | 1.37     |
| 35  | BB    | 2097 | A    | C5-C6   | 7.98  | 1.48        | 1.41     |
| 35  | BB    | 879  | G    | C8-N7   | -7.98 | 1.26        | 1.30     |
| 35  | BB    | 2316 | G    | C8-N7   | -7.98 | 1.26        | 1.30     |
| 1   | AA    | 445  | G    | P-O5'   | 7.97  | 1.67        | 1.59     |
| 1   | AA    | 1374 | A    | C6-N6   | 7.97  | 1.40        | 1.33     |
| 35  | BB    | 213  | A    | N9-C8   | -7.97 | 1.31        | 1.37     |
| 1   | AA    | 1371 | G    | N9-C8   | 7.97  | 1.43        | 1.37     |
| 22  | AV    | 2    | G    | C8-N7   | -7.97 | 1.26        | 1.30     |
| 34  | BA    | 52   | A    | N9-C4   | -7.97 | 1.33        | 1.37     |
| 35  | BB    | 2413 | G    | C8-N7   | 7.97  | 1.35        | 1.30     |
| 1   | AA    | 518  | C    | C2-N3   | 7.97  | 1.42        | 1.35     |
| 35  | BB    | 446  | G    | C2-N3   | 7.97  | 1.39        | 1.32     |
| 35  | BB    | 1739 | A    | P-O5'   | -7.97 | 1.51        | 1.59     |
| 35  | BB    | 734  | A    | C5'-C4' | 7.97  | 1.60        | 1.51     |
| 35  | BB    | 2689 | U    | C4-C5   | 7.97  | 1.50        | 1.43     |
| 35  | BB    | 1414 | C    | N3-C4   | 7.96  | 1.39        | 1.33     |
| 35  | BB    | 2066 | C    | C2-N3   | 7.96  | 1.42        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1533 | C    | N1-C6   | 7.96  | 1.42        | 1.37     |
| 35  | BB    | 1669 | A    | N1-C2   | -7.96 | 1.27        | 1.34     |
| 1   | AA    | 22   | G    | N7-C5   | -7.96 | 1.34        | 1.39     |
| 1   | AA    | 397  | A    | C5-C6   | 7.96  | 1.48        | 1.41     |
| 35  | BB    | 1738 | G    | C5-C4   | 7.96  | 1.44        | 1.38     |
| 35  | BB    | 2782 | G    | C2-N3   | 7.96  | 1.39        | 1.32     |
| 1   | AA    | 1214 | C    | C2-N3   | 7.96  | 1.42        | 1.35     |
| 1   | AA    | 1310 | G    | C6-N1   | 7.96  | 1.45        | 1.39     |
| 35  | BB    | 1182 | G    | C2-N3   | 7.96  | 1.39        | 1.32     |
| 34  | BA    | 69   | G    | C6-N1   | 7.96  | 1.45        | 1.39     |
| 35  | BB    | 68   | G    | N7-C5   | -7.96 | 1.34        | 1.39     |
| 1   | AA    | 705  | G    | C2-N3   | 7.95  | 1.39        | 1.32     |
| 1   | AA    | 994  | A    | C6-N6   | 7.95  | 1.40        | 1.33     |
| 35  | BB    | 374  | A    | N3-C4   | -7.95 | 1.30        | 1.34     |
| 35  | BB    | 612  | G    | C8-N7   | -7.95 | 1.26        | 1.30     |
| 35  | BB    | 1655 | A    | N7-C5   | 7.95  | 1.44        | 1.39     |
| 35  | BB    | 2001 | C    | C2'-C1' | -7.95 | 1.44        | 1.53     |
| 1   | AA    | 1497 | G    | C2-N2   | 7.95  | 1.42        | 1.34     |
| 35  | BB    | 2353 | G    | C2'-C1' | -7.95 | 1.44        | 1.53     |
| 1   | AA    | 24   | U    | N1-C6   | 7.95  | 1.45        | 1.38     |
| 1   | AA    | 297  | G    | C8-N7   | 7.95  | 1.35        | 1.30     |
| 35  | BB    | 1693 | U    | C5-C6   | 7.95  | 1.41        | 1.34     |
| 35  | BB    | 2639 | A    | C5-C6   | -7.95 | 1.33        | 1.41     |
| 1   | AA    | 1039 | G    | N1-C2   | 7.95  | 1.44        | 1.37     |
| 35  | BB    | 971  | G    | C6-N1   | 7.95  | 1.45        | 1.39     |
| 1   | AA    | 1168 | U    | N1-C2   | 7.95  | 1.45        | 1.38     |
| 35  | BB    | 2230 | G    | C2-N3   | 7.95  | 1.39        | 1.32     |
| 1   | AA    | 937  | A    | N7-C5   | -7.95 | 1.34        | 1.39     |
| 35  | BB    | 22   | C    | P-O5'   | -7.95 | 1.51        | 1.59     |
| 35  | BB    | 1334 | G    | C6-N1   | 7.95  | 1.45        | 1.39     |
| 35  | BB    | 2693 | G    | C2-N2   | 7.95  | 1.42        | 1.34     |
| 22  | AV    | 76   | A    | C5-C4   | -7.94 | 1.33        | 1.38     |
| 35  | BB    | 717  | C    | C4-C5   | 7.94  | 1.49        | 1.43     |
| 35  | BB    | 883  | G    | N1-C2   | 7.94  | 1.44        | 1.37     |
| 1   | AA    | 172  | A    | N3-C4   | -7.94 | 1.30        | 1.34     |
| 35  | BB    | 683  | U    | C2'-C1' | -7.94 | 1.44        | 1.53     |
| 35  | BB    | 1015 | U    | P-O5'   | -7.94 | 1.51        | 1.59     |
| 1   | AA    | 979  | C    | N3-C4   | 7.94  | 1.39        | 1.33     |
| 35  | BB    | 1722 | A    | P-O5'   | -7.94 | 1.51        | 1.59     |
| 35  | BB    | 2393 | U    | O3'-P   | -7.94 | 1.51        | 1.61     |
| 35  | BB    | 1612 | C    | N3-C4   | 7.94  | 1.39        | 1.33     |
| 1   | AA    | 1505 | G    | P-O5'   | -7.94 | 1.51        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1195 | C    | C4-N4   | 7.93  | 1.41        | 1.33     |
| 1   | AA    | 1352 | C    | C4-C5   | 7.93  | 1.49        | 1.43     |
| 35  | BB    | 111  | A    | O4'-C1' | -7.93 | 1.31        | 1.41     |
| 35  | BB    | 2003 | A    | C2'-C1' | -7.93 | 1.44        | 1.53     |
| 35  | BB    | 2289 | G    | C2-N3   | 7.93  | 1.39        | 1.32     |
| 35  | BB    | 712  | G    | N1-C2   | 7.93  | 1.44        | 1.37     |
| 35  | BB    | 1032 | A    | C6-N6   | 7.93  | 1.40        | 1.33     |
| 1   | AA    | 1248 | A    | C6-N1   | 7.93  | 1.41        | 1.35     |
| 35  | BB    | 1641 | A    | C8-N7   | -7.93 | 1.25        | 1.31     |
| 35  | BB    | 2516 | A    | C8-N7   | -7.93 | 1.25        | 1.31     |
| 35  | BB    | 2758 | A    | N7-C5   | -7.93 | 1.34        | 1.39     |
| 34  | BA    | 73   | A    | C4'-O4' | -7.93 | 1.35        | 1.45     |
| 35  | BB    | 2360 | G    | N7-C5   | -7.93 | 1.34        | 1.39     |
| 34  | BA    | 104  | A    | C8-N7   | -7.93 | 1.26        | 1.31     |
| 35  | BB    | 1066 | U    | C2-N3   | 7.93  | 1.43        | 1.37     |
| 35  | BB    | 1425 | G    | C6-N1   | 7.93  | 1.45        | 1.39     |
| 35  | BB    | 62   | U    | N3-C4   | 7.92  | 1.45        | 1.38     |
| 35  | BB    | 211  | C    | N1-C6   | -7.92 | 1.32        | 1.37     |
| 35  | BB    | 2104 | C    | C4-N4   | 7.92  | 1.41        | 1.33     |
| 1   | AA    | 427  | U    | C2-N3   | 7.92  | 1.43        | 1.37     |
| 1   | AA    | 755  | G    | C6-N1   | 7.92  | 1.45        | 1.39     |
| 35  | BB    | 643  | A    | N7-C5   | 7.92  | 1.44        | 1.39     |
| 35  | BB    | 1617 | C    | N3-C4   | 7.92  | 1.39        | 1.33     |
| 35  | BB    | 1455 | G    | P-O5'   | -7.92 | 1.51        | 1.59     |
| 35  | BB    | 1530 | G    | C6-N1   | 7.92  | 1.45        | 1.39     |
| 35  | BB    | 1662 | U    | N3-C4   | 7.92  | 1.45        | 1.38     |
| 35  | BB    | 2445 | G    | C4'-C3' | -7.92 | 1.44        | 1.53     |
| 1   | AA    | 1190 | G    | C8-N7   | -7.92 | 1.26        | 1.30     |
| 35  | BB    | 2030 | A    | N3-C4   | -7.92 | 1.30        | 1.34     |
| 1   | AA    | 88   | U    | P-O5'   | -7.92 | 1.51        | 1.59     |
| 1   | AA    | 558  | G    | C2-N3   | 7.92  | 1.39        | 1.32     |
| 1   | AA    | 1336 | C    | C2'-C1' | -7.92 | 1.44        | 1.53     |
| 35  | BB    | 1096 | A    | N9-C4   | 7.92  | 1.42        | 1.37     |
| 35  | BB    | 1601 | G    | C2-N2   | 7.92  | 1.42        | 1.34     |
| 1   | AA    | 1446 | A    | C4'-C3' | 7.92  | 1.61        | 1.53     |
| 35  | BB    | 2274 | A    | N3-C4   | -7.92 | 1.30        | 1.34     |
| 1   | AA    | 1500 | A    | N1-C2   | 7.91  | 1.41        | 1.34     |
| 35  | BB    | 78   | U    | C4'-C3' | -7.91 | 1.44        | 1.53     |
| 35  | BB    | 1223 | G    | N1-C2   | 7.91  | 1.44        | 1.37     |
| 35  | BB    | 2121 | G    | C8-N7   | -7.91 | 1.26        | 1.30     |
| 1   | AA    | 1125 | U    | C2-N3   | 7.91  | 1.43        | 1.37     |
| 22  | AV    | 32   | A    | N9-C8   | 7.91  | 1.44        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2102 | G    | N7-C5   | -7.91 | 1.34        | 1.39     |
| 35  | BB    | 2456 | C    | N3-C4   | 7.91  | 1.39        | 1.33     |
| 1   | AA    | 1184 | G    | C2'-C1' | -7.91 | 1.44        | 1.53     |
| 1   | AA    | 1410 | A    | C6-N6   | 7.91  | 1.40        | 1.33     |
| 35  | BB    | 410  | G    | N7-C5   | -7.91 | 1.34        | 1.39     |
| 35  | BB    | 2693 | G    | C8-N7   | -7.91 | 1.26        | 1.30     |
| 1   | AA    | 1453 | G    | C2-N3   | 7.91  | 1.39        | 1.32     |
| 35  | BB    | 885  | C    | N3-C4   | 7.91  | 1.39        | 1.33     |
| 35  | BB    | 919  | U    | C3'-C2' | 7.91  | 1.61        | 1.52     |
| 1   | AA    | 176  | C    | P-O5'   | -7.91 | 1.51        | 1.59     |
| 1   | AA    | 1196 | A    | C5-C6   | -7.91 | 1.33        | 1.41     |
| 35  | BB    | 735  | A    | C6-N6   | 7.91  | 1.40        | 1.33     |
| 35  | BB    | 1257 | C    | N1-C6   | 7.91  | 1.41        | 1.37     |
| 19  | AS    | 31   | ARG  | CZ-NH2  | 7.90  | 1.43        | 1.33     |
| 35  | BB    | 123  | G    | C2-N2   | 7.90  | 1.42        | 1.34     |
| 35  | BB    | 497  | A    | N1-C2   | 7.90  | 1.41        | 1.34     |
| 35  | BB    | 2193 | G    | C8-N7   | 7.90  | 1.35        | 1.30     |
| 35  | BB    | 2582 | G    | C8-N7   | -7.90 | 1.26        | 1.30     |
| 1   | AA    | 1184 | G    | C5-C4   | 7.90  | 1.43        | 1.38     |
| 35  | BB    | 398  | C    | C2-N3   | 7.90  | 1.42        | 1.35     |
| 35  | BB    | 2124 | G    | C4'-O4' | -7.90 | 1.35        | 1.45     |
| 1   | AA    | 1140 | C    | N3-C4   | 7.90  | 1.39        | 1.33     |
| 35  | BB    | 1889 | A    | C6-N1   | 7.90  | 1.41        | 1.35     |
| 22  | AV    | 73   | A    | C5'-C4' | 7.90  | 1.60        | 1.51     |
| 35  | BB    | 2736 | A    | N3-C4   | -7.90 | 1.30        | 1.34     |
| 1   | AA    | 195  | A    | C6-N6   | 7.90  | 1.40        | 1.33     |
| 1   | AA    | 968  | A    | C5-C4   | 7.90  | 1.44        | 1.38     |
| 1   | AA    | 1111 | A    | C8-N7   | -7.90 | 1.26        | 1.31     |
| 35  | BB    | 301  | G    | C6-N1   | 7.90  | 1.45        | 1.39     |
| 35  | BB    | 1087 | G    | C4'-C3' | 7.89  | 1.61        | 1.53     |
| 35  | BB    | 1933 | G    | N1-C2   | 7.89  | 1.44        | 1.37     |
| 1   | AA    | 1000 | A    | C2'-C1' | -7.89 | 1.44        | 1.53     |
| 35  | BB    | 2557 | G    | C2'-C1' | -7.89 | 1.44        | 1.53     |
| 35  | BB    | 2616 | C    | C2-N3   | 7.89  | 1.42        | 1.35     |
| 35  | BB    | 2735 | G    | C8-N7   | -7.89 | 1.26        | 1.30     |
| 35  | BB    | 428  | A    | C6-N6   | 7.89  | 1.40        | 1.33     |
| 35  | BB    | 1001 | A    | C6-N6   | 7.89  | 1.40        | 1.33     |
| 35  | BB    | 210  | C    | C4-N4   | 7.89  | 1.41        | 1.33     |
| 35  | BB    | 1257 | C    | P-O5'   | -7.89 | 1.51        | 1.59     |
| 35  | BB    | 2186 | G    | C5-C4   | 7.89  | 1.43        | 1.38     |
| 1   | AA    | 747  | A    | C4'-C3' | -7.89 | 1.44        | 1.53     |
| 1   | AA    | 1361 | G    | C5-C6   | -7.89 | 1.34        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 249  | C    | N3-C4   | 7.89  | 1.39        | 1.33     |
| 1   | AA    | 423  | G    | C2'-O2' | -7.88 | 1.31        | 1.41     |
| 1   | AA    | 748  | G    | C2-N3   | 7.88  | 1.39        | 1.32     |
| 1   | AA    | 1394 | A    | C5-C4   | 7.88  | 1.44        | 1.38     |
| 35  | BB    | 495  | G    | N7-C5   | -7.88 | 1.34        | 1.39     |
| 35  | BB    | 780  | G    | C2'-C1' | 7.88  | 1.62        | 1.53     |
| 35  | BB    | 1171 | G    | P-O5'   | 7.88  | 1.67        | 1.59     |
| 1   | AA    | 355  | C    | C4-C5   | -7.88 | 1.36        | 1.43     |
| 35  | BB    | 1403 | A    | C2'-C1' | -7.88 | 1.44        | 1.53     |
| 35  | BB    | 1949 | G    | C8-N7   | -7.88 | 1.26        | 1.30     |
| 35  | BB    | 2058 | A    | N7-C5   | -7.88 | 1.34        | 1.39     |
| 35  | BB    | 2346 | A    | C5-C6   | -7.88 | 1.33        | 1.41     |
| 35  | BB    | 1521 | G    | C6-N1   | 7.88  | 1.45        | 1.39     |
| 35  | BB    | 2153 | C    | C3'-O3' | 7.88  | 1.53        | 1.42     |
| 1   | AA    | 145  | G    | N1-C2   | 7.88  | 1.44        | 1.37     |
| 1   | AA    | 438  | U    | C3'-C2' | 7.88  | 1.61        | 1.52     |
| 32  | B7    | 39   | ARG  | NE-CZ   | 7.88  | 1.43        | 1.33     |
| 34  | BA    | 79   | G    | N1-C2   | 7.88  | 1.44        | 1.37     |
| 1   | AA    | 74   | A    | N3-C4   | 7.88  | 1.39        | 1.34     |
| 1   | AA    | 766  | A    | N7-C5   | -7.88 | 1.34        | 1.39     |
| 1   | AA    | 958  | A    | C6-N6   | 7.88  | 1.40        | 1.33     |
| 35  | BB    | 751  | A    | C6-N1   | 7.88  | 1.41        | 1.35     |
| 35  | BB    | 815  | C    | C5-C6   | 7.88  | 1.40        | 1.34     |
| 35  | BB    | 1048 | A    | C6-N6   | 7.88  | 1.40        | 1.33     |
| 35  | BB    | 1628 | G    | P-O5'   | -7.88 | 1.51        | 1.59     |
| 35  | BB    | 479  | A    | C6-N6   | 7.87  | 1.40        | 1.33     |
| 35  | BB    | 1378 | A    | N3-C4   | -7.87 | 1.30        | 1.34     |
| 35  | BB    | 1392 | A    | C2'-C1' | -7.87 | 1.44        | 1.53     |
| 35  | BB    | 1548 | A    | C6-N1   | 7.87  | 1.41        | 1.35     |
| 35  | BB    | 1584 | U    | C4'-C3' | 7.87  | 1.61        | 1.53     |
| 35  | BB    | 2768 | U    | C2-N3   | 7.87  | 1.43        | 1.37     |
| 1   | AA    | 74   | A    | C6-N1   | 7.87  | 1.41        | 1.35     |
| 1   | AA    | 352  | C    | N3-C4   | 7.87  | 1.39        | 1.33     |
| 1   | AA    | 678  | U    | C2-N3   | 7.87  | 1.43        | 1.37     |
| 35  | BB    | 247  | G    | N9-C4   | -7.87 | 1.31        | 1.38     |
| 35  | BB    | 656  | G    | C6-N1   | 7.87  | 1.45        | 1.39     |
| 35  | BB    | 1593 | A    | C6-N1   | 7.87  | 1.41        | 1.35     |
| 1   | AA    | 518  | C    | C2'-C1' | -7.87 | 1.44        | 1.53     |
| 1   | AA    | 1141 | C    | C3'-C2' | 7.87  | 1.61        | 1.52     |
| 35  | BB    | 1869 | G    | C5'-C4' | 7.87  | 1.60        | 1.51     |
| 35  | BB    | 2867 | G    | N1-C2   | 7.87  | 1.44        | 1.37     |
| 1   | AA    | 65   | A    | C6-N6   | 7.86  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 429  | U    | O3'-P   | -7.86 | 1.51        | 1.61     |
| 35  | BB    | 665  | U    | C2-N3   | 7.86  | 1.43        | 1.37     |
| 35  | BB    | 924  | G    | C2'-C1' | -7.86 | 1.44        | 1.53     |
| 35  | BB    | 2013 | A    | P-O5'   | -7.86 | 1.51        | 1.59     |
| 35  | BB    | 2061 | G    | C3'-C2' | 7.86  | 1.61        | 1.52     |
| 35  | BB    | 2199 | A    | C6-N6   | 7.86  | 1.40        | 1.33     |
| 35  | BB    | 1361 | G    | C6-N1   | 7.86  | 1.45        | 1.39     |
| 35  | BB    | 2898 | U    | C4-O4   | -7.86 | 1.17        | 1.23     |
| 35  | BB    | 119  | A    | N1-C2   | 7.86  | 1.41        | 1.34     |
| 1   | AA    | 832  | G    | C3'-O3' | 7.86  | 1.53        | 1.42     |
| 1   | AA    | 1231 | G    | N3-C4   | -7.86 | 1.29        | 1.35     |
| 35  | BB    | 1177 | G    | N9-C8   | -7.86 | 1.32        | 1.37     |
| 1   | AA    | 329  | A    | N3-C4   | -7.86 | 1.30        | 1.34     |
| 35  | BB    | 516  | C    | N1-C6   | 7.86  | 1.41        | 1.37     |
| 35  | BB    | 939  | G    | C6-N1   | 7.86  | 1.45        | 1.39     |
| 35  | BB    | 1432 | G    | C6-N1   | 7.86  | 1.45        | 1.39     |
| 35  | BB    | 1903 | G    | N9-C8   | -7.86 | 1.32        | 1.37     |
| 35  | BB    | 2798 | U    | O4'-C1' | -7.86 | 1.31        | 1.41     |
| 34  | BA    | 115  | A    | C5-C4   | 7.86  | 1.44        | 1.38     |
| 35  | BB    | 855  | G    | N7-C5   | -7.86 | 1.34        | 1.39     |
| 35  | BB    | 1669 | A    | N7-C5   | -7.86 | 1.34        | 1.39     |
| 35  | BB    | 917  | A    | N9-C8   | -7.85 | 1.31        | 1.37     |
| 35  | BB    | 2732 | G    | C6-N1   | -7.85 | 1.34        | 1.39     |
| 35  | BB    | 344  | A    | C2'-C1' | -7.85 | 1.44        | 1.53     |
| 35  | BB    | 449  | A    | P-O5'   | -7.85 | 1.51        | 1.59     |
| 35  | BB    | 1116 | G    | N3-C4   | 7.85  | 1.41        | 1.35     |
| 35  | BB    | 2030 | A    | N7-C5   | -7.85 | 1.34        | 1.39     |
| 35  | BB    | 745  | G    | P-O5'   | -7.85 | 1.51        | 1.59     |
| 1   | AA    | 1339 | A    | C6-N1   | 7.85  | 1.41        | 1.35     |
| 34  | BA    | 11   | C    | N3-C4   | 7.85  | 1.39        | 1.33     |
| 35  | BB    | 232  | G    | O3'-P   | -7.85 | 1.51        | 1.61     |
| 35  | BB    | 2704 | C    | C4-C5   | 7.85  | 1.49        | 1.43     |
| 35  | BB    | 542  | C    | N1-C6   | 7.85  | 1.41        | 1.37     |
| 35  | BB    | 2253 | G    | C8-N7   | -7.85 | 1.26        | 1.30     |
| 1   | AA    | 113  | G    | N1-C2   | 7.85  | 1.44        | 1.37     |
| 1   | AA    | 1371 | G    | C2'-C1' | -7.85 | 1.44        | 1.53     |
| 1   | AA    | 153  | C    | O4'-C1' | -7.84 | 1.31        | 1.41     |
| 1   | AA    | 553  | A    | C6-N1   | 7.84  | 1.41        | 1.35     |
| 1   | AA    | 1111 | A    | C5-C4   | 7.84  | 1.44        | 1.38     |
| 35  | BB    | 531  | C    | N3-C4   | 7.84  | 1.39        | 1.33     |
| 35  | BB    | 1770 | G    | C3'-C2' | -7.84 | 1.44        | 1.52     |
| 1   | AA    | 1277 | C    | C3'-C2' | -7.84 | 1.44        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1462 | C    | C4-C5   | 7.84  | 1.49        | 1.43     |
| 1   | AA    | 42   | G    | P-O5'   | -7.84 | 1.51        | 1.59     |
| 1   | AA    | 568  | G    | N9-C4   | 7.84  | 1.44        | 1.38     |
| 1   | AA    | 1066 | C    | C2-N3   | 7.84  | 1.42        | 1.35     |
| 3   | AC    | 87   | ARG  | NE-CZ   | 7.84  | 1.43        | 1.33     |
| 35  | BB    | 297  | G    | C5-C4   | 7.84  | 1.43        | 1.38     |
| 35  | BB    | 707  | G    | N7-C5   | -7.84 | 1.34        | 1.39     |
| 35  | BB    | 914  | G    | C2-N2   | 7.84  | 1.42        | 1.34     |
| 35  | BB    | 1873 | G    | C3'-O3' | 7.84  | 1.53        | 1.42     |
| 35  | BB    | 2107 | G    | N9-C4   | -7.84 | 1.31        | 1.38     |
| 35  | BB    | 1527 | G    | O3'-P   | -7.84 | 1.51        | 1.61     |
| 1   | AA    | 315  | A    | N9-C4   | 7.84  | 1.42        | 1.37     |
| 1   | AA    | 799  | G    | C2-N3   | 7.84  | 1.39        | 1.32     |
| 1   | AA    | 1505 | G    | C2-N2   | 7.84  | 1.42        | 1.34     |
| 35  | BB    | 19   | A    | P-O5'   | -7.84 | 1.51        | 1.59     |
| 35  | BB    | 1451 | C    | C4-C5   | 7.84  | 1.49        | 1.43     |
| 35  | BB    | 2323 | G    | N1-C2   | 7.84  | 1.44        | 1.37     |
| 35  | BB    | 2489 | U    | P-O5'   | -7.84 | 1.51        | 1.59     |
| 1   | AA    | 772  | U    | C2-N3   | 7.83  | 1.43        | 1.37     |
| 35  | BB    | 2018 | G    | N3-C4   | -7.83 | 1.29        | 1.35     |
| 1   | AA    | 690  | G    | P-O5'   | -7.83 | 1.51        | 1.59     |
| 35  | BB    | 745  | G    | N9-C8   | 7.83  | 1.43        | 1.37     |
| 35  | BB    | 1661 | G    | N3-C4   | -7.83 | 1.29        | 1.35     |
| 35  | BB    | 2597 | G    | C5'-C4' | 7.83  | 1.60        | 1.51     |
| 1   | AA    | 142  | G    | N9-C4   | 7.83  | 1.44        | 1.38     |
| 1   | AA    | 232  | G    | C1'-N9  | 7.83  | 1.60        | 1.48     |
| 1   | AA    | 836  | G    | C2-N3   | 7.83  | 1.39        | 1.32     |
| 35  | BB    | 1134 | A    | C8-N7   | -7.83 | 1.26        | 1.31     |
| 35  | BB    | 2495 | G    | C2'-C1' | -7.83 | 1.44        | 1.53     |
| 35  | BB    | 2655 | G    | C3'-C2' | 7.83  | 1.61        | 1.52     |
| 35  | BB    | 469  | G    | C2'-C1' | -7.83 | 1.44        | 1.53     |
| 35  | BB    | 2533 | U    | N3-C4   | 7.83  | 1.45        | 1.38     |
| 35  | BB    | 2775 | G    | N9-C4   | -7.83 | 1.31        | 1.38     |
| 1   | AA    | 199  | A    | C8-N7   | -7.83 | 1.26        | 1.31     |
| 1   | AA    | 1175 | G    | C6-N1   | 7.83  | 1.45        | 1.39     |
| 1   | AA    | 1280 | A    | C2'-C1' | -7.83 | 1.44        | 1.53     |
| 35  | BB    | 619  | G    | C8-N7   | 7.83  | 1.35        | 1.30     |
| 35  | BB    | 634  | C    | N3-C4   | 7.83  | 1.39        | 1.33     |
| 35  | BB    | 822  | G    | C5-C6   | -7.83 | 1.34        | 1.42     |
| 1   | AA    | 922  | G    | N3-C4   | 7.83  | 1.41        | 1.35     |
| 1   | AA    | 1051 | C    | C4-N4   | 7.83  | 1.41        | 1.33     |
| 1   | AA    | 1222 | G    | N7-C5   | -7.83 | 1.34        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1206 | G    | C6-N1   | 7.83  | 1.45        | 1.39     |
| 35  | BB    | 931  | U    | C5'-C4' | 7.82  | 1.60        | 1.51     |
| 35  | BB    | 2258 | C    | N3-C4   | 7.82  | 1.39        | 1.33     |
| 35  | BB    | 2833 | U    | N1-C2   | 7.82  | 1.45        | 1.38     |
| 1   | AA    | 746  | A    | C5-C4   | 7.82  | 1.44        | 1.38     |
| 35  | BB    | 503  | A    | N7-C5   | -7.82 | 1.34        | 1.39     |
| 35  | BB    | 1062 | G    | C5-C6   | -7.82 | 1.34        | 1.42     |
| 35  | BB    | 1109 | C    | C4'-C3' | 7.82  | 1.61        | 1.53     |
| 35  | BB    | 401  | A    | C6-N6   | 7.82  | 1.40        | 1.33     |
| 35  | BB    | 933  | A    | N7-C5   | -7.82 | 1.34        | 1.39     |
| 35  | BB    | 1906 | G    | N1-C2   | 7.82  | 1.44        | 1.37     |
| 1   | AA    | 1418 | A    | N7-C5   | -7.82 | 1.34        | 1.39     |
| 35  | BB    | 2279 | G    | C2-N3   | -7.82 | 1.26        | 1.32     |
| 35  | BB    | 2290 | G    | N1-C2   | 7.82  | 1.44        | 1.37     |
| 35  | BB    | 2376 | A    | N7-C5   | -7.82 | 1.34        | 1.39     |
| 35  | BB    | 2398 | U    | N1-C2   | 7.82  | 1.45        | 1.38     |
| 35  | BB    | 2564 | A    | C6-N6   | 7.82  | 1.40        | 1.33     |
| 35  | BB    | 2120 | G    | N1-C2   | 7.81  | 1.44        | 1.37     |
| 1   | AA    | 309  | A    | C6-N1   | 7.81  | 1.41        | 1.35     |
| 35  | BB    | 1421 | G    | N1-C2   | 7.81  | 1.44        | 1.37     |
| 35  | BB    | 1890 | A    | N3-C4   | -7.81 | 1.30        | 1.34     |
| 1   | AA    | 1171 | A    | C5'-C4' | 7.81  | 1.60        | 1.51     |
| 1   | AA    | 636  | U    | C2-N3   | 7.81  | 1.43        | 1.37     |
| 1   | AA    | 787  | A    | C6-N6   | 7.81  | 1.40        | 1.33     |
| 35  | BB    | 1669 | A    | C6-N1   | 7.81  | 1.41        | 1.35     |
| 35  | BB    | 1833 | C    | P-O5'   | -7.81 | 1.51        | 1.59     |
| 1   | AA    | 577  | G    | C5-C4   | -7.81 | 1.32        | 1.38     |
| 1   | AA    | 947  | G    | C2'-C1' | -7.81 | 1.44        | 1.53     |
| 35  | BB    | 997  | G    | C6-N1   | 7.81  | 1.45        | 1.39     |
| 35  | BB    | 1305 | C    | N1-C6   | -7.81 | 1.32        | 1.37     |
| 35  | BB    | 2280 | G    | N7-C5   | -7.81 | 1.34        | 1.39     |
| 35  | BB    | 2846 | G    | N7-C5   | -7.81 | 1.34        | 1.39     |
| 35  | BB    | 1358 | G    | C3'-C2' | 7.81  | 1.61        | 1.52     |
| 35  | BB    | 1392 | A    | P-O5'   | 7.81  | 1.67        | 1.59     |
| 1   | AA    | 674  | G    | N9-C4   | 7.80  | 1.44        | 1.38     |
| 35  | BB    | 396  | G    | C2-N3   | 7.80  | 1.39        | 1.32     |
| 35  | BB    | 409  | G    | C6-N1   | 7.80  | 1.45        | 1.39     |
| 35  | BB    | 546  | U    | C2-N3   | 7.80  | 1.43        | 1.37     |
| 35  | BB    | 2599 | G    | N9-C8   | -7.80 | 1.32        | 1.37     |
| 1   | AA    | 941  | G    | N1-C2   | 7.80  | 1.44        | 1.37     |
| 1   | AA    | 1293 | C    | N3-C4   | 7.80  | 1.39        | 1.33     |
| 35  | BB    | 473  | G    | N9-C8   | -7.80 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 767  | U    | C5-C6   | 7.80  | 1.41        | 1.34     |
| 35  | BB    | 1754 | A    | C6-N1   | 7.80  | 1.41        | 1.35     |
| 35  | BB    | 2418 | A    | C2'-C1' | -7.80 | 1.44        | 1.53     |
| 35  | BB    | 294  | A    | C2'-C1' | -7.80 | 1.44        | 1.53     |
| 1   | AA    | 128  | G    | N1-C2   | 7.80  | 1.44        | 1.37     |
| 1   | AA    | 711  | G    | C6-N1   | 7.80  | 1.45        | 1.39     |
| 1   | AA    | 1276 | G    | P-O5'   | -7.80 | 1.51        | 1.59     |
| 35  | BB    | 1974 | C    | P-O5'   | -7.80 | 1.51        | 1.59     |
| 22  | AV    | 72   | G    | C2'-C1' | -7.80 | 1.44        | 1.53     |
| 35  | BB    | 349  | U    | C4'-O4' | -7.80 | 1.35        | 1.45     |
| 35  | BB    | 2012 | G    | N3-C4   | 7.80  | 1.41        | 1.35     |
| 1   | AA    | 1142 | G    | N9-C8   | 7.79  | 1.43        | 1.37     |
| 1   | AA    | 1327 | C    | N3-C4   | 7.79  | 1.39        | 1.33     |
| 35  | BB    | 1559 | U    | C4-C5   | 7.79  | 1.50        | 1.43     |
| 1   | AA    | 131  | A    | N1-C2   | -7.79 | 1.27        | 1.34     |
| 35  | BB    | 84   | A    | C5-C4   | 7.79  | 1.44        | 1.38     |
| 35  | BB    | 544  | C    | N1-C6   | 7.79  | 1.41        | 1.37     |
| 35  | BB    | 2469 | A    | C6-N1   | 7.79  | 1.41        | 1.35     |
| 1   | AA    | 1388 | C    | O3'-P   | -7.79 | 1.51        | 1.61     |
| 1   | AA    | 1415 | G    | P-O5'   | -7.79 | 1.51        | 1.59     |
| 35  | BB    | 707  | G    | C8-N7   | -7.79 | 1.26        | 1.30     |
| 35  | BB    | 551  | G    | C6-N1   | 7.79  | 1.45        | 1.39     |
| 35  | BB    | 763  | G    | N1-C2   | 7.79  | 1.44        | 1.37     |
| 1   | AA    | 1065 | U    | P-O5'   | 7.79  | 1.67        | 1.59     |
| 35  | BB    | 490  | C    | C2-N3   | 7.79  | 1.42        | 1.35     |
| 35  | BB    | 2725 | A    | N7-C5   | -7.79 | 1.34        | 1.39     |
| 1   | AA    | 1025 | U    | O3'-P   | -7.79 | 1.51        | 1.61     |
| 35  | BB    | 532  | A    | C6-N6   | 7.79  | 1.40        | 1.33     |
| 35  | BB    | 2868 | A    | C5-C4   | 7.79  | 1.44        | 1.38     |
| 35  | BB    | 1093 | G    | C5-C4   | 7.79  | 1.43        | 1.38     |
| 35  | BB    | 38   | A    | C2'-C1' | -7.78 | 1.44        | 1.53     |
| 1   | AA    | 310  | G    | P-O5'   | -7.78 | 1.51        | 1.59     |
| 35  | BB    | 2132 | U    | O3'-P   | -7.78 | 1.51        | 1.61     |
| 35  | BB    | 2900 | A    | C6-N6   | 7.78  | 1.40        | 1.33     |
| 1   | AA    | 813  | U    | C2'-C1' | -7.78 | 1.44        | 1.53     |
| 22  | AV    | 3    | G    | O3'-P   | -7.78 | 1.51        | 1.61     |
| 35  | BB    | 406  | G    | C2'-C1' | -7.78 | 1.44        | 1.53     |
| 35  | BB    | 811  | U    | C2-N3   | 7.78  | 1.43        | 1.37     |
| 35  | BB    | 2029 | G    | C2-N3   | 7.78  | 1.39        | 1.32     |
| 1   | AA    | 585  | G    | C5-C4   | 7.78  | 1.43        | 1.38     |
| 1   | AA    | 837  | U    | N3-C4   | 7.78  | 1.45        | 1.38     |
| 1   | AA    | 1300 | G    | C6-N1   | 7.78  | 1.45        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 708  | G    | N7-C5   | -7.78 | 1.34        | 1.39     |
| 1   | AA    | 115  | G    | C2-N3   | 7.78  | 1.39        | 1.32     |
| 1   | AA    | 1202 | U    | N1-C6   | 7.78  | 1.45        | 1.38     |
| 35  | BB    | 1165 | A    | C5'-C4' | 7.78  | 1.60        | 1.51     |
| 35  | BB    | 1868 | C    | N3-C4   | 7.78  | 1.39        | 1.33     |
| 1   | AA    | 124  | C    | C4-C5   | 7.78  | 1.49        | 1.43     |
| 1   | AA    | 181  | A    | C6-N6   | 7.78  | 1.40        | 1.33     |
| 1   | AA    | 228  | A    | N7-C5   | -7.78 | 1.34        | 1.39     |
| 1   | AA    | 414  | A    | C6-N6   | 7.78  | 1.40        | 1.33     |
| 35  | BB    | 1608 | A    | N9-C4   | -7.78 | 1.33        | 1.37     |
| 35  | BB    | 1735 | A    | C6-N1   | 7.78  | 1.41        | 1.35     |
| 35  | BB    | 2394 | C    | C2'-C1' | -7.78 | 1.44        | 1.53     |
| 35  | BB    | 423  | A    | N9-C4   | -7.77 | 1.33        | 1.37     |
| 35  | BB    | 1373 | A    | C6-N1   | 7.77  | 1.41        | 1.35     |
| 1   | AA    | 985  | C    | O4'-C1' | 7.77  | 1.51        | 1.41     |
| 1   | AA    | 1003 | G    | N9-C8   | 7.77  | 1.43        | 1.37     |
| 35  | BB    | 380  | G    | C2'-C1' | -7.77 | 1.44        | 1.53     |
| 35  | BB    | 1828 | G    | C6-O6   | -7.77 | 1.17        | 1.24     |
| 35  | BB    | 2038 | G    | C2'-C1' | -7.77 | 1.44        | 1.53     |
| 35  | BB    | 2118 | U    | N3-C4   | 7.77  | 1.45        | 1.38     |
| 35  | BB    | 2780 | G    | P-O5'   | -7.77 | 1.51        | 1.59     |
| 35  | BB    | 636  | G    | N7-C5   | -7.77 | 1.34        | 1.39     |
| 35  | BB    | 757  | G    | P-O5'   | -7.77 | 1.51        | 1.59     |
| 35  | BB    | 1128 | G    | N1-C2   | 7.77  | 1.44        | 1.37     |
| 1   | AA    | 859  | G    | C2-N3   | 7.77  | 1.39        | 1.32     |
| 35  | BB    | 137  | U    | P-O5'   | -7.77 | 1.51        | 1.59     |
| 35  | BB    | 220  | G    | C6-N1   | 7.77  | 1.45        | 1.39     |
| 1   | AA    | 7    | A    | C6-N1   | 7.77  | 1.41        | 1.35     |
| 35  | BB    | 220  | G    | N1-C2   | 7.77  | 1.44        | 1.37     |
| 1   | AA    | 523  | A    | C5-C4   | 7.77  | 1.44        | 1.38     |
| 1   | AA    | 1052 | U    | O3'-P   | -7.77 | 1.51        | 1.61     |
| 1   | AA    | 1326 | U    | C2-N3   | 7.77  | 1.43        | 1.37     |
| 35  | BB    | 1600 | C    | C4-N4   | 7.77  | 1.41        | 1.33     |
| 1   | AA    | 384  | G    | C4'-O4' | -7.76 | 1.35        | 1.45     |
| 1   | AA    | 611  | C    | C2-N3   | 7.76  | 1.42        | 1.35     |
| 35  | BB    | 258  | G    | O4'-C1' | 7.76  | 1.51        | 1.41     |
| 35  | BB    | 299  | A    | C6-N6   | 7.76  | 1.40        | 1.33     |
| 35  | BB    | 688  | U    | N3-C4   | 7.76  | 1.45        | 1.38     |
| 35  | BB    | 1233 | C    | C2-N3   | 7.76  | 1.42        | 1.35     |
| 35  | BB    | 2677 | G    | N7-C5   | -7.76 | 1.34        | 1.39     |
| 35  | BB    | 14   | A    | N3-C4   | 7.76  | 1.39        | 1.34     |
| 35  | BB    | 450  | G    | N9-C4   | -7.76 | 1.31        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 517  | G    | C5-C4   | -7.76 | 1.32        | 1.38     |
| 1   | AA    | 1376 | U    | C2-N3   | 7.76  | 1.43        | 1.37     |
| 35  | BB    | 53   | A    | C6-N1   | 7.76  | 1.41        | 1.35     |
| 35  | BB    | 1336 | A    | N9-C4   | -7.76 | 1.33        | 1.37     |
| 35  | BB    | 2114 | A    | C6-N6   | 7.76  | 1.40        | 1.33     |
| 35  | BB    | 2198 | A    | C6-N1   | 7.76  | 1.41        | 1.35     |
| 35  | BB    | 2739 | U    | C2'-C1' | -7.76 | 1.44        | 1.53     |
| 1   | AA    | 916  | U    | N1-C2   | 7.76  | 1.45        | 1.38     |
| 1   | AA    | 1160 | G    | O4'-C1' | 7.76  | 1.51        | 1.41     |
| 35  | BB    | 723  | C    | C4-N4   | 7.76  | 1.41        | 1.33     |
| 35  | BB    | 1017 | G    | C6-N1   | 7.76  | 1.45        | 1.39     |
| 35  | BB    | 2123 | G    | O3'-P   | -7.76 | 1.51        | 1.61     |
| 1   | AA    | 1160 | G    | N9-C8   | 7.76  | 1.43        | 1.37     |
| 1   | AA    | 1363 | A    | O3'-P   | -7.76 | 1.51        | 1.61     |
| 35  | BB    | 1849 | G    | N3-C4   | -7.76 | 1.30        | 1.35     |
| 35  | BB    | 2236 | U    | C2-N3   | 7.76  | 1.43        | 1.37     |
| 1   | AA    | 884  | U    | N1-C6   | -7.76 | 1.30        | 1.38     |
| 1   | AA    | 1231 | G    | N1-C2   | 7.76  | 1.44        | 1.37     |
| 35  | BB    | 124  | G    | C2-N2   | 7.76  | 1.42        | 1.34     |
| 35  | BB    | 277  | G    | N9-C4   | 7.76  | 1.44        | 1.38     |
| 35  | BB    | 1274 | A    | C6-N6   | 7.76  | 1.40        | 1.33     |
| 35  | BB    | 1586 | A    | N7-C5   | -7.76 | 1.34        | 1.39     |
| 35  | BB    | 1989 | G    | C6-N1   | 7.76  | 1.45        | 1.39     |
| 35  | BB    | 2513 | A    | C6-N1   | 7.76  | 1.41        | 1.35     |
| 1   | AA    | 473  | U    | C2-O2   | 7.75  | 1.29        | 1.22     |
| 35  | BB    | 4    | U    | C2-N3   | 7.75  | 1.43        | 1.37     |
| 35  | BB    | 1155 | A    | C5-C4   | -7.75 | 1.33        | 1.38     |
| 1   | AA    | 28   | A    | N3-C4   | -7.75 | 1.30        | 1.34     |
| 34  | BA    | 108  | A    | C4'-C3' | -7.75 | 1.44        | 1.53     |
| 35  | BB    | 2874 | C    | C4'-C3' | -7.75 | 1.44        | 1.53     |
| 1   | AA    | 532  | A    | P-O5'   | -7.75 | 1.51        | 1.59     |
| 1   | AA    | 1215 | G    | C8-N7   | 7.75  | 1.35        | 1.30     |
| 35  | BB    | 2863 | C    | P-O5'   | -7.75 | 1.51        | 1.59     |
| 35  | BB    | 668  | A    | O4'-C1' | -7.75 | 1.31        | 1.41     |
| 35  | BB    | 919  | U    | C2-N3   | 7.75  | 1.43        | 1.37     |
| 1   | AA    | 228  | A    | C8-N7   | -7.75 | 1.26        | 1.31     |
| 1   | AA    | 838  | G    | C5-C4   | 7.75  | 1.43        | 1.38     |
| 35  | BB    | 474  | G    | O3'-P   | -7.75 | 1.51        | 1.61     |
| 35  | BB    | 693  | A    | C8-N7   | -7.75 | 1.26        | 1.31     |
| 35  | BB    | 2251 | G    | C2-N3   | 7.75  | 1.39        | 1.32     |
| 35  | BB    | 2874 | C    | N1-C6   | 7.75  | 1.41        | 1.37     |
| 35  | BB    | 75   | G    | C8-N7   | -7.75 | 1.26        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 799  | G    | N9-C4   | -7.75 | 1.31        | 1.38     |
| 35  | BB    | 2445 | G    | O3'-P   | 7.75  | 1.70        | 1.61     |
| 35  | BB    | 2177 | C    | C4-N4   | 7.75  | 1.41        | 1.33     |
| 35  | BB    | 2136 | G    | C3'-C2' | 7.74  | 1.61        | 1.52     |
| 35  | BB    | 2739 | U    | P-O5'   | 7.74  | 1.67        | 1.59     |
| 35  | BB    | 222  | A    | C6-N1   | 7.74  | 1.41        | 1.35     |
| 35  | BB    | 2009 | A    | P-O5'   | -7.74 | 1.52        | 1.59     |
| 35  | BB    | 2572 | A    | C6-N6   | 7.74  | 1.40        | 1.33     |
| 35  | BB    | 2826 | A    | N3-C4   | -7.74 | 1.30        | 1.34     |
| 35  | BB    | 2881 | U    | N3-C4   | 7.74  | 1.45        | 1.38     |
| 1   | AA    | 556  | C    | N1-C6   | 7.74  | 1.41        | 1.37     |
| 35  | BB    | 24   | G    | C2-N3   | 7.74  | 1.39        | 1.32     |
| 35  | BB    | 454  | A    | N9-C4   | -7.74 | 1.33        | 1.37     |
| 35  | BB    | 1151 | A    | N9-C8   | -7.74 | 1.31        | 1.37     |
| 35  | BB    | 1764 | C    | N1-C6   | 7.74  | 1.41        | 1.37     |
| 35  | BB    | 1836 | C    | N1-C6   | 7.74  | 1.41        | 1.37     |
| 1   | AA    | 674  | G    | C8-N7   | 7.74  | 1.35        | 1.30     |
| 35  | BB    | 1368 | G    | N3-C4   | -7.74 | 1.30        | 1.35     |
| 1   | AA    | 44   | A    | C6-N6   | 7.74  | 1.40        | 1.33     |
| 35  | BB    | 415  | A    | C8-N7   | -7.74 | 1.26        | 1.31     |
| 35  | BB    | 1271 | G    | N1-C2   | 7.74  | 1.44        | 1.37     |
| 35  | BB    | 1678 | A    | N7-C5   | -7.74 | 1.34        | 1.39     |
| 35  | BB    | 2576 | G    | C5-C6   | -7.74 | 1.34        | 1.42     |
| 35  | BB    | 492  | A    | N3-C4   | 7.73  | 1.39        | 1.34     |
| 35  | BB    | 954  | G    | C6-N1   | 7.73  | 1.45        | 1.39     |
| 1   | AA    | 1050 | G    | N7-C5   | -7.73 | 1.34        | 1.39     |
| 1   | AA    | 1228 | C    | O3'-P   | -7.73 | 1.51        | 1.61     |
| 1   | AA    | 1356 | G    | N1-C2   | 7.73  | 1.44        | 1.37     |
| 34  | BA    | 4    | C    | N3-C4   | 7.73  | 1.39        | 1.33     |
| 35  | BB    | 1672 | A    | C8-N7   | -7.73 | 1.26        | 1.31     |
| 35  | BB    | 2331 | G    | C8-N7   | -7.73 | 1.26        | 1.30     |
| 1   | AA    | 581  | G    | C5'-C4' | 7.73  | 1.60        | 1.51     |
| 35  | BB    | 1626 | A    | N7-C5   | -7.73 | 1.34        | 1.39     |
| 1   | AA    | 233  | C    | N3-C4   | 7.73  | 1.39        | 1.33     |
| 35  | BB    | 1897 | G    | C6-N1   | 7.73  | 1.45        | 1.39     |
| 35  | BB    | 2669 | G    | C2-N3   | 7.73  | 1.39        | 1.32     |
| 35  | BB    | 2869 | G    | N1-C2   | 7.73  | 1.44        | 1.37     |
| 1   | AA    | 836  | G    | N7-C5   | -7.73 | 1.34        | 1.39     |
| 35  | BB    | 360  | U    | C2'-C1' | -7.73 | 1.44        | 1.53     |
| 35  | BB    | 1571 | A    | C6-N1   | -7.73 | 1.30        | 1.35     |
| 35  | BB    | 1766 | G    | C8-N7   | -7.73 | 1.26        | 1.30     |
| 1   | AA    | 424  | G    | N3-C4   | -7.72 | 1.30        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1395 | C    | C2-N3   | 7.72  | 1.42        | 1.35     |
| 35  | BB    | 604  | G    | C2'-C1' | -7.72 | 1.44        | 1.53     |
| 35  | BB    | 609  | A    | C5-C6   | -7.72 | 1.34        | 1.41     |
| 35  | BB    | 2242 | G    | C6-N1   | 7.72  | 1.45        | 1.39     |
| 35  | BB    | 2474 | U    | C2'-C1' | -7.72 | 1.44        | 1.53     |
| 35  | BB    | 673  | C    | P-O5'   | -7.72 | 1.52        | 1.59     |
| 35  | BB    | 764  | A    | C5'-C4' | 7.72  | 1.60        | 1.51     |
| 35  | BB    | 2523 | G    | C2'-C1' | -7.72 | 1.44        | 1.53     |
| 1   | AA    | 23   | C    | P-O5'   | -7.72 | 1.52        | 1.59     |
| 1   | AA    | 681  | A    | N9-C8   | 7.72  | 1.44        | 1.37     |
| 35  | BB    | 43   | G    | N1-C2   | 7.72  | 1.44        | 1.37     |
| 35  | BB    | 1074 | G    | C8-N7   | -7.72 | 1.26        | 1.30     |
| 35  | BB    | 1164 | C    | N3-C4   | 7.72  | 1.39        | 1.33     |
| 35  | BB    | 1571 | A    | C2'-C1' | -7.72 | 1.44        | 1.53     |
| 35  | BB    | 1773 | A    | N7-C5   | -7.72 | 1.34        | 1.39     |
| 35  | BB    | 2672 | U    | C4'-C3' | 7.72  | 1.61        | 1.53     |
| 35  | BB    | 2817 | U    | C2-N3   | 7.72  | 1.43        | 1.37     |
| 1   | AA    | 1002 | G    | C2'-C1' | -7.72 | 1.44        | 1.53     |
| 1   | AA    | 1178 | G    | P-O5'   | -7.72 | 1.52        | 1.59     |
| 35  | BB    | 217  | A    | C6-N6   | 7.72  | 1.40        | 1.33     |
| 35  | BB    | 1228 | G    | P-O5'   | 7.72  | 1.67        | 1.59     |
| 35  | BB    | 2450 | A    | C6-N6   | 7.72  | 1.40        | 1.33     |
| 35  | BB    | 2569 | G    | N7-C5   | -7.72 | 1.34        | 1.39     |
| 1   | AA    | 511  | C    | C4-C5   | 7.71  | 1.49        | 1.43     |
| 35  | BB    | 663  | G    | C5-C4   | -7.71 | 1.32        | 1.38     |
| 35  | BB    | 1057 | A    | C4'-C3' | -7.71 | 1.44        | 1.53     |
| 35  | BB    | 1205 | A    | C2'-C1' | -7.71 | 1.44        | 1.53     |
| 35  | BB    | 1490 | A    | N9-C4   | -7.71 | 1.33        | 1.37     |
| 35  | BB    | 2047 | C    | P-O5'   | -7.71 | 1.52        | 1.59     |
| 35  | BB    | 2317 | A    | P-O5'   | -7.71 | 1.52        | 1.59     |
| 35  | BB    | 1755 | A    | C6-N6   | 7.71  | 1.40        | 1.33     |
| 1   | AA    | 537  | G    | C5-C6   | -7.71 | 1.34        | 1.42     |
| 35  | BB    | 38   | A    | C6-N1   | 7.71  | 1.41        | 1.35     |
| 35  | BB    | 128  | C    | N1-C6   | 7.71  | 1.41        | 1.37     |
| 35  | BB    | 1320 | C    | C4-N4   | 7.71  | 1.40        | 1.33     |
| 35  | BB    | 454  | A    | C6-N6   | 7.71  | 1.40        | 1.33     |
| 35  | BB    | 2297 | A    | N3-C4   | 7.71  | 1.39        | 1.34     |
| 35  | BB    | 2346 | A    | C6-N1   | 7.71  | 1.41        | 1.35     |
| 1   | AA    | 497  | G    | C8-N7   | 7.71  | 1.35        | 1.30     |
| 1   | AA    | 607  | A    | C6-N6   | 7.71  | 1.40        | 1.33     |
| 1   | AA    | 1183 | U    | C1'-N1  | 7.71  | 1.60        | 1.48     |
| 1   | AA    | 1197 | A    | N3-C4   | -7.71 | 1.30        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 255  | A    | N9-C4   | 7.71  | 1.42        | 1.37     |
| 35  | BB    | 1317 | G    | N9-C4   | -7.71 | 1.31        | 1.38     |
| 35  | BB    | 1763 | G    | C4'-C3' | 7.71  | 1.61        | 1.53     |
| 35  | BB    | 2045 | C    | C2'-C1' | -7.71 | 1.44        | 1.53     |
| 35  | BB    | 2724 | U    | C4'-C3' | -7.71 | 1.44        | 1.53     |
| 1   | AA    | 1430 | A    | O3'-P   | -7.71 | 1.51        | 1.61     |
| 1   | AA    | 404  | G    | C3'-C2' | 7.70  | 1.61        | 1.52     |
| 1   | AA    | 570  | G    | C6-N1   | 7.70  | 1.45        | 1.39     |
| 1   | AA    | 1164 | G    | C2'-C1' | -7.70 | 1.44        | 1.53     |
| 1   | AA    | 1281 | C    | C4-N4   | 7.70  | 1.40        | 1.33     |
| 34  | BA    | 42   | C    | N1-C6   | -7.70 | 1.32        | 1.37     |
| 35  | BB    | 2744 | G    | N7-C5   | -7.70 | 1.34        | 1.39     |
| 35  | BB    | 2841 | C    | C3'-C2' | -7.70 | 1.44        | 1.52     |
| 1   | AA    | 1242 | G    | C2'-C1' | -7.70 | 1.44        | 1.53     |
| 1   | AA    | 150  | U    | C2-N3   | 7.70  | 1.43        | 1.37     |
| 35  | BB    | 35   | G    | N1-C2   | 7.70  | 1.44        | 1.37     |
| 1   | AA    | 491  | G    | C2'-C1' | -7.70 | 1.44        | 1.53     |
| 1   | AA    | 1166 | G    | N7-C5   | -7.70 | 1.34        | 1.39     |
| 34  | BA    | 46   | A    | C6-N6   | 7.70  | 1.40        | 1.33     |
| 35  | BB    | 132  | G    | C8-N7   | -7.70 | 1.26        | 1.30     |
| 35  | BB    | 489  | G    | N3-C4   | -7.70 | 1.30        | 1.35     |
| 1   | AA    | 97   | G    | C5'-C4' | 7.70  | 1.60        | 1.51     |
| 1   | AA    | 629  | A    | C6-N1   | 7.70  | 1.41        | 1.35     |
| 1   | AA    | 1033 | G    | C4'-C3' | 7.70  | 1.61        | 1.53     |
| 1   | AA    | 1134 | G    | C2-N3   | 7.70  | 1.39        | 1.32     |
| 35  | BB    | 195  | A    | C4'-C3' | 7.70  | 1.61        | 1.53     |
| 35  | BB    | 224  | U    | N1-C2   | -7.70 | 1.31        | 1.38     |
| 35  | BB    | 614  | A    | N3-C4   | 7.70  | 1.39        | 1.34     |
| 35  | BB    | 1235 | G    | N3-C4   | -7.70 | 1.30        | 1.35     |
| 35  | BB    | 1246 | A    | C2'-C1' | -7.70 | 1.44        | 1.53     |
| 35  | BB    | 1871 | A    | C6-N6   | 7.70  | 1.40        | 1.33     |
| 35  | BB    | 539  | G    | C2'-C1' | -7.69 | 1.44        | 1.53     |
| 35  | BB    | 602  | A    | C2-N3   | 7.69  | 1.40        | 1.33     |
| 35  | BB    | 922  | C    | C4-N4   | 7.69  | 1.40        | 1.33     |
| 35  | BB    | 2082 | A    | N9-C4   | -7.69 | 1.33        | 1.37     |
| 1   | AA    | 35   | G    | C6-N1   | 7.69  | 1.45        | 1.39     |
| 35  | BB    | 629  | G    | N7-C5   | -7.69 | 1.34        | 1.39     |
| 35  | BB    | 1283 | G    | C2-N2   | 7.69  | 1.42        | 1.34     |
| 35  | BB    | 1470 | A    | C8-N7   | -7.69 | 1.26        | 1.31     |
| 35  | BB    | 2255 | G    | P-O5'   | -7.69 | 1.52        | 1.59     |
| 8   | AH    | 76   | ARG  | CZ-NH1  | 7.69  | 1.43        | 1.33     |
| 34  | BA    | 42   | C    | C4-C5   | 7.69  | 1.49        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1117 | C    | C5'-C4' | 7.69  | 1.60        | 1.51     |
| 35  | BB    | 1234 | U    | C3'-C2' | -7.69 | 1.44        | 1.52     |
| 35  | BB    | 1320 | C    | O3'-P   | -7.69 | 1.51        | 1.61     |
| 35  | BB    | 1589 | U    | C4'-C3' | 7.69  | 1.61        | 1.53     |
| 35  | BB    | 2157 | G    | C2-N2   | 7.69  | 1.42        | 1.34     |
| 1   | AA    | 807  | A    | C6-N6   | 7.69  | 1.40        | 1.33     |
| 35  | BB    | 1046 | A    | N7-C5   | -7.69 | 1.34        | 1.39     |
| 35  | BB    | 1637 | A    | N9-C8   | 7.69  | 1.44        | 1.37     |
| 35  | BB    | 2453 | A    | P-O5'   | -7.69 | 1.52        | 1.59     |
| 35  | BB    | 2678 | C    | O3'-P   | -7.69 | 1.51        | 1.61     |
| 1   | AA    | 1317 | C    | N3-C4   | 7.69  | 1.39        | 1.33     |
| 35  | BB    | 2784 | U    | C2-N3   | 7.69  | 1.43        | 1.37     |
| 1   | AA    | 57   | G    | N3-C4   | -7.68 | 1.30        | 1.35     |
| 1   | AA    | 276  | G    | C6-N1   | -7.68 | 1.34        | 1.39     |
| 35  | BB    | 1286 | A    | N7-C5   | -7.68 | 1.34        | 1.39     |
| 35  | BB    | 1967 | C    | C4-N4   | 7.68  | 1.40        | 1.33     |
| 35  | BB    | 2080 | A    | C8-N7   | -7.68 | 1.26        | 1.31     |
| 35  | BB    | 2823 | A    | N1-C2   | 7.68  | 1.41        | 1.34     |
| 35  | BB    | 686  | U    | N1-C2   | 7.68  | 1.45        | 1.38     |
| 35  | BB    | 1653 | G    | O3'-P   | -7.68 | 1.51        | 1.61     |
| 1   | AA    | 627  | G    | N9-C8   | 7.68  | 1.43        | 1.37     |
| 35  | BB    | 945  | A    | C6-N1   | 7.68  | 1.41        | 1.35     |
| 35  | BB    | 1341 | G    | C4'-C3' | 7.68  | 1.61        | 1.53     |
| 1   | AA    | 577  | G    | C3'-C2' | -7.68 | 1.44        | 1.52     |
| 35  | BB    | 676  | A    | N9-C4   | -7.68 | 1.33        | 1.37     |
| 35  | BB    | 1471 | G    | C2-N2   | 7.68  | 1.42        | 1.34     |
| 35  | BB    | 1650 | A    | C8-N7   | 7.68  | 1.36        | 1.31     |
| 35  | BB    | 2558 | C    | C4-C5   | 7.68  | 1.49        | 1.43     |
| 1   | AA    | 28   | A    | C5-C4   | 7.68  | 1.44        | 1.38     |
| 1   | AA    | 681  | A    | N7-C5   | -7.68 | 1.34        | 1.39     |
| 1   | AA    | 1011 | C    | C4-N4   | 7.68  | 1.40        | 1.33     |
| 1   | AA    | 806  | C    | N3-C4   | 7.68  | 1.39        | 1.33     |
| 35  | BB    | 293  | U    | O3'-P   | -7.68 | 1.51        | 1.61     |
| 1   | AA    | 1216 | A    | N7-C5   | -7.67 | 1.34        | 1.39     |
| 35  | BB    | 540  | C    | N3-C4   | 7.67  | 1.39        | 1.33     |
| 35  | BB    | 2816 | G    | C5-C4   | 7.67  | 1.43        | 1.38     |
| 35  | BB    | 487  | C    | C4-C5   | -7.67 | 1.36        | 1.43     |
| 35  | BB    | 1684 | G    | N7-C5   | -7.67 | 1.34        | 1.39     |
| 35  | BB    | 1952 | A    | N7-C5   | -7.67 | 1.34        | 1.39     |
| 35  | BB    | 2110 | G    | C8-N7   | 7.67  | 1.35        | 1.30     |
| 1   | AA    | 841  | C    | P-O5'   | 7.67  | 1.67        | 1.59     |
| 35  | BB    | 1379 | U    | C5'-C4' | 7.67  | 1.60        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1021 | A    | C5-C4   | 7.67  | 1.44        | 1.38     |
| 35  | BB    | 659  | G    | N1-C2   | 7.67  | 1.43        | 1.37     |
| 35  | BB    | 1867 | G    | C8-N7   | 7.67  | 1.35        | 1.30     |
| 35  | BB    | 2365 | G    | N9-C8   | -7.67 | 1.32        | 1.37     |
| 1   | AA    | 289  | G    | N9-C8   | 7.67  | 1.43        | 1.37     |
| 1   | AA    | 559  | A    | N9-C8   | 7.67  | 1.43        | 1.37     |
| 1   | AA    | 1050 | G    | N1-C2   | 7.67  | 1.43        | 1.37     |
| 35  | BB    | 650  | C    | C4-N4   | 7.67  | 1.40        | 1.33     |
| 35  | BB    | 2024 | G    | C6-N1   | 7.67  | 1.45        | 1.39     |
| 1   | AA    | 1224 | U    | N3-C4   | 7.67  | 1.45        | 1.38     |
| 35  | BB    | 1097 | U    | C5-C6   | -7.67 | 1.27        | 1.34     |
| 1   | AA    | 1516 | G    | C5'-C4' | 7.66  | 1.60        | 1.51     |
| 35  | BB    | 530  | G    | C4'-C3' | -7.66 | 1.44        | 1.53     |
| 35  | BB    | 1368 | G    | C8-N7   | -7.66 | 1.26        | 1.30     |
| 1   | AA    | 264  | C    | C1'-N1  | 7.66  | 1.60        | 1.48     |
| 35  | BB    | 705  | A    | N7-C5   | -7.66 | 1.34        | 1.39     |
| 35  | BB    | 1465 | G    | N1-C2   | 7.66  | 1.43        | 1.37     |
| 35  | BB    | 2391 | G    | N1-C2   | 7.66  | 1.43        | 1.37     |
| 35  | BB    | 2537 | U    | C2'-C1' | -7.66 | 1.45        | 1.53     |
| 35  | BB    | 2764 | A    | C2-N3   | -7.66 | 1.26        | 1.33     |
| 1   | AA    | 752  | G    | C5-C4   | -7.66 | 1.32        | 1.38     |
| 1   | AA    | 770  | C    | N3-C4   | 7.66  | 1.39        | 1.33     |
| 34  | BA    | 76   | G    | C3'-C2' | 7.66  | 1.61        | 1.52     |
| 35  | BB    | 885  | C    | C3'-C2' | -7.66 | 1.44        | 1.52     |
| 35  | BB    | 2315 | G    | C6-N1   | 7.66  | 1.45        | 1.39     |
| 1   | AA    | 467  | U    | C5-C6   | 7.66  | 1.41        | 1.34     |
| 19  | AS    | 54   | ARG  | NE-CZ   | 7.66  | 1.43        | 1.33     |
| 35  | BB    | 549  | G    | N7-C5   | -7.66 | 1.34        | 1.39     |
| 35  | BB    | 655  | A    | C4'-C3' | 7.66  | 1.61        | 1.53     |
| 35  | BB    | 1355 | G    | C2-N3   | 7.66  | 1.38        | 1.32     |
| 35  | BB    | 1530 | G    | P-O5'   | -7.66 | 1.52        | 1.59     |
| 35  | BB    | 2046 | G    | C2-N3   | 7.66  | 1.38        | 1.32     |
| 1   | AA    | 76   | G    | C6-N1   | 7.65  | 1.45        | 1.39     |
| 1   | AA    | 538  | G    | C2-N2   | 7.65  | 1.42        | 1.34     |
| 35  | BB    | 280  | U    | C2-N3   | 7.65  | 1.43        | 1.37     |
| 35  | BB    | 346  | A    | C8-N7   | -7.65 | 1.26        | 1.31     |
| 35  | BB    | 616  | A    | C2-N3   | 7.65  | 1.40        | 1.33     |
| 35  | BB    | 2012 | G    | N1-C2   | 7.65  | 1.43        | 1.37     |
| 1   | AA    | 226  | G    | N1-C2   | 7.65  | 1.43        | 1.37     |
| 1   | AA    | 634  | C    | C3'-C2' | -7.65 | 1.44        | 1.52     |
| 1   | AA    | 1409 | C    | C4-C5   | 7.65  | 1.49        | 1.43     |
| 35  | BB    | 1577 | C    | N1-C6   | 7.65  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2204 | G    | C2-N2   | 7.65  | 1.42        | 1.34     |
| 1   | AA    | 381  | C    | C4-N4   | 7.65  | 1.40        | 1.33     |
| 1   | AA    | 712  | A    | C6-N1   | 7.65  | 1.41        | 1.35     |
| 35  | BB    | 1631 | G    | P-O5'   | -7.65 | 1.52        | 1.59     |
| 1   | AA    | 69   | G    | N1-C2   | 7.65  | 1.43        | 1.37     |
| 35  | BB    | 946  | C    | C2'-C1' | -7.65 | 1.45        | 1.53     |
| 1   | AA    | 410  | G    | C8-N7   | -7.65 | 1.26        | 1.30     |
| 1   | AA    | 688  | G    | P-O5'   | -7.65 | 1.52        | 1.59     |
| 1   | AA    | 780  | A    | C8-N7   | -7.65 | 1.26        | 1.31     |
| 35  | BB    | 2369 | A    | N7-C5   | -7.65 | 1.34        | 1.39     |
| 1   | AA    | 541  | G    | N9-C4   | -7.65 | 1.31        | 1.38     |
| 1   | AA    | 829  | G    | C2-N3   | 7.65  | 1.38        | 1.32     |
| 35  | BB    | 1678 | A    | O3'-P   | -7.65 | 1.51        | 1.61     |
| 34  | BA    | 16   | G    | N1-C2   | 7.64  | 1.43        | 1.37     |
| 35  | BB    | 350  | G    | O3'-P   | -7.64 | 1.51        | 1.61     |
| 35  | BB    | 1143 | A    | N9-C4   | 7.64  | 1.42        | 1.37     |
| 35  | BB    | 1702 | G    | N1-C2   | 7.64  | 1.43        | 1.37     |
| 35  | BB    | 1787 | A    | C6-N6   | 7.64  | 1.40        | 1.33     |
| 35  | BB    | 2010 | G    | N1-C2   | 7.64  | 1.43        | 1.37     |
| 35  | BB    | 2664 | G    | N1-C2   | 7.64  | 1.43        | 1.37     |
| 1   | AA    | 1361 | G    | O4'-C1' | 7.64  | 1.51        | 1.41     |
| 35  | BB    | 172  | A    | N1-C2   | 7.64  | 1.41        | 1.34     |
| 35  | BB    | 1709 | U    | C2-N3   | 7.64  | 1.43        | 1.37     |
| 35  | BB    | 2168 | G    | C2'-C1' | -7.64 | 1.45        | 1.53     |
| 35  | BB    | 2731 | G    | N7-C5   | -7.64 | 1.34        | 1.39     |
| 34  | BA    | 104  | A    | C6-N6   | 7.64  | 1.40        | 1.33     |
| 35  | BB    | 2611 | C    | C4-N4   | 7.64  | 1.40        | 1.33     |
| 1   | AA    | 457  | G    | C8-N7   | -7.64 | 1.26        | 1.30     |
| 35  | BB    | 350  | G    | N9-C8   | -7.64 | 1.32        | 1.37     |
| 35  | BB    | 2358 | A    | C2'-C1' | -7.64 | 1.45        | 1.53     |
| 35  | BB    | 2487 | G    | C5-C6   | -7.64 | 1.34        | 1.42     |
| 1   | AA    | 74   | A    | N7-C5   | -7.64 | 1.34        | 1.39     |
| 35  | BB    | 107  | G    | C4'-C3' | -7.64 | 1.44        | 1.53     |
| 35  | BB    | 2355 | G    | N1-C2   | 7.64  | 1.43        | 1.37     |
| 35  | BB    | 2561 | U    | N3-C4   | 7.64  | 1.45        | 1.38     |
| 35  | BB    | 620  | G    | N1-C2   | 7.64  | 1.43        | 1.37     |
| 35  | BB    | 1975 | G    | N1-C2   | 7.64  | 1.43        | 1.37     |
| 35  | BB    | 2864 | G    | N1-C2   | 7.64  | 1.43        | 1.37     |
| 35  | BB    | 1628 | G    | C2'-C1' | -7.63 | 1.45        | 1.53     |
| 35  | BB    | 2241 | A    | C2'-C1' | -7.63 | 1.45        | 1.53     |
| 1   | AA    | 968  | A    | N3-C4   | 7.63  | 1.39        | 1.34     |
| 35  | BB    | 22   | C    | N1-C6   | 7.63  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2524 | G    | C6-N1   | 7.63  | 1.44        | 1.39     |
| 1   | AA    | 484  | G    | N7-C5   | -7.63 | 1.34        | 1.39     |
| 1   | AA    | 1402 | C    | C3'-C2' | -7.63 | 1.44        | 1.52     |
| 35  | BB    | 5    | A    | C5-C6   | -7.63 | 1.34        | 1.41     |
| 35  | BB    | 242  | G    | C2-N3   | 7.63  | 1.38        | 1.32     |
| 35  | BB    | 2268 | A    | N9-C4   | -7.63 | 1.33        | 1.37     |
| 1   | AA    | 628  | G    | O3'-P   | -7.63 | 1.51        | 1.61     |
| 35  | BB    | 1309 | G    | N1-C2   | 7.63  | 1.43        | 1.37     |
| 1   | AA    | 293  | G    | C5-C4   | 7.63  | 1.43        | 1.38     |
| 1   | AA    | 643  | C    | N3-C4   | 7.63  | 1.39        | 1.33     |
| 35  | BB    | 217  | A    | C5-C4   | -7.63 | 1.33        | 1.38     |
| 35  | BB    | 638  | G    | C2-N3   | 7.63  | 1.38        | 1.32     |
| 1   | AA    | 344  | A    | C6-N1   | 7.63  | 1.40        | 1.35     |
| 1   | AA    | 844  | G    | N3-C4   | 7.63  | 1.40        | 1.35     |
| 12  | AL    | 69   | GLU  | CD-OE1  | 7.63  | 1.34        | 1.25     |
| 35  | BB    | 2550 | G    | C8-N7   | -7.63 | 1.26        | 1.30     |
| 35  | BB    | 2626 | C    | O3'-P   | -7.63 | 1.51        | 1.61     |
| 35  | BB    | 2696 | U    | C2-N3   | 7.63  | 1.43        | 1.37     |
| 35  | BB    | 896  | A    | C6-N1   | 7.62  | 1.40        | 1.35     |
| 35  | BB    | 1396 | U    | C4-O4   | -7.62 | 1.17        | 1.23     |
| 35  | BB    | 910  | A    | N7-C5   | -7.62 | 1.34        | 1.39     |
| 35  | BB    | 2483 | C    | C2-N3   | 7.62  | 1.41        | 1.35     |
| 1   | AA    | 258  | G    | N7-C5   | -7.62 | 1.34        | 1.39     |
| 1   | AA    | 550  | G    | N9-C4   | 7.62  | 1.44        | 1.38     |
| 1   | AA    | 1205 | U    | C4'-C3' | 7.62  | 1.61        | 1.53     |
| 35  | BB    | 605  | G    | N9-C8   | -7.62 | 1.32        | 1.37     |
| 35  | BB    | 1878 | G    | N7-C5   | -7.62 | 1.34        | 1.39     |
| 35  | BB    | 359  | G    | C2-N3   | 7.62  | 1.38        | 1.32     |
| 35  | BB    | 2590 | A    | N9-C4   | 7.62  | 1.42        | 1.37     |
| 1   | AA    | 59   | A    | C5-C6   | -7.62 | 1.34        | 1.41     |
| 1   | AA    | 428  | G    | C2-N3   | 7.62  | 1.38        | 1.32     |
| 1   | AA    | 1446 | A    | N9-C8   | -7.62 | 1.31        | 1.37     |
| 1   | AA    | 1467 | C    | C3'-O3' | 7.62  | 1.52        | 1.42     |
| 35  | BB    | 555  | G    | N3-C4   | -7.62 | 1.30        | 1.35     |
| 35  | BB    | 1615 | C    | C4-N4   | 7.62  | 1.40        | 1.33     |
| 35  | BB    | 1985 | C    | C4-N4   | 7.62  | 1.40        | 1.33     |
| 35  | BB    | 2686 | G    | N7-C5   | -7.62 | 1.34        | 1.39     |
| 1   | AA    | 558  | G    | N1-C2   | 7.62  | 1.43        | 1.37     |
| 1   | AA    | 346  | G    | N7-C5   | -7.62 | 1.34        | 1.39     |
| 35  | BB    | 74   | A    | N3-C4   | -7.62 | 1.30        | 1.34     |
| 35  | BB    | 845  | A    | N1-C2   | 7.62  | 1.41        | 1.34     |
| 35  | BB    | 300  | A    | C5-C6   | -7.61 | 1.34        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 822  | G    | N7-C5   | -7.61 | 1.34        | 1.39     |
| 35  | BB    | 2391 | G    | C6-N1   | 7.61  | 1.44        | 1.39     |
| 1   | AA    | 183  | C    | O3'-P   | -7.61 | 1.52        | 1.61     |
| 1   | AA    | 609  | A    | N7-C5   | -7.61 | 1.34        | 1.39     |
| 35  | BB    | 697  | G    | C2-N3   | 7.61  | 1.38        | 1.32     |
| 35  | BB    | 2414 | G    | P-O5'   | -7.61 | 1.52        | 1.59     |
| 1   | AA    | 441  | A    | C2'-C1' | -7.61 | 1.45        | 1.53     |
| 35  | BB    | 1278 | C    | O3'-P   | -7.61 | 1.52        | 1.61     |
| 35  | BB    | 1299 | G    | N7-C5   | -7.61 | 1.34        | 1.39     |
| 35  | BB    | 1308 | A    | O3'-P   | -7.61 | 1.52        | 1.61     |
| 35  | BB    | 2639 | A    | C3'-C2' | -7.61 | 1.44        | 1.52     |
| 1   | AA    | 1245 | C    | P-O5'   | -7.61 | 1.52        | 1.59     |
| 35  | BB    | 541  | A    | C5-C4   | 7.61  | 1.44        | 1.38     |
| 35  | BB    | 1609 | A    | C6-N6   | 7.61  | 1.40        | 1.33     |
| 35  | BB    | 1891 | G    | C2-N2   | 7.61  | 1.42        | 1.34     |
| 35  | BB    | 2381 | A    | P-O5'   | -7.61 | 1.52        | 1.59     |
| 1   | AA    | 158  | G    | N9-C4   | -7.60 | 1.31        | 1.38     |
| 35  | BB    | 366  | C    | C2'-C1' | -7.60 | 1.45        | 1.53     |
| 35  | BB    | 1119 | U    | P-O5'   | -7.60 | 1.52        | 1.59     |
| 35  | BB    | 1177 | G    | C6-N1   | 7.60  | 1.44        | 1.39     |
| 1   | AA    | 127  | G    | C5-C6   | -7.60 | 1.34        | 1.42     |
| 1   | AA    | 327  | A    | N7-C5   | -7.60 | 1.34        | 1.39     |
| 1   | AA    | 1186 | G    | C3'-C2' | -7.60 | 1.44        | 1.52     |
| 35  | BB    | 2722 | G    | N1-C2   | 7.60  | 1.43        | 1.37     |
| 35  | BB    | 978  | G    | C2-N3   | 7.60  | 1.38        | 1.32     |
| 35  | BB    | 1663 | G    | N7-C5   | -7.60 | 1.34        | 1.39     |
| 1   | AA    | 162  | A    | C5'-C4' | 7.60  | 1.60        | 1.51     |
| 35  | BB    | 1138 | G    | N7-C5   | -7.60 | 1.34        | 1.39     |
| 35  | BB    | 1456 | G    | N7-C5   | -7.60 | 1.34        | 1.39     |
| 35  | BB    | 2062 | A    | C6-N1   | 7.60  | 1.40        | 1.35     |
| 35  | BB    | 2355 | G    | N7-C5   | -7.60 | 1.34        | 1.39     |
| 1   | AA    | 140  | U    | P-O5'   | -7.60 | 1.52        | 1.59     |
| 35  | BB    | 1020 | A    | C2'-C1' | -7.60 | 1.45        | 1.53     |
| 35  | BB    | 1135 | C    | N3-C4   | 7.60  | 1.39        | 1.33     |
| 35  | BB    | 2097 | A    | C4'-O4' | 7.60  | 1.55        | 1.45     |
| 35  | BB    | 2859 | G    | O3'-P   | -7.60 | 1.52        | 1.61     |
| 35  | BB    | 1075 | C    | C2-N3   | 7.60  | 1.41        | 1.35     |
| 1   | AA    | 1255 | G    | N3-C4   | -7.59 | 1.30        | 1.35     |
| 35  | BB    | 1867 | G    | C2-N3   | 7.59  | 1.38        | 1.32     |
| 35  | BB    | 2488 | G    | N9-C8   | 7.59  | 1.43        | 1.37     |
| 1   | AA    | 434  | U    | N3-C4   | 7.59  | 1.45        | 1.38     |
| 34  | BA    | 35   | C    | N3-C4   | 7.59  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 99   | U    | O3'-P   | -7.59 | 1.52        | 1.61     |
| 35  | BB    | 2822 | G    | N9-C4   | 7.59  | 1.44        | 1.38     |
| 1   | AA    | 455  | G    | P-O5'   | -7.59 | 1.52        | 1.59     |
| 35  | BB    | 108  | G    | C6-N1   | 7.59  | 1.44        | 1.39     |
| 35  | BB    | 2368 | C    | N3-C4   | 7.59  | 1.39        | 1.33     |
| 35  | BB    | 2555 | U    | C4'-O4' | 7.59  | 1.55        | 1.45     |
| 35  | BB    | 350  | G    | P-O5'   | -7.59 | 1.52        | 1.59     |
| 35  | BB    | 1154 | G    | C5-C4   | 7.59  | 1.43        | 1.38     |
| 22  | AV    | 6    | C    | C4-C5   | -7.59 | 1.36        | 1.43     |
| 35  | BB    | 487  | C    | C4-N4   | 7.59  | 1.40        | 1.33     |
| 35  | BB    | 1941 | C    | N3-C4   | 7.59  | 1.39        | 1.33     |
| 1   | AA    | 108  | G    | C2-N3   | 7.59  | 1.38        | 1.32     |
| 35  | BB    | 993  | G    | N9-C8   | 7.59  | 1.43        | 1.37     |
| 35  | BB    | 1208 | C    | N1-C6   | -7.59 | 1.32        | 1.37     |
| 35  | BB    | 2845 | U    | C4-O4   | 7.59  | 1.29        | 1.23     |
| 35  | BB    | 1100 | C    | P-O5'   | 7.58  | 1.67        | 1.59     |
| 35  | BB    | 1420 | A    | C6-N6   | 7.58  | 1.40        | 1.33     |
| 1   | AA    | 214  | C    | N3-C4   | 7.58  | 1.39        | 1.33     |
| 35  | BB    | 747  | U    | C5'-C4' | 7.58  | 1.60        | 1.51     |
| 35  | BB    | 1952 | A    | C6-N1   | 7.58  | 1.40        | 1.35     |
| 35  | BB    | 2708 | G    | C8-N7   | -7.58 | 1.26        | 1.30     |
| 35  | BB    | 518  | G    | C8-N7   | -7.58 | 1.26        | 1.30     |
| 35  | BB    | 823  | C    | N1-C6   | -7.58 | 1.32        | 1.37     |
| 35  | BB    | 1160 | G    | C2'-C1' | -7.58 | 1.45        | 1.53     |
| 35  | BB    | 1864 | U    | N3-C4   | 7.58  | 1.45        | 1.38     |
| 35  | BB    | 2398 | U    | P-O5'   | -7.58 | 1.52        | 1.59     |
| 35  | BB    | 1752 | C    | P-O5'   | -7.58 | 1.52        | 1.59     |
| 1   | AA    | 515  | G    | N1-C2   | 7.58  | 1.43        | 1.37     |
| 35  | BB    | 729  | G    | N7-C5   | -7.58 | 1.34        | 1.39     |
| 35  | BB    | 1664 | A    | N3-C4   | -7.58 | 1.30        | 1.34     |
| 35  | BB    | 1713 | A    | N9-C4   | -7.58 | 1.33        | 1.37     |
| 35  | BB    | 1977 | A    | C2'-C1' | -7.58 | 1.45        | 1.53     |
| 1   | AA    | 428  | G    | C6-N1   | 7.58  | 1.44        | 1.39     |
| 35  | BB    | 196  | A    | N3-C4   | -7.58 | 1.30        | 1.34     |
| 35  | BB    | 648  | G    | C5'-C4' | 7.58  | 1.60        | 1.51     |
| 35  | BB    | 1165 | A    | C2'-C1' | -7.58 | 1.45        | 1.53     |
| 35  | BB    | 2263 | C    | N3-C4   | 7.58  | 1.39        | 1.33     |
| 1   | AA    | 1199 | U    | N3-C4   | 7.57  | 1.45        | 1.38     |
| 35  | BB    | 511  | U    | O3'-P   | -7.57 | 1.52        | 1.61     |
| 35  | BB    | 769  | U    | O3'-P   | -7.57 | 1.52        | 1.61     |
| 35  | BB    | 1081 | U    | C5'-C4' | 7.57  | 1.60        | 1.51     |
| 1   | AA    | 264  | C    | N3-C4   | 7.57  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1360 | A    | C5'-C4' | 7.57  | 1.60        | 1.51     |
| 35  | BB    | 2    | G    | C2'-C1' | -7.57 | 1.45        | 1.53     |
| 35  | BB    | 197  | A    | N7-C5   | -7.57 | 1.34        | 1.39     |
| 35  | BB    | 926  | G    | N7-C5   | -7.57 | 1.34        | 1.39     |
| 35  | BB    | 1369 | G    | N7-C5   | 7.57  | 1.43        | 1.39     |
| 1   | AA    | 1523 | G    | N1-C2   | 7.57  | 1.43        | 1.37     |
| 35  | BB    | 1973 | G    | P-O5'   | -7.57 | 1.52        | 1.59     |
| 35  | BB    | 2434 | A    | C6-N6   | 7.57  | 1.40        | 1.33     |
| 1   | AA    | 476  | U    | P-O5'   | -7.57 | 1.52        | 1.59     |
| 1   | AA    | 938  | A    | C5-C4   | 7.57  | 1.44        | 1.38     |
| 1   | AA    | 946  | A    | C6-N1   | 7.57  | 1.40        | 1.35     |
| 35  | BB    | 1606 | C    | C4-N4   | 7.57  | 1.40        | 1.33     |
| 35  | BB    | 2847 | U    | C2-N3   | 7.57  | 1.43        | 1.37     |
| 1   | AA    | 46   | G    | N9-C8   | 7.56  | 1.43        | 1.37     |
| 1   | AA    | 1462 | C    | C2'-C1' | -7.56 | 1.45        | 1.53     |
| 35  | BB    | 879  | G    | C2-N3   | 7.56  | 1.38        | 1.32     |
| 35  | BB    | 1181 | U    | N1-C2   | 7.56  | 1.45        | 1.38     |
| 35  | BB    | 1785 | A    | N9-C4   | -7.56 | 1.33        | 1.37     |
| 1   | AA    | 130  | A    | C8-N7   | -7.56 | 1.26        | 1.31     |
| 35  | BB    | 255  | A    | N7-C5   | -7.56 | 1.34        | 1.39     |
| 35  | BB    | 2580 | U    | O3'-P   | -7.56 | 1.52        | 1.61     |
| 1   | AA    | 632  | U    | C2-N3   | 7.56  | 1.43        | 1.37     |
| 1   | AA    | 685  | G    | C2-N3   | 7.56  | 1.38        | 1.32     |
| 35  | BB    | 1455 | G    | N9-C8   | -7.56 | 1.32        | 1.37     |
| 35  | BB    | 1831 | G    | N7-C5   | -7.56 | 1.34        | 1.39     |
| 35  | BB    | 1838 | C    | C4-N4   | 7.56  | 1.40        | 1.33     |
| 35  | BB    | 2213 | U    | C2'-C1' | -7.56 | 1.45        | 1.53     |
| 35  | BB    | 2692 | G    | C2-N3   | 7.56  | 1.38        | 1.32     |
| 1   | AA    | 81   | A    | P-O5'   | -7.56 | 1.52        | 1.59     |
| 1   | AA    | 429  | U    | N1-C6   | 7.55  | 1.44        | 1.38     |
| 1   | AA    | 1098 | C    | N3-C4   | 7.55  | 1.39        | 1.33     |
| 22  | AV    | 72   | G    | C2-N2   | 7.55  | 1.42        | 1.34     |
| 35  | BB    | 575  | A    | N3-C4   | -7.55 | 1.30        | 1.34     |
| 35  | BB    | 1787 | A    | C5-C4   | 7.55  | 1.44        | 1.38     |
| 1   | AA    | 512  | U    | N3-C4   | 7.55  | 1.45        | 1.38     |
| 1   | AA    | 1481 | U    | C5'-C4' | 7.55  | 1.60        | 1.51     |
| 35  | BB    | 342  | A    | O3'-P   | -7.55 | 1.52        | 1.61     |
| 35  | BB    | 2102 | G    | P-O5'   | -7.55 | 1.52        | 1.59     |
| 35  | BB    | 2298 | A    | N3-C4   | -7.55 | 1.30        | 1.34     |
| 35  | BB    | 2311 | A    | C4'-O4' | -7.55 | 1.35        | 1.45     |
| 1   | AA    | 466  | A    | N7-C5   | -7.55 | 1.34        | 1.39     |
| 1   | AA    | 667  | G    | C2'-C1' | -7.55 | 1.45        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 858  | G    | C8-N7   | 7.55  | 1.35        | 1.30     |
| 35  | BB    | 1805 | A    | C8-N7   | -7.55 | 1.26        | 1.31     |
| 35  | BB    | 2357 | G    | N3-C4   | -7.55 | 1.30        | 1.35     |
| 35  | BB    | 408  | G    | C6-N1   | 7.55  | 1.44        | 1.39     |
| 35  | BB    | 259  | G    | N1-C2   | 7.55  | 1.43        | 1.37     |
| 35  | BB    | 663  | G    | N9-C4   | 7.55  | 1.44        | 1.38     |
| 35  | BB    | 1359 | A    | C2'-C1' | -7.55 | 1.45        | 1.53     |
| 35  | BB    | 2744 | G    | C5-C4   | -7.55 | 1.33        | 1.38     |
| 35  | BB    | 2790 | U    | P-O5'   | -7.55 | 1.52        | 1.59     |
| 1   | AA    | 910  | C    | C2'-C1' | -7.54 | 1.45        | 1.53     |
| 35  | BB    | 926  | G    | N9-C8   | 7.54  | 1.43        | 1.37     |
| 1   | AA    | 215  | C    | C4'-C3' | 7.54  | 1.61        | 1.53     |
| 1   | AA    | 349  | A    | N1-C2   | 7.54  | 1.41        | 1.34     |
| 1   | AA    | 1141 | C    | C5'-C4' | 7.54  | 1.60        | 1.51     |
| 22  | AV    | 3    | G    | N9-C4   | 7.54  | 1.44        | 1.38     |
| 35  | BB    | 217  | A    | P-O5'   | -7.54 | 1.52        | 1.59     |
| 35  | BB    | 576  | U    | N3-C4   | 7.54  | 1.45        | 1.38     |
| 35  | BB    | 889  | C    | C5'-C4' | 7.54  | 1.60        | 1.51     |
| 1   | AA    | 164  | G    | N9-C8   | -7.54 | 1.32        | 1.37     |
| 1   | AA    | 664  | G    | C8-N7   | 7.54  | 1.35        | 1.30     |
| 1   | AA    | 803  | G    | C4'-C3' | 7.54  | 1.61        | 1.53     |
| 1   | AA    | 1071 | C    | C5'-C4' | 7.54  | 1.60        | 1.51     |
| 35  | BB    | 813  | U    | N1-C2   | 7.54  | 1.45        | 1.38     |
| 35  | BB    | 118  | A    | C5-C4   | 7.54  | 1.44        | 1.38     |
| 35  | BB    | 730  | A    | C5'-C4' | -7.54 | 1.42        | 1.51     |
| 35  | BB    | 2505 | G    | C2'-C1' | -7.54 | 1.45        | 1.53     |
| 35  | BB    | 2567 | G    | N1-C2   | 7.54  | 1.43        | 1.37     |
| 35  | BB    | 1598 | A    | C5-C4   | 7.54  | 1.44        | 1.38     |
| 35  | BB    | 1935 | G    | N1-C2   | 7.54  | 1.43        | 1.37     |
| 1   | AA    | 771  | G    | C2-N3   | 7.54  | 1.38        | 1.32     |
| 1   | AA    | 1259 | C    | C4-N4   | 7.54  | 1.40        | 1.33     |
| 35  | BB    | 1529 | G    | C2-N2   | 7.54  | 1.42        | 1.34     |
| 35  | BB    | 2059 | A    | N3-C4   | -7.54 | 1.30        | 1.34     |
| 1   | AA    | 813  | U    | C4'-C3' | -7.53 | 1.44        | 1.53     |
| 35  | BB    | 878  | A    | C6-N6   | 7.53  | 1.40        | 1.33     |
| 35  | BB    | 1844 | C    | C4-C5   | 7.53  | 1.49        | 1.43     |
| 35  | BB    | 2765 | A    | N7-C5   | -7.53 | 1.34        | 1.39     |
| 1   | AA    | 39   | G    | N1-C2   | 7.53  | 1.43        | 1.37     |
| 34  | BA    | 42   | C    | O4'-C1' | 7.53  | 1.51        | 1.41     |
| 35  | BB    | 2895 | G    | C5-C4   | 7.53  | 1.43        | 1.38     |
| 1   | AA    | 670  | G    | C6-N1   | 7.53  | 1.44        | 1.39     |
| 35  | BB    | 657  | U    | N3-C4   | 7.53  | 1.45        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2528 | U    | C5'-C4' | 7.53  | 1.60        | 1.51     |
| 35  | BB    | 1780 | A    | C5'-C4' | 7.53  | 1.60        | 1.51     |
| 35  | BB    | 1930 | G    | C8-N7   | -7.53 | 1.26        | 1.30     |
| 35  | BB    | 2758 | A    | N9-C8   | -7.53 | 1.31        | 1.37     |
| 1   | AA    | 62   | U    | C2'-C1' | -7.53 | 1.45        | 1.53     |
| 1   | AA    | 477  | C    | N3-C4   | 7.53  | 1.39        | 1.33     |
| 35  | BB    | 1024 | G    | C8-N7   | -7.53 | 1.26        | 1.30     |
| 35  | BB    | 476  | G    | N9-C4   | -7.52 | 1.31        | 1.38     |
| 35  | BB    | 1127 | A    | O3'-P   | -7.52 | 1.52        | 1.61     |
| 35  | BB    | 1424 | G    | C8-N7   | -7.52 | 1.26        | 1.30     |
| 35  | BB    | 2660 | A    | C8-N7   | -7.52 | 1.26        | 1.31     |
| 1   | AA    | 551  | U    | P-O5'   | -7.52 | 1.52        | 1.59     |
| 1   | AA    | 979  | C    | P-O5'   | -7.52 | 1.52        | 1.59     |
| 35  | BB    | 472  | A    | N7-C5   | -7.52 | 1.34        | 1.39     |
| 35  | BB    | 920  | A    | C4'-C3' | 7.52  | 1.61        | 1.53     |
| 35  | BB    | 1682 | G    | N9-C8   | 7.52  | 1.43        | 1.37     |
| 1   | AA    | 959  | A    | C6-N6   | 7.52  | 1.40        | 1.33     |
| 35  | BB    | 633  | A    | C5-C4   | 7.52  | 1.44        | 1.38     |
| 35  | BB    | 1179 | G    | C2-N2   | 7.52  | 1.42        | 1.34     |
| 1   | AA    | 1193 | G    | C2-N3   | 7.52  | 1.38        | 1.32     |
| 1   | AA    | 1263 | C    | C2-O2   | -7.52 | 1.17        | 1.24     |
| 35  | BB    | 739  | A    | C2'-C1' | -7.52 | 1.45        | 1.53     |
| 35  | BB    | 1073 | A    | C3'-C2' | 7.52  | 1.61        | 1.52     |
| 35  | BB    | 1198 | U    | C4'-C3' | 7.52  | 1.61        | 1.53     |
| 35  | BB    | 1593 | A    | C8-N7   | 7.52  | 1.36        | 1.31     |
| 35  | BB    | 1727 | C    | C5'-C4' | 7.52  | 1.60        | 1.51     |
| 1   | AA    | 341  | C    | C2-N3   | -7.52 | 1.29        | 1.35     |
| 1   | AA    | 980  | C    | C4'-C3' | -7.52 | 1.44        | 1.53     |
| 1   | AA    | 971  | G    | N7-C5   | -7.51 | 1.34        | 1.39     |
| 35  | BB    | 2840 | C    | C4'-C3' | 7.51  | 1.61        | 1.53     |
| 35  | BB    | 1419 | A    | N9-C8   | -7.51 | 1.31        | 1.37     |
| 35  | BB    | 1649 | G    | N7-C5   | -7.51 | 1.34        | 1.39     |
| 1   | AA    | 205  | A    | C6-N6   | 7.51  | 1.40        | 1.33     |
| 1   | AA    | 903  | G    | N7-C5   | -7.51 | 1.34        | 1.39     |
| 35  | BB    | 953  | G    | P-O5'   | -7.51 | 1.52        | 1.59     |
| 1   | AA    | 594  | U    | C4-O4   | 7.51  | 1.29        | 1.23     |
| 1   | AA    | 1306 | A    | C8-N7   | -7.51 | 1.26        | 1.31     |
| 1   | AA    | 1317 | C    | C2-N3   | 7.51  | 1.41        | 1.35     |
| 35  | BB    | 2416 | C    | C5'-C4' | 7.51  | 1.60        | 1.51     |
| 35  | BB    | 2589 | A    | C6-N6   | 7.51  | 1.40        | 1.33     |
| 1   | AA    | 221  | C    | N1-C6   | 7.51  | 1.41        | 1.37     |
| 1   | AA    | 1213 | A    | N9-C4   | 7.51  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 468  | G    | O3'-P   | -7.51 | 1.52        | 1.61     |
| 1   | AA    | 1521 | C    | N1-C6   | -7.51 | 1.32        | 1.37     |
| 35  | BB    | 76   | C    | N3-C4   | 7.51  | 1.39        | 1.33     |
| 35  | BB    | 1111 | A    | N7-C5   | -7.51 | 1.34        | 1.39     |
| 35  | BB    | 1133 | A    | O5'-C5' | 7.51  | 1.56        | 1.44     |
| 35  | BB    | 1682 | G    | C5-C6   | -7.51 | 1.34        | 1.42     |
| 35  | BB    | 2236 | U    | P-O5'   | 7.51  | 1.67        | 1.59     |
| 35  | BB    | 2300 | C    | N3-C4   | 7.51  | 1.39        | 1.33     |
| 1   | AA    | 1396 | A    | C5'-C4' | 7.50  | 1.60        | 1.51     |
| 35  | BB    | 1394 | U    | C4-C5   | 7.50  | 1.50        | 1.43     |
| 35  | BB    | 2373 | G    | C5-C6   | 7.50  | 1.49        | 1.42     |
| 35  | BB    | 2508 | G    | N7-C5   | -7.50 | 1.34        | 1.39     |
| 1   | AA    | 731  | G    | C5'-C4' | 7.50  | 1.60        | 1.51     |
| 1   | AA    | 1042 | A    | C8-N7   | -7.50 | 1.26        | 1.31     |
| 35  | BB    | 147  | C    | C4-C5   | -7.50 | 1.36        | 1.43     |
| 35  | BB    | 756  | A    | C6-N1   | 7.50  | 1.40        | 1.35     |
| 35  | BB    | 819  | A    | C2'-C1' | -7.50 | 1.45        | 1.53     |
| 35  | BB    | 1750 | G    | P-O5'   | -7.50 | 1.52        | 1.59     |
| 1   | AA    | 649  | A    | N1-C2   | -7.50 | 1.27        | 1.34     |
| 1   | AA    | 784  | A    | C4'-O4' | -7.50 | 1.35        | 1.45     |
| 35  | BB    | 395  | U    | N1-C2   | 7.50  | 1.45        | 1.38     |
| 50  | BQ    | 91   | ARG  | CZ-NH1  | 7.50  | 1.42        | 1.33     |
| 1   | AA    | 298  | A    | C5'-C4' | 7.50  | 1.60        | 1.51     |
| 1   | AA    | 430  | A    | N9-C4   | -7.50 | 1.33        | 1.37     |
| 1   | AA    | 709  | U    | C2'-C1' | -7.50 | 1.45        | 1.53     |
| 35  | BB    | 2511 | U    | C5'-C4' | 7.50  | 1.60        | 1.51     |
| 35  | BB    | 2517 | C    | C4-C5   | 7.50  | 1.49        | 1.43     |
| 35  | BB    | 2623 | G    | N1-C2   | 7.50  | 1.43        | 1.37     |
| 35  | BB    | 500  | G    | C6-N1   | 7.50  | 1.44        | 1.39     |
| 1   | AA    | 1373 | G    | C6-N1   | 7.49  | 1.44        | 1.39     |
| 1   | AA    | 1381 | U    | P-O5'   | -7.49 | 1.52        | 1.59     |
| 35  | BB    | 149  | A    | N9-C4   | -7.49 | 1.33        | 1.37     |
| 35  | BB    | 1451 | C    | N3-C4   | 7.49  | 1.39        | 1.33     |
| 35  | BB    | 1469 | A    | N1-C2   | 7.49  | 1.41        | 1.34     |
| 35  | BB    | 1552 | A    | C5-C4   | 7.49  | 1.44        | 1.38     |
| 1   | AA    | 27   | G    | C6-N1   | 7.49  | 1.44        | 1.39     |
| 1   | AA    | 1403 | C    | C4-C5   | 7.49  | 1.49        | 1.43     |
| 1   | AA    | 431  | A    | N7-C5   | -7.49 | 1.34        | 1.39     |
| 1   | AA    | 765  | G    | C2'-C1' | -7.49 | 1.45        | 1.53     |
| 1   | AA    | 1348 | U    | C2-N3   | 7.49  | 1.43        | 1.37     |
| 35  | BB    | 340  | A    | N7-C5   | -7.49 | 1.34        | 1.39     |
| 35  | BB    | 1971 | U    | C5'-C4' | 7.49  | 1.60        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 550  | G    | N1-C2   | 7.49  | 1.43        | 1.37     |
| 1   | AA    | 1251 | A    | C5-C4   | -7.49 | 1.33        | 1.38     |
| 35  | BB    | 203  | A    | C2'-C1' | -7.49 | 1.45        | 1.53     |
| 35  | BB    | 1006 | C    | C2-N3   | 7.49  | 1.41        | 1.35     |
| 35  | BB    | 1055 | G    | C5'-C4' | 7.49  | 1.60        | 1.51     |
| 35  | BB    | 1134 | A    | C3'-C2' | 7.49  | 1.61        | 1.52     |
| 35  | BB    | 1431 | A    | C2-N3   | 7.49  | 1.40        | 1.33     |
| 35  | BB    | 2549 | G    | N7-C5   | -7.49 | 1.34        | 1.39     |
| 35  | BB    | 2761 | A    | P-O5'   | -7.49 | 1.52        | 1.59     |
| 35  | BB    | 1323 | C    | P-O5'   | -7.49 | 1.52        | 1.59     |
| 35  | BB    | 2713 | U    | O3'-P   | -7.49 | 1.52        | 1.61     |
| 1   | AA    | 6    | G    | N1-C2   | 7.49  | 1.43        | 1.37     |
| 1   | AA    | 793  | U    | C2-N3   | 7.49  | 1.43        | 1.37     |
| 1   | AA    | 1398 | A    | N9-C4   | 7.49  | 1.42        | 1.37     |
| 35  | BB    | 1354 | A    | N3-C4   | 7.49  | 1.39        | 1.34     |
| 35  | BB    | 1378 | A    | C6-N1   | 7.49  | 1.40        | 1.35     |
| 35  | BB    | 2758 | A    | N3-C4   | -7.49 | 1.30        | 1.34     |
| 1   | AA    | 861  | G    | N9-C4   | -7.48 | 1.31        | 1.38     |
| 1   | AA    | 1093 | A    | C5-C4   | -7.48 | 1.33        | 1.38     |
| 35  | BB    | 1914 | C    | N1-C6   | 7.48  | 1.41        | 1.37     |
| 35  | BB    | 2538 | C    | C4'-C3' | 7.48  | 1.61        | 1.53     |
| 1   | AA    | 394  | G    | C8-N7   | -7.48 | 1.26        | 1.30     |
| 1   | AA    | 1424 | U    | P-O5'   | -7.48 | 1.52        | 1.59     |
| 35  | BB    | 580  | U    | C4'-C3' | 7.48  | 1.61        | 1.53     |
| 1   | AA    | 517  | G    | N7-C5   | -7.48 | 1.34        | 1.39     |
| 1   | AA    | 557  | G    | C4'-C3' | -7.48 | 1.45        | 1.53     |
| 1   | AA    | 646  | G    | C2'-C1' | -7.48 | 1.45        | 1.53     |
| 35  | BB    | 219  | A    | C5'-C4' | 7.48  | 1.60        | 1.51     |
| 35  | BB    | 385  | C    | C4-C5   | 7.48  | 1.49        | 1.43     |
| 1   | AA    | 1444 | U    | C2'-C1' | -7.48 | 1.45        | 1.53     |
| 35  | BB    | 882  | G    | N1-C2   | 7.48  | 1.43        | 1.37     |
| 35  | BB    | 1034 | G    | C5'-C4' | 7.48  | 1.60        | 1.51     |
| 35  | BB    | 1557 | C    | C5-C6   | 7.48  | 1.40        | 1.34     |
| 35  | BB    | 1930 | G    | C4'-C3' | 7.48  | 1.61        | 1.53     |
| 35  | BB    | 1970 | A    | N1-C2   | 7.48  | 1.41        | 1.34     |
| 35  | BB    | 2895 | G    | C5-C6   | -7.48 | 1.34        | 1.42     |
| 1   | AA    | 1329 | A    | N3-C4   | -7.48 | 1.30        | 1.34     |
| 35  | BB    | 1269 | A    | C2'-C1' | -7.48 | 1.45        | 1.53     |
| 1   | AA    | 461  | A    | C4'-C3' | 7.47  | 1.61        | 1.53     |
| 1   | AA    | 823  | C    | C4'-O4' | 7.47  | 1.55        | 1.45     |
| 35  | BB    | 1268 | A    | N3-C4   | 7.47  | 1.39        | 1.34     |
| 35  | BB    | 1430 | G    | N1-C2   | 7.47  | 1.43        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1444 | G    | C5'-C4' | 7.47  | 1.60        | 1.51     |
| 1   | AA    | 589  | U    | P-O5'   | -7.47 | 1.52        | 1.59     |
| 35  | BB    | 1489 | C    | C4-N4   | 7.47  | 1.40        | 1.33     |
| 35  | BB    | 1171 | G    | N3-C4   | 7.47  | 1.40        | 1.35     |
| 35  | BB    | 2703 | C    | N3-C4   | 7.47  | 1.39        | 1.33     |
| 1   | AA    | 529  | G    | C2-N3   | 7.47  | 1.38        | 1.32     |
| 1   | AA    | 1534 | A    | C5-C4   | 7.47  | 1.44        | 1.38     |
| 35  | BB    | 370  | G    | C2-N3   | 7.47  | 1.38        | 1.32     |
| 35  | BB    | 321  | U    | C4'-O4' | -7.47 | 1.35        | 1.45     |
| 35  | BB    | 591  | U    | N1-C6   | 7.47  | 1.44        | 1.38     |
| 35  | BB    | 1445 | G    | C8-N7   | -7.47 | 1.26        | 1.30     |
| 1   | AA    | 309  | A    | C3'-C2' | -7.46 | 1.44        | 1.52     |
| 1   | AA    | 469  | C    | N3-C4   | 7.46  | 1.39        | 1.33     |
| 35  | BB    | 859  | G    | N3-C4   | 7.46  | 1.40        | 1.35     |
| 35  | BB    | 2108 | A    | N3-C4   | 7.46  | 1.39        | 1.34     |
| 35  | BB    | 2439 | A    | C6-N6   | 7.46  | 1.40        | 1.33     |
| 1   | AA    | 581  | G    | N3-C4   | -7.46 | 1.30        | 1.35     |
| 35  | BB    | 2560 | A    | N3-C4   | -7.46 | 1.30        | 1.34     |
| 1   | AA    | 849  | G    | N7-C5   | -7.46 | 1.34        | 1.39     |
| 1   | AA    | 1000 | A    | N9-C8   | -7.46 | 1.31        | 1.37     |
| 1   | AA    | 1053 | G    | C2'-C1' | -7.46 | 1.45        | 1.53     |
| 1   | AA    | 1455 | G    | N9-C8   | -7.46 | 1.32        | 1.37     |
| 35  | BB    | 341  | C    | N3-C4   | 7.46  | 1.39        | 1.33     |
| 1   | AA    | 865  | A    | C3'-O3' | 7.46  | 1.52        | 1.42     |
| 1   | AA    | 511  | C    | N3-C4   | 7.46  | 1.39        | 1.33     |
| 1   | AA    | 1365 | G    | C4'-O4' | -7.46 | 1.35        | 1.45     |
| 35  | BB    | 1031 | G    | C2'-C1' | -7.46 | 1.45        | 1.53     |
| 35  | BB    | 2364 | C    | P-O5'   | -7.46 | 1.52        | 1.59     |
| 1   | AA    | 465  | A    | C2-N3   | -7.46 | 1.26        | 1.33     |
| 1   | AA    | 946  | A    | C8-N7   | -7.46 | 1.26        | 1.31     |
| 35  | BB    | 323  | C    | N3-C4   | 7.46  | 1.39        | 1.33     |
| 35  | BB    | 809  | G    | C6-N1   | 7.46  | 1.44        | 1.39     |
| 35  | BB    | 2427 | C    | C4-N4   | 7.46  | 1.40        | 1.33     |
| 35  | BB    | 2573 | C    | C4-N4   | 7.46  | 1.40        | 1.33     |
| 1   | AA    | 1430 | A    | C2'-C1' | -7.46 | 1.45        | 1.53     |
| 35  | BB    | 2395 | C    | O3'-P   | -7.46 | 1.52        | 1.61     |
| 1   | AA    | 506  | G    | N7-C5   | -7.45 | 1.34        | 1.39     |
| 1   | AA    | 894  | G    | N1-C2   | 7.45  | 1.43        | 1.37     |
| 35  | BB    | 853  | C    | C5'-C4' | 7.45  | 1.60        | 1.51     |
| 35  | BB    | 2677 | G    | C6-N1   | 7.45  | 1.44        | 1.39     |
| 35  | BB    | 794  | A    | N9-C4   | 7.45  | 1.42        | 1.37     |
| 1   | AA    | 27   | G    | N9-C4   | -7.45 | 1.31        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1480 | A    | N9-C4   | -7.45 | 1.33        | 1.37     |
| 35  | BB    | 1779 | U    | C2-N3   | 7.45  | 1.43        | 1.37     |
| 35  | BB    | 1164 | C    | C5-C6   | 7.45  | 1.40        | 1.34     |
| 35  | BB    | 2072 | C    | P-O5'   | -7.45 | 1.52        | 1.59     |
| 35  | BB    | 2627 | G    | C3'-C2' | -7.45 | 1.44        | 1.52     |
| 1   | AA    | 1111 | A    | C4'-C3' | 7.45  | 1.61        | 1.53     |
| 35  | BB    | 665  | U    | N3-C4   | 7.45  | 1.45        | 1.38     |
| 1   | AA    | 142  | G    | C5'-C4' | 7.45  | 1.60        | 1.51     |
| 35  | BB    | 600  | G    | C5-C6   | -7.45 | 1.34        | 1.42     |
| 1   | AA    | 519  | C    | C4-N4   | 7.44  | 1.40        | 1.33     |
| 1   | AA    | 1514 | G    | C5-C4   | -7.44 | 1.33        | 1.38     |
| 1   | AA    | 1426 | G    | C2-N3   | 7.44  | 1.38        | 1.32     |
| 35  | BB    | 832  | U    | C2-N3   | 7.44  | 1.43        | 1.37     |
| 35  | BB    | 1217 | U    | C5'-C4' | 7.44  | 1.60        | 1.51     |
| 35  | BB    | 2838 | G    | C2-N2   | 7.44  | 1.42        | 1.34     |
| 34  | BA    | 76   | G    | N7-C5   | -7.44 | 1.34        | 1.39     |
| 35  | BB    | 1295 | C    | C4-N4   | 7.44  | 1.40        | 1.33     |
| 35  | BB    | 1157 | G    | N3-C4   | -7.44 | 1.30        | 1.35     |
| 35  | BB    | 1238 | G    | C3'-C2' | 7.44  | 1.61        | 1.52     |
| 35  | BB    | 2138 | G    | N3-C4   | 7.44  | 1.40        | 1.35     |
| 1   | AA    | 705  | G    | C5-C4   | -7.44 | 1.33        | 1.38     |
| 35  | BB    | 274  | C    | N3-C4   | 7.44  | 1.39        | 1.33     |
| 35  | BB    | 2116 | G    | C2-N3   | 7.44  | 1.38        | 1.32     |
| 35  | BB    | 479  | A    | C5-C4   | 7.44  | 1.44        | 1.38     |
| 35  | BB    | 1585 | C    | P-O5'   | -7.44 | 1.52        | 1.59     |
| 35  | BB    | 1942 | C    | N1-C6   | -7.44 | 1.32        | 1.37     |
| 1   | AA    | 332  | G    | N7-C5   | -7.43 | 1.34        | 1.39     |
| 1   | AA    | 505  | G    | C2-N3   | 7.43  | 1.38        | 1.32     |
| 1   | AA    | 1190 | G    | C5-C6   | -7.43 | 1.34        | 1.42     |
| 1   | AA    | 1435 | G    | C2-N2   | 7.43  | 1.42        | 1.34     |
| 35  | BB    | 280  | U    | N1-C6   | 7.43  | 1.44        | 1.38     |
| 35  | BB    | 751  | A    | C8-N7   | -7.43 | 1.26        | 1.31     |
| 35  | BB    | 819  | A    | C8-N7   | -7.43 | 1.26        | 1.31     |
| 35  | BB    | 1284 | A    | N7-C5   | -7.43 | 1.34        | 1.39     |
| 1   | AA    | 542  | G    | N3-C4   | -7.43 | 1.30        | 1.35     |
| 1   | AA    | 830  | G    | N9-C8   | 7.43  | 1.43        | 1.37     |
| 35  | BB    | 649  | G    | C2-N3   | 7.43  | 1.38        | 1.32     |
| 35  | BB    | 211  | C    | P-O5'   | -7.43 | 1.52        | 1.59     |
| 35  | BB    | 925  | A    | C6-N6   | 7.43  | 1.39        | 1.33     |
| 34  | BA    | 18   | G    | N1-C2   | 7.43  | 1.43        | 1.37     |
| 35  | BB    | 396  | G    | C2-N2   | 7.43  | 1.42        | 1.34     |
| 35  | BB    | 532  | A    | O3'-P   | -7.43 | 1.52        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1336 | A    | C2-N3   | 7.43  | 1.40        | 1.33     |
| 35  | BB    | 1687 | G    | P-O5'   | -7.43 | 1.52        | 1.59     |
| 35  | BB    | 2483 | C    | C4-N4   | 7.43  | 1.40        | 1.33     |
| 1   | AA    | 298  | A    | C5-C4   | 7.43  | 1.44        | 1.38     |
| 35  | BB    | 2167 | U    | C4-O4   | -7.43 | 1.17        | 1.23     |
| 35  | BB    | 2464 | G    | N3-C4   | -7.43 | 1.30        | 1.35     |
| 1   | AA    | 300  | A    | C2'-C1' | -7.43 | 1.45        | 1.53     |
| 1   | AA    | 864  | A    | C6-N6   | 7.43  | 1.39        | 1.33     |
| 1   | AA    | 1222 | G    | N1-C2   | 7.43  | 1.43        | 1.37     |
| 35  | BB    | 305  | C    | C4-N4   | 7.43  | 1.40        | 1.33     |
| 35  | BB    | 574  | A    | C5'-C4' | 7.43  | 1.60        | 1.51     |
| 35  | BB    | 1938 | A    | O3'-P   | -7.43 | 1.52        | 1.61     |
| 35  | BB    | 2318 | G    | C4'-C3' | 7.43  | 1.61        | 1.53     |
| 1   | AA    | 1036 | A    | C8-N7   | -7.42 | 1.26        | 1.31     |
| 1   | AA    | 1096 | C    | C4-N4   | 7.42  | 1.40        | 1.33     |
| 35  | BB    | 215  | G    | C2-N3   | 7.42  | 1.38        | 1.32     |
| 35  | BB    | 2776 | A    | N9-C8   | -7.42 | 1.31        | 1.37     |
| 35  | BB    | 2856 | A    | N7-C5   | -7.42 | 1.34        | 1.39     |
| 1   | AA    | 703  | G    | C6-N1   | 7.42  | 1.44        | 1.39     |
| 1   | AA    | 976  | G    | C2-N3   | 7.42  | 1.38        | 1.32     |
| 35  | BB    | 730  | A    | N3-C4   | 7.42  | 1.39        | 1.34     |
| 35  | BB    | 2135 | A    | C3'-C2' | -7.42 | 1.44        | 1.52     |
| 1   | AA    | 1164 | G    | N1-C2   | 7.42  | 1.43        | 1.37     |
| 35  | BB    | 1644 | C    | C4-C5   | -7.42 | 1.37        | 1.43     |
| 35  | BB    | 2326 | C    | C4-N4   | 7.42  | 1.40        | 1.33     |
| 35  | BB    | 2823 | A    | C8-N7   | -7.42 | 1.26        | 1.31     |
| 35  | BB    | 173  | A    | C5'-C4' | 7.42  | 1.60        | 1.51     |
| 35  | BB    | 1279 | G    | C2-N3   | 7.42  | 1.38        | 1.32     |
| 1   | AA    | 419  | C    | N1-C6   | 7.42  | 1.41        | 1.37     |
| 1   | AA    | 911  | U    | P-O5'   | -7.42 | 1.52        | 1.59     |
| 35  | BB    | 1471 | G    | C8-N7   | -7.42 | 1.26        | 1.30     |
| 35  | BB    | 1877 | A    | N3-C4   | -7.42 | 1.30        | 1.34     |
| 1   | AA    | 79   | G    | N7-C5   | -7.42 | 1.34        | 1.39     |
| 1   | AA    | 777  | A    | C5-C4   | 7.42  | 1.44        | 1.38     |
| 35  | BB    | 188  | G    | N9-C8   | -7.42 | 1.32        | 1.37     |
| 35  | BB    | 973  | A    | N3-C4   | -7.42 | 1.30        | 1.34     |
| 35  | BB    | 1884 | G    | C6-N1   | 7.42  | 1.44        | 1.39     |
| 35  | BB    | 2592 | G    | N1-C2   | 7.42  | 1.43        | 1.37     |
| 35  | BB    | 2821 | A    | N7-C5   | -7.42 | 1.34        | 1.39     |
| 1   | AA    | 920  | U    | C2-N3   | -7.42 | 1.32        | 1.37     |
| 35  | BB    | 1818 | U    | N3-C4   | 7.42  | 1.45        | 1.38     |
| 1   | AA    | 614  | C    | C3'-C2' | 7.41  | 1.61        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 426  | C    | N3-C4   | 7.41  | 1.39        | 1.33     |
| 35  | BB    | 2009 | A    | N3-C4   | -7.41 | 1.30        | 1.34     |
| 35  | BB    | 2213 | U    | C5'-C4' | 7.41  | 1.60        | 1.51     |
| 35  | BB    | 309  | A    | N7-C5   | -7.41 | 1.34        | 1.39     |
| 35  | BB    | 804  | A    | C5'-C4' | 7.41  | 1.60        | 1.51     |
| 1   | AA    | 481  | G    | N9-C8   | -7.41 | 1.32        | 1.37     |
| 1   | AA    | 1044 | A    | O3'-P   | -7.41 | 1.52        | 1.61     |
| 1   | AA    | 1087 | G    | C8-N7   | 7.41  | 1.35        | 1.30     |
| 1   | AA    | 1280 | A    | C5'-C4' | 7.41  | 1.60        | 1.51     |
| 35  | BB    | 480  | A    | N9-C4   | -7.41 | 1.33        | 1.37     |
| 35  | BB    | 1883 | U    | N3-C4   | 7.41  | 1.45        | 1.38     |
| 1   | AA    | 267  | C    | P-O5'   | -7.41 | 1.52        | 1.59     |
| 1   | AA    | 391  | G    | C6-N1   | 7.41  | 1.44        | 1.39     |
| 15  | AO    | 83   | ARG  | NE-CZ   | 7.41  | 1.42        | 1.33     |
| 35  | BB    | 734  | A    | C6-N1   | 7.41  | 1.40        | 1.35     |
| 35  | BB    | 1529 | G    | C5-C4   | -7.41 | 1.33        | 1.38     |
| 35  | BB    | 2427 | C    | C4-C5   | 7.41  | 1.48        | 1.43     |
| 1   | AA    | 465  | A    | C5'-C4' | 7.41  | 1.60        | 1.51     |
| 35  | BB    | 804  | A    | N7-C5   | -7.41 | 1.34        | 1.39     |
| 35  | BB    | 2032 | G    | C2-N2   | 7.41  | 1.42        | 1.34     |
| 35  | BB    | 2445 | G    | C2'-C1' | -7.41 | 1.45        | 1.53     |
| 1   | AA    | 425  | G    | C2'-C1' | -7.41 | 1.45        | 1.53     |
| 1   | AA    | 968  | A    | N7-C5   | -7.41 | 1.34        | 1.39     |
| 35  | BB    | 270  | A    | N9-C4   | -7.41 | 1.33        | 1.37     |
| 35  | BB    | 275  | C    | C4'-C3' | -7.41 | 1.45        | 1.53     |
| 35  | BB    | 661  | A    | C6-N1   | 7.41  | 1.40        | 1.35     |
| 35  | BB    | 1037 | G    | N7-C5   | -7.41 | 1.34        | 1.39     |
| 35  | BB    | 1660 | G    | N7-C5   | -7.41 | 1.34        | 1.39     |
| 35  | BB    | 2235 | G    | N3-C4   | -7.41 | 1.30        | 1.35     |
| 1   | AA    | 530  | G    | N9-C8   | 7.40  | 1.43        | 1.37     |
| 1   | AA    | 965  | U    | C4-C5   | 7.40  | 1.50        | 1.43     |
| 35  | BB    | 877  | A    | N9-C4   | -7.40 | 1.33        | 1.37     |
| 35  | BB    | 1136 | G    | N7-C5   | 7.40  | 1.43        | 1.39     |
| 35  | BB    | 1505 | A    | N9-C4   | 7.40  | 1.42        | 1.37     |
| 35  | BB    | 2446 | G    | N3-C4   | -7.40 | 1.30        | 1.35     |
| 1   | AA    | 994  | A    | O4'-C1' | 7.40  | 1.51        | 1.41     |
| 1   | AA    | 1118 | U    | C4-C5   | 7.40  | 1.50        | 1.43     |
| 1   | AA    | 1469 | C    | C4-C5   | 7.40  | 1.48        | 1.43     |
| 35  | BB    | 192  | C    | C2'-C1' | -7.40 | 1.45        | 1.53     |
| 35  | BB    | 590  | A    | C3'-C2' | 7.40  | 1.61        | 1.52     |
| 35  | BB    | 1535 | A    | C2'-C1' | -7.40 | 1.45        | 1.53     |
| 35  | BB    | 2056 | G    | C6-N1   | 7.40  | 1.44        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2643 | G    | O3'-P   | -7.40 | 1.52        | 1.61     |
| 35  | BB    | 2734 | A    | C5-C4   | -7.40 | 1.33        | 1.38     |
| 35  | BB    | 407  | G    | C8-N7   | -7.40 | 1.26        | 1.30     |
| 35  | BB    | 2351 | G    | C6-N1   | 7.40  | 1.44        | 1.39     |
| 1   | AA    | 825  | A    | C6-N6   | 7.40  | 1.39        | 1.33     |
| 34  | BA    | 22   | U    | P-O5'   | -7.40 | 1.52        | 1.59     |
| 35  | BB    | 308  | G    | C3'-C2' | -7.40 | 1.44        | 1.52     |
| 1   | AA    | 132  | C    | N1-C6   | 7.40  | 1.41        | 1.37     |
| 34  | BA    | 75   | G    | N9-C4   | -7.40 | 1.32        | 1.38     |
| 35  | BB    | 1576 | U    | C5-C6   | 7.40  | 1.40        | 1.34     |
| 35  | BB    | 2245 | U    | O4'-C1' | -7.40 | 1.32        | 1.41     |
| 35  | BB    | 2319 | G    | N9-C8   | 7.40  | 1.43        | 1.37     |
| 35  | BB    | 2458 | G    | N1-C2   | 7.40  | 1.43        | 1.37     |
| 35  | BB    | 2902 | C    | C2'-C1' | -7.40 | 1.45        | 1.53     |
| 1   | AA    | 1068 | G    | N1-C2   | 7.40  | 1.43        | 1.37     |
| 1   | AA    | 1473 | G    | C6-N1   | 7.40  | 1.44        | 1.39     |
| 34  | BA    | 71   | C    | C2-N3   | 7.40  | 1.41        | 1.35     |
| 35  | BB    | 531  | C    | C2'-C1' | -7.40 | 1.45        | 1.53     |
| 35  | BB    | 2082 | A    | C2'-C1' | -7.40 | 1.45        | 1.53     |
| 35  | BB    | 2135 | A    | N7-C5   | -7.40 | 1.34        | 1.39     |
| 35  | BB    | 2893 | A    | C2-N3   | 7.40  | 1.40        | 1.33     |
| 35  | BB    | 113  | U    | C2-N3   | 7.39  | 1.43        | 1.37     |
| 35  | BB    | 272  | A    | C6-N6   | 7.39  | 1.39        | 1.33     |
| 35  | BB    | 1456 | G    | C5-C4   | 7.39  | 1.43        | 1.38     |
| 1   | AA    | 77   | A    | C6-N6   | 7.39  | 1.39        | 1.33     |
| 35  | BB    | 1070 | A    | N3-C4   | -7.39 | 1.30        | 1.34     |
| 35  | BB    | 2635 | A    | N7-C5   | 7.39  | 1.43        | 1.39     |
| 1   | AA    | 33   | A    | C6-N6   | 7.39  | 1.39        | 1.33     |
| 1   | AA    | 551  | U    | N3-C4   | 7.39  | 1.45        | 1.38     |
| 1   | AA    | 1111 | A    | C6-N1   | 7.39  | 1.40        | 1.35     |
| 1   | AA    | 1285 | A    | N1-C2   | 7.39  | 1.41        | 1.34     |
| 1   | AA    | 621  | A    | C2'-C1' | -7.39 | 1.45        | 1.53     |
| 1   | AA    | 712  | A    | N1-C2   | 7.39  | 1.41        | 1.34     |
| 35  | BB    | 67   | U    | P-O5'   | -7.39 | 1.52        | 1.59     |
| 35  | BB    | 1141 | U    | C2-N3   | 7.39  | 1.43        | 1.37     |
| 35  | BB    | 1975 | G    | N9-C8   | 7.39  | 1.43        | 1.37     |
| 35  | BB    | 364  | C    | N3-C4   | 7.39  | 1.39        | 1.33     |
| 35  | BB    | 2412 | A    | N3-C4   | 7.39  | 1.39        | 1.34     |
| 35  | BB    | 2444 | G    | N1-C2   | -7.39 | 1.31        | 1.37     |
| 35  | BB    | 529  | A    | N7-C5   | -7.39 | 1.34        | 1.39     |
| 35  | BB    | 1496 | A    | N9-C8   | 7.39  | 1.43        | 1.37     |
| 35  | BB    | 2027 | G    | C8-N7   | 7.39  | 1.35        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2718 | G    | C5-C4   | 7.39  | 1.43        | 1.38     |
| 1   | AA    | 1181 | G    | N7-C5   | -7.38 | 1.34        | 1.39     |
| 16  | AP    | 77   | GLU  | CG-CD   | 7.38  | 1.63        | 1.51     |
| 35  | BB    | 159  | G    | C2-N3   | 7.38  | 1.38        | 1.32     |
| 35  | BB    | 261  | G    | N9-C8   | 7.38  | 1.43        | 1.37     |
| 35  | BB    | 1030 | C    | N1-C6   | 7.38  | 1.41        | 1.37     |
| 35  | BB    | 2327 | A    | C3'-C2' | 7.38  | 1.61        | 1.52     |
| 1   | AA    | 1494 | G    | C5-C4   | 7.38  | 1.43        | 1.38     |
| 35  | BB    | 125  | A    | C4'-O4' | 7.38  | 1.55        | 1.45     |
| 35  | BB    | 293  | U    | N3-C4   | 7.38  | 1.45        | 1.38     |
| 35  | BB    | 2073 | C    | C4-N4   | 7.38  | 1.40        | 1.33     |
| 1   | AA    | 7    | A    | C5-C4   | -7.38 | 1.33        | 1.38     |
| 1   | AA    | 1510 | C    | N1-C6   | 7.38  | 1.41        | 1.37     |
| 35  | BB    | 2226 | C    | C4'-C3' | 7.38  | 1.61        | 1.53     |
| 35  | BB    | 2751 | G    | N1-C2   | 7.38  | 1.43        | 1.37     |
| 35  | BB    | 2863 | C    | C2'-C1' | -7.38 | 1.45        | 1.53     |
| 1   | AA    | 34   | C    | C4-N4   | 7.38  | 1.40        | 1.33     |
| 1   | AA    | 1099 | G    | C2'-C1' | -7.38 | 1.45        | 1.53     |
| 1   | AA    | 1302 | C    | C4-C5   | 7.38  | 1.48        | 1.43     |
| 35  | BB    | 2407 | A    | C5-C4   | 7.38  | 1.44        | 1.38     |
| 35  | BB    | 2601 | C    | N1-C2   | 7.38  | 1.47        | 1.40     |
| 34  | BA    | 46   | A    | N3-C4   | 7.38  | 1.39        | 1.34     |
| 35  | BB    | 1724 | G    | C8-N7   | 7.38  | 1.35        | 1.30     |
| 35  | BB    | 1928 | A    | C2'-C1' | -7.38 | 1.45        | 1.53     |
| 35  | BB    | 2836 | U    | P-O5'   | -7.38 | 1.52        | 1.59     |
| 1   | AA    | 213  | G    | N1-C2   | 7.38  | 1.43        | 1.37     |
| 1   | AA    | 391  | G    | C8-N7   | -7.38 | 1.26        | 1.30     |
| 35  | BB    | 1601 | G    | N1-C2   | 7.38  | 1.43        | 1.37     |
| 35  | BB    | 2188 | U    | N3-C4   | 7.38  | 1.45        | 1.38     |
| 35  | BB    | 2702 | G    | C4'-C3' | -7.38 | 1.45        | 1.53     |
| 1   | AA    | 176  | C    | N3-C4   | 7.37  | 1.39        | 1.33     |
| 1   | AA    | 592  | G    | C2'-C1' | -7.37 | 1.45        | 1.53     |
| 1   | AA    | 640  | A    | N9-C4   | 7.37  | 1.42        | 1.37     |
| 1   | AA    | 1505 | G    | C5-C6   | 7.37  | 1.49        | 1.42     |
| 35  | BB    | 623  | C    | N3-C4   | 7.37  | 1.39        | 1.33     |
| 35  | BB    | 1781 | U    | C2-N3   | 7.37  | 1.43        | 1.37     |
| 1   | AA    | 209  | U    | C4'-O4' | -7.37 | 1.35        | 1.45     |
| 1   | AA    | 272  | C    | N3-C4   | 7.37  | 1.39        | 1.33     |
| 1   | AA    | 371  | A    | N7-C5   | -7.37 | 1.34        | 1.39     |
| 1   | AA    | 1082 | A    | C8-N7   | -7.37 | 1.26        | 1.31     |
| 1   | AA    | 1086 | U    | C2'-C1' | -7.37 | 1.45        | 1.53     |
| 35  | BB    | 1423 | G    | N3-C4   | -7.37 | 1.30        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 49   | U    | C4'-C3' | 7.37  | 1.61        | 1.53     |
| 1   | AA    | 297  | G    | C5-C4   | -7.37 | 1.33        | 1.38     |
| 35  | BB    | 148  | U    | N3-C4   | 7.37  | 1.45        | 1.38     |
| 22  | AV    | 33   | U    | C4'-C3' | 7.37  | 1.61        | 1.53     |
| 35  | BB    | 6    | A    | N1-C2   | 7.37  | 1.41        | 1.34     |
| 35  | BB    | 916  | G    | C5-C6   | -7.37 | 1.34        | 1.42     |
| 35  | BB    | 1906 | G    | N3-C4   | -7.37 | 1.30        | 1.35     |
| 35  | BB    | 1938 | A    | C6-N1   | 7.37  | 1.40        | 1.35     |
| 35  | BB    | 2895 | G    | C2-N2   | 7.37  | 1.42        | 1.34     |
| 1   | AA    | 1373 | G    | N7-C5   | -7.37 | 1.34        | 1.39     |
| 1   | AA    | 204  | G    | N1-C2   | 7.37  | 1.43        | 1.37     |
| 1   | AA    | 356  | A    | C6-N1   | 7.37  | 1.40        | 1.35     |
| 1   | AA    | 830  | G    | C2-N3   | 7.37  | 1.38        | 1.32     |
| 1   | AA    | 1373 | G    | C2-N3   | 7.37  | 1.38        | 1.32     |
| 35  | BB    | 752  | A    | C6-N1   | 7.37  | 1.40        | 1.35     |
| 35  | BB    | 844  | A    | N1-C2   | 7.37  | 1.41        | 1.34     |
| 35  | BB    | 1002 | G    | C5'-C4' | 7.37  | 1.60        | 1.51     |
| 35  | BB    | 2021 | C    | N1-C6   | 7.37  | 1.41        | 1.37     |
| 35  | BB    | 2077 | A    | N1-C2   | 7.37  | 1.41        | 1.34     |
| 35  | BB    | 2294 | G    | C5'-C4' | 7.37  | 1.60        | 1.51     |
| 1   | AA    | 881  | G    | C6-N1   | 7.36  | 1.44        | 1.39     |
| 11  | AK    | 127  | ARG  | CD-NE   | 7.36  | 1.58        | 1.46     |
| 35  | BB    | 504  | A    | C5-C4   | 7.36  | 1.44        | 1.38     |
| 35  | BB    | 2217 | G    | P-O5'   | 7.36  | 1.67        | 1.59     |
| 35  | BB    | 2502 | G    | C2-N3   | 7.36  | 1.38        | 1.32     |
| 35  | BB    | 2850 | A    | C2'-C1' | -7.36 | 1.45        | 1.53     |
| 1   | AA    | 39   | G    | C2-N3   | 7.36  | 1.38        | 1.32     |
| 1   | AA    | 704  | A    | N7-C5   | -7.36 | 1.34        | 1.39     |
| 35  | BB    | 597  | G    | C5-C4   | -7.36 | 1.33        | 1.38     |
| 35  | BB    | 616  | A    | N9-C4   | 7.36  | 1.42        | 1.37     |
| 35  | BB    | 1118 | C    | N1-C6   | 7.36  | 1.41        | 1.37     |
| 35  | BB    | 1156 | A    | C3'-C2' | -7.36 | 1.44        | 1.52     |
| 35  | BB    | 1233 | C    | C4-C5   | -7.36 | 1.37        | 1.43     |
| 35  | BB    | 1675 | C    | C5-C6   | 7.36  | 1.40        | 1.34     |
| 35  | BB    | 108  | G    | N7-C5   | -7.36 | 1.34        | 1.39     |
| 35  | BB    | 562  | U    | O3'-P   | -7.36 | 1.52        | 1.61     |
| 35  | BB    | 836  | G    | C5-C4   | 7.36  | 1.43        | 1.38     |
| 35  | BB    | 1035 | U    | C2'-C1' | -7.36 | 1.45        | 1.53     |
| 35  | BB    | 2370 | G    | C2-N3   | 7.36  | 1.38        | 1.32     |
| 35  | BB    | 2448 | A    | N7-C5   | -7.36 | 1.34        | 1.39     |
| 1   | AA    | 127  | G    | C8-N7   | -7.36 | 1.26        | 1.30     |
| 1   | AA    | 134  | G    | C2-N3   | 7.36  | 1.38        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 162  | A    | C6-N6   | 7.36  | 1.39        | 1.33     |
| 34  | BA    | 57   | A    | N7-C5   | -7.36 | 1.34        | 1.39     |
| 35  | BB    | 1541 | C    | C2-N3   | 7.36  | 1.41        | 1.35     |
| 35  | BB    | 1954 | G    | C2-N3   | 7.36  | 1.38        | 1.32     |
| 1   | AA    | 1389 | C    | C4'-C3' | 7.35  | 1.61        | 1.53     |
| 1   | AA    | 1515 | G    | N7-C5   | -7.35 | 1.34        | 1.39     |
| 35  | BB    | 1149 | G    | P-O5'   | -7.35 | 1.52        | 1.59     |
| 1   | AA    | 180  | U    | C2-N3   | 7.35  | 1.42        | 1.37     |
| 35  | BB    | 630  | G    | N7-C5   | -7.35 | 1.34        | 1.39     |
| 35  | BB    | 940  | G    | N1-C2   | 7.35  | 1.43        | 1.37     |
| 35  | BB    | 1267 | U    | C4'-C3' | 7.35  | 1.61        | 1.53     |
| 1   | AA    | 228  | A    | C6-N6   | 7.35  | 1.39        | 1.33     |
| 1   | AA    | 320  | A    | P-O5'   | -7.35 | 1.52        | 1.59     |
| 1   | AA    | 770  | C    | C4'-O4' | 7.35  | 1.55        | 1.45     |
| 1   | AA    | 1344 | C    | P-O5'   | -7.35 | 1.52        | 1.59     |
| 35  | BB    | 567  | U    | C4'-O4' | -7.35 | 1.35        | 1.45     |
| 35  | BB    | 2519 | U    | C5'-C4' | 7.35  | 1.60        | 1.51     |
| 1   | AA    | 255  | G    | C2'-C1' | -7.35 | 1.45        | 1.53     |
| 1   | AA    | 887  | G    | C5'-C4' | 7.35  | 1.60        | 1.51     |
| 1   | AA    | 1496 | C    | O4'-C1' | -7.35 | 1.32        | 1.41     |
| 35  | BB    | 738  | G    | N9-C4   | -7.35 | 1.32        | 1.38     |
| 35  | BB    | 2087 | G    | C6-N1   | 7.35  | 1.44        | 1.39     |
| 1   | AA    | 493  | A    | N9-C4   | 7.35  | 1.42        | 1.37     |
| 35  | BB    | 2588 | G    | C2-N3   | 7.35  | 1.38        | 1.32     |
| 1   | AA    | 1019 | A    | N3-C4   | -7.35 | 1.30        | 1.34     |
| 35  | BB    | 1815 | A    | O4'-C1' | -7.35 | 1.32        | 1.41     |
| 35  | BB    | 2503 | A    | N9-C8   | -7.35 | 1.31        | 1.37     |
| 1   | AA    | 350  | G    | N1-C2   | 7.34  | 1.43        | 1.37     |
| 1   | AA    | 1494 | G    | N1-C2   | 7.34  | 1.43        | 1.37     |
| 12  | AL    | 53   | ARG  | CZ-NH2  | 7.34  | 1.42        | 1.33     |
| 35  | BB    | 277  | G    | N3-C4   | 7.34  | 1.40        | 1.35     |
| 35  | BB    | 560  | C    | C4-C5   | -7.34 | 1.37        | 1.43     |
| 35  | BB    | 2613 | U    | C3'-C2' | -7.34 | 1.44        | 1.52     |
| 35  | BB    | 2858 | C    | C5'-C4' | 7.34  | 1.60        | 1.51     |
| 1   | AA    | 189  | A    | N9-C8   | 7.34  | 1.43        | 1.37     |
| 1   | AA    | 718  | A    | N9-C4   | -7.34 | 1.33        | 1.37     |
| 1   | AA    | 944  | G    | C5'-C4' | 7.34  | 1.60        | 1.51     |
| 35  | BB    | 779  | U    | C5'-C4' | 7.34  | 1.60        | 1.51     |
| 1   | AA    | 974  | A    | C6-N6   | 7.34  | 1.39        | 1.33     |
| 35  | BB    | 1513 | U    | N3-C4   | 7.34  | 1.45        | 1.38     |
| 35  | BB    | 1731 | G    | N1-C2   | 7.34  | 1.43        | 1.37     |
| 35  | BB    | 2358 | A    | C5'-C4' | 7.34  | 1.60        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2594 | C    | N1-C6   | -7.34 | 1.32        | 1.37     |
| 1   | AA    | 457  | G    | N9-C4   | 7.34  | 1.43        | 1.38     |
| 1   | AA    | 1080 | A    | N7-C5   | -7.34 | 1.34        | 1.39     |
| 1   | AA    | 1365 | G    | N9-C8   | 7.34  | 1.43        | 1.37     |
| 35  | BB    | 1768 | C    | C2-O2   | 7.34  | 1.31        | 1.24     |
| 26  | B1    | 47   | ARG  | CZ-NH2  | 7.33  | 1.42        | 1.33     |
| 35  | BB    | 1621 | U    | C4-O4   | 7.33  | 1.29        | 1.23     |
| 1   | AA    | 468  | A    | C6-N1   | -7.33 | 1.30        | 1.35     |
| 1   | AA    | 1048 | G    | N1-C2   | 7.33  | 1.43        | 1.37     |
| 35  | BB    | 507  | A    | C2'-C1' | -7.33 | 1.45        | 1.53     |
| 35  | BB    | 561  | G    | C2-N2   | 7.33  | 1.41        | 1.34     |
| 35  | BB    | 1080 | A    | C5-C4   | 7.33  | 1.43        | 1.38     |
| 35  | BB    | 1252 | G    | N1-C2   | 7.33  | 1.43        | 1.37     |
| 35  | BB    | 1314 | C    | C4'-C3' | -7.33 | 1.45        | 1.53     |
| 35  | BB    | 1695 | G    | C6-N1   | 7.33  | 1.44        | 1.39     |
| 35  | BB    | 2235 | G    | N7-C5   | 7.33  | 1.43        | 1.39     |
| 35  | BB    | 2471 | A    | C4'-C3' | 7.33  | 1.61        | 1.53     |
| 1   | AA    | 1138 | G    | C8-N7   | 7.33  | 1.35        | 1.30     |
| 35  | BB    | 1984 | G    | N1-C2   | 7.33  | 1.43        | 1.37     |
| 35  | BB    | 2679 | A    | C5-C6   | -7.33 | 1.34        | 1.41     |
| 1   | AA    | 194  | C    | C4'-C3' | 7.33  | 1.61        | 1.53     |
| 1   | AA    | 941  | G    | C8-N7   | 7.33  | 1.35        | 1.30     |
| 1   | AA    | 1506 | U    | C4'-C3' | 7.33  | 1.61        | 1.53     |
| 35  | BB    | 2364 | C    | C2'-C1' | -7.33 | 1.45        | 1.53     |
| 35  | BB    | 1249 | U    | C4-O4   | -7.33 | 1.17        | 1.23     |
| 35  | BB    | 1613 | G    | C5'-C4' | 7.33  | 1.60        | 1.51     |
| 35  | BB    | 1751 | U    | N1-C6   | 7.33  | 1.44        | 1.38     |
| 1   | AA    | 417  | G    | N9-C4   | -7.33 | 1.32        | 1.38     |
| 1   | AA    | 455  | G    | O3'-P   | -7.33 | 1.52        | 1.61     |
| 35  | BB    | 2708 | G    | N3-C4   | -7.33 | 1.30        | 1.35     |
| 1   | AA    | 423  | G    | N3-C4   | -7.33 | 1.30        | 1.35     |
| 1   | AA    | 1174 | G    | C5-C4   | -7.33 | 1.33        | 1.38     |
| 17  | AQ    | 13   | SER  | CA-CB   | 7.33  | 1.64        | 1.52     |
| 35  | BB    | 767  | U    | P-O5'   | -7.33 | 1.52        | 1.59     |
| 35  | BB    | 905  | A    | C5-C6   | -7.33 | 1.34        | 1.41     |
| 35  | BB    | 936  | A    | N3-C4   | -7.33 | 1.30        | 1.34     |
| 35  | BB    | 1520 | U    | P-O5'   | -7.33 | 1.52        | 1.59     |
| 35  | BB    | 1549 | A    | C8-N7   | -7.33 | 1.26        | 1.31     |
| 35  | BB    | 1994 | C    | O4'-C1' | -7.33 | 1.32        | 1.41     |
| 35  | BB    | 2211 | A    | C5-C6   | 7.33  | 1.47        | 1.41     |
| 35  | BB    | 2848 | G    | C2-N3   | 7.33  | 1.38        | 1.32     |
| 1   | AA    | 820  | U    | C4-C5   | 7.32  | 1.50        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 855  | G    | C4'-C3' | 7.32  | 1.61        | 1.53     |
| 1   | AA    | 758  | C    | C4-N4   | 7.32  | 1.40        | 1.33     |
| 1   | AA    | 1378 | C    | C4-N4   | 7.32  | 1.40        | 1.33     |
| 35  | BB    | 38   | A    | N9-C4   | 7.32  | 1.42        | 1.37     |
| 35  | BB    | 246  | C    | C4'-C3' | -7.32 | 1.45        | 1.53     |
| 35  | BB    | 1161 | C    | N3-C4   | 7.32  | 1.39        | 1.33     |
| 1   | AA    | 296  | U    | P-O5'   | -7.32 | 1.52        | 1.59     |
| 1   | AA    | 1409 | C    | P-O5'   | 7.32  | 1.67        | 1.59     |
| 34  | BA    | 65   | U    | P-O5'   | -7.32 | 1.52        | 1.59     |
| 35  | BB    | 1444 | G    | N7-C5   | -7.32 | 1.34        | 1.39     |
| 3   | AC    | 87   | ARG  | CD-NE   | 7.32  | 1.58        | 1.46     |
| 35  | BB    | 589  | U    | C2'-O2' | -7.32 | 1.32        | 1.41     |
| 35  | BB    | 2815 | C    | C3'-C2' | 7.32  | 1.61        | 1.52     |
| 35  | BB    | 2487 | G    | N7-C5   | -7.32 | 1.34        | 1.39     |
| 35  | BB    | 2856 | A    | C6-N1   | 7.32  | 1.40        | 1.35     |
| 1   | AA    | 230  | G    | N7-C5   | -7.32 | 1.34        | 1.39     |
| 1   | AA    | 713  | G    | P-O5'   | -7.32 | 1.52        | 1.59     |
| 1   | AA    | 929  | G    | C8-N7   | -7.32 | 1.26        | 1.30     |
| 1   | AA    | 1250 | A    | N9-C4   | 7.32  | 1.42        | 1.37     |
| 35  | BB    | 889  | C    | C2'-C1' | -7.32 | 1.45        | 1.53     |
| 35  | BB    | 2405 | G    | C6-N1   | 7.32  | 1.44        | 1.39     |
| 1   | AA    | 715  | A    | N9-C8   | -7.31 | 1.31        | 1.37     |
| 1   | AA    | 1491 | G    | C2-N3   | 7.31  | 1.38        | 1.32     |
| 35  | BB    | 599  | A    | C2-N3   | 7.31  | 1.40        | 1.33     |
| 35  | BB    | 1421 | G    | C5-C4   | 7.31  | 1.43        | 1.38     |
| 35  | BB    | 1580 | A    | C5-C4   | 7.31  | 1.43        | 1.38     |
| 35  | BB    | 2344 | U    | C2-N3   | 7.31  | 1.42        | 1.37     |
| 35  | BB    | 2372 | U    | C4-C5   | 7.31  | 1.50        | 1.43     |
| 1   | AA    | 140  | U    | C2-N3   | 7.31  | 1.42        | 1.37     |
| 1   | AA    | 383  | A    | C2'-C1' | -7.31 | 1.45        | 1.53     |
| 1   | AA    | 676  | A    | C6-N6   | 7.31  | 1.39        | 1.33     |
| 1   | AA    | 676  | A    | N9-C8   | 7.31  | 1.43        | 1.37     |
| 1   | AA    | 926  | G    | C5-C4   | -7.31 | 1.33        | 1.38     |
| 1   | AA    | 1491 | G    | N7-C5   | -7.31 | 1.34        | 1.39     |
| 35  | BB    | 538  | A    | N3-C4   | -7.31 | 1.30        | 1.34     |
| 1   | AA    | 977  | A    | N9-C4   | -7.31 | 1.33        | 1.37     |
| 1   | AA    | 1019 | A    | C2'-C1' | -7.31 | 1.45        | 1.53     |
| 1   | AA    | 1206 | G    | N7-C5   | 7.31  | 1.43        | 1.39     |
| 1   | AA    | 1330 | U    | C4'-C3' | -7.31 | 1.45        | 1.53     |
| 35  | BB    | 772  | C    | C2-N3   | 7.31  | 1.41        | 1.35     |
| 35  | BB    | 992  | C    | C4-C5   | -7.31 | 1.37        | 1.43     |
| 35  | BB    | 2546 | U    | O3'-P   | -7.31 | 1.52        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 730  | G    | C8-N7   | 7.31  | 1.35        | 1.30     |
| 1   | AA    | 1412 | C    | C3'-C2' | -7.31 | 1.44        | 1.52     |
| 35  | BB    | 914  | G    | N1-C2   | 7.31  | 1.43        | 1.37     |
| 35  | BB    | 2146 | C    | C5'-C4' | 7.31  | 1.60        | 1.51     |
| 35  | BB    | 2168 | G    | N7-C5   | -7.31 | 1.34        | 1.39     |
| 1   | AA    | 586  | C    | N3-C4   | 7.30  | 1.39        | 1.33     |
| 1   | AA    | 661  | G    | C5-C4   | -7.30 | 1.33        | 1.38     |
| 1   | AA    | 1077 | G    | N3-C4   | 7.30  | 1.40        | 1.35     |
| 35  | BB    | 2442 | C    | N1-C6   | 7.30  | 1.41        | 1.37     |
| 1   | AA    | 71   | A    | N9-C4   | 7.30  | 1.42        | 1.37     |
| 35  | BB    | 946  | C    | O3'-P   | -7.30 | 1.52        | 1.61     |
| 35  | BB    | 1331 | G    | C5-C4   | 7.30  | 1.43        | 1.38     |
| 35  | BB    | 147  | C    | C2-N3   | 7.30  | 1.41        | 1.35     |
| 35  | BB    | 2038 | G    | N7-C5   | 7.30  | 1.43        | 1.39     |
| 1   | AA    | 625  | U    | P-O5'   | -7.30 | 1.52        | 1.59     |
| 1   | AA    | 222  | C    | C2'-C1' | -7.30 | 1.45        | 1.53     |
| 1   | AA    | 428  | G    | C2'-C1' | -7.30 | 1.45        | 1.53     |
| 35  | BB    | 129  | C    | C4-N4   | 7.30  | 1.40        | 1.33     |
| 35  | BB    | 625  | G    | C5'-C4' | 7.30  | 1.60        | 1.51     |
| 1   | AA    | 297  | G    | C2-N3   | 7.29  | 1.38        | 1.32     |
| 35  | BB    | 169  | G    | N7-C5   | -7.29 | 1.34        | 1.39     |
| 35  | BB    | 2061 | G    | N9-C8   | -7.29 | 1.32        | 1.37     |
| 35  | BB    | 2442 | C    | C1'-N1  | 7.29  | 1.59        | 1.48     |
| 35  | BB    | 2446 | G    | O3'-P   | -7.29 | 1.52        | 1.61     |
| 1   | AA    | 686  | U    | O3'-P   | -7.29 | 1.52        | 1.61     |
| 34  | BA    | 62   | C    | C4-C5   | -7.29 | 1.37        | 1.43     |
| 35  | BB    | 966  | G    | N1-C2   | 7.29  | 1.43        | 1.37     |
| 35  | BB    | 1038 | G    | C6-N1   | 7.29  | 1.44        | 1.39     |
| 35  | BB    | 1844 | C    | C5-C6   | 7.29  | 1.40        | 1.34     |
| 35  | BB    | 1952 | A    | C5'-C4' | 7.29  | 1.60        | 1.51     |
| 1   | AA    | 954  | G    | C4'-C3' | 7.29  | 1.61        | 1.53     |
| 35  | BB    | 162  | U    | C4'-C3' | 7.29  | 1.61        | 1.53     |
| 35  | BB    | 760  | G    | N9-C8   | 7.29  | 1.43        | 1.37     |
| 1   | AA    | 1310 | G    | N3-C4   | -7.29 | 1.30        | 1.35     |
| 1   | AA    | 10   | A    | N9-C4   | -7.29 | 1.33        | 1.37     |
| 1   | AA    | 60   | A    | C6-N6   | 7.29  | 1.39        | 1.33     |
| 1   | AA    | 151  | A    | P-O5'   | 7.29  | 1.67        | 1.59     |
| 1   | AA    | 338  | A    | N9-C8   | 7.29  | 1.43        | 1.37     |
| 35  | BB    | 1353 | A    | C8-N7   | -7.29 | 1.26        | 1.31     |
| 35  | BB    | 1366 | A    | N1-C2   | 7.29  | 1.41        | 1.34     |
| 35  | BB    | 1564 | C    | C5'-C4' | 7.29  | 1.60        | 1.51     |
| 35  | BB    | 1640 | A    | O3'-P   | -7.29 | 1.52        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1215 | G    | N9-C4   | 7.29  | 1.43        | 1.38     |
| 1   | AA    | 1360 | A    | N7-C5   | -7.29 | 1.34        | 1.39     |
| 35  | BB    | 1877 | A    | C6-N6   | 7.29  | 1.39        | 1.33     |
| 35  | BB    | 1969 | A    | N9-C4   | -7.29 | 1.33        | 1.37     |
| 35  | BB    | 2478 | A    | N9-C8   | 7.29  | 1.43        | 1.37     |
| 1   | AA    | 1425 | U    | C5-C6   | 7.28  | 1.40        | 1.34     |
| 35  | BB    | 822  | G    | P-O5'   | -7.28 | 1.52        | 1.59     |
| 35  | BB    | 919  | U    | N3-C4   | 7.28  | 1.45        | 1.38     |
| 1   | AA    | 1000 | A    | N9-C4   | 7.28  | 1.42        | 1.37     |
| 1   | AA    | 1521 | C    | P-O5'   | -7.28 | 1.52        | 1.59     |
| 35  | BB    | 1491 | G    | C6-N1   | 7.28  | 1.44        | 1.39     |
| 1   | AA    | 253  | A    | N9-C4   | 7.28  | 1.42        | 1.37     |
| 1   | AA    | 305  | G    | N1-C2   | 7.28  | 1.43        | 1.37     |
| 1   | AA    | 607  | A    | C6-N1   | 7.28  | 1.40        | 1.35     |
| 1   | AA    | 1098 | C    | C4'-C3' | 7.28  | 1.61        | 1.53     |
| 1   | AA    | 1223 | C    | P-O5'   | -7.28 | 1.52        | 1.59     |
| 35  | BB    | 1633 | G    | P-O5'   | -7.28 | 1.52        | 1.59     |
| 35  | BB    | 2628 | C    | N1-C6   | -7.28 | 1.32        | 1.37     |
| 1   | AA    | 642  | A    | C5-C4   | -7.28 | 1.33        | 1.38     |
| 1   | AA    | 1399 | C    | N1-C6   | 7.28  | 1.41        | 1.37     |
| 35  | BB    | 842  | U    | N1-C6   | 7.28  | 1.44        | 1.38     |
| 35  | BB    | 1968 | G    | C2-N2   | 7.28  | 1.41        | 1.34     |
| 35  | BB    | 2696 | U    | C2'-C1' | -7.28 | 1.45        | 1.53     |
| 1   | AA    | 157  | U    | N1-C2   | -7.28 | 1.32        | 1.38     |
| 35  | BB    | 793  | A    | C8-N7   | 7.28  | 1.36        | 1.31     |
| 35  | BB    | 1055 | G    | C8-N7   | -7.28 | 1.26        | 1.30     |
| 35  | BB    | 2682 | A    | C8-N7   | -7.28 | 1.26        | 1.31     |
| 1   | AA    | 382  | A    | N9-C4   | -7.28 | 1.33        | 1.37     |
| 35  | BB    | 325  | G    | N9-C4   | -7.28 | 1.32        | 1.38     |
| 1   | AA    | 744  | C    | C4-N4   | 7.27  | 1.40        | 1.33     |
| 35  | BB    | 855  | G    | C3'-C2' | -7.27 | 1.44        | 1.52     |
| 35  | BB    | 2853 | C    | C4-C5   | 7.27  | 1.48        | 1.43     |
| 1   | AA    | 68   | G    | N7-C5   | -7.27 | 1.34        | 1.39     |
| 1   | AA    | 990  | C    | P-O5'   | -7.27 | 1.52        | 1.59     |
| 35  | BB    | 393  | C    | N3-C4   | 7.27  | 1.39        | 1.33     |
| 35  | BB    | 746  | U    | O3'-P   | -7.27 | 1.52        | 1.61     |
| 35  | BB    | 2601 | C    | C4'-C3' | 7.27  | 1.61        | 1.53     |
| 34  | BA    | 74   | U    | N1-C6   | 7.27  | 1.44        | 1.38     |
| 35  | BB    | 354  | A    | N7-C5   | -7.27 | 1.34        | 1.39     |
| 35  | BB    | 458  | G    | N1-C2   | 7.27  | 1.43        | 1.37     |
| 1   | AA    | 843  | U    | C2-N3   | 7.27  | 1.42        | 1.37     |
| 1   | AA    | 1379 | G    | C2-N2   | 7.27  | 1.41        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1167 | C    | N1-C6   | 7.27  | 1.41        | 1.37     |
| 35  | BB    | 2287 | A    | C8-N7   | -7.27 | 1.26        | 1.31     |
| 35  | BB    | 2516 | A    | N9-C4   | 7.27  | 1.42        | 1.37     |
| 1   | AA    | 143  | A    | N3-C4   | -7.27 | 1.30        | 1.34     |
| 1   | AA    | 468  | A    | C8-N7   | -7.27 | 1.26        | 1.31     |
| 35  | BB    | 188  | G    | O3'-P   | -7.27 | 1.52        | 1.61     |
| 35  | BB    | 1192 | G    | N1-C2   | 7.27  | 1.43        | 1.37     |
| 35  | BB    | 1457 | U    | C2-N3   | -7.27 | 1.32        | 1.37     |
| 35  | BB    | 1508 | A    | C5-C6   | -7.27 | 1.34        | 1.41     |
| 1   | AA    | 35   | G    | C2-N2   | 7.27  | 1.41        | 1.34     |
| 1   | AA    | 537  | G    | C2-N3   | 7.27  | 1.38        | 1.32     |
| 1   | AA    | 1243 | C    | C4-N4   | 7.27  | 1.40        | 1.33     |
| 35  | BB    | 705  | A    | C2'-C1' | -7.27 | 1.45        | 1.53     |
| 35  | BB    | 1429 | G    | N7-C5   | -7.27 | 1.34        | 1.39     |
| 1   | AA    | 56   | U    | N3-C4   | 7.26  | 1.45        | 1.38     |
| 1   | AA    | 243  | A    | N1-C2   | 7.26  | 1.40        | 1.34     |
| 1   | AA    | 577  | G    | N9-C8   | -7.26 | 1.32        | 1.37     |
| 1   | AA    | 732  | C    | C2'-C1' | -7.26 | 1.45        | 1.53     |
| 1   | AA    | 993  | G    | C3'-C2' | 7.26  | 1.60        | 1.52     |
| 1   | AA    | 1392 | G    | P-O5'   | -7.26 | 1.52        | 1.59     |
| 35  | BB    | 39   | G    | C5-C4   | 7.26  | 1.43        | 1.38     |
| 35  | BB    | 242  | G    | C2'-C1' | -7.26 | 1.45        | 1.53     |
| 35  | BB    | 505  | A    | C6-N1   | 7.26  | 1.40        | 1.35     |
| 35  | BB    | 645  | C    | C5-C6   | 7.26  | 1.40        | 1.34     |
| 35  | BB    | 639  | U    | P-O5'   | -7.26 | 1.52        | 1.59     |
| 35  | BB    | 2159 | G    | N9-C8   | 7.26  | 1.43        | 1.37     |
| 35  | BB    | 801  | G    | C5-C6   | -7.26 | 1.35        | 1.42     |
| 35  | BB    | 930  | G    | N7-C5   | -7.26 | 1.34        | 1.39     |
| 35  | BB    | 956  | G    | C4'-C3' | 7.26  | 1.61        | 1.53     |
| 35  | BB    | 2473 | U    | C4-C5   | 7.26  | 1.50        | 1.43     |
| 1   | AA    | 847  | G    | C4'-O4' | 7.26  | 1.54        | 1.45     |
| 35  | BB    | 303  | G    | N3-C4   | 7.26  | 1.40        | 1.35     |
| 35  | BB    | 1009 | A    | N7-C5   | -7.26 | 1.34        | 1.39     |
| 35  | BB    | 1453 | A    | C6-N1   | 7.26  | 1.40        | 1.35     |
| 35  | BB    | 1578 | U    | C2'-C1' | -7.26 | 1.45        | 1.53     |
| 35  | BB    | 2150 | C    | C4-C5   | 7.26  | 1.48        | 1.43     |
| 35  | BB    | 2424 | C    | N1-C6   | -7.26 | 1.32        | 1.37     |
| 35  | BB    | 2552 | U    | N3-C4   | 7.26  | 1.45        | 1.38     |
| 35  | BB    | 2603 | G    | C6-N1   | 7.26  | 1.44        | 1.39     |
| 1   | AA    | 170  | U    | C2'-C1' | -7.26 | 1.45        | 1.53     |
| 1   | AA    | 752  | G    | N3-C4   | 7.26  | 1.40        | 1.35     |
| 1   | AA    | 1308 | U    | C4-C5   | 7.26  | 1.50        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 333  | G    | N9-C4   | 7.26  | 1.43        | 1.38     |
| 35  | BB    | 2734 | A    | N3-C4   | -7.26 | 1.30        | 1.34     |
| 1   | AA    | 1475 | G    | P-O5'   | -7.26 | 1.52        | 1.59     |
| 33  | B8    | 27   | CYS  | CB-SG   | 7.26  | 1.94        | 1.82     |
| 35  | BB    | 1250 | G    | N9-C4   | -7.26 | 1.32        | 1.38     |
| 35  | BB    | 2404 | U    | O3'-P   | -7.26 | 1.52        | 1.61     |
| 35  | BB    | 2516 | A    | N3-C4   | -7.26 | 1.30        | 1.34     |
| 35  | BB    | 2811 | G    | N9-C4   | 7.26  | 1.43        | 1.38     |
| 1   | AA    | 1260 | G    | C5-C6   | -7.25 | 1.35        | 1.42     |
| 34  | BA    | 18   | G    | P-O5'   | -7.25 | 1.52        | 1.59     |
| 35  | BB    | 936  | A    | N9-C8   | 7.25  | 1.43        | 1.37     |
| 35  | BB    | 2204 | G    | N9-C8   | -7.25 | 1.32        | 1.37     |
| 1   | AA    | 210  | C    | N3-C4   | 7.25  | 1.39        | 1.33     |
| 1   | AA    | 455  | G    | C6-N1   | 7.25  | 1.44        | 1.39     |
| 1   | AA    | 1005 | A    | N1-C2   | 7.25  | 1.40        | 1.34     |
| 1   | AA    | 1289 | A    | C8-N7   | -7.25 | 1.26        | 1.31     |
| 35  | BB    | 435  | C    | N1-C6   | 7.25  | 1.41        | 1.37     |
| 35  | BB    | 2193 | G    | C2-N3   | 7.25  | 1.38        | 1.32     |
| 35  | BB    | 2883 | A    | N3-C4   | 7.25  | 1.39        | 1.34     |
| 1   | AA    | 1370 | G    | C6-N1   | 7.25  | 1.44        | 1.39     |
| 22  | AV    | 32   | A    | C4'-O4' | -7.25 | 1.36        | 1.45     |
| 35  | BB    | 520  | G    | N1-C2   | 7.25  | 1.43        | 1.37     |
| 35  | BB    | 1164 | C    | N1-C6   | 7.25  | 1.41        | 1.37     |
| 35  | BB    | 1711 | A    | N7-C5   | -7.25 | 1.34        | 1.39     |
| 35  | BB    | 2425 | A    | N7-C5   | -7.25 | 1.34        | 1.39     |
| 35  | BB    | 2273 | A    | C5-C4   | 7.25  | 1.43        | 1.38     |
| 1   | AA    | 1186 | G    | C5-C6   | 7.25  | 1.49        | 1.42     |
| 1   | AA    | 1360 | A    | N9-C8   | 7.25  | 1.43        | 1.37     |
| 35  | BB    | 253  | C    | N3-C4   | 7.25  | 1.39        | 1.33     |
| 35  | BB    | 725  | G    | C6-N1   | 7.25  | 1.44        | 1.39     |
| 35  | BB    | 977  | G    | N3-C4   | -7.25 | 1.30        | 1.35     |
| 35  | BB    | 1608 | A    | C3'-C2' | 7.25  | 1.60        | 1.52     |
| 35  | BB    | 2708 | G    | C2'-C1' | -7.25 | 1.45        | 1.53     |
| 1   | AA    | 905  | U    | C2-N3   | 7.25  | 1.42        | 1.37     |
| 35  | BB    | 1407 | G    | C6-N1   | -7.25 | 1.34        | 1.39     |
| 35  | BB    | 1434 | A    | C4'-C3' | -7.25 | 1.45        | 1.53     |
| 35  | BB    | 2854 | G    | N9-C4   | -7.25 | 1.32        | 1.38     |
| 1   | AA    | 97   | G    | N1-C2   | 7.24  | 1.43        | 1.37     |
| 1   | AA    | 1084 | G    | C6-N1   | 7.24  | 1.44        | 1.39     |
| 35  | BB    | 11   | C    | C4-N4   | 7.24  | 1.40        | 1.33     |
| 35  | BB    | 509  | C    | P-O5'   | -7.24 | 1.52        | 1.59     |
| 35  | BB    | 1634 | A    | N9-C8   | -7.24 | 1.31        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1812 | U    | C2-N3   | 7.24  | 1.42        | 1.37     |
| 35  | BB    | 2575 | C    | O3'-P   | -7.24 | 1.52        | 1.61     |
| 35  | BB    | 2718 | G    | C8-N7   | 7.24  | 1.35        | 1.30     |
| 35  | BB    | 2742 | G    | N1-C2   | 7.24  | 1.43        | 1.37     |
| 1   | AA    | 328  | C    | N1-C6   | -7.24 | 1.32        | 1.37     |
| 11  | AK    | 55   | ARG  | NE-CZ   | 7.24  | 1.42        | 1.33     |
| 35  | BB    | 786  | C    | N3-C4   | 7.24  | 1.39        | 1.33     |
| 35  | BB    | 1560 | G    | C6-N1   | 7.24  | 1.44        | 1.39     |
| 35  | BB    | 71   | A    | C6-N6   | 7.24  | 1.39        | 1.33     |
| 35  | BB    | 1887 | C    | C2'-C1' | -7.24 | 1.45        | 1.53     |
| 1   | AA    | 7    | A    | C6-N6   | 7.24  | 1.39        | 1.33     |
| 1   | AA    | 160  | A    | C6-N1   | 7.24  | 1.40        | 1.35     |
| 1   | AA    | 284  | C    | C4'-O4' | 7.24  | 1.54        | 1.45     |
| 35  | BB    | 1780 | A    | N9-C4   | -7.24 | 1.33        | 1.37     |
| 35  | BB    | 1204 | A    | N9-C4   | 7.24  | 1.42        | 1.37     |
| 35  | BB    | 1772 | A    | C5-C4   | 7.24  | 1.43        | 1.38     |
| 1   | AA    | 222  | C    | C4'-C3' | -7.24 | 1.45        | 1.53     |
| 1   | AA    | 935  | A    | C6-N1   | 7.24  | 1.40        | 1.35     |
| 1   | AA    | 1204 | A    | C5'-C4' | 7.24  | 1.60        | 1.51     |
| 1   | AA    | 1237 | C    | C4-N4   | 7.24  | 1.40        | 1.33     |
| 35  | BB    | 1197 | G    | N9-C4   | -7.24 | 1.32        | 1.38     |
| 35  | BB    | 2341 | G    | N9-C4   | -7.24 | 1.32        | 1.38     |
| 1   | AA    | 750  | C    | C4-N4   | 7.23  | 1.40        | 1.33     |
| 35  | BB    | 1706 | C    | C3'-C2' | -7.23 | 1.44        | 1.52     |
| 35  | BB    | 2810 | A    | N9-C4   | -7.23 | 1.33        | 1.37     |
| 1   | AA    | 71   | A    | C6-N1   | 7.23  | 1.40        | 1.35     |
| 1   | AA    | 452  | A    | C6-N6   | 7.23  | 1.39        | 1.33     |
| 1   | AA    | 1515 | G    | N9-C8   | 7.23  | 1.43        | 1.37     |
| 34  | BA    | 100  | G    | C5-C4   | 7.23  | 1.43        | 1.38     |
| 34  | BA    | 115  | A    | N7-C5   | -7.23 | 1.34        | 1.39     |
| 35  | BB    | 581  | C    | C3'-C2' | 7.23  | 1.60        | 1.52     |
| 35  | BB    | 1739 | A    | C5-C6   | -7.23 | 1.34        | 1.41     |
| 35  | BB    | 2002 | G    | N7-C5   | -7.23 | 1.34        | 1.39     |
| 1   | AA    | 1267 | C    | C4-N4   | 7.23  | 1.40        | 1.33     |
| 35  | BB    | 316  | C    | C4-C5   | -7.23 | 1.37        | 1.43     |
| 35  | BB    | 659  | G    | C2-N3   | 7.23  | 1.38        | 1.32     |
| 1   | AA    | 128  | G    | C5-C4   | -7.23 | 1.33        | 1.38     |
| 35  | BB    | 314  | C    | N3-C4   | 7.23  | 1.39        | 1.33     |
| 35  | BB    | 722  | A    | N9-C4   | 7.23  | 1.42        | 1.37     |
| 1   | AA    | 116  | A    | P-O5'   | -7.23 | 1.52        | 1.59     |
| 1   | AA    | 356  | A    | C8-N7   | -7.23 | 1.26        | 1.31     |
| 1   | AA    | 615  | G    | C2-N3   | 7.23  | 1.38        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 264  | C    | C2-N3   | 7.23  | 1.41        | 1.35     |
| 35  | BB    | 1142 | A    | O3'-P   | -7.23 | 1.52        | 1.61     |
| 1   | AA    | 454  | G    | C2-N3   | 7.23  | 1.38        | 1.32     |
| 1   | AA    | 569  | C    | C4-C5   | 7.23  | 1.48        | 1.43     |
| 35  | BB    | 1003 | G    | N7-C5   | 7.23  | 1.43        | 1.39     |
| 35  | BB    | 2372 | U    | O3'-P   | -7.23 | 1.52        | 1.61     |
| 1   | AA    | 1047 | G    | P-O5'   | -7.22 | 1.52        | 1.59     |
| 35  | BB    | 1617 | C    | C2'-C1' | -7.22 | 1.45        | 1.53     |
| 35  | BB    | 2874 | C    | N3-C4   | 7.22  | 1.39        | 1.33     |
| 1   | AA    | 137  | U    | C2'-C1' | -7.22 | 1.45        | 1.53     |
| 1   | AA    | 716  | A    | N9-C8   | 7.22  | 1.43        | 1.37     |
| 1   | AA    | 785  | G    | N1-C2   | 7.22  | 1.43        | 1.37     |
| 1   | AA    | 1363 | A    | N7-C5   | -7.22 | 1.34        | 1.39     |
| 35  | BB    | 1358 | G    | N7-C5   | -7.22 | 1.34        | 1.39     |
| 35  | BB    | 2251 | G    | C3'-C2' | -7.22 | 1.44        | 1.52     |
| 1   | AA    | 303  | A    | N3-C4   | -7.22 | 1.30        | 1.34     |
| 1   | AA    | 1239 | A    | N7-C5   | -7.22 | 1.34        | 1.39     |
| 1   | AA    | 845  | A    | C2'-C1' | -7.22 | 1.45        | 1.53     |
| 1   | AA    | 1157 | A    | N7-C5   | -7.22 | 1.34        | 1.39     |
| 1   | AA    | 1356 | G    | N7-C5   | -7.22 | 1.34        | 1.39     |
| 35  | BB    | 520  | G    | N9-C8   | 7.22  | 1.43        | 1.37     |
| 35  | BB    | 1131 | G    | N1-C2   | 7.22  | 1.43        | 1.37     |
| 35  | BB    | 1356 | G    | N7-C5   | -7.22 | 1.34        | 1.39     |
| 1   | AA    | 819  | A    | N7-C5   | -7.22 | 1.34        | 1.39     |
| 1   | AA    | 1429 | A    | C6-N1   | 7.22  | 1.40        | 1.35     |
| 34  | BA    | 39   | A    | N9-C8   | 7.22  | 1.43        | 1.37     |
| 35  | BB    | 862  | G    | C3'-C2' | 7.22  | 1.60        | 1.52     |
| 35  | BB    | 513  | A    | C5-C4   | 7.22  | 1.43        | 1.38     |
| 35  | BB    | 1297 | C    | N3-C4   | 7.22  | 1.39        | 1.33     |
| 35  | BB    | 2495 | G    | N7-C5   | -7.22 | 1.34        | 1.39     |
| 34  | BA    | 34   | A    | C6-N1   | 7.21  | 1.40        | 1.35     |
| 35  | BB    | 2345 | G    | C5-C6   | -7.21 | 1.35        | 1.42     |
| 35  | BB    | 1265 | A    | C8-N7   | -7.21 | 1.26        | 1.31     |
| 35  | BB    | 1640 | A    | C6-N1   | 7.21  | 1.40        | 1.35     |
| 35  | BB    | 2035 | G    | N9-C4   | -7.21 | 1.32        | 1.38     |
| 35  | BB    | 2588 | G    | N7-C5   | -7.21 | 1.34        | 1.39     |
| 1   | AA    | 285  | C    | N3-C4   | 7.21  | 1.39        | 1.33     |
| 2   | AB    | 125  | PHE  | CG-CD1  | 7.21  | 1.49        | 1.38     |
| 35  | BB    | 415  | A    | C6-N6   | 7.21  | 1.39        | 1.33     |
| 35  | BB    | 999  | U    | N1-C6   | 7.21  | 1.44        | 1.38     |
| 1   | AA    | 31   | G    | C6-N1   | 7.21  | 1.44        | 1.39     |
| 1   | AA    | 564  | C    | N1-C6   | 7.21  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1287 | A    | N9-C4   | 7.21  | 1.42        | 1.37     |
| 35  | BB    | 959  | A    | C6-N6   | 7.21  | 1.39        | 1.33     |
| 35  | BB    | 1069 | A    | C2'-C1' | -7.21 | 1.45        | 1.53     |
| 35  | BB    | 2462 | C    | C2-N3   | 7.21  | 1.41        | 1.35     |
| 35  | BB    | 2738 | A    | C2'-C1' | -7.21 | 1.45        | 1.53     |
| 1   | AA    | 401  | C    | C3'-C2' | -7.21 | 1.44        | 1.52     |
| 1   | AA    | 670  | G    | C2-N3   | 7.21  | 1.38        | 1.32     |
| 35  | BB    | 2520 | C    | N1-C6   | 7.21  | 1.41        | 1.37     |
| 35  | BB    | 2575 | C    | C4-N4   | 7.21  | 1.40        | 1.33     |
| 1   | AA    | 1327 | C    | C4-N4   | 7.21  | 1.40        | 1.33     |
| 35  | BB    | 970  | U    | C2'-C1' | -7.21 | 1.45        | 1.53     |
| 35  | BB    | 1029 | A    | C6-N1   | 7.21  | 1.40        | 1.35     |
| 35  | BB    | 1680 | U    | C2'-C1' | -7.21 | 1.45        | 1.53     |
| 35  | BB    | 2775 | G    | C2-N2   | -7.21 | 1.27        | 1.34     |
| 35  | BB    | 612  | G    | C6-N1   | 7.21  | 1.44        | 1.39     |
| 35  | BB    | 2811 | G    | N1-C2   | 7.20  | 1.43        | 1.37     |
| 1   | AA    | 1402 | C    | C2'-C1' | -7.20 | 1.45        | 1.53     |
| 35  | BB    | 519  | U    | C2-N3   | 7.20  | 1.42        | 1.37     |
| 35  | BB    | 2835 | A    | N9-C8   | -7.20 | 1.31        | 1.37     |
| 35  | BB    | 215  | G    | N1-C2   | 7.20  | 1.43        | 1.37     |
| 35  | BB    | 364  | C    | C2-N3   | 7.20  | 1.41        | 1.35     |
| 35  | BB    | 695  | G    | C8-N7   | 7.20  | 1.35        | 1.30     |
| 35  | BB    | 987  | C    | N3-C4   | 7.20  | 1.39        | 1.33     |
| 35  | BB    | 1282 | U    | C5'-C4' | 7.20  | 1.59        | 1.51     |
| 35  | BB    | 1556 | C    | O3'-P   | -7.20 | 1.52        | 1.61     |
| 35  | BB    | 1776 | G    | C5'-C4' | 7.20  | 1.59        | 1.51     |
| 35  | BB    | 2055 | C    | O4'-C1' | 7.20  | 1.51        | 1.41     |
| 35  | BB    | 2513 | A    | C5-C4   | -7.20 | 1.33        | 1.38     |
| 34  | BA    | 78   | A    | C6-N1   | 7.20  | 1.40        | 1.35     |
| 35  | BB    | 2340 | A    | P-O5'   | -7.20 | 1.52        | 1.59     |
| 35  | BB    | 676  | A    | N7-C5   | -7.20 | 1.34        | 1.39     |
| 35  | BB    | 1445 | G    | C5-C4   | 7.20  | 1.43        | 1.38     |
| 35  | BB    | 2515 | C    | C4-C5   | -7.20 | 1.37        | 1.43     |
| 1   | AA    | 15   | G    | C6-N1   | 7.19  | 1.44        | 1.39     |
| 1   | AA    | 810  | C    | C4'-C3' | -7.19 | 1.45        | 1.53     |
| 1   | AA    | 1491 | G    | N1-C2   | 7.19  | 1.43        | 1.37     |
| 35  | BB    | 541  | A    | C2-N3   | 7.19  | 1.40        | 1.33     |
| 35  | BB    | 1832 | C    | C4'-O4' | 7.19  | 1.54        | 1.45     |
| 1   | AA    | 696  | A    | C6-N1   | -7.19 | 1.30        | 1.35     |
| 34  | BA    | 100  | G    | C5'-C4' | 7.19  | 1.59        | 1.51     |
| 35  | BB    | 768  | G    | N3-C4   | -7.19 | 1.30        | 1.35     |
| 35  | BB    | 1371 | G    | C2-N2   | 7.19  | 1.41        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1488 | C    | P-O5'   | -7.19 | 1.52        | 1.59     |
| 1   | AA    | 605  | U    | C4'-O4' | -7.19 | 1.36        | 1.45     |
| 35  | BB    | 811  | U    | C5'-C4' | -7.19 | 1.42        | 1.51     |
| 35  | BB    | 1000 | A    | N9-C4   | -7.19 | 1.33        | 1.37     |
| 35  | BB    | 1382 | G    | N7-C5   | -7.19 | 1.34        | 1.39     |
| 35  | BB    | 1850 | G    | C2-N3   | -7.19 | 1.26        | 1.32     |
| 35  | BB    | 1873 | G    | C2'-C1' | -7.19 | 1.45        | 1.53     |
| 1   | AA    | 109  | A    | N7-C5   | -7.19 | 1.34        | 1.39     |
| 1   | AA    | 887  | G    | C8-N7   | 7.19  | 1.35        | 1.30     |
| 35  | BB    | 1599 | U    | N1-C6   | -7.19 | 1.31        | 1.38     |
| 35  | BB    | 1964 | G    | C6-N1   | 7.19  | 1.44        | 1.39     |
| 35  | BB    | 2751 | G    | N3-C4   | 7.19  | 1.40        | 1.35     |
| 1   | AA    | 1040 | U    | C2-N3   | -7.19 | 1.32        | 1.37     |
| 1   | AA    | 1119 | C    | N1-C6   | -7.19 | 1.32        | 1.37     |
| 35  | BB    | 704  | G    | N1-C2   | 7.19  | 1.43        | 1.37     |
| 35  | BB    | 1015 | U    | O3'-P   | -7.19 | 1.52        | 1.61     |
| 35  | BB    | 1891 | G    | N9-C8   | 7.19  | 1.42        | 1.37     |
| 35  | BB    | 2653 | U    | O3'-P   | -7.19 | 1.52        | 1.61     |
| 1   | AA    | 144  | G    | N9-C4   | 7.19  | 1.43        | 1.38     |
| 1   | AA    | 453  | G    | C6-N1   | 7.19  | 1.44        | 1.39     |
| 1   | AA    | 1401 | G    | C2'-C1' | -7.19 | 1.45        | 1.53     |
| 1   | AA    | 1414 | U    | C4-C5   | 7.19  | 1.50        | 1.43     |
| 34  | BA    | 51   | G    | C8-N7   | -7.19 | 1.26        | 1.30     |
| 35  | BB    | 568  | U    | C4'-C3' | -7.19 | 1.45        | 1.53     |
| 35  | BB    | 1059 | G    | C2-N3   | 7.19  | 1.38        | 1.32     |
| 35  | BB    | 1427 | A    | C5-C4   | 7.19  | 1.43        | 1.38     |
| 35  | BB    | 2115 | G    | N7-C5   | -7.19 | 1.34        | 1.39     |
| 45  | BL    | 138  | ALA  | C-N     | 7.19  | 1.46        | 1.33     |
| 1   | AA    | 141  | G    | O3'-P   | -7.18 | 1.52        | 1.61     |
| 34  | BA    | 86   | G    | N1-C2   | 7.18  | 1.43        | 1.37     |
| 35  | BB    | 1449 | G    | N1-C2   | 7.18  | 1.43        | 1.37     |
| 35  | BB    | 2112 | G    | C6-N1   | 7.18  | 1.44        | 1.39     |
| 35  | BB    | 2116 | G    | C5'-C4' | 7.18  | 1.59        | 1.51     |
| 35  | BB    | 2513 | A    | C5'-C4' | -7.18 | 1.42        | 1.51     |
| 35  | BB    | 2731 | G    | C6-N1   | 7.18  | 1.44        | 1.39     |
| 1   | AA    | 165  | G    | C4'-C3' | -7.18 | 1.45        | 1.53     |
| 1   | AA    | 239  | U    | N1-C2   | 7.18  | 1.45        | 1.38     |
| 35  | BB    | 1500 | G    | C8-N7   | -7.18 | 1.26        | 1.30     |
| 1   | AA    | 1471 | U    | C4-C5   | 7.18  | 1.50        | 1.43     |
| 35  | BB    | 236  | C    | O3'-P   | -7.18 | 1.52        | 1.61     |
| 35  | BB    | 1889 | A    | C8-N7   | -7.18 | 1.26        | 1.31     |
| 1   | AA    | 561  | U    | C2-N3   | 7.18  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 631  | C    | C2'-C1' | 7.18  | 1.61        | 1.53     |
| 1   | AA    | 818  | G    | C6-N1   | 7.18  | 1.44        | 1.39     |
| 1   | AA    | 820  | U    | N3-C4   | -7.18 | 1.31        | 1.38     |
| 35  | BB    | 627  | A    | N7-C5   | -7.18 | 1.34        | 1.39     |
| 35  | BB    | 1921 | G    | C5-C4   | 7.18  | 1.43        | 1.38     |
| 35  | BB    | 2142 | A    | C2'-C1' | -7.18 | 1.45        | 1.53     |
| 1   | AA    | 1505 | G    | O3'-P   | -7.18 | 1.52        | 1.61     |
| 35  | BB    | 1791 | A    | N9-C4   | -7.18 | 1.33        | 1.37     |
| 1   | AA    | 331  | G    | C2-N3   | 7.18  | 1.38        | 1.32     |
| 1   | AA    | 713  | G    | N9-C4   | -7.18 | 1.32        | 1.38     |
| 1   | AA    | 1196 | A    | C6-N6   | 7.18  | 1.39        | 1.33     |
| 35  | BB    | 165  | A    | C6-N6   | 7.18  | 1.39        | 1.33     |
| 35  | BB    | 765  | C    | C2'-C1' | -7.18 | 1.45        | 1.53     |
| 35  | BB    | 814  | C    | P-O5'   | -7.18 | 1.52        | 1.59     |
| 35  | BB    | 1192 | G    | C2'-C1' | -7.18 | 1.45        | 1.53     |
| 35  | BB    | 1538 | G    | C2'-C1' | -7.18 | 1.45        | 1.53     |
| 35  | BB    | 1607 | C    | N1-C2   | 7.18  | 1.47        | 1.40     |
| 35  | BB    | 1684 | G    | C6-N1   | 7.18  | 1.44        | 1.39     |
| 35  | BB    | 2435 | A    | C2'-C1' | -7.18 | 1.45        | 1.53     |
| 1   | AA    | 470  | C    | C4-C5   | 7.17  | 1.48        | 1.43     |
| 1   | AA    | 668  | G    | C2-N3   | 7.17  | 1.38        | 1.32     |
| 1   | AA    | 1342 | C    | N3-C4   | 7.17  | 1.39        | 1.33     |
| 35  | BB    | 1065 | U    | N1-C2   | -7.17 | 1.32        | 1.38     |
| 35  | BB    | 2644 | G    | P-O5'   | -7.17 | 1.52        | 1.59     |
| 34  | BA    | 13   | G    | C2-N2   | 7.17  | 1.41        | 1.34     |
| 35  | BB    | 1146 | C    | C2'-C1' | -7.17 | 1.45        | 1.53     |
| 43  | BJ    | 96   | ARG  | CZ-NH1  | 7.17  | 1.42        | 1.33     |
| 35  | BB    | 1093 | G    | N9-C8   | -7.17 | 1.32        | 1.37     |
| 35  | BB    | 1346 | G    | C6-N1   | 7.17  | 1.44        | 1.39     |
| 35  | BB    | 1593 | A    | N3-C4   | 7.17  | 1.39        | 1.34     |
| 35  | BB    | 2367 | G    | N9-C4   | -7.17 | 1.32        | 1.38     |
| 1   | AA    | 1000 | A    | C6-N6   | -7.17 | 1.28        | 1.33     |
| 35  | BB    | 1980 | G    | N9-C4   | -7.17 | 1.32        | 1.38     |
| 35  | BB    | 2357 | G    | N7-C5   | -7.17 | 1.34        | 1.39     |
| 1   | AA    | 831  | A    | C8-N7   | -7.17 | 1.26        | 1.31     |
| 1   | AA    | 1229 | A    | N7-C5   | 7.17  | 1.43        | 1.39     |
| 1   | AA    | 1320 | C    | N1-C6   | -7.17 | 1.32        | 1.37     |
| 35  | BB    | 993  | G    | N3-C4   | 7.17  | 1.40        | 1.35     |
| 35  | BB    | 2033 | A    | C4'-C3' | 7.17  | 1.61        | 1.53     |
| 35  | BB    | 1303 | G    | C5-C6   | 7.17  | 1.49        | 1.42     |
| 35  | BB    | 2267 | A    | N9-C4   | 7.17  | 1.42        | 1.37     |
| 35  | BB    | 2491 | U    | C5'-C4' | 7.17  | 1.59        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2621 | G    | N3-C4   | -7.17 | 1.30        | 1.35     |
| 1   | AA    | 181  | A    | C6-N1   | 7.16  | 1.40        | 1.35     |
| 1   | AA    | 198  | G    | P-O5'   | -7.16 | 1.52        | 1.59     |
| 1   | AA    | 1245 | C    | C2'-C1' | -7.16 | 1.45        | 1.53     |
| 35  | BB    | 1923 | U    | N3-C4   | 7.16  | 1.44        | 1.38     |
| 35  | BB    | 1980 | G    | C2'-O2' | -7.16 | 1.32        | 1.41     |
| 1   | AA    | 240  | G    | C5-C4   | 7.16  | 1.43        | 1.38     |
| 1   | AA    | 823  | C    | N3-C4   | 7.16  | 1.39        | 1.33     |
| 1   | AA    | 1053 | G    | N9-C8   | 7.16  | 1.42        | 1.37     |
| 35  | BB    | 407  | G    | C2-N3   | 7.16  | 1.38        | 1.32     |
| 35  | BB    | 2534 | A    | C5-C4   | 7.16  | 1.43        | 1.38     |
| 35  | BB    | 2856 | A    | C5-C4   | 7.16  | 1.43        | 1.38     |
| 35  | BB    | 2872 | A    | C3'-C2' | 7.16  | 1.60        | 1.52     |
| 1   | AA    | 601  | G    | C8-N7   | 7.16  | 1.35        | 1.30     |
| 1   | AA    | 749  | A    | N3-C4   | -7.16 | 1.30        | 1.34     |
| 1   | AA    | 861  | G    | C5-C4   | 7.16  | 1.43        | 1.38     |
| 35  | BB    | 512  | G    | N9-C8   | 7.16  | 1.42        | 1.37     |
| 35  | BB    | 626  | A    | C5'-C4' | 7.16  | 1.59        | 1.51     |
| 35  | BB    | 1426 | G    | N7-C5   | -7.16 | 1.34        | 1.39     |
| 35  | BB    | 1523 | U    | C1'-N1  | 7.16  | 1.59        | 1.48     |
| 35  | BB    | 1612 | C    | N1-C6   | -7.16 | 1.32        | 1.37     |
| 35  | BB    | 2589 | A    | N3-C4   | -7.16 | 1.30        | 1.34     |
| 1   | AA    | 56   | U    | C5-C6   | -7.16 | 1.27        | 1.34     |
| 1   | AA    | 120  | A    | C6-N6   | 7.16  | 1.39        | 1.33     |
| 1   | AA    | 605  | U    | N3-C4   | 7.16  | 1.44        | 1.38     |
| 35  | BB    | 1793 | C    | N3-C4   | 7.16  | 1.39        | 1.33     |
| 1   | AA    | 16   | A    | C5'-C4' | 7.15  | 1.59        | 1.51     |
| 35  | BB    | 1002 | G    | C4'-C3' | 7.15  | 1.61        | 1.53     |
| 35  | BB    | 2107 | G    | C2'-C1' | -7.15 | 1.45        | 1.53     |
| 35  | BB    | 2301 | C    | C2'-C1' | -7.15 | 1.45        | 1.53     |
| 1   | AA    | 601  | G    | C2'-C1' | -7.15 | 1.45        | 1.53     |
| 1   | AA    | 1308 | U    | C2-N3   | 7.15  | 1.42        | 1.37     |
| 1   | AA    | 1329 | A    | N9-C4   | -7.15 | 1.33        | 1.37     |
| 1   | AA    | 1477 | U    | P-O5'   | -7.15 | 1.52        | 1.59     |
| 35  | BB    | 202  | U    | C4-C5   | -7.15 | 1.37        | 1.43     |
| 35  | BB    | 903  | C    | N3-C4   | 7.15  | 1.39        | 1.33     |
| 35  | BB    | 1139 | G    | C8-N7   | 7.15  | 1.35        | 1.30     |
| 35  | BB    | 2325 | G    | C2-N2   | 7.15  | 1.41        | 1.34     |
| 1   | AA    | 639  | G    | C2-N2   | 7.15  | 1.41        | 1.34     |
| 35  | BB    | 643  | A    | C6-N1   | 7.15  | 1.40        | 1.35     |
| 35  | BB    | 1635 | A    | C6-N6   | 7.15  | 1.39        | 1.33     |
| 1   | AA    | 374  | A    | C6-N1   | 7.15  | 1.40        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 765  | G    | C8-N7   | 7.15  | 1.35        | 1.30     |
| 1   | AA    | 858  | G    | N1-C2   | 7.15  | 1.43        | 1.37     |
| 35  | BB    | 1337 | G    | C4'-C3' | -7.15 | 1.45        | 1.53     |
| 35  | BB    | 1506 | U    | O3'-P   | -7.15 | 1.52        | 1.61     |
| 35  | BB    | 2736 | A    | C5'-C4' | 7.15  | 1.59        | 1.51     |
| 35  | BB    | 2792 | A    | P-O5'   | -7.15 | 1.52        | 1.59     |
| 1   | AA    | 325  | A    | C2'-C1' | -7.15 | 1.45        | 1.53     |
| 1   | AA    | 647  | C    | N1-C6   | -7.15 | 1.32        | 1.37     |
| 35  | BB    | 830  | G    | N9-C4   | -7.15 | 1.32        | 1.38     |
| 35  | BB    | 1445 | G    | C2-N3   | 7.15  | 1.38        | 1.32     |
| 35  | BB    | 1676 | A    | N3-C4   | -7.15 | 1.30        | 1.34     |
| 35  | BB    | 1985 | C    | N1-C6   | -7.15 | 1.32        | 1.37     |
| 1   | AA    | 778  | G    | N1-C2   | 7.15  | 1.43        | 1.37     |
| 35  | BB    | 213  | A    | C6-N6   | 7.15  | 1.39        | 1.33     |
| 35  | BB    | 2159 | G    | N7-C5   | -7.15 | 1.34        | 1.39     |
| 1   | AA    | 147  | G    | C2-N3   | 7.14  | 1.38        | 1.32     |
| 1   | AA    | 728  | A    | C8-N7   | -7.14 | 1.26        | 1.31     |
| 30  | B5    | 159  | GLY  | CA-C    | -7.14 | 1.40        | 1.51     |
| 35  | BB    | 1922 | G    | C2'-C1' | -7.14 | 1.45        | 1.53     |
| 35  | BB    | 2789 | C    | N1-C2   | 7.14  | 1.47        | 1.40     |
| 1   | AA    | 1241 | G    | C6-N1   | 7.14  | 1.44        | 1.39     |
| 35  | BB    | 1616 | A    | C2'-C1' | -7.14 | 1.45        | 1.53     |
| 35  | BB    | 1675 | C    | C3'-C2' | 7.14  | 1.60        | 1.52     |
| 35  | BB    | 105  | C    | C4-C5   | -7.14 | 1.37        | 1.43     |
| 35  | BB    | 689  | A    | N7-C5   | 7.14  | 1.43        | 1.39     |
| 35  | BB    | 208  | C    | P-O5'   | -7.14 | 1.52        | 1.59     |
| 35  | BB    | 472  | A    | C6-N1   | 7.14  | 1.40        | 1.35     |
| 35  | BB    | 1138 | G    | N1-C2   | 7.14  | 1.43        | 1.37     |
| 35  | BB    | 1395 | A    | N9-C4   | 7.14  | 1.42        | 1.37     |
| 35  | BB    | 2557 | G    | N1-C2   | 7.14  | 1.43        | 1.37     |
| 35  | BB    | 782  | A    | C5'-C4' | 7.14  | 1.59        | 1.51     |
| 35  | BB    | 2848 | G    | P-O5'   | -7.14 | 1.52        | 1.59     |
| 1   | AA    | 31   | G    | C4'-C3' | -7.14 | 1.45        | 1.53     |
| 1   | AA    | 294  | U    | N3-C4   | 7.14  | 1.44        | 1.38     |
| 1   | AA    | 1367 | C    | C2'-C1' | -7.14 | 1.45        | 1.53     |
| 35  | BB    | 1149 | G    | N9-C4   | -7.14 | 1.32        | 1.38     |
| 35  | BB    | 1168 | G    | C6-N1   | 7.14  | 1.44        | 1.39     |
| 35  | BB    | 1696 | G    | N1-C2   | 7.14  | 1.43        | 1.37     |
| 35  | BB    | 1817 | G    | C6-N1   | 7.14  | 1.44        | 1.39     |
| 35  | BB    | 2399 | G    | C6-N1   | 7.14  | 1.44        | 1.39     |
| 1   | AA    | 131  | A    | N3-C4   | -7.13 | 1.30        | 1.34     |
| 1   | AA    | 177  | G    | N1-C2   | 7.13  | 1.43        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 588  | G    | N9-C4   | -7.13 | 1.32        | 1.38     |
| 1   | AA    | 699  | C    | N1-C6   | 7.13  | 1.41        | 1.37     |
| 35  | BB    | 1047 | G    | C2-N3   | 7.13  | 1.38        | 1.32     |
| 35  | BB    | 1475 | G    | C2-N3   | 7.13  | 1.38        | 1.32     |
| 35  | BB    | 2479 | U    | N3-C4   | 7.13  | 1.44        | 1.38     |
| 35  | BB    | 1183 | U    | C5'-C4' | 7.13  | 1.59        | 1.51     |
| 35  | BB    | 1927 | A    | P-O5'   | -7.13 | 1.52        | 1.59     |
| 1   | AA    | 662  | U    | N3-C4   | 7.13  | 1.44        | 1.38     |
| 1   | AA    | 747  | A    | C8-N7   | -7.13 | 1.26        | 1.31     |
| 1   | AA    | 1456 | A    | C6-N6   | 7.13  | 1.39        | 1.33     |
| 35  | BB    | 1916 | A    | C6-N6   | 7.13  | 1.39        | 1.33     |
| 35  | BB    | 2399 | G    | N7-C5   | -7.13 | 1.34        | 1.39     |
| 1   | AA    | 139  | A    | N7-C5   | -7.13 | 1.34        | 1.39     |
| 35  | BB    | 2659 | G    | N3-C4   | -7.13 | 1.30        | 1.35     |
| 1   | AA    | 121  | U    | N3-C4   | 7.13  | 1.44        | 1.38     |
| 35  | BB    | 1655 | A    | N9-C8   | 7.13  | 1.43        | 1.37     |
| 35  | BB    | 380  | G    | C6-O6   | -7.12 | 1.17        | 1.24     |
| 35  | BB    | 1724 | G    | N7-C5   | -7.12 | 1.34        | 1.39     |
| 35  | BB    | 1962 | C    | C3'-C2' | -7.12 | 1.45        | 1.52     |
| 1   | AA    | 541  | G    | C2'-C1' | -7.12 | 1.45        | 1.53     |
| 13  | AM    | 86   | ARG  | CZ-NH2  | 7.12  | 1.42        | 1.33     |
| 35  | BB    | 82   | U    | O3'-P   | -7.12 | 1.52        | 1.61     |
| 35  | BB    | 580  | U    | C3'-C2' | -7.12 | 1.45        | 1.52     |
| 35  | BB    | 2837 | A    | C6-N1   | -7.12 | 1.30        | 1.35     |
| 1   | AA    | 957  | U    | C4'-C3' | 7.12  | 1.60        | 1.53     |
| 1   | AA    | 1362 | A    | N7-C5   | -7.12 | 1.34        | 1.39     |
| 35  | BB    | 337  | C    | N1-C6   | 7.12  | 1.41        | 1.37     |
| 1   | AA    | 394  | G    | N7-C5   | -7.12 | 1.34        | 1.39     |
| 35  | BB    | 2476 | A    | O4'-C1' | 7.12  | 1.50        | 1.41     |
| 35  | BB    | 2801 | G    | P-O5'   | -7.12 | 1.52        | 1.59     |
| 1   | AA    | 219  | U    | O3'-P   | -7.12 | 1.52        | 1.61     |
| 1   | AA    | 508  | U    | C4-C5   | 7.12  | 1.50        | 1.43     |
| 1   | AA    | 1248 | A    | N3-C4   | -7.12 | 1.30        | 1.34     |
| 34  | BA    | 4    | C    | C4'-C3' | 7.12  | 1.60        | 1.53     |
| 35  | BB    | 640  | C    | O3'-P   | -7.12 | 1.52        | 1.61     |
| 35  | BB    | 1594 | U    | C2-O2   | 7.12  | 1.28        | 1.22     |
| 35  | BB    | 1613 | G    | C4'-C3' | 7.12  | 1.60        | 1.53     |
| 35  | BB    | 2322 | A    | N7-C5   | -7.12 | 1.34        | 1.39     |
| 35  | BB    | 1235 | G    | C4'-C3' | -7.12 | 1.45        | 1.53     |
| 1   | AA    | 1350 | A    | N7-C5   | -7.12 | 1.34        | 1.39     |
| 35  | BB    | 661  | A    | P-O5'   | -7.12 | 1.52        | 1.59     |
| 35  | BB    | 1793 | C    | C4-N4   | 7.12  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1974 | C    | C4-N4   | 7.12  | 1.40        | 1.33     |
| 1   | AA    | 1360 | A    | C5-C4   | 7.11  | 1.43        | 1.38     |
| 35  | BB    | 287  | G    | C5-C4   | 7.11  | 1.43        | 1.38     |
| 35  | BB    | 2102 | G    | N9-C8   | -7.11 | 1.32        | 1.37     |
| 35  | BB    | 2251 | G    | C4'-C3' | -7.11 | 1.45        | 1.53     |
| 1   | AA    | 901  | A    | N9-C4   | -7.11 | 1.33        | 1.37     |
| 35  | BB    | 1829 | A    | N3-C4   | 7.11  | 1.39        | 1.34     |
| 35  | BB    | 2285 | C    | C4-N4   | 7.11  | 1.40        | 1.33     |
| 35  | BB    | 672  | C    | C2-N3   | 7.11  | 1.41        | 1.35     |
| 35  | BB    | 1425 | G    | N9-C8   | 7.11  | 1.42        | 1.37     |
| 35  | BB    | 1744 | A    | N9-C8   | 7.11  | 1.43        | 1.37     |
| 1   | AA    | 1432 | G    | C2-N3   | 7.11  | 1.38        | 1.32     |
| 1   | AA    | 94   | G    | C5-C6   | -7.11 | 1.35        | 1.42     |
| 1   | AA    | 938  | A    | C6-N1   | 7.11  | 1.40        | 1.35     |
| 1   | AA    | 1181 | G    | C6-N1   | 7.11  | 1.44        | 1.39     |
| 35  | BB    | 654  | A    | C6-N6   | 7.11  | 1.39        | 1.33     |
| 4   | AD    | 187  | ARG  | CZ-NH1  | 7.11  | 1.42        | 1.33     |
| 35  | BB    | 1203 | U    | P-O5'   | -7.11 | 1.52        | 1.59     |
| 35  | BB    | 2022 | U    | C2'-C1' | -7.11 | 1.45        | 1.53     |
| 35  | BB    | 2792 | A    | C6-N6   | 7.11  | 1.39        | 1.33     |
| 35  | BB    | 2893 | A    | O3'-P   | -7.11 | 1.52        | 1.61     |
| 1   | AA    | 501  | C    | N3-C4   | 7.10  | 1.39        | 1.33     |
| 1   | AA    | 533  | A    | C2-N3   | 7.10  | 1.40        | 1.33     |
| 1   | AA    | 716  | A    | C2'-C1' | -7.10 | 1.45        | 1.53     |
| 35  | BB    | 1776 | G    | C6-N1   | 7.10  | 1.44        | 1.39     |
| 35  | BB    | 1901 | A    | N9-C4   | 7.10  | 1.42        | 1.37     |
| 1   | AA    | 264  | C    | C4-N4   | 7.10  | 1.40        | 1.33     |
| 1   | AA    | 521  | G    | C2-N3   | 7.10  | 1.38        | 1.32     |
| 35  | BB    | 1573 | G    | N7-C5   | -7.10 | 1.34        | 1.39     |
| 35  | BB    | 2143 | C    | C4-C5   | 7.10  | 1.48        | 1.43     |
| 1   | AA    | 449  | G    | C5'-C4' | 7.10  | 1.59        | 1.51     |
| 1   | AA    | 568  | G    | O4'-C1' | 7.10  | 1.50        | 1.41     |
| 35  | BB    | 1992 | G    | N9-C8   | 7.10  | 1.42        | 1.37     |
| 1   | AA    | 761  | G    | C2-N3   | 7.10  | 1.38        | 1.32     |
| 1   | AA    | 873  | A    | N9-C4   | 7.10  | 1.42        | 1.37     |
| 35  | BB    | 226  | A    | N9-C4   | 7.10  | 1.42        | 1.37     |
| 35  | BB    | 624  | C    | C4'-C3' | 7.10  | 1.60        | 1.53     |
| 35  | BB    | 989  | G    | C6-N1   | 7.10  | 1.44        | 1.39     |
| 35  | BB    | 1222 | U    | O3'-P   | -7.10 | 1.52        | 1.61     |
| 1   | AA    | 114  | U    | C2'-C1' | -7.10 | 1.45        | 1.53     |
| 1   | AA    | 603  | U    | N3-C4   | 7.10  | 1.44        | 1.38     |
| 1   | AA    | 1041 | G    | N1-C2   | 7.10  | 1.43        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 182  | A    | C5-C6   | -7.10 | 1.34        | 1.41     |
| 35  | BB    | 779  | U    | N1-C6   | -7.10 | 1.31        | 1.38     |
| 35  | BB    | 924  | G    | N9-C4   | -7.10 | 1.32        | 1.38     |
| 35  | BB    | 2325 | G    | C8-N7   | -7.10 | 1.26        | 1.30     |
| 1   | AA    | 1179 | A    | N3-C4   | 7.10  | 1.39        | 1.34     |
| 1   | AA    | 722  | G    | P-O5'   | -7.09 | 1.52        | 1.59     |
| 1   | AA    | 1130 | A    | N3-C4   | -7.09 | 1.30        | 1.34     |
| 1   | AA    | 1408 | A    | N7-C5   | -7.09 | 1.34        | 1.39     |
| 35  | BB    | 63   | A    | N9-C4   | -7.09 | 1.33        | 1.37     |
| 35  | BB    | 319  | G    | N1-C2   | 7.09  | 1.43        | 1.37     |
| 35  | BB    | 407  | G    | C6-N1   | 7.09  | 1.44        | 1.39     |
| 35  | BB    | 905  | A    | C6-N6   | 7.09  | 1.39        | 1.33     |
| 35  | BB    | 1250 | G    | C6-N1   | 7.09  | 1.44        | 1.39     |
| 35  | BB    | 1259 | G    | C8-N7   | 7.09  | 1.35        | 1.30     |
| 1   | AA    | 680  | C    | C4-C5   | -7.09 | 1.37        | 1.43     |
| 1   | AA    | 1135 | U    | N3-C4   | 7.09  | 1.44        | 1.38     |
| 1   | AA    | 1296 | C    | C4-C5   | 7.09  | 1.48        | 1.43     |
| 35  | BB    | 959  | A    | N9-C8   | -7.09 | 1.32        | 1.37     |
| 35  | BB    | 1439 | A    | N7-C5   | -7.09 | 1.34        | 1.39     |
| 35  | BB    | 1586 | A    | O3'-P   | -7.09 | 1.52        | 1.61     |
| 35  | BB    | 1881 | C    | P-O5'   | -7.09 | 1.52        | 1.59     |
| 1   | AA    | 55   | A    | N7-C5   | -7.09 | 1.34        | 1.39     |
| 35  | BB    | 681  | G    | C8-N7   | -7.09 | 1.26        | 1.30     |
| 35  | BB    | 1516 | G    | C4'-C3' | -7.09 | 1.45        | 1.53     |
| 35  | BB    | 1999 | C    | C3'-C2' | -7.09 | 1.45        | 1.52     |
| 35  | BB    | 2803 | G    | N9-C8   | 7.09  | 1.42        | 1.37     |
| 35  | BB    | 424  | G    | N7-C5   | 7.09  | 1.43        | 1.39     |
| 35  | BB    | 821  | A    | O3'-P   | -7.09 | 1.52        | 1.61     |
| 35  | BB    | 1396 | U    | N1-C2   | 7.09  | 1.45        | 1.38     |
| 35  | BB    | 1776 | G    | C8-N7   | 7.09  | 1.35        | 1.30     |
| 35  | BB    | 2705 | A    | N7-C5   | -7.09 | 1.34        | 1.39     |
| 1   | AA    | 1410 | A    | C2'-C1' | -7.09 | 1.45        | 1.53     |
| 1   | AA    | 1427 | C    | N3-C4   | 7.09  | 1.39        | 1.33     |
| 35  | BB    | 1698 | A    | C6-N6   | 7.09  | 1.39        | 1.33     |
| 1   | AA    | 285  | C    | N1-C6   | 7.09  | 1.41        | 1.37     |
| 1   | AA    | 591  | U    | C2'-C1' | -7.09 | 1.45        | 1.53     |
| 1   | AA    | 1431 | A    | N9-C4   | -7.09 | 1.33        | 1.37     |
| 9   | AI    | 98   | ARG  | CZ-NH1  | 7.09  | 1.42        | 1.33     |
| 35  | BB    | 1197 | G    | N9-C8   | -7.09 | 1.32        | 1.37     |
| 35  | BB    | 1291 | C    | C2'-C1' | -7.09 | 1.45        | 1.53     |
| 35  | BB    | 2124 | G    | N9-C8   | 7.09  | 1.42        | 1.37     |
| 1   | AA    | 877  | G    | C6-N1   | 7.08  | 1.44        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 297  | G    | C6-N1   | 7.08  | 1.44        | 1.39     |
| 35  | BB    | 825  | A    | C2'-C1' | -7.08 | 1.45        | 1.53     |
| 35  | BB    | 1246 | A    | N9-C4   | 7.08  | 1.42        | 1.37     |
| 35  | BB    | 2079 | U    | N3-C4   | 7.08  | 1.44        | 1.38     |
| 1   | AA    | 303  | A    | N7-C5   | 7.08  | 1.43        | 1.39     |
| 1   | AA    | 442  | G    | C8-N7   | 7.08  | 1.35        | 1.30     |
| 1   | AA    | 1051 | C    | N3-C4   | 7.08  | 1.39        | 1.33     |
| 35  | BB    | 1598 | A    | C6-N6   | 7.08  | 1.39        | 1.33     |
| 35  | BB    | 1619 | G    | C2-N3   | 7.08  | 1.38        | 1.32     |
| 35  | BB    | 2472 | G    | C8-N7   | -7.08 | 1.26        | 1.30     |
| 1   | AA    | 61   | G    | C6-N1   | 7.08  | 1.44        | 1.39     |
| 1   | AA    | 1300 | G    | N1-C2   | 7.08  | 1.43        | 1.37     |
| 35  | BB    | 844  | A    | C5'-C4' | 7.08  | 1.59        | 1.51     |
| 35  | BB    | 1473 | G    | C5-C4   | -7.08 | 1.33        | 1.38     |
| 35  | BB    | 2135 | A    | O3'-P   | -7.08 | 1.52        | 1.61     |
| 35  | BB    | 2217 | G    | C4'-C3' | 7.08  | 1.60        | 1.53     |
| 35  | BB    | 2282 | G    | C8-N7   | -7.08 | 1.26        | 1.30     |
| 1   | AA    | 635  | A    | C2'-C1' | -7.08 | 1.45        | 1.53     |
| 1   | AA    | 1451 | U    | N3-C4   | 7.08  | 1.44        | 1.38     |
| 35  | BB    | 1345 | C    | N1-C6   | -7.08 | 1.32        | 1.37     |
| 35  | BB    | 1492 | G    | C2-N2   | 7.08  | 1.41        | 1.34     |
| 1   | AA    | 1489 | G    | C2-N3   | 7.08  | 1.38        | 1.32     |
| 1   | AA    | 1513 | A    | N9-C4   | -7.08 | 1.33        | 1.37     |
| 35  | BB    | 1457 | U    | P-O5'   | -7.08 | 1.52        | 1.59     |
| 35  | BB    | 1552 | A    | N9-C4   | -7.08 | 1.33        | 1.37     |
| 35  | BB    | 1619 | G    | P-O5'   | -7.08 | 1.52        | 1.59     |
| 35  | BB    | 1866 | A    | N9-C4   | -7.08 | 1.33        | 1.37     |
| 35  | BB    | 1918 | A    | C6-N1   | 7.08  | 1.40        | 1.35     |
| 35  | BB    | 2469 | A    | C8-N7   | 7.08  | 1.36        | 1.31     |
| 35  | BB    | 1205 | A    | N7-C5   | 7.08  | 1.43        | 1.39     |
| 35  | BB    | 1464 | G    | N1-C2   | 7.08  | 1.43        | 1.37     |
| 35  | BB    | 2511 | U    | N1-C2   | 7.08  | 1.45        | 1.38     |
| 35  | BB    | 2629 | U    | C5-C6   | 7.08  | 1.40        | 1.34     |
| 35  | BB    | 2819 | G    | C5-C6   | -7.08 | 1.35        | 1.42     |
| 1   | AA    | 479  | U    | N3-C4   | 7.08  | 1.44        | 1.38     |
| 1   | AA    | 566  | G    | C6-N1   | 7.08  | 1.44        | 1.39     |
| 34  | BA    | 8    | C    | N3-C4   | 7.08  | 1.39        | 1.33     |
| 35  | BB    | 1250 | G    | C2-N3   | 7.08  | 1.38        | 1.32     |
| 35  | BB    | 1577 | C    | O3'-P   | -7.08 | 1.52        | 1.61     |
| 35  | BB    | 1872 | A    | N7-C5   | -7.08 | 1.35        | 1.39     |
| 1   | AA    | 520  | A    | C6-N1   | 7.07  | 1.40        | 1.35     |
| 1   | AA    | 972  | C    | O3'-P   | -7.07 | 1.52        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10  | AJ    | 9    | ARG  | CD-NE   | 7.07  | 1.58        | 1.46     |
| 35  | BB    | 2476 | A    | C6-N6   | 7.07  | 1.39        | 1.33     |
| 37  | BD    | 45   | TYR  | CE1-CZ  | 7.07  | 1.47        | 1.38     |
| 35  | BB    | 386  | G    | N7-C5   | -7.07 | 1.35        | 1.39     |
| 35  | BB    | 799  | G    | C5-C4   | 7.07  | 1.43        | 1.38     |
| 35  | BB    | 1776 | G    | N3-C4   | 7.07  | 1.40        | 1.35     |
| 35  | BB    | 2244 | U    | O3'-P   | -7.07 | 1.52        | 1.61     |
| 35  | BB    | 2786 | U    | C2'-C1' | -7.07 | 1.45        | 1.53     |
| 35  | BB    | 1611 | C    | N1-C6   | 7.07  | 1.41        | 1.37     |
| 35  | BB    | 1649 | G    | N3-C4   | 7.07  | 1.40        | 1.35     |
| 1   | AA    | 1484 | C    | N3-C4   | 7.07  | 1.38        | 1.33     |
| 35  | BB    | 1458 | U    | N3-C4   | 7.07  | 1.44        | 1.38     |
| 35  | BB    | 1596 | A    | N7-C5   | -7.07 | 1.35        | 1.39     |
| 35  | BB    | 1767 | G    | C2-N2   | 7.07  | 1.41        | 1.34     |
| 35  | BB    | 2721 | A    | P-O5'   | -7.07 | 1.52        | 1.59     |
| 1   | AA    | 93   | U    | C3'-C2' | 7.07  | 1.60        | 1.52     |
| 1   | AA    | 258  | G    | C2-N3   | 7.07  | 1.38        | 1.32     |
| 1   | AA    | 788  | U    | C3'-C2' | 7.07  | 1.60        | 1.52     |
| 1   | AA    | 1338 | G    | C6-N1   | 7.07  | 1.44        | 1.39     |
| 35  | BB    | 229  | C    | C4-N4   | 7.07  | 1.40        | 1.33     |
| 35  | BB    | 506  | G    | O3'-P   | -7.07 | 1.52        | 1.61     |
| 35  | BB    | 1357 | C    | N3-C4   | 7.07  | 1.38        | 1.33     |
| 35  | BB    | 2061 | G    | C4'-C3' | 7.07  | 1.60        | 1.53     |
| 35  | BB    | 1060 | U    | N3-C4   | 7.06  | 1.44        | 1.38     |
| 35  | BB    | 2742 | G    | C2'-C1' | -7.06 | 1.45        | 1.53     |
| 1   | AA    | 154  | U    | N3-C4   | 7.06  | 1.44        | 1.38     |
| 1   | AA    | 802  | A    | N7-C5   | -7.06 | 1.35        | 1.39     |
| 1   | AA    | 1415 | G    | C6-N1   | 7.06  | 1.44        | 1.39     |
| 35  | BB    | 311  | A    | N7-C5   | -7.06 | 1.35        | 1.39     |
| 35  | BB    | 317  | G    | C3'-C2' | -7.06 | 1.45        | 1.52     |
| 1   | AA    | 231  | U    | C2-N3   | 7.06  | 1.42        | 1.37     |
| 35  | BB    | 563  | A    | C5-C4   | 7.06  | 1.43        | 1.38     |
| 35  | BB    | 1103 | A    | N9-C4   | 7.06  | 1.42        | 1.37     |
| 35  | BB    | 1668 | A    | N9-C8   | -7.06 | 1.32        | 1.37     |
| 35  | BB    | 1918 | A    | O3'-P   | -7.06 | 1.52        | 1.61     |
| 35  | BB    | 2123 | G    | N9-C4   | -7.06 | 1.32        | 1.38     |
| 35  | BB    | 2475 | C    | C4-C5   | 7.06  | 1.48        | 1.43     |
| 35  | BB    | 826  | U    | N3-C4   | 7.06  | 1.44        | 1.38     |
| 35  | BB    | 2527 | C    | C4-N4   | 7.06  | 1.40        | 1.33     |
| 35  | BB    | 909  | A    | C5-C4   | 7.06  | 1.43        | 1.38     |
| 1   | AA    | 675  | A    | C5-C4   | 7.05  | 1.43        | 1.38     |
| 4   | AD    | 171  | GLU  | CD-OE2  | 7.05  | 1.33        | 1.25     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 79   | C    | C4-N4   | 7.05  | 1.40        | 1.33     |
| 35  | BB    | 1949 | G    | N7-C5   | -7.05 | 1.35        | 1.39     |
| 1   | AA    | 229  | U    | C5'-C4' | 7.05  | 1.59        | 1.51     |
| 35  | BB    | 2184 | A    | N9-C4   | 7.05  | 1.42        | 1.37     |
| 31  | B6    | 12   | ARG  | CD-NE   | 7.05  | 1.58        | 1.46     |
| 35  | BB    | 2768 | U    | N3-C4   | 7.05  | 1.44        | 1.38     |
| 1   | AA    | 932  | C    | C4-C5   | 7.05  | 1.48        | 1.43     |
| 1   | AA    | 1162 | C    | N1-C2   | -7.05 | 1.33        | 1.40     |
| 35  | BB    | 126  | A    | C6-N6   | 7.05  | 1.39        | 1.33     |
| 35  | BB    | 1516 | G    | N7-C5   | 7.05  | 1.43        | 1.39     |
| 35  | BB    | 1695 | G    | O4'-C1' | -7.05 | 1.32        | 1.41     |
| 35  | BB    | 2292 | U    | O3'-P   | -7.05 | 1.52        | 1.61     |
| 35  | BB    | 2405 | G    | C8-N7   | 7.05  | 1.35        | 1.30     |
| 1   | AA    | 1261 | A    | N9-C4   | 7.05  | 1.42        | 1.37     |
| 35  | BB    | 1304 | A    | C5-C4   | -7.05 | 1.33        | 1.38     |
| 35  | BB    | 1575 | C    | O3'-P   | -7.05 | 1.52        | 1.61     |
| 35  | BB    | 1924 | C    | N1-C6   | 7.05  | 1.41        | 1.37     |
| 35  | BB    | 1959 | G    | N9-C4   | -7.05 | 1.32        | 1.38     |
| 1   | AA    | 1127 | G    | C5'-C4' | 7.05  | 1.59        | 1.51     |
| 35  | BB    | 457  | A    | N3-C4   | 7.05  | 1.39        | 1.34     |
| 35  | BB    | 572  | A    | N7-C5   | -7.05 | 1.35        | 1.39     |
| 35  | BB    | 1774 | C    | C5-C6   | 7.05  | 1.40        | 1.34     |
| 35  | BB    | 2051 | A    | C6-N1   | 7.05  | 1.40        | 1.35     |
| 35  | BB    | 398  | C    | C4-N4   | 7.04  | 1.40        | 1.33     |
| 35  | BB    | 1677 | A    | P-O5'   | -7.04 | 1.52        | 1.59     |
| 35  | BB    | 1856 | U    | N3-C4   | 7.04  | 1.44        | 1.38     |
| 1   | AA    | 496  | A    | C6-N1   | 7.04  | 1.40        | 1.35     |
| 34  | BA    | 24   | G    | C8-N7   | -7.04 | 1.26        | 1.30     |
| 34  | BA    | 52   | A    | N3-C4   | -7.04 | 1.30        | 1.34     |
| 35  | BB    | 543  | G    | N9-C8   | -7.04 | 1.32        | 1.37     |
| 35  | BB    | 2087 | G    | C2-N3   | 7.04  | 1.38        | 1.32     |
| 35  | BB    | 2398 | U    | N1-C6   | 7.04  | 1.44        | 1.38     |
| 35  | BB    | 758  | C    | O3'-P   | -7.04 | 1.52        | 1.61     |
| 35  | BB    | 2733 | A    | C6-N1   | 7.04  | 1.40        | 1.35     |
| 35  | BB    | 2760 | C    | N3-C4   | 7.04  | 1.38        | 1.33     |
| 1   | AA    | 431  | A    | N9-C4   | 7.04  | 1.42        | 1.37     |
| 35  | BB    | 1120 | G    | C5-C6   | -7.04 | 1.35        | 1.42     |
| 35  | BB    | 1706 | C    | N1-C6   | 7.04  | 1.41        | 1.37     |
| 1   | AA    | 172  | A    | C6-N6   | 7.04  | 1.39        | 1.33     |
| 35  | BB    | 1147 | A    | C6-N1   | 7.04  | 1.40        | 1.35     |
| 35  | BB    | 1696 | G    | C2-N3   | 7.04  | 1.38        | 1.32     |
| 35  | BB    | 2524 | G    | C2-N3   | 7.04  | 1.38        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2803 | G    | C2-N2   | 7.04  | 1.41        | 1.34     |
| 1   | AA    | 88   | U    | N1-C2   | 7.04  | 1.44        | 1.38     |
| 35  | BB    | 1042 | G    | C5'-C4' | 7.04  | 1.59        | 1.51     |
| 1   | AA    | 134  | G    | N3-C4   | -7.04 | 1.30        | 1.35     |
| 1   | AA    | 1052 | U    | N1-C6   | 7.04  | 1.44        | 1.38     |
| 34  | BA    | 46   | A    | N9-C8   | -7.04 | 1.32        | 1.37     |
| 35  | BB    | 371  | A    | O3'-P   | -7.04 | 1.52        | 1.61     |
| 35  | BB    | 458  | G    | N9-C4   | -7.04 | 1.32        | 1.38     |
| 35  | BB    | 1978 | A    | C6-N1   | 7.04  | 1.40        | 1.35     |
| 1   | AA    | 1325 | C    | C4-C5   | 7.03  | 1.48        | 1.43     |
| 35  | BB    | 297  | G    | N1-C2   | 7.03  | 1.43        | 1.37     |
| 35  | BB    | 438  | G    | C2-N2   | 7.03  | 1.41        | 1.34     |
| 35  | BB    | 1046 | A    | C5'-C4' | 7.03  | 1.59        | 1.51     |
| 35  | BB    | 2414 | G    | N1-C2   | 7.03  | 1.43        | 1.37     |
| 35  | BB    | 2718 | G    | C2-N2   | 7.03  | 1.41        | 1.34     |
| 1   | AA    | 1279 | G    | C4'-C3' | -7.03 | 1.45        | 1.53     |
| 35  | BB    | 2459 | A    | C5'-C4' | 7.03  | 1.59        | 1.51     |
| 1   | AA    | 808  | C    | P-O5'   | -7.03 | 1.52        | 1.59     |
| 1   | AA    | 927  | G    | N3-C4   | -7.03 | 1.30        | 1.35     |
| 22  | AV    | 75   | C    | N3-C4   | 7.03  | 1.38        | 1.33     |
| 35  | BB    | 601  | C    | C2'-C1' | -7.03 | 1.45        | 1.53     |
| 35  | BB    | 669  | G    | C8-N7   | 7.03  | 1.35        | 1.30     |
| 35  | BB    | 2136 | G    | C3'-O3' | 7.03  | 1.51        | 1.42     |
| 35  | BB    | 2328 | A    | C3'-C2' | -7.03 | 1.45        | 1.52     |
| 35  | BB    | 2726 | A    | N7-C5   | -7.03 | 1.35        | 1.39     |
| 39  | BF    | 111  | ARG  | CZ-NH1  | 7.03  | 1.42        | 1.33     |
| 35  | BB    | 1771 | C    | C1'-N1  | 7.03  | 1.59        | 1.48     |
| 35  | BB    | 2081 | U    | C2'-C1' | -7.03 | 1.45        | 1.53     |
| 1   | AA    | 180  | U    | C2'-C1' | -7.03 | 1.45        | 1.53     |
| 1   | AA    | 475  | C    | O3'-P   | -7.03 | 1.52        | 1.61     |
| 1   | AA    | 545  | C    | N1-C2   | 7.03  | 1.47        | 1.40     |
| 1   | AA    | 754  | C    | N3-C4   | 7.03  | 1.38        | 1.33     |
| 1   | AA    | 916  | U    | N3-C4   | 7.03  | 1.44        | 1.38     |
| 1   | AA    | 1210 | C    | N3-C4   | 7.03  | 1.38        | 1.33     |
| 35  | BB    | 132  | G    | C2-N3   | 7.03  | 1.38        | 1.32     |
| 35  | BB    | 1574 | C    | N1-C6   | 7.03  | 1.41        | 1.37     |
| 35  | BB    | 1709 | U    | P-O5'   | -7.03 | 1.52        | 1.59     |
| 35  | BB    | 2740 | A    | C5'-C4' | 7.03  | 1.59        | 1.51     |
| 1   | AA    | 941  | G    | C5-C4   | 7.03  | 1.43        | 1.38     |
| 35  | BB    | 967  | U    | C2-N3   | 7.03  | 1.42        | 1.37     |
| 35  | BB    | 2289 | G    | N7-C5   | -7.03 | 1.35        | 1.39     |
| 22  | AV    | 13   | C    | C4'-O4' | 7.02  | 1.54        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2528 | U    | C2-N3   | 7.02  | 1.42        | 1.37     |
| 1   | AA    | 1191 | A    | N7-C5   | -7.02 | 1.35        | 1.39     |
| 1   | AA    | 1433 | A    | C5-C4   | 7.02  | 1.43        | 1.38     |
| 35  | BB    | 111  | A    | C8-N7   | 7.02  | 1.36        | 1.31     |
| 35  | BB    | 1365 | A    | C6-N1   | 7.02  | 1.40        | 1.35     |
| 35  | BB    | 1787 | A    | C8-N7   | -7.02 | 1.26        | 1.31     |
| 35  | BB    | 1861 | G    | N9-C4   | -7.02 | 1.32        | 1.38     |
| 35  | BB    | 2547 | A    | C2'-C1' | -7.02 | 1.45        | 1.53     |
| 35  | BB    | 2759 | G    | C2-N3   | 7.02  | 1.38        | 1.32     |
| 1   | AA    | 196  | A    | C5-C4   | 7.02  | 1.43        | 1.38     |
| 1   | AA    | 1105 | A    | C6-N1   | 7.02  | 1.40        | 1.35     |
| 35  | BB    | 62   | U    | C4'-C3' | 7.02  | 1.60        | 1.53     |
| 35  | BB    | 2484 | G    | C2-N2   | 7.02  | 1.41        | 1.34     |
| 1   | AA    | 164  | G    | N1-C2   | 7.02  | 1.43        | 1.37     |
| 1   | AA    | 484  | G    | N3-C4   | -7.02 | 1.30        | 1.35     |
| 34  | BA    | 44   | G    | N3-C4   | -7.02 | 1.30        | 1.35     |
| 35  | BB    | 1    | G    | P-O5'   | 7.02  | 1.66        | 1.59     |
| 35  | BB    | 191  | A    | C6-N6   | 7.02  | 1.39        | 1.33     |
| 35  | BB    | 536  | G    | C2-N3   | 7.02  | 1.38        | 1.32     |
| 35  | BB    | 1522 | A    | C2'-C1' | -7.02 | 1.45        | 1.53     |
| 35  | BB    | 2166 | U    | C2-N3   | 7.02  | 1.42        | 1.37     |
| 35  | BB    | 2728 | U    | P-O5'   | -7.02 | 1.52        | 1.59     |
| 1   | AA    | 901  | A    | C2'-C1' | -7.02 | 1.45        | 1.53     |
| 34  | BA    | 100  | G    | C6-N1   | 7.02  | 1.44        | 1.39     |
| 35  | BB    | 687  | C    | C2-N3   | 7.02  | 1.41        | 1.35     |
| 35  | BB    | 2392 | A    | N9-C8   | -7.02 | 1.32        | 1.37     |
| 35  | BB    | 2743 | U    | P-O5'   | -7.02 | 1.52        | 1.59     |
| 35  | BB    | 2898 | U    | C4-C5   | 7.02  | 1.49        | 1.43     |
| 34  | BA    | 116  | G    | C6-N1   | 7.02  | 1.44        | 1.39     |
| 1   | AA    | 109  | A    | N9-C8   | 7.01  | 1.43        | 1.37     |
| 35  | BB    | 333  | G    | N7-C5   | -7.01 | 1.35        | 1.39     |
| 35  | BB    | 458  | G    | C2-N3   | 7.01  | 1.38        | 1.32     |
| 35  | BB    | 962  | G    | C2-N3   | 7.01  | 1.38        | 1.32     |
| 35  | BB    | 1250 | G    | C8-N7   | -7.01 | 1.26        | 1.30     |
| 35  | BB    | 1381 | G    | O4'-C1' | -7.01 | 1.32        | 1.41     |
| 1   | AA    | 361  | G    | C2-N2   | 7.01  | 1.41        | 1.34     |
| 1   | AA    | 1414 | U    | N1-C2   | 7.01  | 1.44        | 1.38     |
| 1   | AA    | 85   | U    | P-O5'   | -7.01 | 1.52        | 1.59     |
| 1   | AA    | 170  | U    | C4'-O4' | -7.01 | 1.36        | 1.45     |
| 1   | AA    | 1011 | C    | N3-C4   | 7.01  | 1.38        | 1.33     |
| 15  | AO    | 16   | ARG  | NE-CZ   | 7.01  | 1.42        | 1.33     |
| 35  | BB    | 1144 | A    | N3-C4   | -7.01 | 1.30        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1930 | G    | C2-N3   | 7.01  | 1.38        | 1.32     |
| 35  | BB    | 2391 | G    | N7-C5   | -7.01 | 1.35        | 1.39     |
| 35  | BB    | 2608 | G    | C2-N3   | 7.01  | 1.38        | 1.32     |
| 50  | BQ    | 31   | TYR  | CG-CD1  | 7.01  | 1.48        | 1.39     |
| 1   | AA    | 955  | U    | C3'-O3' | 7.01  | 1.51        | 1.42     |
| 35  | BB    | 125  | A    | C5-C4   | 7.01  | 1.43        | 1.38     |
| 35  | BB    | 644  | A    | N9-C4   | 7.01  | 1.42        | 1.37     |
| 35  | BB    | 2536 | G    | N3-C4   | -7.01 | 1.30        | 1.35     |
| 44  | BK    | 70   | ARG  | CD-NE   | 7.01  | 1.58        | 1.46     |
| 1   | AA    | 198  | G    | C6-N1   | 7.01  | 1.44        | 1.39     |
| 35  | BB    | 2033 | A    | C6-N1   | 7.01  | 1.40        | 1.35     |
| 1   | AA    | 706  | A    | N9-C4   | -7.01 | 1.33        | 1.37     |
| 1   | AA    | 852  | G    | N7-C5   | -7.01 | 1.35        | 1.39     |
| 35  | BB    | 247  | G    | C2-N2   | -7.01 | 1.27        | 1.34     |
| 35  | BB    | 624  | C    | N3-C4   | 7.01  | 1.38        | 1.33     |
| 35  | BB    | 1799 | G    | N9-C8   | -7.01 | 1.32        | 1.37     |
| 35  | BB    | 2666 | C    | N3-C4   | 7.01  | 1.38        | 1.33     |
| 35  | BB    | 2857 | G    | P-O5'   | -7.01 | 1.52        | 1.59     |
| 1   | AA    | 794  | A    | N9-C4   | 7.00  | 1.42        | 1.37     |
| 35  | BB    | 523  | C    | C3'-C2' | 7.00  | 1.60        | 1.52     |
| 1   | AA    | 443  | C    | N1-C6   | 7.00  | 1.41        | 1.37     |
| 1   | AA    | 939  | G    | C2-N2   | 7.00  | 1.41        | 1.34     |
| 1   | AA    | 1412 | C    | C5-C6   | -7.00 | 1.28        | 1.34     |
| 35  | BB    | 252  | G    | C6-N1   | 7.00  | 1.44        | 1.39     |
| 35  | BB    | 1698 | A    | C2-N3   | 7.00  | 1.39        | 1.33     |
| 35  | BB    | 2853 | C    | C2-N3   | 7.00  | 1.41        | 1.35     |
| 35  | BB    | 2862 | G    | N1-C2   | 7.00  | 1.43        | 1.37     |
| 1   | AA    | 360  | G    | N9-C4   | 7.00  | 1.43        | 1.38     |
| 1   | AA    | 364  | A    | N3-C4   | -7.00 | 1.30        | 1.34     |
| 1   | AA    | 1174 | G    | N7-C5   | -7.00 | 1.35        | 1.39     |
| 1   | AA    | 1265 | C    | C2'-C1' | -7.00 | 1.45        | 1.53     |
| 35  | BB    | 1257 | C    | C4'-C3' | -7.00 | 1.45        | 1.53     |
| 35  | BB    | 2035 | G    | O3'-P   | -7.00 | 1.52        | 1.61     |
| 5   | AE    | 49   | TYR  | CE1-CZ  | 7.00  | 1.47        | 1.38     |
| 1   | AA    | 1185 | G    | C4'-O4' | 7.00  | 1.54        | 1.45     |
| 34  | BA    | 96   | G    | N9-C4   | 7.00  | 1.43        | 1.38     |
| 34  | BA    | 100  | G    | N9-C8   | 7.00  | 1.42        | 1.37     |
| 35  | BB    | 302  | C    | C2'-C1' | -7.00 | 1.45        | 1.53     |
| 35  | BB    | 476  | G    | N3-C4   | -7.00 | 1.30        | 1.35     |
| 35  | BB    | 477  | A    | C6-N6   | 7.00  | 1.39        | 1.33     |
| 35  | BB    | 1745 | A    | N7-C5   | -7.00 | 1.35        | 1.39     |
| 1   | AA    | 129  | A    | N3-C4   | -7.00 | 1.30        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 168  | G    | N9-C4   | -7.00 | 1.32        | 1.38     |
| 35  | BB    | 452  | G    | C8-N7   | -7.00 | 1.26        | 1.30     |
| 35  | BB    | 710  | U    | N3-C4   | 7.00  | 1.44        | 1.38     |
| 35  | BB    | 711  | G    | C8-N7   | 7.00  | 1.35        | 1.30     |
| 35  | BB    | 1803 | A    | O3'-P   | -7.00 | 1.52        | 1.61     |
| 35  | BB    | 2069 | G    | C4'-C3' | -7.00 | 1.45        | 1.53     |
| 1   | AA    | 666  | G    | C2-N3   | 7.00  | 1.38        | 1.32     |
| 1   | AA    | 1391 | U    | N1-C6   | 7.00  | 1.44        | 1.38     |
| 35  | BB    | 1302 | A    | N3-C4   | -7.00 | 1.30        | 1.34     |
| 1   | AA    | 454  | G    | N7-C5   | -6.99 | 1.35        | 1.39     |
| 1   | AA    | 1237 | C    | C2-N3   | 6.99  | 1.41        | 1.35     |
| 35  | BB    | 984  | A    | C5-C4   | 6.99  | 1.43        | 1.38     |
| 35  | BB    | 1517 | G    | N9-C8   | 6.99  | 1.42        | 1.37     |
| 35  | BB    | 1748 | C    | N1-C6   | 6.99  | 1.41        | 1.37     |
| 35  | BB    | 2672 | U    | N1-C6   | 6.99  | 1.44        | 1.38     |
| 1   | AA    | 289  | G    | C5-C6   | -6.99 | 1.35        | 1.42     |
| 1   | AA    | 791  | G    | C8-N7   | -6.99 | 1.26        | 1.30     |
| 1   | AA    | 1453 | G    | C5'-C4' | 6.99  | 1.59        | 1.51     |
| 1   | AA    | 1475 | G    | C2-N3   | 6.99  | 1.38        | 1.32     |
| 35  | BB    | 1349 | C    | N1-C6   | 6.99  | 1.41        | 1.37     |
| 35  | BB    | 1549 | A    | C5'-C4' | 6.99  | 1.59        | 1.51     |
| 35  | BB    | 1804 | C    | C4'-C3' | -6.99 | 1.45        | 1.53     |
| 35  | BB    | 2877 | G    | N7-C5   | -6.99 | 1.35        | 1.39     |
| 1   | AA    | 221  | C    | C3'-C2' | -6.99 | 1.45        | 1.52     |
| 1   | AA    | 271  | C    | N1-C6   | -6.99 | 1.32        | 1.37     |
| 1   | AA    | 1421 | G    | C4'-C3' | 6.99  | 1.60        | 1.53     |
| 1   | AA    | 1483 | A    | N9-C8   | 6.99  | 1.43        | 1.37     |
| 35  | BB    | 846  | U    | C2-N3   | 6.99  | 1.42        | 1.37     |
| 35  | BB    | 2607 | G    | C2-N3   | 6.99  | 1.38        | 1.32     |
| 1   | AA    | 353  | A    | C5-C6   | -6.99 | 1.34        | 1.41     |
| 1   | AA    | 1227 | A    | N9-C4   | 6.99  | 1.42        | 1.37     |
| 1   | AA    | 1459 | G    | C6-N1   | 6.99  | 1.44        | 1.39     |
| 35  | BB    | 2107 | G    | C6-N1   | 6.99  | 1.44        | 1.39     |
| 1   | AA    | 417  | G    | C8-N7   | -6.99 | 1.26        | 1.30     |
| 1   | AA    | 951  | G    | C8-N7   | -6.99 | 1.26        | 1.30     |
| 35  | BB    | 1239 | G    | C5-C6   | -6.99 | 1.35        | 1.42     |
| 35  | BB    | 1333 | G    | C2-N2   | 6.99  | 1.41        | 1.34     |
| 35  | BB    | 1439 | A    | C5'-C4' | 6.99  | 1.59        | 1.51     |
| 35  | BB    | 1919 | A    | N9-C8   | -6.99 | 1.32        | 1.37     |
| 35  | BB    | 2475 | C    | N3-C4   | 6.99  | 1.38        | 1.33     |
| 35  | BB    | 1707 | G    | C5-C4   | 6.98  | 1.43        | 1.38     |
| 35  | BB    | 2002 | G    | O3'-P   | -6.98 | 1.52        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2669 | G    | N3-C4   | -6.98 | 1.30        | 1.35     |
| 1   | AA    | 589  | U    | O3'-P   | -6.98 | 1.52        | 1.61     |
| 34  | BA    | 104  | A    | N9-C4   | -6.98 | 1.33        | 1.37     |
| 35  | BB    | 2210 | U    | N3-C4   | 6.98  | 1.44        | 1.38     |
| 35  | BB    | 2329 | U    | C2-N3   | 6.98  | 1.42        | 1.37     |
| 1   | AA    | 1208 | C    | N3-C4   | 6.98  | 1.38        | 1.33     |
| 35  | BB    | 708  | G    | C6-N1   | 6.98  | 1.44        | 1.39     |
| 35  | BB    | 1265 | A    | N9-C4   | -6.98 | 1.33        | 1.37     |
| 35  | BB    | 2324 | U    | O3'-P   | -6.98 | 1.52        | 1.61     |
| 35  | BB    | 2447 | G    | C5-C4   | -6.98 | 1.33        | 1.38     |
| 25  | B0    | 71   | ARG  | NE-CZ   | 6.98  | 1.42        | 1.33     |
| 10  | AJ    | 89   | ARG  | CZ-NH1  | 6.98  | 1.42        | 1.33     |
| 35  | BB    | 142  | A    | C3'-C2' | 6.98  | 1.60        | 1.52     |
| 35  | BB    | 1130 | U    | C4'-C3' | 6.98  | 1.60        | 1.53     |
| 35  | BB    | 1502 | A    | N7-C5   | 6.98  | 1.43        | 1.39     |
| 35  | BB    | 1594 | U    | C2-N3   | 6.98  | 1.42        | 1.37     |
| 35  | BB    | 1973 | G    | N7-C5   | -6.98 | 1.35        | 1.39     |
| 35  | BB    | 2466 | C    | C4'-O4' | 6.98  | 1.54        | 1.45     |
| 1   | AA    | 686  | U    | C5'-C4' | 6.98  | 1.59        | 1.51     |
| 35  | BB    | 730  | A    | N9-C4   | 6.98  | 1.42        | 1.37     |
| 1   | AA    | 356  | A    | C2'-O2' | 6.97  | 1.50        | 1.41     |
| 1   | AA    | 380  | G    | N1-C2   | 6.97  | 1.43        | 1.37     |
| 1   | AA    | 776  | G    | C6-N1   | 6.97  | 1.44        | 1.39     |
| 35  | BB    | 745  | G    | O3'-P   | -6.97 | 1.52        | 1.61     |
| 35  | BB    | 1437 | C    | C2-N3   | 6.97  | 1.41        | 1.35     |
| 35  | BB    | 2142 | A    | N9-C4   | 6.97  | 1.42        | 1.37     |
| 35  | BB    | 2834 | G    | C6-N1   | 6.97  | 1.44        | 1.39     |
| 1   | AA    | 288  | A    | N3-C4   | -6.97 | 1.30        | 1.34     |
| 1   | AA    | 514  | C    | C3'-C2' | -6.97 | 1.45        | 1.52     |
| 34  | BA    | 75   | G    | C6-N1   | 6.97  | 1.44        | 1.39     |
| 35  | BB    | 2123 | G    | C5'-C4' | 6.97  | 1.59        | 1.51     |
| 1   | AA    | 261  | U    | N1-C2   | 6.97  | 1.44        | 1.38     |
| 34  | BA    | 58   | A    | C5-C4   | 6.97  | 1.43        | 1.38     |
| 35  | BB    | 1345 | C    | C2-N3   | 6.97  | 1.41        | 1.35     |
| 1   | AA    | 720  | C    | O3'-P   | -6.97 | 1.52        | 1.61     |
| 35  | BB    | 53   | A    | N3-C4   | -6.97 | 1.30        | 1.34     |
| 35  | BB    | 873  | C    | C4'-C3' | -6.97 | 1.45        | 1.53     |
| 35  | BB    | 1302 | A    | C5'-C4' | 6.97  | 1.59        | 1.51     |
| 35  | BB    | 1636 | U    | P-O5'   | -6.97 | 1.52        | 1.59     |
| 35  | BB    | 1772 | A    | N9-C8   | 6.97  | 1.43        | 1.37     |
| 35  | BB    | 2648 | G    | C2-N2   | 6.97  | 1.41        | 1.34     |
| 1   | AA    | 1369 | C    | C3'-C2' | -6.96 | 1.45        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2167 | U    | N1-C2   | 6.96  | 1.44        | 1.38     |
| 35  | BB    | 2360 | G    | N1-C2   | 6.96  | 1.43        | 1.37     |
| 35  | BB    | 1433 | A    | N9-C4   | -6.96 | 1.33        | 1.37     |
| 35  | BB    | 1564 | C    | C2-N3   | 6.96  | 1.41        | 1.35     |
| 35  | BB    | 2017 | U    | C2-N3   | 6.96  | 1.42        | 1.37     |
| 35  | BB    | 2358 | A    | C6-N6   | 6.96  | 1.39        | 1.33     |
| 35  | BB    | 2567 | G    | N9-C8   | 6.96  | 1.42        | 1.37     |
| 1   | AA    | 95   | C    | C4'-C3' | -6.96 | 1.45        | 1.53     |
| 1   | AA    | 271  | C    | O4'-C1' | 6.96  | 1.50        | 1.41     |
| 1   | AA    | 1265 | C    | P-O5'   | -6.96 | 1.52        | 1.59     |
| 35  | BB    | 482  | A    | C2-N3   | 6.96  | 1.39        | 1.33     |
| 35  | BB    | 660  | C    | C4-N4   | 6.96  | 1.40        | 1.33     |
| 35  | BB    | 1857 | G    | N1-C2   | 6.96  | 1.43        | 1.37     |
| 35  | BB    | 2503 | A    | C8-N7   | -6.96 | 1.26        | 1.31     |
| 1   | AA    | 454  | G    | C2-N2   | 6.96  | 1.41        | 1.34     |
| 35  | BB    | 189  | G    | N9-C4   | -6.96 | 1.32        | 1.38     |
| 1   | AA    | 178  | C    | C2'-C1' | -6.96 | 1.45        | 1.53     |
| 35  | BB    | 612  | G    | N9-C4   | -6.96 | 1.32        | 1.38     |
| 35  | BB    | 1252 | G    | N9-C4   | -6.96 | 1.32        | 1.38     |
| 35  | BB    | 1266 | G    | C2-N3   | 6.96  | 1.38        | 1.32     |
| 1   | AA    | 394  | G    | N1-C2   | 6.96  | 1.43        | 1.37     |
| 1   | AA    | 472  | U    | N1-C6   | 6.96  | 1.44        | 1.38     |
| 1   | AA    | 484  | G    | C2'-C1' | -6.96 | 1.45        | 1.53     |
| 1   | AA    | 1016 | A    | C4'-C3' | -6.96 | 1.45        | 1.53     |
| 35  | BB    | 205  | G    | N9-C8   | -6.96 | 1.32        | 1.37     |
| 35  | BB    | 2148 | G    | C5'-C4' | 6.96  | 1.59        | 1.51     |
| 35  | BB    | 2224 | G    | C5-C6   | -6.96 | 1.35        | 1.42     |
| 35  | BB    | 2670 | A    | C8-N7   | -6.96 | 1.26        | 1.31     |
| 35  | BB    | 2777 | G    | N7-C5   | -6.96 | 1.35        | 1.39     |
| 1   | AA    | 780  | A    | C5'-C4' | 6.96  | 1.59        | 1.51     |
| 35  | BB    | 2384 | U    | O3'-P   | -6.96 | 1.52        | 1.61     |
| 35  | BB    | 2727 | A    | C2'-O2' | -6.96 | 1.32        | 1.41     |
| 1   | AA    | 529  | G    | C6-N1   | -6.95 | 1.34        | 1.39     |
| 1   | AA    | 651  | C    | C3'-C2' | -6.95 | 1.45        | 1.52     |
| 1   | AA    | 1324 | A    | N9-C4   | 6.95  | 1.42        | 1.37     |
| 9   | AI    | 6    | TYR  | CB-CG   | -6.95 | 1.41        | 1.51     |
| 34  | BA    | 71   | C    | P-O5'   | -6.95 | 1.52        | 1.59     |
| 35  | BB    | 87   | U    | C2'-C1' | -6.95 | 1.45        | 1.53     |
| 35  | BB    | 2275 | C    | C5'-C4' | 6.95  | 1.59        | 1.51     |
| 35  | BB    | 2658 | C    | N3-C4   | 6.95  | 1.38        | 1.33     |
| 35  | BB    | 2534 | A    | C8-N7   | -6.95 | 1.26        | 1.31     |
| 35  | BB    | 541  | A    | N7-C5   | -6.95 | 1.35        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2488 | G    | C6-N1   | 6.95  | 1.44        | 1.39     |
| 1   | AA    | 1489 | G    | P-O5'   | -6.95 | 1.52        | 1.59     |
| 35  | BB    | 298  | G    | N3-C4   | 6.95  | 1.40        | 1.35     |
| 35  | BB    | 1287 | A    | O3'-P   | -6.95 | 1.52        | 1.61     |
| 1   | AA    | 806  | C    | P-O5'   | -6.95 | 1.52        | 1.59     |
| 34  | BA    | 53   | A    | C5'-C4' | 6.95  | 1.59        | 1.51     |
| 35  | BB    | 1374 | G    | O3'-P   | -6.95 | 1.52        | 1.61     |
| 35  | BB    | 1773 | A    | P-O5'   | -6.95 | 1.52        | 1.59     |
| 1   | AA    | 457  | G    | N1-C2   | 6.95  | 1.43        | 1.37     |
| 35  | BB    | 352  | A    | N7-C5   | -6.95 | 1.35        | 1.39     |
| 35  | BB    | 564  | C    | N1-C6   | 6.95  | 1.41        | 1.37     |
| 35  | BB    | 850  | U    | P-O5'   | -6.95 | 1.52        | 1.59     |
| 35  | BB    | 2379 | G    | N1-C2   | 6.95  | 1.43        | 1.37     |
| 35  | BB    | 64   | A    | C6-N6   | 6.94  | 1.39        | 1.33     |
| 35  | BB    | 1128 | G    | C4'-C3' | 6.94  | 1.60        | 1.53     |
| 1   | AA    | 367  | U    | C3'-C2' | -6.94 | 1.45        | 1.52     |
| 35  | BB    | 1378 | A    | C6-N6   | 6.94  | 1.39        | 1.33     |
| 35  | BB    | 1778 | U    | P-O5'   | -6.94 | 1.52        | 1.59     |
| 35  | BB    | 2159 | G    | C2-N3   | 6.94  | 1.38        | 1.32     |
| 35  | BB    | 2669 | G    | P-O5'   | 6.94  | 1.66        | 1.59     |
| 1   | AA    | 143  | A    | C2'-C1' | 6.94  | 1.60        | 1.53     |
| 35  | BB    | 1098 | A    | P-O5'   | -6.94 | 1.52        | 1.59     |
| 35  | BB    | 1177 | G    | N1-C2   | 6.94  | 1.43        | 1.37     |
| 35  | BB    | 1250 | G    | O3'-P   | -6.94 | 1.52        | 1.61     |
| 35  | BB    | 1638 | C    | C2'-O2' | -6.94 | 1.32        | 1.41     |
| 35  | BB    | 2195 | U    | O3'-P   | -6.94 | 1.52        | 1.61     |
| 1   | AA    | 415  | A    | C6-N6   | 6.94  | 1.39        | 1.33     |
| 1   | AA    | 568  | G    | C5'-C4' | 6.94  | 1.59        | 1.51     |
| 1   | AA    | 851  | G    | C2-N3   | 6.94  | 1.38        | 1.32     |
| 35  | BB    | 1095 | A    | N9-C4   | 6.94  | 1.42        | 1.37     |
| 35  | BB    | 1206 | G    | O3'-P   | -6.94 | 1.52        | 1.61     |
| 35  | BB    | 1894 | C    | C2-N3   | 6.94  | 1.41        | 1.35     |
| 35  | BB    | 870  | U    | P-O5'   | -6.94 | 1.52        | 1.59     |
| 35  | BB    | 1055 | G    | C6-N1   | 6.94  | 1.44        | 1.39     |
| 35  | BB    | 1409 | U    | N1-C2   | 6.94  | 1.44        | 1.38     |
| 35  | BB    | 1844 | C    | P-O5'   | -6.94 | 1.52        | 1.59     |
| 35  | BB    | 2134 | A    | C5'-C4' | 6.94  | 1.59        | 1.51     |
| 35  | BB    | 2851 | A    | N3-C4   | -6.94 | 1.30        | 1.34     |
| 1   | AA    | 408  | A    | N7-C5   | -6.94 | 1.35        | 1.39     |
| 1   | AA    | 931  | C    | C4-N4   | 6.94  | 1.40        | 1.33     |
| 34  | BA    | 36   | C    | C3'-C2' | -6.94 | 1.45        | 1.52     |
| 35  | BB    | 644  | A    | O4'-C1' | 6.94  | 1.50        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1853 | A    | C5'-C4' | 6.94  | 1.59        | 1.51     |
| 35  | BB    | 1888 | G    | C2-N3   | 6.94  | 1.38        | 1.32     |
| 1   | AA    | 1045 | C    | N3-C4   | 6.93  | 1.38        | 1.33     |
| 35  | BB    | 1213 | A    | C6-N1   | 6.93  | 1.40        | 1.35     |
| 1   | AA    | 129  | A    | C2-N3   | 6.93  | 1.39        | 1.33     |
| 34  | BA    | 96   | G    | C2-N3   | 6.93  | 1.38        | 1.32     |
| 35  | BB    | 216  | A    | N9-C4   | 6.93  | 1.42        | 1.37     |
| 35  | BB    | 1262 | A    | C6-N6   | 6.93  | 1.39        | 1.33     |
| 35  | BB    | 1434 | A    | C2'-C1' | -6.93 | 1.45        | 1.53     |
| 35  | BB    | 1900 | A    | O3'-P   | -6.93 | 1.52        | 1.61     |
| 35  | BB    | 1928 | A    | C6-N6   | 6.93  | 1.39        | 1.33     |
| 1   | AA    | 587  | G    | N9-C8   | -6.93 | 1.32        | 1.37     |
| 35  | BB    | 184  | C    | N1-C6   | 6.93  | 1.41        | 1.37     |
| 35  | BB    | 361  | G    | N1-C2   | 6.93  | 1.43        | 1.37     |
| 35  | BB    | 881  | G    | N7-C5   | -6.93 | 1.35        | 1.39     |
| 1   | AA    | 1471 | U    | O4'-C1' | -6.93 | 1.32        | 1.41     |
| 35  | BB    | 176  | A    | C5-C4   | -6.93 | 1.33        | 1.38     |
| 35  | BB    | 346  | A    | N3-C4   | -6.93 | 1.30        | 1.34     |
| 35  | BB    | 507  | A    | N9-C4   | -6.93 | 1.33        | 1.37     |
| 35  | BB    | 1705 | A    | C5-C6   | 6.93  | 1.47        | 1.41     |
| 35  | BB    | 2015 | A    | N1-C2   | -6.93 | 1.28        | 1.34     |
| 1   | AA    | 886  | G    | N1-C2   | 6.93  | 1.43        | 1.37     |
| 34  | BA    | 24   | G    | O3'-P   | -6.93 | 1.52        | 1.61     |
| 34  | BA    | 43   | C    | C4-N4   | 6.93  | 1.40        | 1.33     |
| 35  | BB    | 2214 | C    | C5'-C4' | 6.93  | 1.59        | 1.51     |
| 35  | BB    | 2446 | G    | N1-C2   | 6.93  | 1.43        | 1.37     |
| 1   | AA    | 237  | G    | C2-N3   | 6.93  | 1.38        | 1.32     |
| 1   | AA    | 371  | A    | C5-C4   | 6.93  | 1.43        | 1.38     |
| 1   | AA    | 487  | A    | N3-C4   | -6.93 | 1.30        | 1.34     |
| 35  | BB    | 537  | G    | P-O5'   | -6.93 | 1.52        | 1.59     |
| 1   | AA    | 41   | G    | C8-N7   | -6.92 | 1.26        | 1.30     |
| 1   | AA    | 423  | G    | C6-N1   | 6.92  | 1.44        | 1.39     |
| 1   | AA    | 1248 | A    | C2'-C1' | -6.92 | 1.45        | 1.53     |
| 34  | BA    | 4    | C    | N1-C6   | -6.92 | 1.32        | 1.37     |
| 35  | BB    | 414  | C    | C3'-C2' | -6.92 | 1.45        | 1.52     |
| 35  | BB    | 761  | A    | C4'-O4' | 6.92  | 1.54        | 1.45     |
| 35  | BB    | 836  | G    | N1-C2   | 6.92  | 1.43        | 1.37     |
| 35  | BB    | 1252 | G    | C6-N1   | 6.92  | 1.44        | 1.39     |
| 35  | BB    | 1548 | A    | N7-C5   | 6.92  | 1.43        | 1.39     |
| 35  | BB    | 2199 | A    | N7-C5   | -6.92 | 1.35        | 1.39     |
| 35  | BB    | 2545 | G    | C5'-C4' | -6.92 | 1.43        | 1.51     |
| 35  | BB    | 2806 | C    | N1-C6   | -6.92 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 587  | G    | C6-N1   | 6.92  | 1.44        | 1.39     |
| 35  | BB    | 380  | G    | C4'-O4' | -6.92 | 1.36        | 1.45     |
| 34  | BA    | 16   | G    | C2'-C1' | -6.92 | 1.45        | 1.53     |
| 35  | BB    | 1818 | U    | C4'-O4' | -6.92 | 1.36        | 1.45     |
| 1   | AA    | 1458 | G    | C4'-C3' | 6.92  | 1.60        | 1.53     |
| 35  | BB    | 290  | U    | C2-N3   | -6.92 | 1.32        | 1.37     |
| 35  | BB    | 1860 | G    | N1-C2   | 6.92  | 1.43        | 1.37     |
| 35  | BB    | 2093 | G    | C4'-O4' | -6.92 | 1.36        | 1.45     |
| 36  | BC    | 62   | ARG  | CD-NE   | 6.92  | 1.58        | 1.46     |
| 1   | AA    | 367  | U    | C2'-C1' | -6.92 | 1.45        | 1.53     |
| 1   | AA    | 954  | G    | N7-C5   | -6.92 | 1.35        | 1.39     |
| 35  | BB    | 1093 | G    | C2-N2   | 6.92  | 1.41        | 1.34     |
| 35  | BB    | 2435 | A    | N7-C5   | -6.92 | 1.35        | 1.39     |
| 35  | BB    | 2764 | A    | N7-C5   | -6.92 | 1.35        | 1.39     |
| 1   | AA    | 314  | C    | C4-N4   | 6.92  | 1.40        | 1.33     |
| 1   | AA    | 926  | G    | N9-C8   | -6.92 | 1.33        | 1.37     |
| 35  | BB    | 323  | C    | P-O5'   | -6.92 | 1.52        | 1.59     |
| 35  | BB    | 2489 | U    | C4-O4   | -6.92 | 1.18        | 1.23     |
| 1   | AA    | 539  | A    | N3-C4   | -6.91 | 1.30        | 1.34     |
| 1   | AA    | 1463 | U    | C4-C5   | 6.91  | 1.49        | 1.43     |
| 35  | BB    | 53   | A    | C5-C4   | 6.91  | 1.43        | 1.38     |
| 35  | BB    | 1241 | A    | C5-C4   | 6.91  | 1.43        | 1.38     |
| 35  | BB    | 2049 | G    | P-O5'   | -6.91 | 1.52        | 1.59     |
| 35  | BB    | 2819 | G    | N7-C5   | -6.91 | 1.35        | 1.39     |
| 35  | BB    | 2873 | A    | N3-C4   | 6.91  | 1.39        | 1.34     |
| 1   | AA    | 300  | A    | C5'-C4' | 6.91  | 1.59        | 1.51     |
| 1   | AA    | 1117 | A    | N7-C5   | -6.91 | 1.35        | 1.39     |
| 35  | BB    | 1134 | A    | N9-C4   | -6.91 | 1.33        | 1.37     |
| 1   | AA    | 94   | G    | C2-N3   | 6.91  | 1.38        | 1.32     |
| 1   | AA    | 1416 | G    | C5'-C4' | -6.91 | 1.43        | 1.51     |
| 35  | BB    | 218  | A    | N7-C5   | -6.91 | 1.35        | 1.39     |
| 35  | BB    | 2815 | C    | C2-N3   | 6.91  | 1.41        | 1.35     |
| 1   | AA    | 215  | C    | C4-N4   | 6.91  | 1.40        | 1.33     |
| 1   | AA    | 288  | A    | C8-N7   | 6.91  | 1.36        | 1.31     |
| 1   | AA    | 710  | G    | C8-N7   | -6.91 | 1.26        | 1.30     |
| 1   | AA    | 941  | G    | C6-N1   | 6.91  | 1.44        | 1.39     |
| 1   | AA    | 1430 | A    | C2-N3   | 6.91  | 1.39        | 1.33     |
| 35  | BB    | 493  | G    | N1-C2   | 6.91  | 1.43        | 1.37     |
| 35  | BB    | 2854 | G    | C5-C4   | -6.91 | 1.33        | 1.38     |
| 1   | AA    | 643  | C    | N1-C6   | 6.91  | 1.41        | 1.37     |
| 6   | AF    | 79   | ARG  | CZ-NH1  | 6.91  | 1.42        | 1.33     |
| 35  | BB    | 363  | G    | N7-C5   | -6.91 | 1.35        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 762  | U    | C4-C5   | 6.91  | 1.49        | 1.43     |
| 35  | BB    | 2703 | C    | C5-C6   | -6.91 | 1.28        | 1.34     |
| 1   | AA    | 1257 | A    | N9-C8   | 6.90  | 1.43        | 1.37     |
| 35  | BB    | 323  | C    | C5-C6   | -6.90 | 1.28        | 1.34     |
| 1   | AA    | 1170 | A    | N7-C5   | -6.90 | 1.35        | 1.39     |
| 1   | AA    | 1236 | A    | N3-C4   | 6.90  | 1.39        | 1.34     |
| 35  | BB    | 797  | G    | C2-N3   | 6.90  | 1.38        | 1.32     |
| 35  | BB    | 1927 | A    | C6-N6   | 6.90  | 1.39        | 1.33     |
| 35  | BB    | 2182 | U    | C5-C6   | -6.90 | 1.27        | 1.34     |
| 1   | AA    | 201  | G    | N3-C4   | 6.90  | 1.40        | 1.35     |
| 34  | BA    | 112  | G    | N1-C2   | 6.90  | 1.43        | 1.37     |
| 35  | BB    | 708  | G    | N3-C4   | 6.90  | 1.40        | 1.35     |
| 35  | BB    | 1432 | G    | P-O5'   | -6.90 | 1.52        | 1.59     |
| 35  | BB    | 456  | C    | N1-C6   | -6.90 | 1.33        | 1.37     |
| 35  | BB    | 738  | G    | C2-N2   | 6.90  | 1.41        | 1.34     |
| 1   | AA    | 414  | A    | N9-C4   | -6.90 | 1.33        | 1.37     |
| 1   | AA    | 540  | G    | N1-C2   | 6.90  | 1.43        | 1.37     |
| 1   | AA    | 586  | C    | C3'-C2' | -6.90 | 1.45        | 1.52     |
| 1   | AA    | 1020 | G    | N1-C2   | 6.90  | 1.43        | 1.37     |
| 35  | BB    | 506  | G    | C6-N1   | 6.90  | 1.44        | 1.39     |
| 35  | BB    | 517  | C    | C4-N4   | 6.90  | 1.40        | 1.33     |
| 35  | BB    | 681  | G    | C2'-C1' | -6.90 | 1.45        | 1.53     |
| 35  | BB    | 1311 | G    | C6-N1   | 6.90  | 1.44        | 1.39     |
| 35  | BB    | 1412 | U    | C5'-C4' | 6.90  | 1.59        | 1.51     |
| 35  | BB    | 800  | A    | C8-N7   | -6.90 | 1.26        | 1.31     |
| 35  | BB    | 1958 | C    | N3-C4   | 6.90  | 1.38        | 1.33     |
| 35  | BB    | 415  | A    | C6-N1   | 6.89  | 1.40        | 1.35     |
| 35  | BB    | 1650 | A    | P-O5'   | -6.89 | 1.52        | 1.59     |
| 35  | BB    | 1887 | C    | C4-C5   | 6.89  | 1.48        | 1.43     |
| 35  | BB    | 2886 | A    | C5-C4   | 6.89  | 1.43        | 1.38     |
| 1   | AA    | 59   | A    | N9-C4   | 6.89  | 1.42        | 1.37     |
| 1   | AA    | 89   | U    | C2'-C1' | -6.89 | 1.45        | 1.53     |
| 1   | AA    | 134  | G    | N9-C4   | -6.89 | 1.32        | 1.38     |
| 1   | AA    | 739  | C    | N1-C6   | -6.89 | 1.33        | 1.37     |
| 1   | AA    | 1142 | G    | C2'-C1' | -6.89 | 1.45        | 1.53     |
| 1   | AA    | 1431 | A    | C6-N1   | 6.89  | 1.40        | 1.35     |
| 35  | BB    | 595  | C    | N3-C4   | 6.89  | 1.38        | 1.33     |
| 35  | BB    | 756  | A    | C6-N6   | 6.89  | 1.39        | 1.33     |
| 35  | BB    | 2860 | A    | C5-C4   | 6.89  | 1.43        | 1.38     |
| 35  | BB    | 477  | A    | N7-C5   | -6.89 | 1.35        | 1.39     |
| 1   | AA    | 264  | C    | C2'-C1' | -6.89 | 1.45        | 1.53     |
| 35  | BB    | 1051 | G    | N7-C5   | 6.89  | 1.43        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2220 | U    | C4-O4   | -6.89 | 1.18        | 1.23     |
| 35  | BB    | 2673 | G    | C4'-C3' | -6.89 | 1.45        | 1.53     |
| 35  | BB    | 2881 | U    | N1-C6   | -6.89 | 1.31        | 1.38     |
| 35  | BB    | 521  | U    | P-O5'   | -6.89 | 1.52        | 1.59     |
| 35  | BB    | 1644 | C    | N1-C6   | 6.89  | 1.41        | 1.37     |
| 35  | BB    | 2465 | C    | C2'-C1' | -6.89 | 1.45        | 1.53     |
| 1   | AA    | 441  | A    | C8-N7   | -6.89 | 1.26        | 1.31     |
| 1   | AA    | 1292 | G    | P-O5'   | -6.89 | 1.52        | 1.59     |
| 35  | BB    | 31   | C    | N1-C6   | -6.89 | 1.33        | 1.37     |
| 35  | BB    | 2078 | C    | O3'-P   | -6.89 | 1.52        | 1.61     |
| 35  | BB    | 2325 | G    | P-O5'   | -6.89 | 1.52        | 1.59     |
| 1   | AA    | 319  | G    | N3-C4   | 6.88  | 1.40        | 1.35     |
| 34  | BA    | 10   | G    | N1-C2   | 6.88  | 1.43        | 1.37     |
| 35  | BB    | 508  | A    | P-O5'   | -6.88 | 1.52        | 1.59     |
| 35  | BB    | 2690 | U    | P-O5'   | -6.88 | 1.52        | 1.59     |
| 1   | AA    | 1129 | C    | C5-C6   | -6.88 | 1.28        | 1.34     |
| 34  | BA    | 15   | A    | C5-C6   | -6.88 | 1.34        | 1.41     |
| 35  | BB    | 103  | A    | C2'-C1' | -6.88 | 1.45        | 1.53     |
| 35  | BB    | 1460 | U    | C2-O2   | 6.88  | 1.28        | 1.22     |
| 35  | BB    | 1697 | G    | C6-N1   | 6.88  | 1.44        | 1.39     |
| 35  | BB    | 1015 | U    | C4-C5   | 6.88  | 1.49        | 1.43     |
| 35  | BB    | 1609 | A    | C8-N7   | -6.88 | 1.26        | 1.31     |
| 35  | BB    | 185  | G    | N1-C2   | 6.88  | 1.43        | 1.37     |
| 35  | BB    | 249  | C    | C2'-C1' | 6.88  | 1.60        | 1.53     |
| 35  | BB    | 857  | G    | N9-C8   | 6.88  | 1.42        | 1.37     |
| 35  | BB    | 985  | C    | P-O5'   | -6.88 | 1.52        | 1.59     |
| 1   | AA    | 357  | G    | N9-C8   | 6.88  | 1.42        | 1.37     |
| 35  | BB    | 381  | G    | C5'-C4' | 6.88  | 1.59        | 1.51     |
| 35  | BB    | 845  | A    | C3'-O3' | 6.88  | 1.51        | 1.42     |
| 35  | BB    | 1196 | C    | N1-C2   | 6.88  | 1.47        | 1.40     |
| 1   | AA    | 848  | C    | O3'-P   | -6.88 | 1.52        | 1.61     |
| 1   | AA    | 1090 | U    | C2'-C1' | -6.88 | 1.45        | 1.53     |
| 35  | BB    | 121  | G    | C6-N1   | 6.88  | 1.44        | 1.39     |
| 35  | BB    | 442  | G    | N1-C2   | 6.88  | 1.43        | 1.37     |
| 35  | BB    | 845  | A    | C2-N3   | -6.88 | 1.27        | 1.33     |
| 35  | BB    | 2638 | G    | O3'-P   | -6.88 | 1.52        | 1.61     |
| 35  | BB    | 2705 | A    | N9-C8   | 6.88  | 1.43        | 1.37     |
| 1   | AA    | 461  | A    | C6-N1   | 6.87  | 1.40        | 1.35     |
| 1   | AA    | 500  | G    | C2-N3   | 6.87  | 1.38        | 1.32     |
| 31  | B6    | 28   | ARG  | CD-NE   | 6.87  | 1.58        | 1.46     |
| 35  | BB    | 959  | A    | N3-C4   | -6.87 | 1.30        | 1.34     |
| 1   | AA    | 139  | A    | N1-C2   | 6.87  | 1.40        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1242 | G    | C4'-C3' | 6.87  | 1.60        | 1.53     |
| 35  | BB    | 761  | A    | N3-C4   | -6.87 | 1.30        | 1.34     |
| 35  | BB    | 2143 | C    | C4'-O4' | -6.87 | 1.36        | 1.45     |
| 1   | AA    | 244  | U    | N1-C6   | 6.87  | 1.44        | 1.38     |
| 1   | AA    | 626  | G    | C2-N3   | 6.87  | 1.38        | 1.32     |
| 1   | AA    | 1311 | A    | C8-N7   | -6.87 | 1.26        | 1.31     |
| 35  | BB    | 493  | G    | C2-N3   | 6.87  | 1.38        | 1.32     |
| 35  | BB    | 964  | C    | C3'-C2' | -6.87 | 1.45        | 1.52     |
| 35  | BB    | 1189 | A    | O3'-P   | -6.87 | 1.52        | 1.61     |
| 1   | AA    | 255  | G    | C2-N3   | 6.87  | 1.38        | 1.32     |
| 1   | AA    | 275  | G    | N9-C8   | 6.87  | 1.42        | 1.37     |
| 1   | AA    | 1192 | C    | P-O5'   | -6.87 | 1.52        | 1.59     |
| 35  | BB    | 1084 | A    | C2'-C1' | -6.87 | 1.45        | 1.53     |
| 35  | BB    | 1212 | G    | C2-N3   | 6.87  | 1.38        | 1.32     |
| 35  | BB    | 2547 | A    | N9-C4   | -6.87 | 1.33        | 1.37     |
| 41  | BH    | 27   | ARG  | NE-CZ   | 6.87  | 1.42        | 1.33     |
| 1   | AA    | 558  | G    | C6-O6   | -6.87 | 1.18        | 1.24     |
| 35  | BB    | 448  | U    | C2'-C1' | -6.87 | 1.45        | 1.53     |
| 35  | BB    | 1966 | A    | C2'-C1' | -6.87 | 1.45        | 1.53     |
| 1   | AA    | 1091 | U    | P-O5'   | -6.87 | 1.52        | 1.59     |
| 1   | AA    | 1186 | G    | N7-C5   | -6.87 | 1.35        | 1.39     |
| 30  | B5    | 21   | TYR  | CG-CD2  | 6.87  | 1.48        | 1.39     |
| 35  | BB    | 405  | U    | C4-O4   | -6.87 | 1.18        | 1.23     |
| 35  | BB    | 707  | G    | P-O5'   | -6.87 | 1.52        | 1.59     |
| 35  | BB    | 969  | G    | C6-N1   | 6.87  | 1.44        | 1.39     |
| 35  | BB    | 1017 | G    | C4'-C3' | 6.87  | 1.60        | 1.53     |
| 35  | BB    | 2425 | A    | N9-C4   | -6.87 | 1.33        | 1.37     |
| 1   | AA    | 55   | A    | N9-C4   | 6.86  | 1.42        | 1.37     |
| 1   | AA    | 251  | G    | C5-C4   | 6.86  | 1.43        | 1.38     |
| 1   | AA    | 450  | G    | N3-C4   | 6.86  | 1.40        | 1.35     |
| 14  | AN    | 68   | ARG  | NE-CZ   | 6.86  | 1.42        | 1.33     |
| 35  | BB    | 456  | C    | C4-C5   | 6.86  | 1.48        | 1.43     |
| 35  | BB    | 1580 | A    | N7-C5   | -6.86 | 1.35        | 1.39     |
| 35  | BB    | 1987 | A    | C2-N3   | -6.86 | 1.27        | 1.33     |
| 35  | BB    | 2429 | G    | C6-N1   | 6.86  | 1.44        | 1.39     |
| 35  | BB    | 2639 | A    | N7-C5   | -6.86 | 1.35        | 1.39     |
| 1   | AA    | 813  | U    | C2-N3   | 6.86  | 1.42        | 1.37     |
| 1   | AA    | 978  | A    | N9-C4   | -6.86 | 1.33        | 1.37     |
| 35  | BB    | 2462 | C    | C4-N4   | 6.86  | 1.40        | 1.33     |
| 1   | AA    | 358  | U    | N3-C4   | 6.86  | 1.44        | 1.38     |
| 1   | AA    | 1157 | A    | O4'-C1' | 6.86  | 1.50        | 1.41     |
| 35  | BB    | 1652 | A    | C4'-O4' | 6.86  | 1.54        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 36  | BC    | 213  | ARG  | NE-CZ   | 6.86  | 1.42        | 1.33     |
| 1   | AA    | 397  | A    | C6-N1   | 6.86  | 1.40        | 1.35     |
| 1   | AA    | 128  | G    | P-O5'   | -6.86 | 1.52        | 1.59     |
| 1   | AA    | 1288 | A    | C5-C4   | 6.86  | 1.43        | 1.38     |
| 35  | BB    | 438  | G    | N1-C2   | 6.86  | 1.43        | 1.37     |
| 35  | BB    | 1486 | U    | P-O5'   | -6.86 | 1.52        | 1.59     |
| 35  | BB    | 204  | A    | C6-N6   | 6.86  | 1.39        | 1.33     |
| 35  | BB    | 1858 | A    | C2-N3   | -6.86 | 1.27        | 1.33     |
| 35  | BB    | 1337 | G    | C5-C4   | -6.85 | 1.33        | 1.38     |
| 35  | BB    | 2621 | G    | C2-N3   | 6.85  | 1.38        | 1.32     |
| 1   | AA    | 535  | A    | N7-C5   | 6.85  | 1.43        | 1.39     |
| 1   | AA    | 1126 | U    | C4'-O4' | -6.85 | 1.36        | 1.45     |
| 1   | AA    | 1163 | A    | N7-C5   | -6.85 | 1.35        | 1.39     |
| 35  | BB    | 304  | U    | N1-C6   | 6.85  | 1.44        | 1.38     |
| 35  | BB    | 1854 | A    | C8-N7   | 6.85  | 1.36        | 1.31     |
| 35  | BB    | 2482 | A    | C5-C4   | 6.85  | 1.43        | 1.38     |
| 35  | BB    | 2669 | G    | C2-N2   | 6.85  | 1.41        | 1.34     |
| 1   | AA    | 872  | A    | C4'-C3' | 6.85  | 1.60        | 1.53     |
| 35  | BB    | 410  | G    | C6-N1   | 6.85  | 1.44        | 1.39     |
| 35  | BB    | 1509 | A    | N1-C2   | 6.85  | 1.40        | 1.34     |
| 1   | AA    | 482  | A    | C2'-C1' | -6.85 | 1.45        | 1.53     |
| 35  | BB    | 508  | A    | N7-C5   | -6.85 | 1.35        | 1.39     |
| 35  | BB    | 895  | U    | C5'-C4' | 6.85  | 1.59        | 1.51     |
| 35  | BB    | 1027 | A    | C5'-C4' | 6.85  | 1.59        | 1.51     |
| 35  | BB    | 1546 | G    | N1-C2   | 6.85  | 1.43        | 1.37     |
| 35  | BB    | 2046 | G    | C5-C4   | -6.85 | 1.33        | 1.38     |
| 35  | BB    | 2144 | G    | N3-C4   | 6.85  | 1.40        | 1.35     |
| 35  | BB    | 2519 | U    | N1-C6   | -6.85 | 1.31        | 1.38     |
| 35  | BB    | 2843 | G    | N3-C4   | -6.85 | 1.30        | 1.35     |
| 35  | BB    | 2857 | G    | C5'-C4' | 6.85  | 1.59        | 1.51     |
| 1   | AA    | 24   | U    | C2-N3   | 6.85  | 1.42        | 1.37     |
| 1   | AA    | 227  | G    | C5-C6   | -6.85 | 1.35        | 1.42     |
| 1   | AA    | 258  | G    | N9-C4   | -6.85 | 1.32        | 1.38     |
| 1   | AA    | 565  | U    | C2-N3   | 6.85  | 1.42        | 1.37     |
| 1   | AA    | 1312 | G    | C5-C4   | 6.85  | 1.43        | 1.38     |
| 34  | BA    | 80   | U    | P-O5'   | -6.85 | 1.52        | 1.59     |
| 35  | BB    | 130  | C    | N3-C4   | 6.85  | 1.38        | 1.33     |
| 35  | BB    | 1846 | G    | N7-C5   | -6.85 | 1.35        | 1.39     |
| 35  | BB    | 2219 | U    | C4'-C3' | 6.85  | 1.60        | 1.53     |
| 35  | BB    | 2901 | C    | C4-N4   | 6.85  | 1.40        | 1.33     |
| 10  | AJ    | 68   | ARG  | CZ-NH1  | 6.85  | 1.42        | 1.33     |
| 35  | BB    | 638  | G    | N1-C2   | 6.85  | 1.43        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 233  | C    | C4-C5   | 6.84  | 1.48        | 1.43     |
| 1   | AA    | 853  | C    | C2-N3   | 6.84  | 1.41        | 1.35     |
| 1   | AA    | 998  | C    | N1-C6   | 6.84  | 1.41        | 1.37     |
| 1   | AA    | 1532 | U    | C4-C5   | 6.84  | 1.49        | 1.43     |
| 34  | BA    | 112  | G    | C2-N3   | 6.84  | 1.38        | 1.32     |
| 35  | BB    | 13   | A    | C4'-C3' | 6.84  | 1.60        | 1.53     |
| 35  | BB    | 159  | G    | C4'-O4' | -6.84 | 1.36        | 1.45     |
| 35  | BB    | 356  | G    | N7-C5   | -6.84 | 1.35        | 1.39     |
| 35  | BB    | 601  | C    | O3'-P   | -6.84 | 1.52        | 1.61     |
| 35  | BB    | 1107 | G    | N9-C8   | 6.84  | 1.42        | 1.37     |
| 35  | BB    | 2105 | U    | C3'-C2' | 6.84  | 1.60        | 1.52     |
| 18  | AR    | 35   | SER  | C-N     | 6.84  | 1.45        | 1.33     |
| 35  | BB    | 974  | G    | C2'-C1' | -6.84 | 1.45        | 1.53     |
| 35  | BB    | 1364 | G    | P-O5'   | -6.84 | 1.52        | 1.59     |
| 35  | BB    | 2213 | U    | N3-C4   | 6.84  | 1.44        | 1.38     |
| 1   | AA    | 411  | A    | N9-C8   | -6.84 | 1.32        | 1.37     |
| 1   | AA    | 1105 | A    | C6-N6   | 6.84  | 1.39        | 1.33     |
| 34  | BA    | 81   | G    | C3'-C2' | -6.84 | 1.45        | 1.52     |
| 35  | BB    | 1086 | A    | N3-C4   | -6.84 | 1.30        | 1.34     |
| 35  | BB    | 1411 | U    | C2-N3   | -6.84 | 1.32        | 1.37     |
| 35  | BB    | 1858 | A    | N7-C5   | -6.84 | 1.35        | 1.39     |
| 35  | BB    | 2422 | C    | C3'-C2' | -6.84 | 1.45        | 1.52     |
| 1   | AA    | 57   | G    | C2-N3   | 6.84  | 1.38        | 1.32     |
| 15  | AO    | 88   | ARG  | CZ-NH1  | 6.84  | 1.42        | 1.33     |
| 35  | BB    | 637  | A    | C2-N3   | 6.84  | 1.39        | 1.33     |
| 35  | BB    | 921  | C    | N3-C4   | 6.84  | 1.38        | 1.33     |
| 35  | BB    | 1304 | A    | N7-C5   | -6.84 | 1.35        | 1.39     |
| 35  | BB    | 1399 | C    | C2-N3   | 6.84  | 1.41        | 1.35     |
| 35  | BB    | 2077 | A    | C6-N6   | 6.84  | 1.39        | 1.33     |
| 35  | BB    | 2508 | G    | N1-C2   | 6.84  | 1.43        | 1.37     |
| 1   | AA    | 80   | A    | N9-C8   | 6.84  | 1.43        | 1.37     |
| 1   | AA    | 1192 | C    | N3-C4   | 6.84  | 1.38        | 1.33     |
| 35  | BB    | 1494 | A    | C5-C6   | -6.84 | 1.34        | 1.41     |
| 1   | AA    | 243  | A    | N7-C5   | -6.84 | 1.35        | 1.39     |
| 1   | AA    | 496  | A    | C8-N7   | -6.84 | 1.26        | 1.31     |
| 35  | BB    | 396  | G    | C6-N1   | 6.84  | 1.44        | 1.39     |
| 35  | BB    | 415  | A    | N9-C8   | 6.84  | 1.43        | 1.37     |
| 35  | BB    | 684  | G    | C2-N3   | 6.84  | 1.38        | 1.32     |
| 35  | BB    | 977  | G    | N1-C2   | 6.84  | 1.43        | 1.37     |
| 35  | BB    | 2870 | C    | C5'-C4' | 6.84  | 1.59        | 1.51     |
| 1   | AA    | 1322 | C    | C4-C5   | 6.83  | 1.48        | 1.43     |
| 35  | BB    | 2415 | G    | C2-N3   | 6.83  | 1.38        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 98   | A    | O3'-P   | -6.83 | 1.52        | 1.61     |
| 35  | BB    | 620  | G    | N9-C4   | 6.83  | 1.43        | 1.38     |
| 35  | BB    | 750  | A    | C6-N1   | 6.83  | 1.40        | 1.35     |
| 35  | BB    | 2500 | U    | C2'-C1' | -6.83 | 1.45        | 1.53     |
| 35  | BB    | 2857 | G    | C5-C4   | 6.83  | 1.43        | 1.38     |
| 1   | AA    | 361  | G    | N9-C8   | 6.83  | 1.42        | 1.37     |
| 1   | AA    | 471  | U    | C2-N3   | 6.83  | 1.42        | 1.37     |
| 35  | BB    | 1216 | G    | N1-C2   | 6.83  | 1.43        | 1.37     |
| 35  | BB    | 1508 | A    | C6-N6   | 6.83  | 1.39        | 1.33     |
| 35  | BB    | 1923 | U    | N1-C6   | 6.83  | 1.44        | 1.38     |
| 35  | BB    | 2341 | G    | C5'-C4' | 6.83  | 1.59        | 1.51     |
| 1   | AA    | 66   | A    | P-O5'   | -6.83 | 1.52        | 1.59     |
| 1   | AA    | 515  | G    | C5-C4   | 6.83  | 1.43        | 1.38     |
| 34  | BA    | 66   | A    | O3'-P   | -6.83 | 1.52        | 1.61     |
| 35  | BB    | 1115 | G    | N7-C5   | -6.83 | 1.35        | 1.39     |
| 35  | BB    | 1521 | G    | N9-C8   | 6.83  | 1.42        | 1.37     |
| 35  | BB    | 548  | G    | C4'-O4' | 6.83  | 1.54        | 1.45     |
| 35  | BB    | 2353 | G    | C2-N3   | 6.83  | 1.38        | 1.32     |
| 1   | AA    | 863  | U    | N1-C6   | -6.83 | 1.31        | 1.38     |
| 1   | AA    | 1092 | A    | C5'-C4' | 6.83  | 1.59        | 1.51     |
| 35  | BB    | 622  | G    | C4'-C3' | -6.83 | 1.45        | 1.53     |
| 1   | AA    | 1105 | A    | N7-C5   | -6.82 | 1.35        | 1.39     |
| 1   | AA    | 1372 | U    | N3-C4   | -6.82 | 1.32        | 1.38     |
| 35  | BB    | 2    | G    | N7-C5   | -6.82 | 1.35        | 1.39     |
| 35  | BB    | 26   | G    | C2-N3   | 6.82  | 1.38        | 1.32     |
| 35  | BB    | 193  | U    | C2-N3   | 6.82  | 1.42        | 1.37     |
| 35  | BB    | 219  | A    | C6-N6   | 6.82  | 1.39        | 1.33     |
| 35  | BB    | 499  | U    | P-O5'   | -6.82 | 1.52        | 1.59     |
| 35  | BB    | 1405 | U    | C2'-C1' | -6.82 | 1.45        | 1.53     |
| 35  | BB    | 2440 | C    | C4-C5   | 6.82  | 1.48        | 1.43     |
| 35  | BB    | 2806 | C    | O3'-P   | -6.82 | 1.52        | 1.61     |
| 35  | BB    | 2846 | G    | C6-N1   | 6.82  | 1.44        | 1.39     |
| 1   | AA    | 1476 | A    | N9-C8   | 6.82  | 1.43        | 1.37     |
| 35  | BB    | 1722 | A    | N7-C5   | -6.82 | 1.35        | 1.39     |
| 35  | BB    | 2732 | G    | N1-C2   | 6.82  | 1.43        | 1.37     |
| 1   | AA    | 790  | A    | C2'-C1' | -6.82 | 1.45        | 1.53     |
| 35  | BB    | 1815 | A    | C8-N7   | -6.82 | 1.26        | 1.31     |
| 35  | BB    | 2112 | G    | N7-C5   | -6.82 | 1.35        | 1.39     |
| 1   | AA    | 1070 | U    | O4'-C1' | 6.82  | 1.50        | 1.41     |
| 1   | AA    | 1109 | C    | C2-N3   | 6.82  | 1.41        | 1.35     |
| 1   | AA    | 1358 | U    | N3-C4   | 6.82  | 1.44        | 1.38     |
| 35  | BB    | 1671 | U    | C1'-N1  | 6.82  | 1.58        | 1.48     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2058 | A    | C8-N7   | -6.82 | 1.26        | 1.31     |
| 1   | AA    | 193  | C    | N1-C2   | 6.82  | 1.47        | 1.40     |
| 35  | BB    | 2111 | U    | C2-N3   | 6.82  | 1.42        | 1.37     |
| 35  | BB    | 2492 | U    | C4-O4   | 6.82  | 1.29        | 1.23     |
| 35  | BB    | 60   | G    | C2-N2   | 6.82  | 1.41        | 1.34     |
| 35  | BB    | 1463 | C    | P-O5'   | -6.82 | 1.52        | 1.59     |
| 35  | BB    | 1574 | C    | N3-C4   | 6.82  | 1.38        | 1.33     |
| 1   | AA    | 759  | A    | P-O5'   | -6.81 | 1.52        | 1.59     |
| 1   | AA    | 1442 | G    | C6-N1   | -6.81 | 1.34        | 1.39     |
| 22  | AV    | 76   | A    | C6-N6   | 6.81  | 1.39        | 1.33     |
| 35  | BB    | 1576 | U    | C2'-C1' | 6.81  | 1.60        | 1.53     |
| 35  | BB    | 2034 | U    | C2-N3   | 6.81  | 1.42        | 1.37     |
| 1   | AA    | 776  | G    | N9-C4   | -6.81 | 1.32        | 1.38     |
| 35  | BB    | 80   | G    | C2-N3   | 6.81  | 1.38        | 1.32     |
| 35  | BB    | 459  | U    | C2-N3   | 6.81  | 1.42        | 1.37     |
| 35  | BB    | 2144 | G    | C2'-C1' | 6.81  | 1.60        | 1.53     |
| 1   | AA    | 1388 | C    | C2-N3   | 6.81  | 1.41        | 1.35     |
| 35  | BB    | 365  | U    | C4'-C3' | 6.81  | 1.60        | 1.53     |
| 35  | BB    | 581  | C    | N1-C6   | 6.81  | 1.41        | 1.37     |
| 35  | BB    | 737  | C    | C2'-C1' | -6.81 | 1.45        | 1.53     |
| 35  | BB    | 1538 | G    | C2-N3   | 6.81  | 1.38        | 1.32     |
| 1   | AA    | 795  | C    | C5'-C4' | 6.81  | 1.59        | 1.51     |
| 1   | AA    | 1163 | A    | N9-C4   | -6.81 | 1.33        | 1.37     |
| 35  | BB    | 682  | G    | N1-C2   | 6.81  | 1.43        | 1.37     |
| 35  | BB    | 2291 | U    | C3'-C2' | -6.81 | 1.45        | 1.52     |
| 1   | AA    | 452  | A    | N7-C5   | -6.81 | 1.35        | 1.39     |
| 35  | BB    | 1120 | G    | C3'-C2' | 6.81  | 1.60        | 1.52     |
| 35  | BB    | 1819 | A    | C6-N6   | 6.81  | 1.39        | 1.33     |
| 35  | BB    | 1889 | A    | C3'-C2' | 6.81  | 1.60        | 1.52     |
| 35  | BB    | 2320 | U    | N1-C2   | 6.81  | 1.44        | 1.38     |
| 1   | AA    | 6    | G    | O3'-P   | -6.81 | 1.52        | 1.61     |
| 1   | AA    | 1506 | U    | N1-C2   | 6.81  | 1.44        | 1.38     |
| 9   | AI    | 112  | ARG  | CZ-NH1  | 6.81  | 1.41        | 1.33     |
| 35  | BB    | 356  | G    | N1-C2   | 6.81  | 1.43        | 1.37     |
| 35  | BB    | 1649 | G    | N9-C4   | -6.81 | 1.32        | 1.38     |
| 35  | BB    | 2415 | G    | C6-N1   | 6.81  | 1.44        | 1.39     |
| 1   | AA    | 1101 | A    | C6-N1   | 6.80  | 1.40        | 1.35     |
| 1   | AA    | 1207 | G    | N7-C5   | -6.80 | 1.35        | 1.39     |
| 1   | AA    | 1308 | U    | N1-C6   | 6.80  | 1.44        | 1.38     |
| 35  | BB    | 16   | C    | C2-O2   | -6.80 | 1.18        | 1.24     |
| 35  | BB    | 2123 | G    | N3-C4   | -6.80 | 1.30        | 1.35     |
| 50  | BQ    | 32   | ARG  | NE-CZ   | 6.80  | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 249  | C    | C2-N3   | -6.80 | 1.30        | 1.35     |
| 1   | AA    | 579  | A    | N9-C4   | -6.80 | 1.33        | 1.37     |
| 1   | AA    | 656  | G    | C5-C6   | -6.80 | 1.35        | 1.42     |
| 10  | AJ    | 5    | ARG  | CZ-NH1  | 6.80  | 1.41        | 1.33     |
| 35  | BB    | 781  | A    | N9-C8   | 6.80  | 1.43        | 1.37     |
| 35  | BB    | 1447 | C    | C2-N3   | -6.80 | 1.30        | 1.35     |
| 35  | BB    | 1448 | G    | C2-N2   | 6.80  | 1.41        | 1.34     |
| 35  | BB    | 1798 | U    | C4-C5   | 6.80  | 1.49        | 1.43     |
| 35  | BB    | 1899 | A    | C6-N1   | 6.80  | 1.40        | 1.35     |
| 35  | BB    | 2064 | C    | C4-C5   | 6.80  | 1.48        | 1.43     |
| 35  | BB    | 173  | A    | C5-C4   | 6.80  | 1.43        | 1.38     |
| 35  | BB    | 1164 | C    | C2'-C1' | -6.80 | 1.45        | 1.53     |
| 35  | BB    | 2128 | G    | C2-N3   | 6.80  | 1.38        | 1.32     |
| 35  | BB    | 2603 | G    | C5-C6   | -6.80 | 1.35        | 1.42     |
| 1   | AA    | 641  | U    | N3-C4   | 6.80  | 1.44        | 1.38     |
| 1   | AA    | 832  | G    | C8-N7   | -6.80 | 1.26        | 1.30     |
| 35  | BB    | 958  | U    | N3-C4   | 6.80  | 1.44        | 1.38     |
| 35  | BB    | 1052 | C    | C4'-C3' | -6.80 | 1.45        | 1.53     |
| 35  | BB    | 2401 | U    | N3-C4   | 6.80  | 1.44        | 1.38     |
| 1   | AA    | 1149 | C    | C5'-C4' | 6.80  | 1.59        | 1.51     |
| 35  | BB    | 795  | C    | C2'-C1' | -6.80 | 1.45        | 1.53     |
| 35  | BB    | 1492 | G    | P-O5'   | -6.80 | 1.52        | 1.59     |
| 35  | BB    | 2030 | A    | N9-C4   | -6.80 | 1.33        | 1.37     |
| 35  | BB    | 2437 | G    | C2-N3   | 6.80  | 1.38        | 1.32     |
| 1   | AA    | 115  | G    | C2-N2   | 6.79  | 1.41        | 1.34     |
| 35  | BB    | 2900 | A    | C5'-C4' | 6.79  | 1.59        | 1.51     |
| 4   | AD    | 22   | SER  | CA-CB   | 6.79  | 1.63        | 1.52     |
| 35  | BB    | 904  | G    | C2-N3   | 6.79  | 1.38        | 1.32     |
| 35  | BB    | 2156 | G    | N9-C8   | 6.79  | 1.42        | 1.37     |
| 35  | BB    | 2225 | A    | N9-C4   | -6.79 | 1.33        | 1.37     |
| 45  | BL    | 37   | GLY  | CA-C    | -6.79 | 1.41        | 1.51     |
| 1   | AA    | 55   | A    | C5'-C4' | 6.79  | 1.59        | 1.51     |
| 1   | AA    | 94   | G    | C5-C4   | 6.79  | 1.43        | 1.38     |
| 1   | AA    | 1080 | A    | O3'-P   | -6.79 | 1.52        | 1.61     |
| 35  | BB    | 551  | G    | C2-N3   | 6.79  | 1.38        | 1.32     |
| 35  | BB    | 764  | A    | C5-C6   | -6.79 | 1.34        | 1.41     |
| 35  | BB    | 1078 | U    | C2-N3   | 6.79  | 1.42        | 1.37     |
| 35  | BB    | 1497 | U    | C2-N3   | 6.79  | 1.42        | 1.37     |
| 35  | BB    | 2324 | U    | C5'-C4' | 6.79  | 1.59        | 1.51     |
| 1   | AA    | 22   | G    | C6-N1   | 6.79  | 1.44        | 1.39     |
| 13  | AM    | 70   | ARG  | CZ-NH1  | 6.79  | 1.41        | 1.33     |
| 32  | B7    | 12   | ARG  | CZ-NH1  | 6.79  | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 184  | C    | C5'-C4' | 6.79  | 1.59        | 1.51     |
| 35  | BB    | 188  | G    | C6-N1   | 6.79  | 1.44        | 1.39     |
| 35  | BB    | 394  | C    | O3'-P   | -6.79 | 1.53        | 1.61     |
| 35  | BB    | 2242 | G    | N3-C4   | -6.79 | 1.30        | 1.35     |
| 35  | BB    | 2783 | U    | C5'-C4' | 6.79  | 1.59        | 1.51     |
| 1   | AA    | 192  | A    | O3'-P   | -6.79 | 1.53        | 1.61     |
| 1   | AA    | 1156 | G    | N7-C5   | 6.79  | 1.43        | 1.39     |
| 35  | BB    | 518  | G    | P-O5'   | 6.79  | 1.66        | 1.59     |
| 1   | AA    | 610  | U    | C4'-C3' | 6.79  | 1.60        | 1.53     |
| 1   | AA    | 681  | A    | C6-N1   | 6.79  | 1.40        | 1.35     |
| 1   | AA    | 1082 | A    | C6-N6   | 6.79  | 1.39        | 1.33     |
| 1   | AA    | 1463 | U    | N1-C6   | 6.79  | 1.44        | 1.38     |
| 1   | AA    | 404  | G    | N3-C4   | 6.79  | 1.40        | 1.35     |
| 1   | AA    | 806  | C    | N1-C6   | 6.79  | 1.41        | 1.37     |
| 1   | AA    | 847  | G    | O4'-C1' | -6.79 | 1.32        | 1.41     |
| 1   | AA    | 1342 | C    | O3'-P   | -6.79 | 1.53        | 1.61     |
| 35  | BB    | 443  | A    | C6-N6   | 6.79  | 1.39        | 1.33     |
| 35  | BB    | 1074 | G    | O3'-P   | -6.79 | 1.53        | 1.61     |
| 35  | BB    | 2342 | C    | C4-N4   | 6.79  | 1.40        | 1.33     |
| 35  | BB    | 2755 | C    | C4-C5   | -6.79 | 1.37        | 1.43     |
| 1   | AA    | 1101 | A    | C6-N6   | 6.78  | 1.39        | 1.33     |
| 35  | BB    | 1062 | G    | C6-O6   | -6.78 | 1.18        | 1.24     |
| 1   | AA    | 18   | C    | C4-N4   | 6.78  | 1.40        | 1.33     |
| 35  | BB    | 648  | G    | C2-N3   | 6.78  | 1.38        | 1.32     |
| 35  | BB    | 659  | G    | C5-C6   | -6.78 | 1.35        | 1.42     |
| 35  | BB    | 971  | G    | C5-C6   | -6.78 | 1.35        | 1.42     |
| 35  | BB    | 1299 | G    | N1-C2   | 6.78  | 1.43        | 1.37     |
| 35  | BB    | 1312 | U    | C1'-N1  | 6.78  | 1.58        | 1.48     |
| 35  | BB    | 1639 | C    | C2'-C1' | -6.78 | 1.45        | 1.53     |
| 35  | BB    | 1651 | G    | C3'-O3' | 6.78  | 1.51        | 1.42     |
| 35  | BB    | 2174 | C    | C5-C6   | 6.78  | 1.39        | 1.34     |
| 4   | AD    | 169  | TRP  | CD2-CE2 | 6.78  | 1.49        | 1.41     |
| 35  | BB    | 2546 | U    | P-O5'   | -6.78 | 1.52        | 1.59     |
| 35  | BB    | 78   | U    | C2-N3   | 6.78  | 1.42        | 1.37     |
| 35  | BB    | 1063 | G    | C6-N1   | 6.78  | 1.44        | 1.39     |
| 1   | AA    | 209  | U    | C4-O4   | 6.78  | 1.29        | 1.23     |
| 1   | AA    | 496  | A    | N9-C4   | 6.78  | 1.42        | 1.37     |
| 1   | AA    | 992  | U    | C4'-C3' | -6.78 | 1.45        | 1.53     |
| 35  | BB    | 327  | G    | C5-C4   | 6.78  | 1.43        | 1.38     |
| 35  | BB    | 513  | A    | N1-C2   | 6.78  | 1.40        | 1.34     |
| 35  | BB    | 1945 | G    | O3'-P   | -6.78 | 1.53        | 1.61     |
| 35  | BB    | 2055 | C    | N3-C4   | 6.78  | 1.38        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2333 | A    | C2'-C1' | -6.78 | 1.45        | 1.53     |
| 35  | BB    | 2700 | A    | C4'-O4' | 6.78  | 1.54        | 1.45     |
| 35  | BB    | 877  | A    | C6-N6   | 6.77  | 1.39        | 1.33     |
| 41  | BH    | 131  | SER  | CA-CB   | 6.77  | 1.63        | 1.52     |
| 1   | AA    | 1199 | U    | P-O5'   | -6.77 | 1.52        | 1.59     |
| 35  | BB    | 242  | G    | P-O5'   | 6.77  | 1.66        | 1.59     |
| 35  | BB    | 339  | U    | C3'-O3' | 6.77  | 1.51        | 1.42     |
| 35  | BB    | 1140 | C    | C4-C5   | 6.77  | 1.48        | 1.43     |
| 1   | AA    | 65   | A    | N7-C5   | -6.77 | 1.35        | 1.39     |
| 1   | AA    | 853  | C    | P-O5'   | -6.77 | 1.52        | 1.59     |
| 35  | BB    | 604  | G    | C6-N1   | 6.77  | 1.44        | 1.39     |
| 1   | AA    | 917  | G    | N9-C8   | 6.77  | 1.42        | 1.37     |
| 35  | BB    | 1245 | G    | N9-C8   | -6.77 | 1.33        | 1.37     |
| 35  | BB    | 2382 | G    | N7-C5   | -6.77 | 1.35        | 1.39     |
| 35  | BB    | 2404 | U    | N1-C2   | 6.77  | 1.44        | 1.38     |
| 1   | AA    | 509  | A    | N1-C2   | 6.77  | 1.40        | 1.34     |
| 35  | BB    | 178  | G    | N3-C4   | -6.77 | 1.30        | 1.35     |
| 35  | BB    | 222  | A    | C4'-C3' | 6.77  | 1.60        | 1.53     |
| 35  | BB    | 866  | A    | N9-C4   | 6.77  | 1.42        | 1.37     |
| 35  | BB    | 1805 | A    | N7-C5   | 6.77  | 1.43        | 1.39     |
| 35  | BB    | 2612 | C    | C3'-C2' | 6.77  | 1.60        | 1.52     |
| 1   | AA    | 236  | A    | C6-N1   | 6.77  | 1.40        | 1.35     |
| 1   | AA    | 758  | C    | N3-C4   | 6.77  | 1.38        | 1.33     |
| 35  | BB    | 935  | C    | N3-C4   | 6.77  | 1.38        | 1.33     |
| 35  | BB    | 2635 | A    | N9-C4   | 6.77  | 1.42        | 1.37     |
| 1   | AA    | 505  | G    | N3-C4   | -6.76 | 1.30        | 1.35     |
| 1   | AA    | 941  | G    | C2'-C1' | -6.76 | 1.46        | 1.53     |
| 1   | AA    | 1496 | C    | N3-C4   | 6.76  | 1.38        | 1.33     |
| 35  | BB    | 674  | G    | C8-N7   | -6.76 | 1.26        | 1.30     |
| 35  | BB    | 1642 | G    | C6-N1   | 6.76  | 1.44        | 1.39     |
| 35  | BB    | 1723 | G    | N9-C4   | 6.76  | 1.43        | 1.38     |
| 35  | BB    | 2799 | A    | C6-N1   | 6.76  | 1.40        | 1.35     |
| 35  | BB    | 331  | C    | P-O5'   | -6.76 | 1.52        | 1.59     |
| 35  | BB    | 1237 | A    | C5-C4   | -6.76 | 1.34        | 1.38     |
| 1   | AA    | 158  | G    | N3-C4   | -6.76 | 1.30        | 1.35     |
| 1   | AA    | 261  | U    | C2-N3   | 6.76  | 1.42        | 1.37     |
| 1   | AA    | 1064 | G    | C4'-C3' | 6.76  | 1.60        | 1.53     |
| 1   | AA    | 1316 | G    | C6-N1   | -6.76 | 1.34        | 1.39     |
| 35  | BB    | 79   | C    | N3-C4   | 6.76  | 1.38        | 1.33     |
| 35  | BB    | 498  | G    | N3-C4   | 6.76  | 1.40        | 1.35     |
| 35  | BB    | 931  | U    | C5-C6   | 6.76  | 1.40        | 1.34     |
| 35  | BB    | 1973 | G    | O3'-P   | -6.76 | 1.53        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2791 | G    | C4'-O4' | 6.76  | 1.54        | 1.45     |
| 1   | AA    | 929  | G    | C6-N1   | 6.76  | 1.44        | 1.39     |
| 35  | BB    | 562  | U    | C2'-C1' | -6.76 | 1.46        | 1.53     |
| 35  | BB    | 591  | U    | C3'-O3' | 6.76  | 1.51        | 1.42     |
| 35  | BB    | 2345 | G    | C6-N1   | 6.76  | 1.44        | 1.39     |
| 35  | BB    | 2536 | G    | C8-N7   | -6.76 | 1.26        | 1.30     |
| 35  | BB    | 2826 | A    | C6-N1   | 6.76  | 1.40        | 1.35     |
| 1   | AA    | 247  | G    | N9-C8   | -6.76 | 1.33        | 1.37     |
| 13  | AM    | 89   | ARG  | NE-CZ   | 6.76  | 1.41        | 1.33     |
| 35  | BB    | 858  | G    | C5-C4   | 6.76  | 1.43        | 1.38     |
| 36  | BC    | 269  | ARG  | NE-CZ   | 6.76  | 1.41        | 1.33     |
| 1   | AA    | 48   | C    | C4-C5   | 6.76  | 1.48        | 1.43     |
| 1   | AA    | 122  | G    | N7-C5   | -6.76 | 1.35        | 1.39     |
| 1   | AA    | 213  | G    | C5-C4   | -6.76 | 1.33        | 1.38     |
| 1   | AA    | 389  | A    | C5-C4   | 6.76  | 1.43        | 1.38     |
| 13  | AM    | 69   | ARG  | CZ-NH1  | 6.76  | 1.41        | 1.33     |
| 35  | BB    | 1395 | A    | C2'-C1' | -6.76 | 1.46        | 1.53     |
| 35  | BB    | 1817 | G    | P-O5'   | -6.76 | 1.52        | 1.59     |
| 35  | BB    | 2142 | A    | O3'-P   | -6.76 | 1.53        | 1.61     |
| 35  | BB    | 2401 | U    | C4'-C3' | 6.76  | 1.60        | 1.53     |
| 35  | BB    | 941  | A    | C6-N1   | 6.75  | 1.40        | 1.35     |
| 1   | AA    | 240  | G    | C2'-C1' | -6.75 | 1.46        | 1.53     |
| 1   | AA    | 680  | C    | C2-N3   | 6.75  | 1.41        | 1.35     |
| 1   | AA    | 801  | U    | C3'-C2' | 6.75  | 1.60        | 1.52     |
| 1   | AA    | 1256 | A    | C2'-C1' | -6.75 | 1.46        | 1.53     |
| 35  | BB    | 771  | G    | C4'-C3' | -6.75 | 1.45        | 1.53     |
| 35  | BB    | 2251 | G    | N1-C2   | 6.75  | 1.43        | 1.37     |
| 1   | AA    | 1426 | G    | N7-C5   | -6.75 | 1.35        | 1.39     |
| 35  | BB    | 152  | A    | C6-N1   | 6.75  | 1.40        | 1.35     |
| 35  | BB    | 288  | U    | C4'-C3' | -6.75 | 1.45        | 1.53     |
| 35  | BB    | 384  | A    | C5'-C4' | -6.75 | 1.43        | 1.51     |
| 35  | BB    | 1853 | A    | C2-N3   | 6.75  | 1.39        | 1.33     |
| 35  | BB    | 1392 | A    | N1-C2   | 6.75  | 1.40        | 1.34     |
| 35  | BB    | 1522 | A    | N9-C4   | -6.75 | 1.33        | 1.37     |
| 35  | BB    | 2370 | G    | N7-C5   | -6.75 | 1.35        | 1.39     |
| 35  | BB    | 2608 | G    | C6-O6   | -6.75 | 1.18        | 1.24     |
| 35  | BB    | 2804 | U    | O3'-P   | -6.75 | 1.53        | 1.61     |
| 1   | AA    | 263  | A    | C8-N7   | -6.75 | 1.26        | 1.31     |
| 1   | AA    | 280  | C    | C4-C5   | 6.75  | 1.48        | 1.43     |
| 1   | AA    | 492  | C    | C4'-C3' | 6.75  | 1.60        | 1.53     |
| 1   | AA    | 788  | U    | N1-C6   | -6.75 | 1.31        | 1.38     |
| 35  | BB    | 107  | G    | C5'-C4' | 6.75  | 1.59        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 614  | A    | C2-N3   | 6.75  | 1.39        | 1.33     |
| 35  | BB    | 750  | A    | N9-C4   | 6.75  | 1.41        | 1.37     |
| 35  | BB    | 911  | A    | P-O5'   | 6.75  | 1.66        | 1.59     |
| 35  | BB    | 1791 | A    | C4'-O4' | -6.75 | 1.36        | 1.45     |
| 35  | BB    | 2357 | G    | P-O5'   | -6.75 | 1.53        | 1.59     |
| 35  | BB    | 2669 | G    | C6-N1   | 6.75  | 1.44        | 1.39     |
| 34  | BA    | 34   | A    | C2'-C1' | -6.75 | 1.46        | 1.53     |
| 35  | BB    | 400  | G    | C8-N7   | -6.75 | 1.26        | 1.30     |
| 35  | BB    | 1057 | A    | C5-C4   | -6.75 | 1.34        | 1.38     |
| 35  | BB    | 1367 | A    | C2-N3   | 6.75  | 1.39        | 1.33     |
| 35  | BB    | 1429 | G    | C2-N2   | 6.75  | 1.41        | 1.34     |
| 35  | BB    | 1460 | U    | C2-N3   | 6.75  | 1.42        | 1.37     |
| 35  | BB    | 2100 | G    | N3-C4   | -6.75 | 1.30        | 1.35     |
| 35  | BB    | 2284 | A    | C6-N6   | 6.75  | 1.39        | 1.33     |
| 35  | BB    | 2310 | C    | C2-N3   | 6.75  | 1.41        | 1.35     |
| 35  | BB    | 500  | G    | C2'-C1' | -6.75 | 1.46        | 1.53     |
| 35  | BB    | 838  | C    | N3-C4   | 6.75  | 1.38        | 1.33     |
| 1   | AA    | 267  | C    | O3'-P   | -6.74 | 1.53        | 1.61     |
| 1   | AA    | 1014 | A    | C8-N7   | -6.74 | 1.26        | 1.31     |
| 35  | BB    | 402  | A    | C3'-C2' | -6.74 | 1.45        | 1.52     |
| 35  | BB    | 533  | G    | N7-C5   | -6.74 | 1.35        | 1.39     |
| 35  | BB    | 618  | G    | P-O5'   | -6.74 | 1.53        | 1.59     |
| 35  | BB    | 632  | A    | C4'-C3' | 6.74  | 1.60        | 1.53     |
| 35  | BB    | 1517 | G    | C5-C6   | -6.74 | 1.35        | 1.42     |
| 35  | BB    | 1844 | C    | N1-C2   | -6.74 | 1.33        | 1.40     |
| 35  | BB    | 2379 | G    | C2-N3   | 6.74  | 1.38        | 1.32     |
| 35  | BB    | 2595 | G    | C6-N1   | 6.74  | 1.44        | 1.39     |
| 1   | AA    | 319  | G    | O3'-P   | -6.74 | 1.53        | 1.61     |
| 1   | AA    | 1025 | U    | N3-C4   | 6.74  | 1.44        | 1.38     |
| 1   | AA    | 1397 | C    | N1-C6   | -6.74 | 1.33        | 1.37     |
| 35  | BB    | 1843 | C    | N3-C4   | 6.74  | 1.38        | 1.33     |
| 1   | AA    | 324  | G    | C2'-C1' | -6.74 | 1.46        | 1.53     |
| 1   | AA    | 886  | G    | N7-C5   | -6.74 | 1.35        | 1.39     |
| 1   | AA    | 1369 | C    | C4'-C3' | 6.74  | 1.60        | 1.53     |
| 35  | BB    | 1370 | C    | P-O5'   | -6.74 | 1.53        | 1.59     |
| 35  | BB    | 1811 | G    | O3'-P   | -6.74 | 1.53        | 1.61     |
| 35  | BB    | 2303 | G    | N7-C5   | -6.74 | 1.35        | 1.39     |
| 35  | BB    | 2852 | G    | C2-N3   | 6.74  | 1.38        | 1.32     |
| 1   | AA    | 271  | C    | N3-C4   | 6.74  | 1.38        | 1.33     |
| 1   | AA    | 759  | A    | C6-N6   | 6.74  | 1.39        | 1.33     |
| 1   | AA    | 947  | G    | C2-N3   | 6.74  | 1.38        | 1.32     |
| 1   | AA    | 1531 | A    | C5-C6   | 6.74  | 1.47        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 61   | C    | N1-C6   | -6.74 | 1.33        | 1.37     |
| 35  | BB    | 761  | A    | C5-C4   | 6.74  | 1.43        | 1.38     |
| 35  | BB    | 1678 | A    | C4'-O4' | 6.74  | 1.54        | 1.45     |
| 35  | BB    | 2117 | A    | C6-N6   | 6.74  | 1.39        | 1.33     |
| 1   | AA    | 270  | A    | C5-C4   | 6.74  | 1.43        | 1.38     |
| 1   | AA    | 856  | C    | C5-C6   | -6.74 | 1.28        | 1.34     |
| 1   | AA    | 1408 | A    | N3-C4   | 6.74  | 1.38        | 1.34     |
| 35  | BB    | 1969 | A    | C6-N1   | 6.74  | 1.40        | 1.35     |
| 1   | AA    | 62   | U    | P-O5'   | -6.74 | 1.53        | 1.59     |
| 1   | AA    | 746  | A    | C2-N3   | 6.74  | 1.39        | 1.33     |
| 35  | BB    | 333  | G    | C8-N7   | 6.74  | 1.34        | 1.30     |
| 35  | BB    | 360  | U    | N3-C4   | 6.74  | 1.44        | 1.38     |
| 35  | BB    | 704  | G    | O3'-P   | -6.74 | 1.53        | 1.61     |
| 35  | BB    | 1249 | U    | C4'-O4' | -6.74 | 1.36        | 1.45     |
| 35  | BB    | 1254 | A    | C4'-C3' | 6.74  | 1.60        | 1.53     |
| 35  | BB    | 1935 | G    | P-O5'   | -6.73 | 1.53        | 1.59     |
| 1   | AA    | 299  | G    | C2'-C1' | -6.73 | 1.46        | 1.53     |
| 34  | BA    | 99   | A    | C5-C4   | 6.73  | 1.43        | 1.38     |
| 35  | BB    | 291  | G    | N3-C4   | -6.73 | 1.30        | 1.35     |
| 35  | BB    | 342  | A    | N9-C8   | -6.73 | 1.32        | 1.37     |
| 35  | BB    | 857  | G    | N7-C5   | -6.73 | 1.35        | 1.39     |
| 35  | BB    | 1241 | A    | N7-C5   | -6.73 | 1.35        | 1.39     |
| 35  | BB    | 1544 | A    | N3-C4   | -6.73 | 1.30        | 1.34     |
| 35  | BB    | 1737 | G    | C4'-O4' | -6.73 | 1.36        | 1.45     |
| 35  | BB    | 2177 | C    | C4'-C3' | -6.73 | 1.45        | 1.53     |
| 35  | BB    | 2331 | G    | C2-N2   | 6.73  | 1.41        | 1.34     |
| 35  | BB    | 2576 | G    | P-O5'   | -6.73 | 1.53        | 1.59     |
| 35  | BB    | 2700 | A    | N3-C4   | 6.73  | 1.38        | 1.34     |
| 35  | BB    | 2799 | A    | C2'-C1' | -6.73 | 1.46        | 1.53     |
| 1   | AA    | 22   | G    | N9-C4   | -6.73 | 1.32        | 1.38     |
| 1   | AA    | 79   | G    | C6-N1   | 6.73  | 1.44        | 1.39     |
| 1   | AA    | 859  | G    | N9-C8   | -6.73 | 1.33        | 1.37     |
| 35  | BB    | 71   | A    | C3'-C2' | 6.73  | 1.60        | 1.52     |
| 35  | BB    | 74   | A    | N9-C4   | 6.73  | 1.41        | 1.37     |
| 35  | BB    | 589  | U    | C5'-C4' | 6.73  | 1.59        | 1.51     |
| 35  | BB    | 2155 | U    | C2-N3   | 6.73  | 1.42        | 1.37     |
| 35  | BB    | 2158 | A    | N9-C8   | -6.73 | 1.32        | 1.37     |
| 35  | BB    | 2474 | U    | C3'-O3' | 6.73  | 1.51        | 1.42     |
| 1   | AA    | 28   | A    | C6-N6   | 6.73  | 1.39        | 1.33     |
| 1   | AA    | 278  | G    | N7-C5   | 6.73  | 1.43        | 1.39     |
| 1   | AA    | 1335 | U    | P-O5'   | -6.73 | 1.53        | 1.59     |
| 35  | BB    | 670  | A    | C6-N6   | 6.73  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1357 | C    | C4-N4   | 6.73  | 1.40        | 1.33     |
| 35  | BB    | 1517 | G    | P-O5'   | -6.73 | 1.53        | 1.59     |
| 1   | AA    | 310  | G    | C4'-C3' | 6.73  | 1.60        | 1.53     |
| 1   | AA    | 606  | G    | C2-N3   | 6.73  | 1.38        | 1.32     |
| 35  | BB    | 65   | U    | C2'-C1' | -6.73 | 1.46        | 1.53     |
| 35  | BB    | 91   | A    | C6-N1   | 6.73  | 1.40        | 1.35     |
| 35  | BB    | 488  | G    | N9-C8   | 6.73  | 1.42        | 1.37     |
| 35  | BB    | 799  | G    | C4'-C3' | -6.73 | 1.45        | 1.53     |
| 35  | BB    | 1601 | G    | C6-N1   | 6.73  | 1.44        | 1.39     |
| 35  | BB    | 1727 | C    | N1-C6   | 6.73  | 1.41        | 1.37     |
| 35  | BB    | 2582 | G    | O4'-C1' | 6.73  | 1.50        | 1.41     |
| 35  | BB    | 2860 | A    | N9-C4   | -6.73 | 1.33        | 1.37     |
| 1   | AA    | 251  | G    | C2-N2   | 6.73  | 1.41        | 1.34     |
| 1   | AA    | 818  | G    | C5-C4   | 6.73  | 1.43        | 1.38     |
| 1   | AA    | 969  | A    | C6-N6   | 6.73  | 1.39        | 1.33     |
| 35  | BB    | 774  | G    | C2-N3   | 6.73  | 1.38        | 1.32     |
| 35  | BB    | 2330 | G    | N7-C5   | -6.73 | 1.35        | 1.39     |
| 1   | AA    | 223  | A    | C5-C4   | 6.72  | 1.43        | 1.38     |
| 35  | BB    | 1645 | G    | O3'-P   | -6.72 | 1.53        | 1.61     |
| 35  | BB    | 2513 | A    | P-O5'   | -6.72 | 1.53        | 1.59     |
| 1   | AA    | 400  | C    | N1-C2   | -6.72 | 1.33        | 1.40     |
| 1   | AA    | 899  | C    | C2'-C1' | -6.72 | 1.46        | 1.53     |
| 35  | BB    | 281  | C    | C2-N3   | 6.72  | 1.41        | 1.35     |
| 35  | BB    | 731  | C    | C5'-C4' | 6.72  | 1.59        | 1.51     |
| 35  | BB    | 1259 | G    | C6-N1   | 6.72  | 1.44        | 1.39     |
| 35  | BB    | 1522 | A    | N7-C5   | -6.72 | 1.35        | 1.39     |
| 1   | AA    | 1094 | G    | O4'-C1' | -6.72 | 1.32        | 1.41     |
| 1   | AA    | 100  | G    | C5-C4   | 6.72  | 1.43        | 1.38     |
| 1   | AA    | 781  | A    | C2-N3   | 6.72  | 1.39        | 1.33     |
| 35  | BB    | 862  | G    | N1-C2   | 6.72  | 1.43        | 1.37     |
| 35  | BB    | 1026 | G    | C4'-O4' | -6.72 | 1.36        | 1.45     |
| 35  | BB    | 1538 | G    | N9-C4   | -6.72 | 1.32        | 1.38     |
| 35  | BB    | 2337 | G    | C6-N1   | 6.72  | 1.44        | 1.39     |
| 35  | BB    | 93   | G    | P-O5'   | 6.72  | 1.66        | 1.59     |
| 35  | BB    | 706  | A    | N3-C4   | -6.72 | 1.30        | 1.34     |
| 35  | BB    | 2147 | A    | C2'-C1' | -6.72 | 1.46        | 1.53     |
| 35  | BB    | 686  | U    | P-O5'   | -6.71 | 1.53        | 1.59     |
| 35  | BB    | 770  | G    | C6-N1   | 6.71  | 1.44        | 1.39     |
| 35  | BB    | 1156 | A    | O3'-P   | -6.71 | 1.53        | 1.61     |
| 35  | BB    | 1479 | G    | P-O5'   | -6.71 | 1.53        | 1.59     |
| 35  | BB    | 2641 | G    | P-O5'   | -6.71 | 1.53        | 1.59     |
| 1   | AA    | 134  | G    | O3'-P   | -6.71 | 1.53        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 400  | C    | N3-C4   | 6.71  | 1.38        | 1.33     |
| 4   | AD    | 61   | ARG  | NE-CZ   | 6.71  | 1.41        | 1.33     |
| 22  | AV    | 6    | C    | C4-N4   | 6.71  | 1.40        | 1.33     |
| 35  | BB    | 112  | U    | C2-N3   | 6.71  | 1.42        | 1.37     |
| 1   | AA    | 9    | G    | N9-C8   | -6.71 | 1.33        | 1.37     |
| 1   | AA    | 179  | A    | N3-C4   | -6.71 | 1.30        | 1.34     |
| 1   | AA    | 320  | A    | N3-C4   | -6.71 | 1.30        | 1.34     |
| 1   | AA    | 1331 | G    | N3-C4   | 6.71  | 1.40        | 1.35     |
| 35  | BB    | 105  | C    | C2'-C1' | -6.71 | 1.46        | 1.53     |
| 35  | BB    | 1128 | G    | C6-N1   | 6.71  | 1.44        | 1.39     |
| 35  | BB    | 1157 | G    | C8-N7   | -6.71 | 1.26        | 1.30     |
| 35  | BB    | 1509 | A    | C6-N6   | 6.71  | 1.39        | 1.33     |
| 35  | BB    | 1615 | C    | C4'-O4' | 6.71  | 1.54        | 1.45     |
| 35  | BB    | 2162 | G    | C6-N1   | 6.71  | 1.44        | 1.39     |
| 35  | BB    | 2875 | C    | P-O5'   | -6.71 | 1.53        | 1.59     |
| 36  | BC    | 81   | GLU  | N-CA    | -6.71 | 1.32        | 1.46     |
| 35  | BB    | 641  | U    | N1-C6   | -6.71 | 1.31        | 1.38     |
| 1   | AA    | 222  | C    | N1-C2   | 6.71  | 1.46        | 1.40     |
| 1   | AA    | 921  | U    | C2-N3   | 6.71  | 1.42        | 1.37     |
| 1   | AA    | 1291 | U    | C1'-N1  | 6.71  | 1.58        | 1.48     |
| 35  | BB    | 263  | G    | N1-C2   | 6.71  | 1.43        | 1.37     |
| 35  | BB    | 583  | G    | P-O5'   | -6.71 | 1.53        | 1.59     |
| 35  | BB    | 1295 | C    | O3'-P   | -6.71 | 1.53        | 1.61     |
| 7   | AG    | 114  | SER  | CA-CB   | 6.71  | 1.63        | 1.52     |
| 35  | BB    | 1136 | G    | C6-N1   | 6.71  | 1.44        | 1.39     |
| 35  | BB    | 1718 | G    | N7-C5   | 6.71  | 1.43        | 1.39     |
| 35  | BB    | 2251 | G    | C8-N7   | 6.71  | 1.34        | 1.30     |
| 1   | AA    | 1409 | C    | N1-C6   | 6.71  | 1.41        | 1.37     |
| 35  | BB    | 910  | A    | C6-N1   | 6.71  | 1.40        | 1.35     |
| 35  | BB    | 1431 | A    | N7-C5   | -6.71 | 1.35        | 1.39     |
| 1   | AA    | 499  | A    | C5-C4   | 6.70  | 1.43        | 1.38     |
| 1   | AA    | 901  | A    | N3-C4   | -6.70 | 1.30        | 1.34     |
| 35  | BB    | 192  | C    | P-O5'   | -6.70 | 1.53        | 1.59     |
| 35  | BB    | 325  | G    | C8-N7   | -6.70 | 1.26        | 1.30     |
| 35  | BB    | 1084 | A    | P-O5'   | -6.70 | 1.53        | 1.59     |
| 35  | BB    | 2256 | G    | N7-C5   | -6.70 | 1.35        | 1.39     |
| 1   | AA    | 372  | C    | C4-N4   | 6.70  | 1.40        | 1.33     |
| 1   | AA    | 595  | A    | N9-C8   | -6.70 | 1.32        | 1.37     |
| 3   | AC    | 64   | ARG  | CZ-NH1  | 6.70  | 1.41        | 1.33     |
| 35  | BB    | 2648 | G    | C6-O6   | 6.70  | 1.30        | 1.24     |
| 1   | AA    | 139  | A    | C8-N7   | 6.70  | 1.36        | 1.31     |
| 1   | AA    | 651  | C    | C2-N3   | 6.70  | 1.41        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 864  | G    | N9-C8   | -6.70 | 1.33        | 1.37     |
| 35  | BB    | 1162 | G    | N7-C5   | -6.70 | 1.35        | 1.39     |
| 35  | BB    | 1613 | G    | N7-C5   | -6.70 | 1.35        | 1.39     |
| 1   | AA    | 1325 | C    | P-O5'   | -6.70 | 1.53        | 1.59     |
| 35  | BB    | 1890 | A    | N7-C5   | -6.70 | 1.35        | 1.39     |
| 35  | BB    | 2153 | C    | C2-N3   | -6.70 | 1.30        | 1.35     |
| 35  | BB    | 833  | A    | C6-N6   | 6.70  | 1.39        | 1.33     |
| 1   | AA    | 720  | C    | C2'-C1' | -6.70 | 1.46        | 1.53     |
| 1   | AA    | 1048 | G    | O3'-P   | -6.70 | 1.53        | 1.61     |
| 34  | BA    | 7    | G    | C2-N3   | 6.70  | 1.38        | 1.32     |
| 35  | BB    | 226  | A    | O4'-C1' | -6.70 | 1.32        | 1.41     |
| 35  | BB    | 1547 | C    | N1-C6   | 6.70  | 1.41        | 1.37     |
| 35  | BB    | 39   | G    | P-O5'   | -6.69 | 1.53        | 1.59     |
| 35  | BB    | 51   | G    | N7-C5   | 6.69  | 1.43        | 1.39     |
| 35  | BB    | 2059 | A    | N9-C4   | -6.69 | 1.33        | 1.37     |
| 35  | BB    | 2876 | G    | C8-N7   | -6.69 | 1.26        | 1.30     |
| 1   | AA    | 222  | C    | C4-N4   | 6.69  | 1.40        | 1.33     |
| 1   | AA    | 276  | G    | N1-C2   | 6.69  | 1.43        | 1.37     |
| 1   | AA    | 323  | U    | C5'-C4' | 6.69  | 1.59        | 1.51     |
| 1   | AA    | 1372 | U    | C5-C6   | 6.69  | 1.40        | 1.34     |
| 35  | BB    | 495  | G    | C5-C6   | -6.69 | 1.35        | 1.42     |
| 35  | BB    | 903  | C    | C4-N4   | 6.69  | 1.40        | 1.33     |
| 35  | BB    | 1704 | C    | C4-C5   | 6.69  | 1.48        | 1.43     |
| 35  | BB    | 1978 | A    | P-O5'   | -6.69 | 1.53        | 1.59     |
| 1   | AA    | 1034 | G    | N9-C8   | 6.69  | 1.42        | 1.37     |
| 1   | AA    | 1111 | A    | C6-N6   | 6.69  | 1.39        | 1.33     |
| 35  | BB    | 11   | C    | N3-C4   | 6.69  | 1.38        | 1.33     |
| 35  | BB    | 966  | G    | C2'-C1' | -6.69 | 1.46        | 1.53     |
| 1   | AA    | 322  | C    | C4'-C3' | 6.69  | 1.60        | 1.53     |
| 35  | BB    | 725  | G    | O3'-P   | -6.69 | 1.53        | 1.61     |
| 1   | AA    | 881  | G    | C2'-C1' | -6.69 | 1.46        | 1.53     |
| 35  | BB    | 512  | G    | N1-C2   | 6.69  | 1.43        | 1.37     |
| 35  | BB    | 857  | G    | N1-C2   | 6.69  | 1.43        | 1.37     |
| 35  | BB    | 1248 | G    | N7-C5   | -6.69 | 1.35        | 1.39     |
| 35  | BB    | 1334 | G    | C2-N3   | 6.69  | 1.38        | 1.32     |
| 35  | BB    | 1586 | A    | C6-N6   | 6.69  | 1.39        | 1.33     |
| 1   | AA    | 592  | G    | C5'-C4' | 6.69  | 1.59        | 1.51     |
| 1   | AA    | 1332 | A    | C8-N7   | -6.69 | 1.26        | 1.31     |
| 1   | AA    | 1494 | G    | C2-N2   | 6.69  | 1.41        | 1.34     |
| 5   | AE    | 156  | ARG  | CD-NE   | 6.69  | 1.57        | 1.46     |
| 35  | BB    | 330  | A    | N7-C5   | -6.69 | 1.35        | 1.39     |
| 35  | BB    | 1292 | G    | N9-C8   | -6.69 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 269  | C    | C2'-C1' | -6.68 | 1.46        | 1.53     |
| 13  | AM    | 100  | ARG  | CD-NE   | 6.68  | 1.57        | 1.46     |
| 35  | BB    | 392  | U    | P-O5'   | -6.68 | 1.53        | 1.59     |
| 35  | BB    | 990  | A    | N3-C4   | -6.68 | 1.30        | 1.34     |
| 35  | BB    | 1810 | A    | C5-C4   | 6.68  | 1.43        | 1.38     |
| 35  | BB    | 1853 | A    | N9-C4   | -6.68 | 1.33        | 1.37     |
| 1   | AA    | 1323 | G    | C4'-C3' | -6.68 | 1.45        | 1.53     |
| 34  | BA    | 80   | U    | C2-N3   | 6.68  | 1.42        | 1.37     |
| 35  | BB    | 198  | C    | N1-C6   | -6.68 | 1.33        | 1.37     |
| 35  | BB    | 565  | C    | C4'-C3' | 6.68  | 1.60        | 1.53     |
| 35  | BB    | 937  | C    | C4-N4   | 6.68  | 1.40        | 1.33     |
| 35  | BB    | 1247 | A    | N3-C4   | -6.68 | 1.30        | 1.34     |
| 35  | BB    | 2006 | C    | C3'-C2' | -6.68 | 1.45        | 1.52     |
| 1   | AA    | 1336 | C    | C5'-C4' | 6.68  | 1.59        | 1.51     |
| 35  | BB    | 706  | A    | N9-C8   | 6.68  | 1.43        | 1.37     |
| 35  | BB    | 1367 | A    | O3'-P   | -6.68 | 1.53        | 1.61     |
| 1   | AA    | 50   | A    | N9-C4   | -6.68 | 1.33        | 1.37     |
| 1   | AA    | 240  | G    | N7-C5   | 6.68  | 1.43        | 1.39     |
| 1   | AA    | 400  | C    | C3'-O3' | 6.68  | 1.51        | 1.42     |
| 1   | AA    | 407  | U    | C2-N3   | 6.68  | 1.42        | 1.37     |
| 1   | AA    | 1353 | G    | N9-C4   | -6.68 | 1.32        | 1.38     |
| 35  | BB    | 858  | G    | C6-N1   | 6.68  | 1.44        | 1.39     |
| 35  | BB    | 1786 | A    | C4'-C3' | -6.68 | 1.45        | 1.53     |
| 35  | BB    | 2057 | G    | N7-C5   | -6.68 | 1.35        | 1.39     |
| 35  | BB    | 2711 | A    | N9-C4   | 6.68  | 1.41        | 1.37     |
| 1   | AA    | 505  | G    | C2-N2   | 6.68  | 1.41        | 1.34     |
| 7   | AG    | 78   | ARG  | NE-CZ   | 6.68  | 1.41        | 1.33     |
| 35  | BB    | 323  | C    | O3'-P   | -6.68 | 1.53        | 1.61     |
| 35  | BB    | 466  | A    | C5'-C4' | 6.68  | 1.59        | 1.51     |
| 35  | BB    | 1469 | A    | C5-C4   | 6.68  | 1.43        | 1.38     |
| 35  | BB    | 2151 | U    | O3'-P   | -6.68 | 1.53        | 1.61     |
| 1   | AA    | 1483 | A    | C3'-C2' | 6.68  | 1.60        | 1.52     |
| 34  | BA    | 61   | G    | C2-N2   | -6.68 | 1.27        | 1.34     |
| 35  | BB    | 587  | C    | N3-C4   | 6.68  | 1.38        | 1.33     |
| 35  | BB    | 619  | G    | C6-N1   | 6.68  | 1.44        | 1.39     |
| 35  | BB    | 839  | U    | N3-C4   | 6.68  | 1.44        | 1.38     |
| 35  | BB    | 1219 | U    | N1-C6   | 6.68  | 1.44        | 1.38     |
| 35  | BB    | 2616 | C    | C4-C5   | -6.68 | 1.37        | 1.43     |
| 1   | AA    | 1152 | A    | N7-C5   | -6.67 | 1.35        | 1.39     |
| 35  | BB    | 1077 | A    | C8-N7   | 6.67  | 1.36        | 1.31     |
| 35  | BB    | 1155 | A    | C6-N6   | 6.67  | 1.39        | 1.33     |
| 35  | BB    | 1180 | U    | C3'-C2' | -6.67 | 1.45        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1387 | A    | N9-C8   | 6.67  | 1.43        | 1.37     |
| 35  | BB    | 1652 | A    | C3'-C2' | -6.67 | 1.45        | 1.52     |
| 35  | BB    | 1663 | G    | N3-C4   | -6.67 | 1.30        | 1.35     |
| 35  | BB    | 1989 | G    | C5-C4   | 6.67  | 1.43        | 1.38     |
| 35  | BB    | 2574 | G    | C4'-O4' | 6.67  | 1.54        | 1.45     |
| 35  | BB    | 2760 | C    | C4-C5   | 6.67  | 1.48        | 1.43     |
| 1   | AA    | 969  | A    | C5-C6   | -6.67 | 1.35        | 1.41     |
| 5   | AE    | 49   | TYR  | CZ-OH   | 6.67  | 1.49        | 1.37     |
| 35  | BB    | 917  | A    | C5-C4   | -6.67 | 1.34        | 1.38     |
| 35  | BB    | 1202 | G    | C2-N2   | 6.67  | 1.41        | 1.34     |
| 35  | BB    | 2693 | G    | N7-C5   | -6.67 | 1.35        | 1.39     |
| 35  | BB    | 150  | U    | P-O5'   | -6.67 | 1.53        | 1.59     |
| 35  | BB    | 2038 | G    | C8-N7   | 6.67  | 1.34        | 1.30     |
| 1   | AA    | 81   | A    | C6-N6   | 6.67  | 1.39        | 1.33     |
| 22  | AV    | 7    | G    | N9-C8   | 6.67  | 1.42        | 1.37     |
| 1   | AA    | 337  | G    | C4'-C3' | 6.67  | 1.60        | 1.53     |
| 1   | AA    | 1253 | G    | C6-N1   | 6.67  | 1.44        | 1.39     |
| 35  | BB    | 473  | G    | C2-N3   | 6.67  | 1.38        | 1.32     |
| 35  | BB    | 1373 | A    | C2'-C1' | -6.67 | 1.46        | 1.53     |
| 35  | BB    | 1435 | G    | C2-N3   | 6.67  | 1.38        | 1.32     |
| 35  | BB    | 2777 | G    | C6-N1   | 6.67  | 1.44        | 1.39     |
| 34  | BA    | 41   | G    | N9-C8   | 6.67  | 1.42        | 1.37     |
| 35  | BB    | 647  | G    | C2-N3   | -6.67 | 1.27        | 1.32     |
| 35  | BB    | 1099 | G    | C6-N1   | 6.67  | 1.44        | 1.39     |
| 35  | BB    | 1345 | C    | P-O5'   | -6.67 | 1.53        | 1.59     |
| 35  | BB    | 2035 | G    | C2'-C1' | -6.67 | 1.46        | 1.53     |
| 35  | BB    | 2184 | A    | C8-N7   | -6.67 | 1.26        | 1.31     |
| 1   | AA    | 530  | G    | P-O5'   | -6.67 | 1.53        | 1.59     |
| 1   | AA    | 1480 | A    | N7-C5   | 6.67  | 1.43        | 1.39     |
| 1   | AA    | 102  | G    | N9-C8   | -6.66 | 1.33        | 1.37     |
| 1   | AA    | 467  | U    | N1-C2   | -6.66 | 1.32        | 1.38     |
| 1   | AA    | 1045 | C    | N1-C6   | 6.66  | 1.41        | 1.37     |
| 35  | BB    | 952  | G    | N7-C5   | -6.66 | 1.35        | 1.39     |
| 35  | BB    | 1935 | G    | N3-C4   | -6.66 | 1.30        | 1.35     |
| 35  | BB    | 2145 | C    | C4-N4   | 6.66  | 1.40        | 1.33     |
| 35  | BB    | 2437 | G    | N9-C8   | -6.66 | 1.33        | 1.37     |
| 1   | AA    | 386  | C    | C4-N4   | 6.66  | 1.40        | 1.33     |
| 35  | BB    | 1062 | G    | C2-N3   | 6.66  | 1.38        | 1.32     |
| 35  | BB    | 2717 | C    | C4-C5   | -6.66 | 1.37        | 1.43     |
| 1   | AA    | 227  | G    | C5'-C4' | 6.66  | 1.59        | 1.51     |
| 47  | BN    | 45   | ARG  | CD-NE   | 6.66  | 1.57        | 1.46     |
| 1   | AA    | 326  | G    | C2-N3   | 6.66  | 1.38        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1733 | G    | N3-C4   | -6.66 | 1.30        | 1.35     |
| 1   | AA    | 1066 | C    | C4-C5   | -6.66 | 1.37        | 1.43     |
| 1   | AA    | 1115 | U    | P-O5'   | -6.66 | 1.53        | 1.59     |
| 35  | BB    | 2100 | G    | C2-N3   | 6.66  | 1.38        | 1.32     |
| 1   | AA    | 225  | C    | C2'-C1' | -6.66 | 1.46        | 1.53     |
| 1   | AA    | 925  | G    | P-O5'   | -6.66 | 1.53        | 1.59     |
| 35  | BB    | 127  | A    | N3-C4   | -6.66 | 1.30        | 1.34     |
| 35  | BB    | 529  | A    | C6-N1   | 6.66  | 1.40        | 1.35     |
| 35  | BB    | 1454 | C    | C4'-C3' | -6.66 | 1.45        | 1.53     |
| 35  | BB    | 1907 | G    | C5-C4   | 6.66  | 1.43        | 1.38     |
| 35  | BB    | 2579 | C    | C5'-C4' | 6.66  | 1.59        | 1.51     |
| 35  | BB    | 2709 | G    | N3-C4   | -6.66 | 1.30        | 1.35     |
| 1   | AA    | 513  | C    | C4-N4   | 6.65  | 1.40        | 1.33     |
| 1   | AA    | 669  | G    | C8-N7   | -6.65 | 1.26        | 1.30     |
| 35  | BB    | 796  | C    | C2'-C1' | -6.65 | 1.46        | 1.53     |
| 35  | BB    | 1347 | A    | N3-C4   | -6.65 | 1.30        | 1.34     |
| 35  | BB    | 1385 | A    | N9-C4   | 6.65  | 1.41        | 1.37     |
| 48  | BO    | 16   | ARG  | CD-NE   | 6.65  | 1.57        | 1.46     |
| 1   | AA    | 98   | A    | C6-N1   | 6.65  | 1.40        | 1.35     |
| 35  | BB    | 382  | A    | O3'-P   | -6.65 | 1.53        | 1.61     |
| 35  | BB    | 1442 | U    | C5'-C4' | 6.65  | 1.59        | 1.51     |
| 35  | BB    | 1473 | G    | O4'-C1' | 6.65  | 1.50        | 1.41     |
| 35  | BB    | 1807 | G    | N1-C2   | 6.65  | 1.43        | 1.37     |
| 35  | BB    | 2136 | G    | C5-C4   | 6.65  | 1.43        | 1.38     |
| 35  | BB    | 2495 | G    | N3-C4   | -6.65 | 1.30        | 1.35     |
| 34  | BA    | 99   | A    | C8-N7   | -6.65 | 1.26        | 1.31     |
| 35  | BB    | 147  | C    | N1-C6   | -6.65 | 1.33        | 1.37     |
| 35  | BB    | 232  | G    | N9-C8   | -6.65 | 1.33        | 1.37     |
| 35  | BB    | 340  | A    | C5-C4   | 6.65  | 1.43        | 1.38     |
| 35  | BB    | 760  | G    | N9-C4   | 6.65  | 1.43        | 1.38     |
| 37  | BD    | 83   | ARG  | NE-CZ   | 6.65  | 1.41        | 1.33     |
| 1   | AA    | 156  | C    | O3'-P   | -6.65 | 1.53        | 1.61     |
| 35  | BB    | 84   | A    | N9-C4   | -6.65 | 1.33        | 1.37     |
| 35  | BB    | 1637 | A    | C2'-C1' | -6.65 | 1.46        | 1.53     |
| 35  | BB    | 1959 | G    | N1-C2   | 6.65  | 1.43        | 1.37     |
| 1   | AA    | 383  | A    | O3'-P   | -6.65 | 1.53        | 1.61     |
| 1   | AA    | 617  | G    | C6-O6   | -6.65 | 1.18        | 1.24     |
| 1   | AA    | 1523 | G    | C5-C4   | -6.65 | 1.33        | 1.38     |
| 35  | BB    | 1272 | A    | N3-C4   | 6.65  | 1.38        | 1.34     |
| 35  | BB    | 1499 | C    | P-O5'   | -6.65 | 1.53        | 1.59     |
| 35  | BB    | 1661 | G    | P-O5'   | -6.65 | 1.53        | 1.59     |
| 35  | BB    | 1667 | G    | N9-C4   | -6.65 | 1.32        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2291 | U    | C5'-C4' | 6.65  | 1.59        | 1.51     |
| 35  | BB    | 2598 | A    | N9-C4   | -6.65 | 1.33        | 1.37     |
| 1   | AA    | 864  | A    | N3-C4   | -6.65 | 1.30        | 1.34     |
| 35  | BB    | 2257 | U    | N1-C6   | 6.65  | 1.44        | 1.38     |
| 35  | BB    | 2861 | U    | C2'-C1' | -6.65 | 1.46        | 1.53     |
| 1   | AA    | 305  | G    | N7-C5   | -6.64 | 1.35        | 1.39     |
| 1   | AA    | 370  | C    | O3'-P   | -6.64 | 1.53        | 1.61     |
| 1   | AA    | 1008 | U    | C4-C5   | 6.64  | 1.49        | 1.43     |
| 35  | BB    | 444  | C    | C2'-O2' | 6.64  | 1.50        | 1.41     |
| 35  | BB    | 568  | U    | P-O5'   | -6.64 | 1.53        | 1.59     |
| 35  | BB    | 1666 | G    | O4'-C1' | -6.64 | 1.33        | 1.41     |
| 35  | BB    | 2618 | G    | N1-C2   | 6.64  | 1.43        | 1.37     |
| 1   | AA    | 160  | A    | C2'-C1' | -6.64 | 1.46        | 1.53     |
| 1   | AA    | 470  | C    | N3-C4   | 6.64  | 1.38        | 1.33     |
| 1   | AA    | 681  | A    | C5'-C4' | 6.64  | 1.59        | 1.51     |
| 1   | AA    | 1128 | C    | C4-N4   | 6.64  | 1.40        | 1.33     |
| 1   | AA    | 1450 | U    | C5'-C4' | 6.64  | 1.59        | 1.51     |
| 34  | BA    | 28   | C    | N3-C4   | 6.64  | 1.38        | 1.33     |
| 35  | BB    | 297  | G    | N3-C4   | -6.64 | 1.30        | 1.35     |
| 35  | BB    | 301  | G    | C2-N3   | 6.64  | 1.38        | 1.32     |
| 35  | BB    | 726  | G    | C5-C6   | 6.64  | 1.49        | 1.42     |
| 35  | BB    | 1533 | C    | C5'-C4' | 6.64  | 1.59        | 1.51     |
| 35  | BB    | 1677 | A    | C3'-O3' | 6.64  | 1.51        | 1.42     |
| 35  | BB    | 2832 | U    | N1-C6   | 6.64  | 1.44        | 1.38     |
| 1   | AA    | 60   | A    | P-O5'   | -6.64 | 1.53        | 1.59     |
| 35  | BB    | 1168 | G    | N7-C5   | -6.64 | 1.35        | 1.39     |
| 35  | BB    | 1480 | C    | N3-C4   | 6.64  | 1.38        | 1.33     |
| 1   | AA    | 498  | A    | N7-C5   | -6.64 | 1.35        | 1.39     |
| 1   | AA    | 608  | A    | P-O5'   | -6.64 | 1.53        | 1.59     |
| 1   | AA    | 1316 | G    | N3-C4   | 6.64  | 1.40        | 1.35     |
| 35  | BB    | 753  | A    | N9-C4   | 6.64  | 1.41        | 1.37     |
| 35  | BB    | 1091 | G    | C6-N1   | 6.64  | 1.44        | 1.39     |
| 35  | BB    | 1695 | G    | N1-C2   | 6.64  | 1.43        | 1.37     |
| 35  | BB    | 1941 | C    | C5-C6   | 6.64  | 1.39        | 1.34     |
| 35  | BB    | 2023 | C    | C4-N4   | 6.64  | 1.40        | 1.33     |
| 35  | BB    | 2868 | A    | N9-C4   | -6.64 | 1.33        | 1.37     |
| 1   | AA    | 583  | A    | N9-C4   | 6.64  | 1.41        | 1.37     |
| 1   | AA    | 1169 | A    | C8-N7   | -6.64 | 1.26        | 1.31     |
| 1   | AA    | 1440 | U    | O3'-P   | -6.64 | 1.53        | 1.61     |
| 35  | BB    | 260  | G    | C6-N1   | 6.64  | 1.44        | 1.39     |
| 35  | BB    | 2281 | A    | C8-N7   | -6.64 | 1.26        | 1.31     |
| 1   | AA    | 583  | A    | C2'-C1' | -6.64 | 1.46        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 890  | G    | C5-C6   | -6.64 | 1.35        | 1.42     |
| 1   | AA    | 1176 | A    | C5-C4   | 6.64  | 1.43        | 1.38     |
| 1   | AA    | 1268 | G    | C5-C4   | 6.64  | 1.43        | 1.38     |
| 34  | BA    | 9    | G    | N1-C2   | 6.64  | 1.43        | 1.37     |
| 35  | BB    | 121  | G    | C2-N2   | 6.64  | 1.41        | 1.34     |
| 35  | BB    | 745  | G    | C8-N7   | -6.64 | 1.26        | 1.30     |
| 35  | BB    | 1863 | G    | N9-C8   | -6.64 | 1.33        | 1.37     |
| 35  | BB    | 2640 | G    | C6-O6   | -6.64 | 1.18        | 1.24     |
| 1   | AA    | 482  | A    | C6-N6   | 6.63  | 1.39        | 1.33     |
| 22  | AV    | 71   | C    | C4'-O4' | 6.63  | 1.54        | 1.45     |
| 35  | BB    | 1115 | G    | O3'-P   | -6.63 | 1.53        | 1.61     |
| 35  | BB    | 1532 | A    | N9-C4   | -6.63 | 1.33        | 1.37     |
| 35  | BB    | 1936 | A    | C6-N1   | 6.63  | 1.40        | 1.35     |
| 35  | BB    | 2423 | U    | C5'-C4' | 6.63  | 1.59        | 1.51     |
| 35  | BB    | 2887 | A    | C6-N1   | 6.63  | 1.40        | 1.35     |
| 35  | BB    | 748  | G    | O3'-P   | -6.63 | 1.53        | 1.61     |
| 35  | BB    | 991  | C    | C4'-O4' | 6.63  | 1.54        | 1.45     |
| 35  | BB    | 1447 | C    | N1-C2   | 6.63  | 1.46        | 1.40     |
| 35  | BB    | 1982 | U    | O3'-P   | 6.63  | 1.69        | 1.61     |
| 1   | AA    | 623  | C    | P-O5'   | -6.63 | 1.53        | 1.59     |
| 34  | BA    | 46   | A    | C3'-C2' | -6.63 | 1.45        | 1.52     |
| 35  | BB    | 1979 | U    | C4'-C3' | 6.63  | 1.60        | 1.53     |
| 35  | BB    | 2432 | A    | N7-C5   | -6.63 | 1.35        | 1.39     |
| 35  | BB    | 2600 | A    | C5-C4   | 6.63  | 1.43        | 1.38     |
| 35  | BB    | 2641 | G    | N1-C2   | 6.63  | 1.43        | 1.37     |
| 35  | BB    | 2771 | C    | C2-N3   | 6.63  | 1.41        | 1.35     |
| 40  | BG    | 51   | PHE  | CB-CG   | -6.63 | 1.40        | 1.51     |
| 34  | BA    | 84   | G    | C2-N3   | 6.63  | 1.38        | 1.32     |
| 35  | BB    | 496  | G    | N7-C5   | -6.63 | 1.35        | 1.39     |
| 35  | BB    | 1666 | G    | C5'-C4' | 6.63  | 1.59        | 1.51     |
| 1   | AA    | 1064 | G    | C6-N1   | 6.63  | 1.44        | 1.39     |
| 1   | AA    | 1200 | C    | C4-C5   | -6.63 | 1.37        | 1.43     |
| 35  | BB    | 74   | A    | C6-N6   | 6.63  | 1.39        | 1.33     |
| 35  | BB    | 504  | A    | N9-C8   | 6.63  | 1.43        | 1.37     |
| 35  | BB    | 1136 | G    | C2'-C1' | -6.63 | 1.46        | 1.53     |
| 35  | BB    | 1775 | U    | C5'-C4' | 6.63  | 1.59        | 1.51     |
| 35  | BB    | 2799 | A    | N9-C8   | -6.63 | 1.32        | 1.37     |
| 1   | AA    | 62   | U    | C5-C6   | 6.63  | 1.40        | 1.34     |
| 1   | AA    | 400  | C    | C4-C5   | 6.63  | 1.48        | 1.43     |
| 1   | AA    | 1280 | A    | C8-N7   | -6.63 | 1.26        | 1.31     |
| 35  | BB    | 312  | G    | C2-N2   | 6.63  | 1.41        | 1.34     |
| 35  | BB    | 900  | A    | C6-N1   | 6.63  | 1.40        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1667 | G    | N7-C5   | -6.63 | 1.35        | 1.39     |
| 35  | BB    | 1745 | A    | C6-N1   | 6.63  | 1.40        | 1.35     |
| 35  | BB    | 1965 | C    | C3'-O3' | 6.63  | 1.51        | 1.42     |
| 35  | BB    | 2048 | G    | C5-C4   | -6.63 | 1.33        | 1.38     |
| 35  | BB    | 2318 | G    | C6-O6   | -6.63 | 1.18        | 1.24     |
| 1   | AA    | 1014 | A    | C5'-C4' | 6.62  | 1.59        | 1.51     |
| 1   | AA    | 1188 | A    | N9-C8   | 6.62  | 1.43        | 1.37     |
| 35  | BB    | 2249 | U    | O3'-P   | -6.62 | 1.53        | 1.61     |
| 35  | BB    | 2749 | A    | O3'-P   | -6.62 | 1.53        | 1.61     |
| 36  | BC    | 220  | ARG  | CD-NE   | 6.62  | 1.57        | 1.46     |
| 1   | AA    | 1423 | G    | P-O5'   | -6.62 | 1.53        | 1.59     |
| 35  | BB    | 555  | G    | C4'-O4' | -6.62 | 1.36        | 1.45     |
| 35  | BB    | 2326 | C    | O3'-P   | -6.62 | 1.53        | 1.61     |
| 35  | BB    | 2473 | U    | C2-N3   | 6.62  | 1.42        | 1.37     |
| 1   | AA    | 473  | U    | N3-C4   | 6.62  | 1.44        | 1.38     |
| 1   | AA    | 714  | G    | C2-N3   | 6.62  | 1.38        | 1.32     |
| 28  | B3    | 49   | ARG  | NE-CZ   | 6.62  | 1.41        | 1.33     |
| 35  | BB    | 1391 | U    | N3-C4   | 6.62  | 1.44        | 1.38     |
| 35  | BB    | 1452 | G    | C5-C4   | -6.62 | 1.33        | 1.38     |
| 35  | BB    | 1537 | G    | C8-N7   | -6.62 | 1.26        | 1.30     |
| 35  | BB    | 2613 | U    | O3'-P   | -6.62 | 1.53        | 1.61     |
| 35  | BB    | 2823 | A    | O3'-P   | -6.62 | 1.53        | 1.61     |
| 47  | BN    | 90   | ARG  | CZ-NH2  | 6.62  | 1.41        | 1.33     |
| 35  | BB    | 342  | A    | N3-C4   | -6.62 | 1.30        | 1.34     |
| 35  | BB    | 691  | C    | C5'-C4' | 6.62  | 1.59        | 1.51     |
| 35  | BB    | 2742 | G    | C6-N1   | 6.62  | 1.44        | 1.39     |
| 35  | BB    | 152  | A    | N9-C8   | -6.62 | 1.32        | 1.37     |
| 35  | BB    | 345  | A    | C2-N3   | 6.62  | 1.39        | 1.33     |
| 35  | BB    | 406  | G    | N7-C5   | -6.62 | 1.35        | 1.39     |
| 35  | BB    | 2803 | G    | C6-N1   | 6.62  | 1.44        | 1.39     |
| 1   | AA    | 299  | G    | N1-C2   | 6.62  | 1.43        | 1.37     |
| 1   | AA    | 1068 | G    | C2-N3   | 6.62  | 1.38        | 1.32     |
| 29  | B4    | 19   | PHE  | CG-CD1  | 6.62  | 1.48        | 1.38     |
| 35  | BB    | 324  | A    | N3-C4   | -6.62 | 1.30        | 1.34     |
| 35  | BB    | 194  | G    | C2'-O2' | -6.62 | 1.33        | 1.41     |
| 35  | BB    | 1422 | G    | C2-N2   | 6.62  | 1.41        | 1.34     |
| 1   | AA    | 560  | A    | C5-C4   | -6.61 | 1.34        | 1.38     |
| 1   | AA    | 851  | G    | C3'-C2' | -6.61 | 1.45        | 1.52     |
| 1   | AA    | 1341 | U    | C5'-C4' | 6.61  | 1.59        | 1.51     |
| 35  | BB    | 766  | U    | N1-C6   | -6.61 | 1.31        | 1.38     |
| 35  | BB    | 974  | G    | C2-N2   | 6.61  | 1.41        | 1.34     |
| 35  | BB    | 1540 | G    | C5'-C4' | 6.61  | 1.59        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1710 | G    | C6-N1   | 6.61  | 1.44        | 1.39     |
| 35  | BB    | 1900 | A    | C2-N3   | 6.61  | 1.39        | 1.33     |
| 35  | BB    | 2896 | C    | N3-C4   | 6.61  | 1.38        | 1.33     |
| 35  | BB    | 266  | G    | C6-N1   | -6.61 | 1.34        | 1.39     |
| 35  | BB    | 1450 | G    | C6-N1   | 6.61  | 1.44        | 1.39     |
| 35  | BB    | 2281 | A    | N9-C4   | -6.61 | 1.33        | 1.37     |
| 35  | BB    | 2280 | G    | C5-C4   | 6.61  | 1.43        | 1.38     |
| 34  | BA    | 95   | U    | N1-C2   | 6.61  | 1.44        | 1.38     |
| 35  | BB    | 1530 | G    | C8-N7   | -6.61 | 1.26        | 1.30     |
| 35  | BB    | 2820 | A    | C2'-C1' | -6.61 | 1.46        | 1.53     |
| 1   | AA    | 1057 | G    | N7-C5   | -6.61 | 1.35        | 1.39     |
| 1   | AA    | 1168 | U    | C5'-C4' | 6.61  | 1.59        | 1.51     |
| 1   | AA    | 1235 | U    | N1-C2   | 6.61  | 1.44        | 1.38     |
| 35  | BB    | 688  | U    | C5'-C4' | 6.61  | 1.59        | 1.51     |
| 35  | BB    | 752  | A    | C2'-C1' | -6.61 | 1.46        | 1.53     |
| 35  | BB    | 988  | A    | C5-C6   | 6.61  | 1.47        | 1.41     |
| 35  | BB    | 993  | G    | C8-N7   | 6.61  | 1.34        | 1.30     |
| 35  | BB    | 1116 | G    | C5-C4   | 6.61  | 1.43        | 1.38     |
| 35  | BB    | 2571 | U    | C2-N3   | 6.61  | 1.42        | 1.37     |
| 35  | BB    | 2644 | G    | N7-C5   | -6.61 | 1.35        | 1.39     |
| 1   | AA    | 219  | U    | C2'-C1' | -6.61 | 1.46        | 1.53     |
| 1   | AA    | 394  | G    | N9-C8   | 6.61  | 1.42        | 1.37     |
| 1   | AA    | 997  | U    | C4'-C3' | -6.61 | 1.45        | 1.53     |
| 1   | AA    | 1473 | G    | O3'-P   | -6.61 | 1.53        | 1.61     |
| 35  | BB    | 470  | A    | C5'-C4' | 6.61  | 1.59        | 1.51     |
| 35  | BB    | 900  | A    | C3'-O3' | 6.61  | 1.51        | 1.42     |
| 35  | BB    | 945  | A    | C5'-C4' | 6.61  | 1.59        | 1.51     |
| 35  | BB    | 1035 | U    | N3-C4   | 6.61  | 1.44        | 1.38     |
| 35  | BB    | 1437 | C    | C4'-C3' | -6.61 | 1.45        | 1.53     |
| 35  | BB    | 1505 | A    | P-O5'   | -6.61 | 1.53        | 1.59     |
| 35  | BB    | 1604 | C    | C5'-C4' | 6.61  | 1.59        | 1.51     |
| 35  | BB    | 1775 | U    | N3-C4   | 6.61  | 1.44        | 1.38     |
| 35  | BB    | 484  | C    | C4-N4   | 6.60  | 1.39        | 1.33     |
| 1   | AA    | 215  | C    | O4'-C1' | -6.60 | 1.33        | 1.41     |
| 1   | AA    | 234  | C    | N1-C6   | 6.60  | 1.41        | 1.37     |
| 1   | AA    | 378  | G    | C4'-C3' | 6.60  | 1.60        | 1.53     |
| 35  | BB    | 920  | A    | C5-C4   | -6.60 | 1.34        | 1.38     |
| 35  | BB    | 1266 | G    | N9-C8   | 6.60  | 1.42        | 1.37     |
| 35  | BB    | 1321 | A    | C6-N6   | 6.60  | 1.39        | 1.33     |
| 1   | AA    | 347  | G    | C2-N3   | 6.60  | 1.38        | 1.32     |
| 1   | AA    | 373  | A    | C6-N6   | -6.60 | 1.28        | 1.33     |
| 1   | AA    | 415  | A    | C8-N7   | -6.60 | 1.26        | 1.31     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 439  | U    | N3-C4   | 6.60  | 1.44        | 1.38     |
| 1   | AA    | 337  | G    | O3'-P   | -6.60 | 1.53        | 1.61     |
| 1   | AA    | 971  | G    | C6-N1   | 6.60  | 1.44        | 1.39     |
| 22  | AV    | 37   | G    | C5-C4   | -6.60 | 1.33        | 1.38     |
| 35  | BB    | 391  | A    | C6-N1   | 6.60  | 1.40        | 1.35     |
| 35  | BB    | 727  | A    | N7-C5   | -6.60 | 1.35        | 1.39     |
| 35  | BB    | 758  | C    | C5-C6   | 6.60  | 1.39        | 1.34     |
| 35  | BB    | 1378 | A    | N9-C8   | -6.60 | 1.32        | 1.37     |
| 35  | BB    | 1875 | G    | N1-C2   | 6.60  | 1.43        | 1.37     |
| 39  | BF    | 99   | PHE  | CB-CG   | -6.60 | 1.40        | 1.51     |
| 1   | AA    | 649  | A    | N9-C4   | -6.60 | 1.33        | 1.37     |
| 1   | AA    | 1231 | G    | C5-C6   | -6.60 | 1.35        | 1.42     |
| 35  | BB    | 139  | U    | N1-C6   | 6.60  | 1.43        | 1.38     |
| 35  | BB    | 997  | G    | N7-C5   | -6.60 | 1.35        | 1.39     |
| 35  | BB    | 1360 | G    | N3-C4   | -6.60 | 1.30        | 1.35     |
| 1   | AA    | 445  | G    | O3'-P   | -6.60 | 1.53        | 1.61     |
| 1   | AA    | 927  | G    | C8-N7   | -6.60 | 1.26        | 1.30     |
| 35  | BB    | 156  | A    | C2'-C1' | -6.60 | 1.46        | 1.53     |
| 1   | AA    | 684  | U    | C2-N3   | 6.59  | 1.42        | 1.37     |
| 1   | AA    | 1033 | G    | C2'-C1' | -6.59 | 1.46        | 1.53     |
| 1   | AA    | 1219 | A    | N3-C4   | -6.59 | 1.30        | 1.34     |
| 35  | BB    | 104  | A    | C2-N3   | 6.59  | 1.39        | 1.33     |
| 35  | BB    | 243  | U    | C4-C5   | -6.59 | 1.37        | 1.43     |
| 35  | BB    | 940  | G    | C8-N7   | -6.59 | 1.26        | 1.30     |
| 35  | BB    | 1431 | A    | C6-N1   | 6.59  | 1.40        | 1.35     |
| 35  | BB    | 1826 | G    | N7-C5   | -6.59 | 1.35        | 1.39     |
| 35  | BB    | 1903 | G    | N7-C5   | -6.59 | 1.35        | 1.39     |
| 35  | BB    | 2067 | G    | N7-C5   | -6.59 | 1.35        | 1.39     |
| 1   | AA    | 696  | A    | C5-C4   | -6.59 | 1.34        | 1.38     |
| 35  | BB    | 320  | A    | C8-N7   | -6.59 | 1.26        | 1.31     |
| 1   | AA    | 517  | G    | C5'-C4' | 6.59  | 1.59        | 1.51     |
| 1   | AA    | 557  | G    | C6-N1   | 6.59  | 1.44        | 1.39     |
| 35  | BB    | 109  | C    | P-O5'   | -6.59 | 1.53        | 1.59     |
| 35  | BB    | 1756 | G    | N1-C2   | 6.59  | 1.43        | 1.37     |
| 35  | BB    | 1767 | G    | C6-N1   | 6.59  | 1.44        | 1.39     |
| 35  | BB    | 2061 | G    | N7-C5   | -6.59 | 1.35        | 1.39     |
| 35  | BB    | 2533 | U    | N1-C6   | 6.59  | 1.43        | 1.38     |
| 35  | BB    | 2802 | G    | C5'-C4' | 6.59  | 1.59        | 1.51     |
| 1   | AA    | 641  | U    | C2-N3   | 6.59  | 1.42        | 1.37     |
| 1   | AA    | 945  | G    | O3'-P   | -6.59 | 1.53        | 1.61     |
| 1   | AA    | 1136 | C    | C2-N3   | 6.59  | 1.41        | 1.35     |
| 35  | BB    | 1455 | G    | N1-C2   | 6.59  | 1.43        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2194 | U    | N3-C4   | 6.59  | 1.44        | 1.38     |
| 35  | BB    | 1742 | U    | C2-N3   | 6.59  | 1.42        | 1.37     |
| 35  | BB    | 1913 | A    | C2-N3   | -6.59 | 1.27        | 1.33     |
| 35  | BB    | 2699 | C    | N3-C4   | 6.59  | 1.38        | 1.33     |
| 35  | BB    | 2815 | C    | C2'-C1' | -6.59 | 1.46        | 1.53     |
| 1   | AA    | 1488 | G    | C4'-O4' | -6.59 | 1.36        | 1.45     |
| 35  | BB    | 675  | A    | P-O5'   | -6.59 | 1.53        | 1.59     |
| 35  | BB    | 745  | G    | N7-C5   | 6.59  | 1.43        | 1.39     |
| 35  | BB    | 1001 | A    | N9-C8   | 6.59  | 1.43        | 1.37     |
| 35  | BB    | 1878 | G    | C2'-C1' | -6.59 | 1.46        | 1.53     |
| 35  | BB    | 2670 | A    | N9-C8   | -6.59 | 1.32        | 1.37     |
| 35  | BB    | 2125 | G    | C5'-C4' | 6.58  | 1.59        | 1.51     |
| 1   | AA    | 80   | A    | N3-C4   | -6.58 | 1.30        | 1.34     |
| 1   | AA    | 1423 | G    | C2-N2   | 6.58  | 1.41        | 1.34     |
| 35  | BB    | 229  | C    | C4'-C3' | -6.58 | 1.46        | 1.53     |
| 35  | BB    | 1187 | G    | C2-N3   | 6.58  | 1.38        | 1.32     |
| 35  | BB    | 2569 | G    | C2'-C1' | -6.58 | 1.46        | 1.53     |
| 1   | AA    | 129  | A    | C6-N6   | 6.58  | 1.39        | 1.33     |
| 35  | BB    | 267  | C    | O3'-P   | -6.58 | 1.53        | 1.61     |
| 35  | BB    | 1300 | G    | O4'-C1' | -6.58 | 1.33        | 1.41     |
| 35  | BB    | 1694 | C    | C4-N4   | 6.58  | 1.39        | 1.33     |
| 35  | BB    | 1745 | A    | C4'-O4' | 6.58  | 1.54        | 1.45     |
| 35  | BB    | 1815 | A    | C6-N6   | 6.58  | 1.39        | 1.33     |
| 35  | BB    | 1861 | G    | C2-N3   | 6.58  | 1.38        | 1.32     |
| 35  | BB    | 2336 | A    | C6-N1   | 6.58  | 1.40        | 1.35     |
| 35  | BB    | 2674 | G    | C5-C6   | -6.58 | 1.35        | 1.42     |
| 1   | AA    | 145  | G    | C2-N3   | 6.58  | 1.38        | 1.32     |
| 1   | AA    | 1057 | G    | N3-C4   | -6.58 | 1.30        | 1.35     |
| 35  | BB    | 43   | G    | N7-C5   | -6.58 | 1.35        | 1.39     |
| 35  | BB    | 714  | U    | C3'-C2' | -6.58 | 1.45        | 1.52     |
| 35  | BB    | 2136 | G    | N7-C5   | -6.58 | 1.35        | 1.39     |
| 35  | BB    | 240  | C    | O3'-P   | -6.58 | 1.53        | 1.61     |
| 35  | BB    | 793  | A    | C6-N1   | 6.58  | 1.40        | 1.35     |
| 35  | BB    | 1166 | G    | C2-N3   | 6.58  | 1.38        | 1.32     |
| 35  | BB    | 1271 | G    | N3-C4   | -6.58 | 1.30        | 1.35     |
| 35  | BB    | 2108 | A    | N1-C2   | 6.58  | 1.40        | 1.34     |
| 35  | BB    | 2383 | G    | C6-N1   | 6.58  | 1.44        | 1.39     |
| 35  | BB    | 2504 | U    | N3-C4   | 6.58  | 1.44        | 1.38     |
| 35  | BB    | 2631 | G    | N7-C5   | -6.58 | 1.35        | 1.39     |
| 1   | AA    | 1012 | A    | C6-N1   | 6.58  | 1.40        | 1.35     |
| 35  | BB    | 945  | A    | C2'-C1' | -6.58 | 1.46        | 1.53     |
| 52  | BS    | 88   | ARG  | CZ-NH2  | 6.58  | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 257  | G    | N7-C5   | -6.58 | 1.35        | 1.39     |
| 1   | AA    | 459  | A    | N3-C4   | 6.58  | 1.38        | 1.34     |
| 35  | BB    | 7    | G    | C2'-C1' | -6.58 | 1.46        | 1.53     |
| 35  | BB    | 901  | C    | P-O5'   | -6.58 | 1.53        | 1.59     |
| 35  | BB    | 1628 | G    | N1-C2   | 6.58  | 1.43        | 1.37     |
| 35  | BB    | 2005 | A    | C5'-C4' | 6.58  | 1.59        | 1.51     |
| 35  | BB    | 2339 | C    | C4-N4   | 6.58  | 1.39        | 1.33     |
| 1   | AA    | 1196 | A    | C5'-C4' | 6.57  | 1.59        | 1.51     |
| 35  | BB    | 247  | G    | O4'-C1' | -6.57 | 1.33        | 1.41     |
| 35  | BB    | 1046 | A    | C5-C4   | 6.57  | 1.43        | 1.38     |
| 35  | BB    | 1379 | U    | P-O5'   | -6.57 | 1.53        | 1.59     |
| 35  | BB    | 1613 | G    | N9-C8   | 6.57  | 1.42        | 1.37     |
| 35  | BB    | 2280 | G    | C3'-C2' | -6.57 | 1.45        | 1.52     |
| 35  | BB    | 2392 | A    | C6-N6   | 6.57  | 1.39        | 1.33     |
| 1   | AA    | 203  | G    | C6-N1   | 6.57  | 1.44        | 1.39     |
| 1   | AA    | 1503 | A    | C6-N6   | 6.57  | 1.39        | 1.33     |
| 35  | BB    | 570  | G    | C2'-C1' | -6.57 | 1.46        | 1.53     |
| 35  | BB    | 1963 | U    | C3'-C2' | 6.57  | 1.60        | 1.52     |
| 35  | BB    | 219  | A    | C5-C6   | 6.57  | 1.47        | 1.41     |
| 35  | BB    | 227  | A    | N9-C8   | -6.57 | 1.32        | 1.37     |
| 35  | BB    | 1041 | G    | N1-C2   | 6.57  | 1.43        | 1.37     |
| 35  | BB    | 2748 | A    | N9-C8   | -6.57 | 1.32        | 1.37     |
| 35  | BB    | 2751 | G    | C5'-C4' | 6.57  | 1.59        | 1.51     |
| 1   | AA    | 1329 | A    | C5-C4   | 6.57  | 1.43        | 1.38     |
| 34  | BA    | 96   | G    | C8-N7   | -6.57 | 1.27        | 1.30     |
| 35  | BB    | 458  | G    | C5-C4   | -6.57 | 1.33        | 1.38     |
| 35  | BB    | 1718 | G    | C2-N3   | 6.57  | 1.38        | 1.32     |
| 35  | BB    | 2414 | G    | C8-N7   | 6.57  | 1.34        | 1.30     |
| 35  | BB    | 2615 | U    | N3-C4   | 6.57  | 1.44        | 1.38     |
| 1   | AA    | 139  | A    | O3'-P   | -6.57 | 1.53        | 1.61     |
| 1   | AA    | 171  | A    | C6-N1   | 6.57  | 1.40        | 1.35     |
| 35  | BB    | 1439 | A    | N9-C4   | 6.57  | 1.41        | 1.37     |
| 35  | BB    | 2345 | G    | N1-C2   | 6.57  | 1.43        | 1.37     |
| 1   | AA    | 126  | G    | N3-C4   | -6.57 | 1.30        | 1.35     |
| 1   | AA    | 138  | G    | C6-N1   | 6.57  | 1.44        | 1.39     |
| 1   | AA    | 691  | G    | N7-C5   | -6.57 | 1.35        | 1.39     |
| 1   | AA    | 1221 | G    | N9-C4   | -6.57 | 1.32        | 1.38     |
| 35  | BB    | 349  | U    | N3-C4   | 6.57  | 1.44        | 1.38     |
| 35  | BB    | 949  | G    | C2'-C1' | -6.57 | 1.46        | 1.53     |
| 35  | BB    | 1271 | G    | C3'-O3' | 6.57  | 1.51        | 1.42     |
| 35  | BB    | 2410 | G    | C5-C6   | -6.57 | 1.35        | 1.42     |
| 35  | BB    | 2432 | A    | C5-C4   | 6.57  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 698  | G    | N3-C4   | -6.56 | 1.30        | 1.35     |
| 46  | BM    | 103  | TYR  | CZ-OH   | 6.56  | 1.49        | 1.37     |
| 1   | AA    | 459  | A    | N7-C5   | 6.56  | 1.43        | 1.39     |
| 35  | BB    | 1184 | U    | C3'-C2' | -6.56 | 1.45        | 1.52     |
| 35  | BB    | 1293 | C    | C5'-C4' | 6.56  | 1.59        | 1.51     |
| 35  | BB    | 1407 | G    | N3-C4   | 6.56  | 1.40        | 1.35     |
| 35  | BB    | 1424 | G    | C2-N3   | 6.56  | 1.38        | 1.32     |
| 35  | BB    | 1987 | A    | C2'-C1' | -6.56 | 1.46        | 1.53     |
| 1   | AA    | 580  | C    | N1-C6   | 6.56  | 1.41        | 1.37     |
| 1   | AA    | 847  | G    | N7-C5   | -6.56 | 1.35        | 1.39     |
| 1   | AA    | 1049 | U    | C4'-C3' | 6.56  | 1.60        | 1.53     |
| 1   | AA    | 1423 | G    | C2-N3   | 6.56  | 1.38        | 1.32     |
| 35  | BB    | 1785 | A    | C5-C4   | -6.56 | 1.34        | 1.38     |
| 1   | AA    | 1413 | A    | P-O5'   | -6.56 | 1.53        | 1.59     |
| 35  | BB    | 1130 | U    | N1-C6   | 6.56  | 1.43        | 1.38     |
| 1   | AA    | 574  | A    | C6-N1   | 6.56  | 1.40        | 1.35     |
| 1   | AA    | 703  | G    | C4'-C3' | -6.56 | 1.46        | 1.53     |
| 1   | AA    | 1368 | A    | C5'-C4' | 6.56  | 1.59        | 1.51     |
| 35  | BB    | 671  | C    | C4-N4   | 6.56  | 1.39        | 1.33     |
| 35  | BB    | 2488 | G    | C5-C4   | -6.56 | 1.33        | 1.38     |
| 35  | BB    | 2844 | G    | C5-C4   | 6.56  | 1.43        | 1.38     |
| 51  | BR    | 13   | ARG  | NE-CZ   | 6.56  | 1.41        | 1.33     |
| 35  | BB    | 678  | C    | C4-C5   | -6.56 | 1.37        | 1.43     |
| 1   | AA    | 885  | G    | C2-N3   | 6.55  | 1.38        | 1.32     |
| 1   | AA    | 1075 | U    | N1-C2   | -6.55 | 1.32        | 1.38     |
| 35  | BB    | 332  | A    | N3-C4   | -6.55 | 1.30        | 1.34     |
| 35  | BB    | 1441 | G    | P-O5'   | -6.55 | 1.53        | 1.59     |
| 35  | BB    | 1586 | A    | C8-N7   | -6.55 | 1.26        | 1.31     |
| 9   | AI    | 79   | ARG  | NE-CZ   | 6.55  | 1.41        | 1.33     |
| 35  | BB    | 909  | A    | N9-C4   | 6.55  | 1.41        | 1.37     |
| 35  | BB    | 1074 | G    | C5-C6   | -6.55 | 1.35        | 1.42     |
| 35  | BB    | 1482 | G    | C8-N7   | -6.55 | 1.27        | 1.30     |
| 35  | BB    | 1550 | C    | N3-C4   | 6.55  | 1.38        | 1.33     |
| 35  | BB    | 2019 | A    | N1-C2   | 6.55  | 1.40        | 1.34     |
| 1   | AA    | 123  | U    | C2'-C1' | -6.55 | 1.46        | 1.53     |
| 1   | AA    | 544  | G    | C2-N3   | 6.55  | 1.38        | 1.32     |
| 1   | AA    | 926  | G    | C6-N1   | 6.55  | 1.44        | 1.39     |
| 35  | BB    | 83   | A    | N7-C5   | -6.55 | 1.35        | 1.39     |
| 35  | BB    | 188  | G    | C2-N3   | 6.55  | 1.38        | 1.32     |
| 35  | BB    | 1112 | G    | C5-C4   | -6.55 | 1.33        | 1.38     |
| 35  | BB    | 1311 | G    | C8-N7   | 6.55  | 1.34        | 1.30     |
| 35  | BB    | 1377 | G    | N3-C4   | -6.55 | 1.30        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2852 | G    | C2'-C1' | -6.55 | 1.46        | 1.53     |
| 1   | AA    | 664  | G    | N9-C4   | 6.55  | 1.43        | 1.38     |
| 1   | AA    | 1039 | G    | C2-N3   | 6.55  | 1.38        | 1.32     |
| 22  | AV    | 3    | G    | C2'-C1' | -6.55 | 1.46        | 1.53     |
| 35  | BB    | 153  | U    | C5'-C4' | 6.55  | 1.59        | 1.51     |
| 35  | BB    | 226  | A    | O3'-P   | -6.55 | 1.53        | 1.61     |
| 35  | BB    | 333  | G    | P-O5'   | -6.55 | 1.53        | 1.59     |
| 35  | BB    | 977  | G    | C2'-C1' | -6.55 | 1.46        | 1.53     |
| 35  | BB    | 1051 | G    | C6-N1   | 6.55  | 1.44        | 1.39     |
| 35  | BB    | 1569 | A    | C2'-C1' | -6.55 | 1.46        | 1.53     |
| 35  | BB    | 600  | G    | N9-C8   | 6.55  | 1.42        | 1.37     |
| 35  | BB    | 856  | G    | C2-N3   | 6.55  | 1.38        | 1.32     |
| 35  | BB    | 1117 | C    | C2'-C1' | -6.55 | 1.46        | 1.53     |
| 35  | BB    | 1916 | A    | C8-N7   | 6.55  | 1.36        | 1.31     |
| 35  | BB    | 2071 | A    | C5-C4   | 6.55  | 1.43        | 1.38     |
| 35  | BB    | 2189 | U    | C4-C5   | 6.55  | 1.49        | 1.43     |
| 35  | BB    | 2731 | G    | N9-C8   | -6.55 | 1.33        | 1.37     |
| 1   | AA    | 527  | G    | N7-C5   | -6.55 | 1.35        | 1.39     |
| 1   | AA    | 1160 | G    | C2'-C1' | -6.55 | 1.46        | 1.53     |
| 15  | AO    | 13   | GLU  | CD-OE2  | 6.55  | 1.32        | 1.25     |
| 35  | BB    | 254  | G    | C5-C4   | 6.55  | 1.43        | 1.38     |
| 35  | BB    | 804  | A    | C6-N6   | 6.55  | 1.39        | 1.33     |
| 35  | BB    | 1554 | U    | C2-N3   | 6.55  | 1.42        | 1.37     |
| 35  | BB    | 1896 | G    | C5'-C4' | 6.55  | 1.59        | 1.51     |
| 35  | BB    | 1522 | A    | P-O5'   | -6.54 | 1.53        | 1.59     |
| 35  | BB    | 1989 | G    | C2-N2   | 6.54  | 1.41        | 1.34     |
| 1   | AA    | 359  | G    | N3-C4   | -6.54 | 1.30        | 1.35     |
| 1   | AA    | 753  | A    | C6-N6   | 6.54  | 1.39        | 1.33     |
| 1   | AA    | 1329 | A    | O4'-C1' | 6.54  | 1.50        | 1.41     |
| 35  | BB    | 1579 | A    | C8-N7   | -6.54 | 1.26        | 1.31     |
| 35  | BB    | 2266 | A    | C6-N1   | 6.54  | 1.40        | 1.35     |
| 1   | AA    | 41   | G    | O3'-P   | -6.54 | 1.53        | 1.61     |
| 1   | AA    | 180  | U    | N1-C6   | -6.54 | 1.32        | 1.38     |
| 1   | AA    | 988  | G    | N7-C5   | -6.54 | 1.35        | 1.39     |
| 35  | BB    | 83   | A    | N3-C4   | 6.54  | 1.38        | 1.34     |
| 35  | BB    | 380  | G    | N9-C8   | 6.54  | 1.42        | 1.37     |
| 35  | BB    | 1896 | G    | C4'-C3' | 6.54  | 1.60        | 1.53     |
| 35  | BB    | 2194 | U    | C2-N3   | 6.54  | 1.42        | 1.37     |
| 1   | AA    | 1267 | C    | N1-C6   | 6.54  | 1.41        | 1.37     |
| 35  | BB    | 1926 | U    | C4-C5   | 6.54  | 1.49        | 1.43     |
| 35  | BB    | 2491 | U    | N1-C6   | 6.54  | 1.43        | 1.38     |
| 1   | AA    | 396  | C    | N1-C6   | 6.54  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 974  | A    | N3-C4   | 6.54  | 1.38        | 1.34     |
| 1   | AA    | 1354 | U    | C2'-C1' | -6.54 | 1.46        | 1.53     |
| 35  | BB    | 490  | C    | C3'-O3' | 6.54  | 1.51        | 1.42     |
| 35  | BB    | 866  | A    | C2'-C1' | -6.54 | 1.46        | 1.53     |
| 35  | BB    | 969  | G    | O3'-P   | -6.54 | 1.53        | 1.61     |
| 35  | BB    | 1003 | G    | C6-O6   | 6.54  | 1.30        | 1.24     |
| 35  | BB    | 1061 | U    | C2-N3   | 6.54  | 1.42        | 1.37     |
| 35  | BB    | 2792 | A    | C6-N1   | 6.54  | 1.40        | 1.35     |
| 35  | BB    | 1670 | C    | P-O5'   | 6.54  | 1.66        | 1.59     |
| 1   | AA    | 465  | A    | C6-N6   | 6.54  | 1.39        | 1.33     |
| 1   | AA    | 1387 | G    | N7-C5   | -6.54 | 1.35        | 1.39     |
| 1   | AA    | 1408 | A    | C6-N1   | 6.54  | 1.40        | 1.35     |
| 35  | BB    | 489  | G    | C2-N2   | 6.54  | 1.41        | 1.34     |
| 35  | BB    | 791  | C    | C4'-C3' | 6.54  | 1.60        | 1.53     |
| 35  | BB    | 1081 | U    | N3-C4   | -6.54 | 1.32        | 1.38     |
| 35  | BB    | 1479 | G    | N1-C2   | 6.54  | 1.43        | 1.37     |
| 35  | BB    | 1929 | G    | C5-C4   | 6.54  | 1.43        | 1.38     |
| 35  | BB    | 2799 | A    | N7-C5   | 6.54  | 1.43        | 1.39     |
| 1   | AA    | 1483 | A    | N3-C4   | -6.53 | 1.30        | 1.34     |
| 35  | BB    | 918  | A    | N7-C5   | -6.53 | 1.35        | 1.39     |
| 35  | BB    | 1405 | U    | P-O5'   | -6.53 | 1.53        | 1.59     |
| 35  | BB    | 2667 | C    | C2-O2   | 6.53  | 1.30        | 1.24     |
| 35  | BB    | 2816 | G    | C2-N3   | 6.53  | 1.38        | 1.32     |
| 37  | BD    | 117  | GLY  | CA-C    | -6.53 | 1.41        | 1.51     |
| 27  | B2    | 30   | ARG  | CZ-NH1  | 6.53  | 1.41        | 1.33     |
| 35  | BB    | 2577 | A    | O4'-C1' | -6.53 | 1.33        | 1.41     |
| 1   | AA    | 77   | A    | N9-C4   | 6.53  | 1.41        | 1.37     |
| 1   | AA    | 799  | G    | P-O5'   | -6.53 | 1.53        | 1.59     |
| 1   | AA    | 963  | G    | O4'-C1' | 6.53  | 1.50        | 1.41     |
| 35  | BB    | 1056 | G    | C4'-C3' | -6.53 | 1.46        | 1.53     |
| 35  | BB    | 1455 | G    | N3-C4   | 6.53  | 1.40        | 1.35     |
| 35  | BB    | 2453 | A    | C5-C4   | 6.53  | 1.43        | 1.38     |
| 35  | BB    | 2800 | A    | C4'-O4' | 6.53  | 1.54        | 1.45     |
| 1   | AA    | 310  | G    | N7-C5   | -6.53 | 1.35        | 1.39     |
| 35  | BB    | 793  | A    | C3'-C2' | 6.53  | 1.60        | 1.52     |
| 35  | BB    | 1503 | A    | C8-N7   | -6.53 | 1.26        | 1.31     |
| 35  | BB    | 1901 | A    | O3'-P   | -6.53 | 1.53        | 1.61     |
| 34  | BA    | 31   | C    | C4-N4   | 6.53  | 1.39        | 1.33     |
| 35  | BB    | 283  | G    | C2-N2   | 6.53  | 1.41        | 1.34     |
| 35  | BB    | 693  | A    | C6-N6   | 6.53  | 1.39        | 1.33     |
| 35  | BB    | 855  | G    | C6-N1   | 6.53  | 1.44        | 1.39     |
| 35  | BB    | 1510 | G    | C5-C6   | -6.53 | 1.35        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 33   | A    | C4'-C3' | 6.53  | 1.60        | 1.53     |
| 1   | AA    | 868  | C    | N1-C6   | 6.53  | 1.41        | 1.37     |
| 1   | AA    | 1170 | A    | N3-C4   | -6.53 | 1.30        | 1.34     |
| 35  | BB    | 44   | A    | C6-N6   | 6.53  | 1.39        | 1.33     |
| 35  | BB    | 48   | G    | C5-C4   | 6.53  | 1.43        | 1.38     |
| 35  | BB    | 1546 | G    | C6-N1   | 6.53  | 1.44        | 1.39     |
| 35  | BB    | 1651 | G    | C4'-C3' | 6.53  | 1.60        | 1.53     |
| 35  | BB    | 2720 | U    | N3-C4   | -6.53 | 1.32        | 1.38     |
| 35  | BB    | 818  | G    | C8-N7   | -6.52 | 1.27        | 1.30     |
| 35  | BB    | 1979 | U    | C2-O2   | 6.52  | 1.28        | 1.22     |
| 1   | AA    | 649  | A    | C2-N3   | 6.52  | 1.39        | 1.33     |
| 1   | AA    | 791  | G    | N9-C8   | -6.52 | 1.33        | 1.37     |
| 1   | AA    | 1309 | G    | C4'-O4' | 6.52  | 1.54        | 1.45     |
| 35  | BB    | 55   | G    | P-O5'   | -6.52 | 1.53        | 1.59     |
| 35  | BB    | 452  | G    | C5'-C4' | 6.52  | 1.59        | 1.51     |
| 35  | BB    | 906  | U    | C2'-C1' | -6.52 | 1.46        | 1.53     |
| 35  | BB    | 1275 | A    | C5-C6   | -6.52 | 1.35        | 1.41     |
| 35  | BB    | 2784 | U    | P-O5'   | -6.52 | 1.53        | 1.59     |
| 35  | BB    | 2868 | A    | C8-N7   | -6.52 | 1.26        | 1.31     |
| 1   | AA    | 1129 | C    | N3-C4   | 6.52  | 1.38        | 1.33     |
| 35  | BB    | 2868 | A    | P-O5'   | -6.52 | 1.53        | 1.59     |
| 1   | AA    | 323  | U    | N1-C6   | -6.52 | 1.32        | 1.38     |
| 1   | AA    | 987  | G    | C1'-N9  | -6.52 | 1.37        | 1.46     |
| 1   | AA    | 1212 | U    | C4'-C3' | 6.52  | 1.60        | 1.53     |
| 1   | AA    | 1245 | C    | C4-C5   | 6.52  | 1.48        | 1.43     |
| 3   | AC    | 163  | ARG  | NE-CZ   | 6.52  | 1.41        | 1.33     |
| 35  | BB    | 307  | G    | C4'-C3' | 6.52  | 1.60        | 1.53     |
| 35  | BB    | 475  | C    | C4-N4   | 6.52  | 1.39        | 1.33     |
| 35  | BB    | 1034 | G    | O4'-C1' | 6.52  | 1.50        | 1.41     |
| 35  | BB    | 1213 | A    | C6-N6   | 6.52  | 1.39        | 1.33     |
| 35  | BB    | 2394 | C    | N1-C6   | -6.52 | 1.33        | 1.37     |
| 35  | BB    | 2453 | A    | C3'-C2' | -6.52 | 1.45        | 1.52     |
| 1   | AA    | 441  | A    | C5-C4   | -6.52 | 1.34        | 1.38     |
| 1   | AA    | 733  | G    | N9-C8   | 6.52  | 1.42        | 1.37     |
| 1   | AA    | 1126 | U    | C2'-C1' | -6.52 | 1.46        | 1.53     |
| 1   | AA    | 1136 | C    | C2-O2   | -6.52 | 1.18        | 1.24     |
| 34  | BA    | 15   | A    | N9-C4   | -6.52 | 1.33        | 1.37     |
| 35  | BB    | 1476 | U    | C5'-C4' | 6.52  | 1.59        | 1.51     |
| 1   | AA    | 234  | C    | C1'-N1  | 6.52  | 1.58        | 1.48     |
| 1   | AA    | 845  | A    | C6-N1   | 6.52  | 1.40        | 1.35     |
| 1   | AA    | 1286 | U    | C5-C6   | 6.52  | 1.40        | 1.34     |
| 35  | BB    | 711  | G    | C4'-C3' | -6.52 | 1.46        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 278  | G    | N9-C8   | -6.51 | 1.33        | 1.37     |
| 1   | AA    | 1016 | A    | N3-C4   | 6.51  | 1.38        | 1.34     |
| 22  | AV    | 68   | U    | C4-O4   | -6.51 | 1.18        | 1.23     |
| 35  | BB    | 492  | A    | N9-C4   | 6.51  | 1.41        | 1.37     |
| 1   | AA    | 143  | A    | O3'-P   | -6.51 | 1.53        | 1.61     |
| 1   | AA    | 148  | G    | N9-C4   | -6.51 | 1.32        | 1.38     |
| 1   | AA    | 526  | C    | N1-C6   | 6.51  | 1.41        | 1.37     |
| 1   | AA    | 969  | A    | C4'-O4' | 6.51  | 1.54        | 1.45     |
| 34  | BA    | 4    | C    | C5-C6   | -6.51 | 1.29        | 1.34     |
| 35  | BB    | 696  | G    | C5'-C4' | 6.51  | 1.59        | 1.51     |
| 35  | BB    | 1170 | C    | P-O5'   | -6.51 | 1.53        | 1.59     |
| 35  | BB    | 1753 | G    | C8-N7   | 6.51  | 1.34        | 1.30     |
| 1   | AA    | 252  | U    | C2-N3   | 6.51  | 1.42        | 1.37     |
| 1   | AA    | 279  | A    | C2'-C1' | -6.51 | 1.46        | 1.53     |
| 1   | AA    | 1431 | A    | N3-C4   | -6.51 | 1.30        | 1.34     |
| 34  | BA    | 61   | G    | N3-C4   | -6.51 | 1.30        | 1.35     |
| 35  | BB    | 676  | A    | N1-C2   | 6.51  | 1.40        | 1.34     |
| 35  | BB    | 1653 | G    | C2-N3   | 6.51  | 1.38        | 1.32     |
| 35  | BB    | 1790 | C    | P-O5'   | -6.51 | 1.53        | 1.59     |
| 35  | BB    | 2525 | G    | C6-N1   | -6.51 | 1.34        | 1.39     |
| 35  | BB    | 2770 | G    | C2'-C1' | -6.51 | 1.46        | 1.53     |
| 35  | BB    | 2785 | C    | C5-C6   | -6.51 | 1.29        | 1.34     |
| 34  | BA    | 23   | G    | N3-C4   | 6.51  | 1.40        | 1.35     |
| 35  | BB    | 264  | C    | O3'-P   | -6.51 | 1.53        | 1.61     |
| 35  | BB    | 1431 | A    | N9-C4   | -6.51 | 1.33        | 1.37     |
| 35  | BB    | 2351 | G    | O3'-P   | -6.51 | 1.53        | 1.61     |
| 35  | BB    | 2511 | U    | N3-C4   | 6.51  | 1.44        | 1.38     |
| 48  | BO    | 55   | GLU  | CG-CD   | 6.51  | 1.61        | 1.51     |
| 35  | BB    | 2494 | G    | O3'-P   | -6.51 | 1.53        | 1.61     |
| 35  | BB    | 2886 | A    | N9-C8   | 6.51  | 1.43        | 1.37     |
| 1   | AA    | 544  | G    | O3'-P   | -6.51 | 1.53        | 1.61     |
| 1   | AA    | 1189 | U    | O3'-P   | -6.51 | 1.53        | 1.61     |
| 1   | AA    | 1198 | G    | C6-N1   | 6.51  | 1.44        | 1.39     |
| 35  | BB    | 42   | A    | N9-C4   | 6.51  | 1.41        | 1.37     |
| 35  | BB    | 1504 | A    | N9-C4   | 6.51  | 1.41        | 1.37     |
| 35  | BB    | 1875 | G    | C2-N3   | 6.51  | 1.38        | 1.32     |
| 35  | BB    | 1952 | A    | C6-N6   | 6.51  | 1.39        | 1.33     |
| 35  | BB    | 2161 | C    | N1-C6   | -6.51 | 1.33        | 1.37     |
| 35  | BB    | 2255 | G    | N3-C4   | -6.51 | 1.30        | 1.35     |
| 35  | BB    | 2568 | U    | P-O5'   | -6.51 | 1.53        | 1.59     |
| 35  | BB    | 66   | C    | C5-C6   | -6.50 | 1.29        | 1.34     |
| 35  | BB    | 1651 | G    | C5-C6   | -6.50 | 1.35        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2161 | C    | C4-N4   | 6.50  | 1.39        | 1.33     |
| 1   | AA    | 539  | A    | C8-N7   | -6.50 | 1.26        | 1.31     |
| 1   | AA    | 636  | U    | N1-C6   | -6.50 | 1.32        | 1.38     |
| 1   | AA    | 882  | C    | C4'-C3' | -6.50 | 1.46        | 1.53     |
| 1   | AA    | 1070 | U    | C2'-C1' | -6.50 | 1.46        | 1.53     |
| 1   | AA    | 1299 | A    | C3'-C2' | 6.50  | 1.60        | 1.52     |
| 35  | BB    | 266  | G    | N7-C5   | 6.50  | 1.43        | 1.39     |
| 35  | BB    | 322  | A    | N9-C4   | -6.50 | 1.33        | 1.37     |
| 35  | BB    | 1204 | A    | C6-N1   | 6.50  | 1.40        | 1.35     |
| 35  | BB    | 2821 | A    | C6-N6   | 6.50  | 1.39        | 1.33     |
| 1   | AA    | 538  | G    | N7-C5   | -6.50 | 1.35        | 1.39     |
| 1   | AA    | 768  | A    | N3-C4   | -6.50 | 1.30        | 1.34     |
| 35  | BB    | 111  | A    | C5-C4   | 6.50  | 1.43        | 1.38     |
| 35  | BB    | 838  | C    | C4-N4   | 6.50  | 1.39        | 1.33     |
| 35  | BB    | 1028 | A    | C2'-C1' | -6.50 | 1.46        | 1.53     |
| 34  | BA    | 99   | A    | N1-C2   | 6.50  | 1.40        | 1.34     |
| 35  | BB    | 728  | G    | N9-C8   | 6.50  | 1.42        | 1.37     |
| 1   | AA    | 487  | A    | C6-N6   | 6.50  | 1.39        | 1.33     |
| 35  | BB    | 522  | A    | C5-C4   | 6.50  | 1.43        | 1.38     |
| 35  | BB    | 1091 | G    | C2'-C1' | -6.50 | 1.46        | 1.53     |
| 35  | BB    | 1566 | A    | C5'-C4' | 6.50  | 1.59        | 1.51     |
| 35  | BB    | 2520 | C    | C2-N3   | 6.50  | 1.41        | 1.35     |
| 35  | BB    | 2692 | G    | C3'-C2' | 6.50  | 1.60        | 1.52     |
| 1   | AA    | 80   | A    | C6-N1   | 6.50  | 1.40        | 1.35     |
| 1   | AA    | 856  | C    | P-O5'   | 6.50  | 1.66        | 1.59     |
| 1   | AA    | 1275 | A    | C8-N7   | -6.50 | 1.27        | 1.31     |
| 35  | BB    | 162  | U    | C2-N3   | 6.50  | 1.42        | 1.37     |
| 35  | BB    | 249  | C    | N1-C6   | 6.50  | 1.41        | 1.37     |
| 35  | BB    | 1189 | A    | C5'-C4' | 6.50  | 1.59        | 1.51     |
| 35  | BB    | 1212 | G    | N7-C5   | -6.50 | 1.35        | 1.39     |
| 35  | BB    | 1465 | G    | O3'-P   | -6.50 | 1.53        | 1.61     |
| 35  | BB    | 1764 | C    | C4-N4   | 6.50  | 1.39        | 1.33     |
| 35  | BB    | 2059 | A    | N9-C8   | 6.50  | 1.43        | 1.37     |
| 35  | BB    | 106  | C    | C4-N4   | 6.49  | 1.39        | 1.33     |
| 35  | BB    | 1225 | G    | N9-C8   | 6.49  | 1.42        | 1.37     |
| 35  | BB    | 1970 | A    | P-O5'   | -6.49 | 1.53        | 1.59     |
| 35  | BB    | 2653 | U    | P-O5'   | -6.49 | 1.53        | 1.59     |
| 45  | BL    | 78   | ARG  | CD-NE   | 6.49  | 1.57        | 1.46     |
| 35  | BB    | 372  | G    | C5-C4   | -6.49 | 1.33        | 1.38     |
| 35  | BB    | 1669 | A    | C8-N7   | -6.49 | 1.27        | 1.31     |
| 35  | BB    | 2431 | U    | C2'-C1' | -6.49 | 1.46        | 1.53     |
| 1   | AA    | 942  | G    | C2-N3   | 6.49  | 1.38        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 955  | U    | C4-O4   | 6.49  | 1.28        | 1.23     |
| 35  | BB    | 1554 | U    | C4-C5   | 6.49  | 1.49        | 1.43     |
| 35  | BB    | 531  | C    | P-O5'   | -6.49 | 1.53        | 1.59     |
| 35  | BB    | 1021 | A    | C8-N7   | -6.49 | 1.27        | 1.31     |
| 35  | BB    | 1356 | G    | C8-N7   | -6.49 | 1.27        | 1.30     |
| 35  | BB    | 1683 | U    | C4-C5   | 6.49  | 1.49        | 1.43     |
| 35  | BB    | 2199 | A    | N9-C4   | -6.49 | 1.33        | 1.37     |
| 35  | BB    | 2897 | U    | N1-C6   | 6.49  | 1.43        | 1.38     |
| 35  | BB    | 2583 | G    | N7-C5   | -6.49 | 1.35        | 1.39     |
| 1   | AA    | 1167 | A    | C6-N6   | 6.49  | 1.39        | 1.33     |
| 1   | AA    | 1434 | A    | N9-C4   | -6.49 | 1.33        | 1.37     |
| 35  | BB    | 165  | A    | O3'-P   | -6.49 | 1.53        | 1.61     |
| 35  | BB    | 405  | U    | O4'-C1' | 6.49  | 1.50        | 1.41     |
| 35  | BB    | 429  | A    | O3'-P   | -6.49 | 1.53        | 1.61     |
| 35  | BB    | 470  | A    | C2-N3   | 6.49  | 1.39        | 1.33     |
| 35  | BB    | 1116 | G    | C6-N1   | 6.49  | 1.44        | 1.39     |
| 35  | BB    | 2234 | G    | C8-N7   | 6.49  | 1.34        | 1.30     |
| 35  | BB    | 2476 | A    | C2'-C1' | -6.49 | 1.46        | 1.53     |
| 40  | BG    | 94   | ARG  | NE-CZ   | 6.49  | 1.41        | 1.33     |
| 1   | AA    | 275  | G    | N1-C2   | 6.48  | 1.43        | 1.37     |
| 1   | AA    | 977  | A    | C2-N3   | 6.48  | 1.39        | 1.33     |
| 35  | BB    | 307  | G    | C6-N1   | 6.48  | 1.44        | 1.39     |
| 35  | BB    | 335  | C    | C4-C5   | 6.48  | 1.48        | 1.43     |
| 35  | BB    | 1680 | U    | N1-C6   | 6.48  | 1.43        | 1.38     |
| 35  | BB    | 2428 | G    | C4'-C3' | 6.48  | 1.60        | 1.53     |
| 1   | AA    | 1052 | U    | C3'-O3' | 6.48  | 1.51        | 1.42     |
| 35  | BB    | 373  | U    | C4'-O4' | -6.48 | 1.37        | 1.45     |
| 35  | BB    | 956  | G    | C5'-C4' | 6.48  | 1.59        | 1.51     |
| 35  | BB    | 1827 | U    | C4-O4   | 6.48  | 1.28        | 1.23     |
| 1   | AA    | 329  | A    | O3'-P   | -6.48 | 1.53        | 1.61     |
| 1   | AA    | 1409 | C    | C4'-C3' | 6.48  | 1.60        | 1.53     |
| 1   | AA    | 1442 | G    | N1-C2   | 6.48  | 1.43        | 1.37     |
| 35  | BB    | 862  | G    | C8-N7   | -6.48 | 1.27        | 1.30     |
| 35  | BB    | 146  | A    | C3'-C2' | -6.48 | 1.45        | 1.52     |
| 35  | BB    | 948  | C    | N1-C6   | 6.48  | 1.41        | 1.37     |
| 35  | BB    | 1931 | U    | C5-C6   | 6.48  | 1.40        | 1.34     |
| 35  | BB    | 2308 | G    | C5-C6   | -6.48 | 1.35        | 1.42     |
| 1   | AA    | 19   | A    | C6-N6   | 6.48  | 1.39        | 1.33     |
| 1   | AA    | 1448 | C    | N3-C4   | 6.48  | 1.38        | 1.33     |
| 35  | BB    | 780  | G    | O3'-P   | -6.48 | 1.53        | 1.61     |
| 35  | BB    | 1510 | G    | C6-N1   | 6.48  | 1.44        | 1.39     |
| 35  | BB    | 1884 | G    | C4'-C3' | 6.48  | 1.60        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2018 | G    | N1-C2   | 6.48  | 1.43        | 1.37     |
| 35  | BB    | 2458 | G    | C6-N1   | 6.48  | 1.44        | 1.39     |
| 1   | AA    | 46   | G    | C3'-C2' | -6.48 | 1.45        | 1.52     |
| 1   | AA    | 996  | A    | N7-C5   | -6.48 | 1.35        | 1.39     |
| 4   | AD    | 46   | ARG  | NE-CZ   | 6.48  | 1.41        | 1.33     |
| 35  | BB    | 1121 | C    | N3-C4   | 6.48  | 1.38        | 1.33     |
| 35  | BB    | 1490 | A    | N9-C8   | 6.48  | 1.43        | 1.37     |
| 35  | BB    | 1630 | A    | C6-N6   | 6.48  | 1.39        | 1.33     |
| 35  | BB    | 1873 | G    | C5'-C4' | 6.48  | 1.59        | 1.51     |
| 35  | BB    | 2431 | U    | C3'-C2' | -6.48 | 1.45        | 1.52     |
| 35  | BB    | 2795 | C    | N3-C4   | 6.48  | 1.38        | 1.33     |
| 1   | AA    | 262  | A    | C2'-C1' | -6.47 | 1.46        | 1.53     |
| 1   | AA    | 537  | G    | N1-C2   | 6.47  | 1.43        | 1.37     |
| 1   | AA    | 1487 | G    | C8-N7   | -6.47 | 1.27        | 1.30     |
| 35  | BB    | 1771 | C    | N3-C4   | 6.47  | 1.38        | 1.33     |
| 1   | AA    | 318  | G    | C5-C4   | 6.47  | 1.42        | 1.38     |
| 1   | AA    | 1356 | G    | C2-N3   | 6.47  | 1.38        | 1.32     |
| 35  | BB    | 331  | C    | C3'-C2' | -6.47 | 1.45        | 1.52     |
| 35  | BB    | 782  | A    | C6-N6   | 6.47  | 1.39        | 1.33     |
| 35  | BB    | 1210 | G    | C2-N3   | 6.47  | 1.38        | 1.32     |
| 35  | BB    | 1277 | G    | C6-N1   | -6.47 | 1.35        | 1.39     |
| 35  | BB    | 1324 | G    | C2'-C1' | -6.47 | 1.46        | 1.53     |
| 35  | BB    | 1892 | C    | C3'-C2' | -6.47 | 1.45        | 1.52     |
| 35  | BB    | 2750 | A    | P-O5'   | -6.47 | 1.53        | 1.59     |
| 1   | AA    | 1209 | C    | P-O5'   | 6.47  | 1.66        | 1.59     |
| 1   | AA    | 1528 | U    | N3-C4   | 6.47  | 1.44        | 1.38     |
| 35  | BB    | 496  | G    | N3-C4   | 6.47  | 1.40        | 1.35     |
| 35  | BB    | 678  | C    | N3-C4   | 6.47  | 1.38        | 1.33     |
| 1   | AA    | 499  | A    | C3'-O3' | 6.47  | 1.51        | 1.42     |
| 1   | AA    | 1496 | C    | N1-C6   | 6.47  | 1.41        | 1.37     |
| 35  | BB    | 990  | A    | N7-C5   | -6.47 | 1.35        | 1.39     |
| 35  | BB    | 1704 | C    | N1-C6   | 6.47  | 1.41        | 1.37     |
| 35  | BB    | 2024 | G    | N1-C2   | 6.47  | 1.43        | 1.37     |
| 35  | BB    | 2564 | A    | N3-C4   | 6.47  | 1.38        | 1.34     |
| 35  | BB    | 2688 | G    | C8-N7   | -6.47 | 1.27        | 1.30     |
| 1   | AA    | 72   | A    | C6-N1   | 6.47  | 1.40        | 1.35     |
| 1   | AA    | 1466 | C    | C4'-O4' | 6.47  | 1.53        | 1.45     |
| 35  | BB    | 718  | A    | C5-C4   | 6.47  | 1.43        | 1.38     |
| 35  | BB    | 1385 | A    | O3'-P   | -6.47 | 1.53        | 1.61     |
| 43  | BJ    | 74   | TYR  | CG-CD1  | 6.47  | 1.47        | 1.39     |
| 35  | BB    | 1217 | U    | C2-N3   | 6.47  | 1.42        | 1.37     |
| 35  | BB    | 1253 | A    | N3-C4   | 6.47  | 1.38        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2152 | G    | N9-C4   | 6.47  | 1.43        | 1.38     |
| 35  | BB    | 2193 | G    | C2'-C1' | -6.47 | 1.46        | 1.53     |
| 35  | BB    | 2233 | U    | N1-C6   | -6.47 | 1.32        | 1.38     |
| 1   | AA    | 665  | A    | N3-C4   | -6.46 | 1.30        | 1.34     |
| 1   | AA    | 1435 | G    | C2-N3   | 6.46  | 1.38        | 1.32     |
| 35  | BB    | 1076 | C    | C4-C5   | 6.46  | 1.48        | 1.43     |
| 35  | BB    | 2200 | C    | P-O5'   | -6.46 | 1.53        | 1.59     |
| 1   | AA    | 406  | G    | N9-C4   | 6.46  | 1.43        | 1.38     |
| 1   | AA    | 996  | A    | O3'-P   | -6.46 | 1.53        | 1.61     |
| 1   | AA    | 1121 | U    | C4'-C3' | 6.46  | 1.60        | 1.53     |
| 23  | AX    | 19   | A    | C6-N6   | 6.46  | 1.39        | 1.33     |
| 34  | BA    | 111  | U    | C2'-C1' | -6.46 | 1.46        | 1.53     |
| 35  | BB    | 109  | C    | C4-N4   | 6.46  | 1.39        | 1.33     |
| 35  | BB    | 226  | A    | C6-N1   | 6.46  | 1.40        | 1.35     |
| 35  | BB    | 475  | C    | C3'-C2' | -6.46 | 1.45        | 1.52     |
| 35  | BB    | 795  | C    | O3'-P   | 6.46  | 1.69        | 1.61     |
| 35  | BB    | 807  | U    | C2-N3   | 6.46  | 1.42        | 1.37     |
| 35  | BB    | 818  | G    | C6-N1   | 6.46  | 1.44        | 1.39     |
| 35  | BB    | 1111 | A    | N3-C4   | 6.46  | 1.38        | 1.34     |
| 35  | BB    | 1298 | C    | C2'-C1' | -6.46 | 1.46        | 1.53     |
| 35  | BB    | 1674 | G    | N1-C2   | 6.46  | 1.43        | 1.37     |
| 35  | BB    | 2293 | G    | N7-C5   | -6.46 | 1.35        | 1.39     |
| 2   | AB    | 181  | PRO  | N-CD    | -6.46 | 1.38        | 1.47     |
| 35  | BB    | 48   | G    | C2-N2   | 6.46  | 1.41        | 1.34     |
| 35  | BB    | 249  | C    | C4'-C3' | -6.46 | 1.46        | 1.53     |
| 35  | BB    | 2298 | A    | C6-N1   | 6.46  | 1.40        | 1.35     |
| 35  | BB    | 2869 | G    | C2'-C1' | -6.46 | 1.46        | 1.53     |
| 1   | AA    | 241  | G    | N7-C5   | -6.46 | 1.35        | 1.39     |
| 1   | AA    | 373  | A    | C3'-O3' | 6.46  | 1.51        | 1.42     |
| 1   | AA    | 1151 | A    | C5-C4   | 6.46  | 1.43        | 1.38     |
| 1   | AA    | 1511 | G    | N9-C4   | -6.46 | 1.32        | 1.38     |
| 30  | B5    | 74   | ARG  | NE-CZ   | 6.46  | 1.41        | 1.33     |
| 35  | BB    | 408  | G    | C5-C4   | 6.46  | 1.42        | 1.38     |
| 35  | BB    | 942  | G    | C6-N1   | 6.46  | 1.44        | 1.39     |
| 1   | AA    | 700  | G    | C8-N7   | 6.46  | 1.34        | 1.30     |
| 1   | AA    | 732  | C    | P-O5'   | -6.46 | 1.53        | 1.59     |
| 1   | AA    | 869  | G    | C5-C6   | -6.46 | 1.35        | 1.42     |
| 1   | AA    | 1481 | U    | C2-N3   | 6.46  | 1.42        | 1.37     |
| 35  | BB    | 71   | A    | N1-C2   | -6.46 | 1.28        | 1.34     |
| 35  | BB    | 262  | A    | N9-C4   | 6.46  | 1.41        | 1.37     |
| 35  | BB    | 659  | G    | C1'-N9  | 6.46  | 1.58        | 1.48     |
| 35  | BB    | 2003 | A    | C6-N6   | 6.46  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 831  | A    | C6-N6   | 6.46  | 1.39        | 1.33     |
| 1   | AA    | 1363 | A    | P-O5'   | -6.46 | 1.53        | 1.59     |
| 35  | BB    | 1853 | A    | N9-C8   | -6.46 | 1.32        | 1.37     |
| 35  | BB    | 2467 | C    | C4'-O4' | -6.46 | 1.37        | 1.45     |
| 35  | BB    | 2672 | U    | C3'-C2' | -6.46 | 1.45        | 1.52     |
| 1   | AA    | 251  | G    | N1-C2   | 6.45  | 1.43        | 1.37     |
| 1   | AA    | 309  | A    | P-O5'   | -6.45 | 1.53        | 1.59     |
| 1   | AA    | 549  | C    | C5-C6   | 6.45  | 1.39        | 1.34     |
| 1   | AA    | 648  | A    | C6-N6   | 6.45  | 1.39        | 1.33     |
| 1   | AA    | 1022 | A    | C6-N6   | 6.45  | 1.39        | 1.33     |
| 1   | AA    | 1397 | C    | C4-C5   | 6.45  | 1.48        | 1.43     |
| 35  | BB    | 804  | A    | N9-C4   | 6.45  | 1.41        | 1.37     |
| 35  | BB    | 1011 | G    | C5'-C4' | 6.45  | 1.59        | 1.51     |
| 35  | BB    | 1324 | G    | C8-N7   | -6.45 | 1.27        | 1.30     |
| 35  | BB    | 1580 | A    | N3-C4   | -6.45 | 1.30        | 1.34     |
| 35  | BB    | 2343 | U    | C4'-C3' | -6.45 | 1.46        | 1.53     |
| 35  | BB    | 2473 | U    | C4'-O4' | 6.45  | 1.53        | 1.45     |
| 35  | BB    | 347  | A    | N1-C2   | 6.45  | 1.40        | 1.34     |
| 35  | BB    | 1095 | A    | O4'-C1' | 6.45  | 1.50        | 1.41     |
| 35  | BB    | 1482 | G    | C2-N3   | 6.45  | 1.38        | 1.32     |
| 35  | BB    | 1896 | G    | C4'-O4' | -6.45 | 1.37        | 1.45     |
| 35  | BB    | 2180 | U    | C4-C5   | 6.45  | 1.49        | 1.43     |
| 1   | AA    | 622  | A    | C4'-C3' | 6.45  | 1.60        | 1.53     |
| 35  | BB    | 587  | C    | C5-C6   | 6.45  | 1.39        | 1.34     |
| 35  | BB    | 1158 | C    | P-O5'   | -6.45 | 1.53        | 1.59     |
| 35  | BB    | 1849 | G    | C8-N7   | -6.45 | 1.27        | 1.30     |
| 35  | BB    | 2158 | A    | N9-C4   | 6.45  | 1.41        | 1.37     |
| 35  | BB    | 2515 | C    | C2'-C1' | -6.45 | 1.46        | 1.53     |
| 35  | BB    | 2721 | A    | N1-C2   | 6.45  | 1.40        | 1.34     |
| 35  | BB    | 2846 | G    | P-O5'   | -6.45 | 1.53        | 1.59     |
| 1   | AA    | 872  | A    | O3'-P   | -6.45 | 1.53        | 1.61     |
| 1   | AA    | 1372 | U    | C2'-C1' | -6.45 | 1.46        | 1.53     |
| 35  | BB    | 808  | G    | N1-C2   | 6.45  | 1.43        | 1.37     |
| 35  | BB    | 928  | A    | C2-N3   | 6.45  | 1.39        | 1.33     |
| 35  | BB    | 988  | A    | C6-N1   | 6.45  | 1.40        | 1.35     |
| 35  | BB    | 1242 | U    | N3-C4   | 6.45  | 1.44        | 1.38     |
| 35  | BB    | 1434 | A    | C4'-O4' | -6.45 | 1.37        | 1.45     |
| 35  | BB    | 1775 | U    | N1-C2   | 6.45  | 1.44        | 1.38     |
| 35  | BB    | 2390 | U    | C2-N3   | 6.45  | 1.42        | 1.37     |
| 1   | AA    | 1407 | C    | C2-N3   | 6.45  | 1.41        | 1.35     |
| 35  | BB    | 847  | U    | C1'-N1  | 6.45  | 1.58        | 1.48     |
| 35  | BB    | 2179 | C    | C5'-C4' | 6.45  | 1.59        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 540  | G    | C2-N2   | -6.45 | 1.28        | 1.34     |
| 1   | AA    | 895  | G    | C3'-C2' | 6.45  | 1.60        | 1.52     |
| 1   | AA    | 1163 | A    | C8-N7   | -6.45 | 1.27        | 1.31     |
| 1   | AA    | 1430 | A    | C6-N6   | 6.45  | 1.39        | 1.33     |
| 1   | AA    | 1492 | A    | N3-C4   | 6.45  | 1.38        | 1.34     |
| 14  | AN    | 40   | ARG  | CZ-NH1  | 6.45  | 1.41        | 1.33     |
| 34  | BA    | 52   | A    | C3'-C2' | 6.45  | 1.60        | 1.52     |
| 35  | BB    | 335  | C    | C4'-O4' | 6.45  | 1.53        | 1.45     |
| 35  | BB    | 473  | G    | C5'-C4' | 6.45  | 1.59        | 1.51     |
| 35  | BB    | 606  | U    | C2-N3   | -6.45 | 1.33        | 1.37     |
| 35  | BB    | 709  | U    | P-O5'   | -6.45 | 1.53        | 1.59     |
| 35  | BB    | 1751 | U    | C4'-C3' | 6.45  | 1.60        | 1.53     |
| 35  | BB    | 1870 | C    | C4'-O4' | -6.45 | 1.37        | 1.45     |
| 35  | BB    | 2144 | G    | C3'-O3' | 6.45  | 1.51        | 1.42     |
| 35  | BB    | 2288 | A    | N9-C4   | -6.45 | 1.33        | 1.37     |
| 35  | BB    | 2767 | C    | N1-C2   | 6.45  | 1.46        | 1.40     |
| 1   | AA    | 413  | G    | C8-N7   | 6.44  | 1.34        | 1.30     |
| 1   | AA    | 1020 | G    | N9-C4   | 6.44  | 1.43        | 1.38     |
| 35  | BB    | 1225 | G    | C3'-C2' | -6.44 | 1.45        | 1.52     |
| 35  | BB    | 2709 | G    | C6-N1   | 6.44  | 1.44        | 1.39     |
| 1   | AA    | 389  | A    | N9-C4   | 6.44  | 1.41        | 1.37     |
| 1   | AA    | 429  | U    | C5'-C4' | 6.44  | 1.59        | 1.51     |
| 9   | AI    | 68   | GLY  | CA-C    | -6.44 | 1.41        | 1.51     |
| 34  | BA    | 89   | U    | C5'-C4' | 6.44  | 1.59        | 1.51     |
| 35  | BB    | 492  | A    | C2-N3   | -6.44 | 1.27        | 1.33     |
| 35  | BB    | 677  | A    | C5'-C4' | 6.44  | 1.59        | 1.51     |
| 35  | BB    | 895  | U    | C2-O2   | 6.44  | 1.28        | 1.22     |
| 35  | BB    | 1082 | U    | C1'-N1  | 6.44  | 1.58        | 1.48     |
| 35  | BB    | 1550 | C    | C5-C6   | 6.44  | 1.39        | 1.34     |
| 35  | BB    | 2080 | A    | N7-C5   | -6.44 | 1.35        | 1.39     |
| 35  | BB    | 2174 | C    | C4'-O4' | -6.44 | 1.37        | 1.45     |
| 1   | AA    | 163  | C    | N3-C4   | 6.44  | 1.38        | 1.33     |
| 1   | AA    | 1487 | G    | C2'-C1' | -6.44 | 1.46        | 1.53     |
| 1   | AA    | 1529 | G    | C2-N2   | 6.44  | 1.41        | 1.34     |
| 22  | AV    | 38   | U    | C4'-C3' | -6.44 | 1.46        | 1.53     |
| 35  | BB    | 825  | A    | C2-N3   | -6.44 | 1.27        | 1.33     |
| 35  | BB    | 1141 | U    | C5'-C4' | 6.44  | 1.59        | 1.51     |
| 35  | BB    | 1215 | G    | N9-C8   | 6.44  | 1.42        | 1.37     |
| 35  | BB    | 2186 | G    | N9-C4   | 6.44  | 1.43        | 1.38     |
| 35  | BB    | 2291 | U    | N3-C4   | 6.44  | 1.44        | 1.38     |
| 1   | AA    | 284  | C    | N1-C6   | -6.44 | 1.33        | 1.37     |
| 1   | AA    | 1244 | G    | C2-N3   | 6.44  | 1.38        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 957  | C    | C5-C6   | 6.44  | 1.39        | 1.34     |
| 35  | BB    | 1875 | G    | N9-C4   | -6.44 | 1.32        | 1.38     |
| 35  | BB    | 711  | G    | C5-C4   | 6.44  | 1.42        | 1.38     |
| 35  | BB    | 1039 | A    | N9-C4   | -6.44 | 1.33        | 1.37     |
| 35  | BB    | 2397 | G    | N7-C5   | -6.44 | 1.35        | 1.39     |
| 37  | BD    | 44   | GLY  | N-CA    | -6.44 | 1.36        | 1.46     |
| 1   | AA    | 63   | C    | N1-C6   | 6.44  | 1.41        | 1.37     |
| 35  | BB    | 1616 | A    | C5-C6   | -6.44 | 1.35        | 1.41     |
| 35  | BB    | 2246 | G    | C2-N3   | 6.44  | 1.37        | 1.32     |
| 35  | BB    | 2322 | A    | O3'-P   | -6.44 | 1.53        | 1.61     |
| 35  | BB    | 2534 | A    | C6-N6   | 6.44  | 1.39        | 1.33     |
| 35  | BB    | 2569 | G    | N3-C4   | -6.44 | 1.30        | 1.35     |
| 32  | B7    | 39   | ARG  | CZ-NH1  | 6.43  | 1.41        | 1.33     |
| 35  | BB    | 227  | A    | C5-C4   | -6.43 | 1.34        | 1.38     |
| 35  | BB    | 381  | G    | N7-C5   | 6.43  | 1.43        | 1.39     |
| 35  | BB    | 426  | C    | C2'-O2' | -6.43 | 1.33        | 1.41     |
| 35  | BB    | 915  | C    | N3-C4   | 6.43  | 1.38        | 1.33     |
| 1   | AA    | 558  | G    | C2-N2   | 6.43  | 1.41        | 1.34     |
| 1   | AA    | 1220 | G    | C2'-C1' | 6.43  | 1.60        | 1.53     |
| 1   | AA    | 1466 | C    | C2-N3   | 6.43  | 1.40        | 1.35     |
| 35  | BB    | 1161 | C    | C5'-C4' | 6.43  | 1.59        | 1.51     |
| 35  | BB    | 1345 | C    | C2-O2   | 6.43  | 1.30        | 1.24     |
| 35  | BB    | 1608 | A    | C6-N6   | 6.43  | 1.39        | 1.33     |
| 35  | BB    | 2033 | A    | C5'-C4' | 6.43  | 1.59        | 1.51     |
| 35  | BB    | 2155 | U    | N3-C4   | 6.43  | 1.44        | 1.38     |
| 1   | AA    | 705  | G    | C8-N7   | 6.43  | 1.34        | 1.30     |
| 1   | AA    | 718  | A    | N7-C5   | -6.43 | 1.35        | 1.39     |
| 1   | AA    | 957  | U    | C5-C6   | 6.43  | 1.40        | 1.34     |
| 35  | BB    | 2292 | U    | C2-N3   | 6.43  | 1.42        | 1.37     |
| 35  | BB    | 2895 | G    | C2-N3   | 6.43  | 1.37        | 1.32     |
| 1   | AA    | 161  | A    | C2-N3   | 6.43  | 1.39        | 1.33     |
| 1   | AA    | 611  | C    | C3'-O3' | 6.43  | 1.51        | 1.42     |
| 1   | AA    | 1156 | G    | O3'-P   | -6.43 | 1.53        | 1.61     |
| 1   | AA    | 1505 | G    | N3-C4   | 6.43  | 1.40        | 1.35     |
| 35  | BB    | 493  | G    | O4'-C1' | -6.43 | 1.33        | 1.41     |
| 35  | BB    | 1354 | A    | C6-N1   | 6.43  | 1.40        | 1.35     |
| 35  | BB    | 1459 | G    | N1-C2   | 6.43  | 1.42        | 1.37     |
| 35  | BB    | 1675 | C    | N3-C4   | 6.43  | 1.38        | 1.33     |
| 35  | BB    | 2091 | C    | C4'-O4' | -6.43 | 1.37        | 1.45     |
| 35  | BB    | 2259 | U    | C2-N3   | -6.43 | 1.33        | 1.37     |
| 47  | BN    | 4    | ARG  | CZ-NH1  | 6.43  | 1.41        | 1.33     |
| 1   | AA    | 128  | G    | N9-C4   | -6.43 | 1.32        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 892  | A    | C5'-C4' | -6.43 | 1.43        | 1.51     |
| 35  | BB    | 1860 | G    | N7-C5   | -6.43 | 1.35        | 1.39     |
| 35  | BB    | 2517 | C    | C2-O2   | 6.43  | 1.30        | 1.24     |
| 1   | AA    | 712  | A    | N7-C5   | -6.43 | 1.35        | 1.39     |
| 1   | AA    | 932  | C    | N3-C4   | 6.43  | 1.38        | 1.33     |
| 1   | AA    | 1157 | A    | C6-N6   | 6.43  | 1.39        | 1.33     |
| 1   | AA    | 1388 | C    | P-O5'   | -6.43 | 1.53        | 1.59     |
| 12  | AL    | 116  | TYR  | CE1-CZ  | 6.43  | 1.47        | 1.38     |
| 35  | BB    | 191  | A    | C5'-C4' | 6.43  | 1.59        | 1.51     |
| 35  | BB    | 775  | G    | C6-N1   | 6.43  | 1.44        | 1.39     |
| 1   | AA    | 441  | A    | C6-N1   | 6.42  | 1.40        | 1.35     |
| 1   | AA    | 564  | C    | C4-N4   | 6.42  | 1.39        | 1.33     |
| 1   | AA    | 613  | C    | N3-C4   | 6.42  | 1.38        | 1.33     |
| 1   | AA    | 766  | A    | N1-C2   | -6.42 | 1.28        | 1.34     |
| 1   | AA    | 1018 | G    | C2-N3   | 6.42  | 1.37        | 1.32     |
| 1   | AA    | 1055 | A    | N1-C2   | -6.42 | 1.28        | 1.34     |
| 1   | AA    | 1064 | G    | C2-N3   | 6.42  | 1.37        | 1.32     |
| 34  | BA    | 54   | G    | C5-C4   | 6.42  | 1.42        | 1.38     |
| 35  | BB    | 213  | A    | N7-C5   | -6.42 | 1.35        | 1.39     |
| 35  | BB    | 638  | G    | C5-C4   | -6.42 | 1.33        | 1.38     |
| 35  | BB    | 2632 | A    | C5-C4   | 6.42  | 1.43        | 1.38     |
| 35  | BB    | 2800 | A    | C6-N6   | 6.42  | 1.39        | 1.33     |
| 35  | BB    | 432  | A    | N3-C4   | -6.42 | 1.30        | 1.34     |
| 35  | BB    | 2156 | G    | C5-C4   | -6.42 | 1.33        | 1.38     |
| 1   | AA    | 100  | G    | C6-N1   | 6.42  | 1.44        | 1.39     |
| 1   | AA    | 491  | G    | C5-C6   | -6.42 | 1.35        | 1.42     |
| 1   | AA    | 989  | U    | C2'-C1' | -6.42 | 1.46        | 1.53     |
| 22  | AV    | 32   | A    | O3'-P   | -6.42 | 1.53        | 1.61     |
| 35  | BB    | 1023 | U    | O3'-P   | -6.42 | 1.53        | 1.61     |
| 35  | BB    | 1093 | G    | C2'-O2' | -6.42 | 1.33        | 1.41     |
| 35  | BB    | 1237 | A    | C8-N7   | -6.42 | 1.27        | 1.31     |
| 35  | BB    | 1491 | G    | C2'-C1' | -6.42 | 1.46        | 1.53     |
| 35  | BB    | 2150 | C    | N3-C4   | 6.42  | 1.38        | 1.33     |
| 35  | BB    | 2674 | G    | C2-N3   | -6.42 | 1.27        | 1.32     |
| 35  | BB    | 2745 | C    | C5-C6   | -6.42 | 1.29        | 1.34     |
| 35  | BB    | 1596 | A    | N9-C8   | -6.42 | 1.32        | 1.37     |
| 48  | BO    | 30   | ARG  | NE-CZ   | 6.42  | 1.41        | 1.33     |
| 1   | AA    | 511  | C    | O3'-P   | -6.42 | 1.53        | 1.61     |
| 35  | BB    | 1434 | A    | N3-C4   | -6.42 | 1.30        | 1.34     |
| 35  | BB    | 1510 | G    | C8-N7   | -6.42 | 1.27        | 1.30     |
| 35  | BB    | 1883 | U    | O4'-C1' | 6.42  | 1.50        | 1.41     |
| 35  | BB    | 2814 | A    | N7-C5   | -6.42 | 1.35        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 76   | G    | N1-C2   | 6.42  | 1.42        | 1.37     |
| 1   | AA    | 787  | A    | N7-C5   | -6.42 | 1.35        | 1.39     |
| 1   | AA    | 988  | G    | N9-C4   | 6.42  | 1.43        | 1.38     |
| 1   | AA    | 1278 | G    | C5-C4   | -6.42 | 1.33        | 1.38     |
| 35  | BB    | 1420 | A    | O3'-P   | -6.42 | 1.53        | 1.61     |
| 35  | BB    | 1687 | G    | C2-N3   | 6.42  | 1.37        | 1.32     |
| 35  | BB    | 2145 | C    | N3-C4   | 6.42  | 1.38        | 1.33     |
| 35  | BB    | 2434 | A    | C5-C4   | -6.42 | 1.34        | 1.38     |
| 1   | AA    | 1163 | A    | N3-C4   | -6.42 | 1.31        | 1.34     |
| 35  | BB    | 371  | A    | N3-C4   | 6.42  | 1.38        | 1.34     |
| 35  | BB    | 926  | G    | C8-N7   | -6.42 | 1.27        | 1.30     |
| 35  | BB    | 2056 | G    | C2-N3   | 6.42  | 1.37        | 1.32     |
| 1   | AA    | 394  | G    | C2'-O2' | -6.41 | 1.33        | 1.41     |
| 35  | BB    | 238  | C    | C4-N4   | 6.41  | 1.39        | 1.33     |
| 35  | BB    | 1230 | A    | C5-C6   | -6.41 | 1.35        | 1.41     |
| 35  | BB    | 1377 | G    | C4'-C3' | 6.41  | 1.60        | 1.53     |
| 35  | BB    | 1690 | A    | C5-C4   | 6.41  | 1.43        | 1.38     |
| 35  | BB    | 2770 | G    | O4'-C1' | 6.41  | 1.50        | 1.41     |
| 1   | AA    | 71   | A    | C3'-O3' | 6.41  | 1.51        | 1.42     |
| 1   | AA    | 320  | A    | N9-C4   | -6.41 | 1.34        | 1.37     |
| 1   | AA    | 694  | A    | N3-C4   | 6.41  | 1.38        | 1.34     |
| 35  | BB    | 971  | G    | C2'-C1' | -6.41 | 1.46        | 1.53     |
| 35  | BB    | 1794 | A    | C5'-C4' | 6.41  | 1.59        | 1.51     |
| 35  | BB    | 2259 | U    | O3'-P   | -6.41 | 1.53        | 1.61     |
| 1   | AA    | 513  | C    | N3-C4   | 6.41  | 1.38        | 1.33     |
| 1   | AA    | 706  | A    | C2'-C1' | -6.41 | 1.46        | 1.53     |
| 1   | AA    | 857  | C    | C3'-C2' | -6.41 | 1.45        | 1.52     |
| 35  | BB    | 465  | G    | N1-C2   | 6.41  | 1.42        | 1.37     |
| 35  | BB    | 1358 | G    | N3-C4   | 6.41  | 1.40        | 1.35     |
| 35  | BB    | 2350 | C    | P-O5'   | -6.41 | 1.53        | 1.59     |
| 35  | BB    | 2869 | G    | N9-C4   | 6.41  | 1.43        | 1.38     |
| 1   | AA    | 292  | G    | C5-C4   | 6.41  | 1.42        | 1.38     |
| 1   | AA    | 672  | U    | C5'-C4' | -6.41 | 1.43        | 1.51     |
| 1   | AA    | 854  | U    | N1-C6   | -6.41 | 1.32        | 1.38     |
| 1   | AA    | 942  | G    | N3-C4   | 6.41  | 1.40        | 1.35     |
| 35  | BB    | 94   | A    | C2'-C1' | -6.41 | 1.46        | 1.53     |
| 35  | BB    | 517  | C    | C2'-C1' | -6.41 | 1.46        | 1.53     |
| 35  | BB    | 1331 | G    | C2-N3   | 6.41  | 1.37        | 1.32     |
| 35  | BB    | 1581 | G    | C4'-O4' | -6.41 | 1.37        | 1.45     |
| 35  | BB    | 1600 | C    | C5-C6   | 6.41  | 1.39        | 1.34     |
| 35  | BB    | 2878 | U    | C5'-C4' | 6.41  | 1.59        | 1.51     |
| 1   | AA    | 581  | G    | N7-C5   | -6.41 | 1.35        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 391  | G    | C4'-C3' | -6.41 | 1.46        | 1.53     |
| 1   | AA    | 420  | U    | C5-C6   | 6.41  | 1.40        | 1.34     |
| 1   | AA    | 615  | G    | N7-C5   | -6.41 | 1.35        | 1.39     |
| 1   | AA    | 1163 | A    | O3'-P   | -6.41 | 1.53        | 1.61     |
| 35  | BB    | 520  | G    | C5-C4   | 6.41  | 1.42        | 1.38     |
| 35  | BB    | 557  | C    | C4-C5   | 6.41  | 1.48        | 1.43     |
| 35  | BB    | 1080 | A    | O3'-P   | -6.41 | 1.53        | 1.61     |
| 35  | BB    | 1361 | G    | C3'-C2' | -6.41 | 1.45        | 1.52     |
| 35  | BB    | 1501 | G    | C2'-C1' | -6.41 | 1.46        | 1.53     |
| 35  | BB    | 2632 | A    | N3-C4   | -6.41 | 1.31        | 1.34     |
| 1   | AA    | 1421 | G    | N9-C8   | 6.40  | 1.42        | 1.37     |
| 35  | BB    | 2042 | A    | C1'-N9  | 6.40  | 1.58        | 1.48     |
| 1   | AA    | 840  | C    | P-O5'   | -6.40 | 1.53        | 1.59     |
| 1   | AA    | 1071 | C    | O3'-P   | -6.40 | 1.53        | 1.61     |
| 1   | AA    | 1136 | C    | C4-C5   | 6.40  | 1.48        | 1.43     |
| 1   | AA    | 1189 | U    | N3-C4   | 6.40  | 1.44        | 1.38     |
| 1   | AA    | 1258 | G    | C2-N3   | 6.40  | 1.37        | 1.32     |
| 35  | BB    | 782  | A    | C6-N1   | 6.40  | 1.40        | 1.35     |
| 35  | BB    | 1219 | U    | C2-N3   | 6.40  | 1.42        | 1.37     |
| 35  | BB    | 1303 | G    | P-O5'   | -6.40 | 1.53        | 1.59     |
| 1   | AA    | 781  | A    | P-O5'   | -6.40 | 1.53        | 1.59     |
| 35  | BB    | 52   | A    | C2-N3   | 6.40  | 1.39        | 1.33     |
| 35  | BB    | 359  | G    | N9-C8   | -6.40 | 1.33        | 1.37     |
| 35  | BB    | 470  | A    | C6-N1   | 6.40  | 1.40        | 1.35     |
| 35  | BB    | 785  | G    | C4'-C3' | -6.40 | 1.46        | 1.53     |
| 35  | BB    | 1211 | C    | N1-C6   | 6.40  | 1.41        | 1.37     |
| 35  | BB    | 1676 | A    | N1-C2   | 6.40  | 1.40        | 1.34     |
| 1   | AA    | 1151 | A    | N7-C5   | -6.40 | 1.35        | 1.39     |
| 35  | BB    | 136  | G    | C4'-O4' | 6.40  | 1.53        | 1.45     |
| 35  | BB    | 641  | U    | P-O5'   | -6.40 | 1.53        | 1.59     |
| 35  | BB    | 1377 | G    | N9-C4   | 6.40  | 1.43        | 1.38     |
| 35  | BB    | 1410 | G    | O3'-P   | 6.40  | 1.68        | 1.61     |
| 35  | BB    | 2558 | C    | C5'-C4' | 6.40  | 1.59        | 1.51     |
| 1   | AA    | 1499 | A    | N9-C4   | 6.40  | 1.41        | 1.37     |
| 20  | AT    | 23   | ARG  | CZ-NH1  | 6.40  | 1.41        | 1.33     |
| 35  | BB    | 125  | A    | C5-C6   | -6.40 | 1.35        | 1.41     |
| 35  | BB    | 1514 | G    | C8-N7   | -6.40 | 1.27        | 1.30     |
| 35  | BB    | 1684 | G    | C8-N7   | -6.40 | 1.27        | 1.30     |
| 35  | BB    | 2141 | G    | C5'-C4' | 6.40  | 1.59        | 1.51     |
| 35  | BB    | 2457 | U    | N1-C2   | 6.40  | 1.44        | 1.38     |
| 36  | BC    | 147  | PRO  | N-CD    | -6.40 | 1.38        | 1.47     |
| 1   | AA    | 298  | A    | O3'-P   | -6.39 | 1.53        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 420  | U    | O3'-P   | -6.39 | 1.53        | 1.61     |
| 1   | AA    | 606  | G    | C6-N1   | 6.39  | 1.44        | 1.39     |
| 35  | BB    | 213  | A    | C3'-C2' | -6.39 | 1.45        | 1.52     |
| 35  | BB    | 435  | C    | C2'-C1' | -6.39 | 1.46        | 1.53     |
| 35  | BB    | 724  | U    | N3-C4   | 6.39  | 1.44        | 1.38     |
| 35  | BB    | 1133 | A    | N9-C4   | 6.39  | 1.41        | 1.37     |
| 35  | BB    | 1133 | A    | C6-N6   | 6.39  | 1.39        | 1.33     |
| 35  | BB    | 1795 | C    | N3-C4   | 6.39  | 1.38        | 1.33     |
| 35  | BB    | 2666 | C    | C1'-N1  | 6.39  | 1.58        | 1.48     |
| 1   | AA    | 315  | A    | C2'-C1' | -6.39 | 1.46        | 1.53     |
| 1   | AA    | 839  | C    | N1-C6   | 6.39  | 1.41        | 1.37     |
| 1   | AA    | 840  | C    | C2-N3   | 6.39  | 1.40        | 1.35     |
| 1   | AA    | 1288 | A    | C2'-C1' | -6.39 | 1.46        | 1.53     |
| 1   | AA    | 1349 | A    | O3'-P   | -6.39 | 1.53        | 1.61     |
| 1   | AA    | 1473 | G    | C2-N3   | -6.39 | 1.27        | 1.32     |
| 35  | BB    | 102  | U    | C4-C5   | 6.39  | 1.49        | 1.43     |
| 35  | BB    | 1206 | G    | N9-C8   | -6.39 | 1.33        | 1.37     |
| 35  | BB    | 1990 | C    | O4'-C1' | -6.39 | 1.33        | 1.41     |
| 35  | BB    | 2345 | G    | C2-N3   | 6.39  | 1.37        | 1.32     |
| 35  | BB    | 2848 | G    | C2'-C1' | -6.39 | 1.46        | 1.53     |
| 35  | BB    | 638  | G    | C5-C6   | -6.39 | 1.35        | 1.42     |
| 1   | AA    | 149  | A    | N9-C8   | -6.39 | 1.32        | 1.37     |
| 1   | AA    | 265  | G    | N7-C5   | 6.39  | 1.43        | 1.39     |
| 1   | AA    | 334  | C    | N3-C4   | 6.39  | 1.38        | 1.33     |
| 1   | AA    | 390  | U    | C4-C5   | -6.39 | 1.37        | 1.43     |
| 1   | AA    | 415  | A    | N3-C4   | 6.39  | 1.38        | 1.34     |
| 1   | AA    | 1160 | G    | N7-C5   | 6.39  | 1.43        | 1.39     |
| 35  | BB    | 287  | G    | C2-N3   | 6.39  | 1.37        | 1.32     |
| 35  | BB    | 738  | G    | O3'-P   | -6.39 | 1.53        | 1.61     |
| 35  | BB    | 750  | A    | C5'-C4' | 6.39  | 1.59        | 1.51     |
| 35  | BB    | 761  | A    | N7-C5   | -6.39 | 1.35        | 1.39     |
| 35  | BB    | 2805 | C    | P-O5'   | -6.39 | 1.53        | 1.59     |
| 1   | AA    | 211  | G    | C8-N7   | 6.39  | 1.34        | 1.30     |
| 1   | AA    | 567  | G    | C2-N3   | 6.39  | 1.37        | 1.32     |
| 1   | AA    | 642  | A    | C2-N3   | 6.39  | 1.39        | 1.33     |
| 1   | AA    | 833  | G    | C8-N7   | -6.39 | 1.27        | 1.30     |
| 35  | BB    | 88   | G    | C5-C6   | -6.39 | 1.35        | 1.42     |
| 35  | BB    | 2465 | C    | C5'-C4' | 6.39  | 1.59        | 1.51     |
| 1   | AA    | 1016 | A    | C2'-C1' | -6.39 | 1.46        | 1.53     |
| 1   | AA    | 1392 | G    | C5'-C4' | 6.39  | 1.59        | 1.51     |
| 35  | BB    | 264  | C    | C4-C5   | 6.39  | 1.48        | 1.43     |
| 35  | BB    | 315  | G    | N7-C5   | 6.39  | 1.43        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 953  | G    | N9-C8   | 6.39  | 1.42        | 1.37     |
| 35  | BB    | 2257 | U    | C2'-C1' | -6.39 | 1.46        | 1.53     |
| 35  | BB    | 2764 | A    | N3-C4   | -6.39 | 1.31        | 1.34     |
| 1   | AA    | 109  | A    | C6-N6   | 6.38  | 1.39        | 1.33     |
| 1   | AA    | 266  | G    | C2-N3   | 6.38  | 1.37        | 1.32     |
| 1   | AA    | 1282 | C    | C2-O2   | 6.38  | 1.30        | 1.24     |
| 35  | BB    | 248  | G    | C2-N2   | 6.38  | 1.41        | 1.34     |
| 35  | BB    | 1131 | G    | O3'-P   | -6.38 | 1.53        | 1.61     |
| 35  | BB    | 2246 | G    | N1-C2   | 6.38  | 1.42        | 1.37     |
| 35  | BB    | 2411 | A    | N3-C4   | 6.38  | 1.38        | 1.34     |
| 35  | BB    | 1369 | G    | P-O5'   | -6.38 | 1.53        | 1.59     |
| 35  | BB    | 42   | A    | C4'-O4' | -6.38 | 1.37        | 1.45     |
| 35  | BB    | 1226 | A    | C5-C4   | -6.38 | 1.34        | 1.38     |
| 35  | BB    | 1849 | G    | C5-C6   | -6.38 | 1.35        | 1.42     |
| 35  | BB    | 2052 | A    | C6-N1   | 6.38  | 1.40        | 1.35     |
| 35  | BB    | 2567 | G    | C5-C6   | -6.38 | 1.35        | 1.42     |
| 1   | AA    | 322  | C    | N3-C4   | 6.38  | 1.38        | 1.33     |
| 35  | BB    | 752  | A    | O3'-P   | -6.38 | 1.53        | 1.61     |
| 35  | BB    | 1507 | C    | C4-C5   | 6.38  | 1.48        | 1.43     |
| 35  | BB    | 1799 | G    | C6-N1   | 6.38  | 1.44        | 1.39     |
| 35  | BB    | 1871 | A    | C5-C4   | 6.38  | 1.43        | 1.38     |
| 35  | BB    | 2120 | G    | N9-C8   | -6.38 | 1.33        | 1.37     |
| 35  | BB    | 2175 | C    | N1-C2   | 6.38  | 1.46        | 1.40     |
| 1   | AA    | 114  | U    | P-O5'   | 6.38  | 1.66        | 1.59     |
| 1   | AA    | 1208 | C    | N1-C6   | 6.38  | 1.41        | 1.37     |
| 34  | BA    | 78   | A    | C6-N6   | 6.38  | 1.39        | 1.33     |
| 35  | BB    | 1169 | A    | C2'-C1' | -6.38 | 1.46        | 1.53     |
| 35  | BB    | 1536 | C    | O4'-C1' | 6.38  | 1.50        | 1.41     |
| 35  | BB    | 2067 | G    | C5-C4   | 6.38  | 1.42        | 1.38     |
| 50  | BQ    | 29   | ARG  | CZ-NH1  | 6.38  | 1.41        | 1.33     |
| 1   | AA    | 325  | A    | N3-C4   | -6.38 | 1.31        | 1.34     |
| 1   | AA    | 525  | C    | N3-C4   | 6.38  | 1.38        | 1.33     |
| 1   | AA    | 1062 | U    | C2-N3   | 6.38  | 1.42        | 1.37     |
| 35  | BB    | 1465 | G    | C2'-O2' | -6.38 | 1.33        | 1.41     |
| 35  | BB    | 1813 | G    | C2'-C1' | -6.38 | 1.46        | 1.53     |
| 1   | AA    | 800  | G    | N7-C5   | -6.37 | 1.35        | 1.39     |
| 1   | AA    | 845  | A    | C8-N7   | -6.37 | 1.27        | 1.31     |
| 1   | AA    | 1127 | G    | C5-C4   | -6.37 | 1.33        | 1.38     |
| 1   | AA    | 1319 | A    | N9-C4   | -6.37 | 1.34        | 1.37     |
| 1   | AA    | 1357 | A    | N7-C5   | -6.37 | 1.35        | 1.39     |
| 1   | AA    | 1405 | G    | C2'-C1' | -6.37 | 1.46        | 1.53     |
| 33  | B8    | 24   | ARG  | CD-NE   | 6.37  | 1.57        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 127  | A    | C2-N3   | 6.37  | 1.39        | 1.33     |
| 35  | BB    | 1322 | A    | C5-C4   | 6.37  | 1.43        | 1.38     |
| 35  | BB    | 1510 | G    | N9-C4   | -6.37 | 1.32        | 1.38     |
| 35  | BB    | 1564 | C    | N1-C6   | 6.37  | 1.41        | 1.37     |
| 35  | BB    | 1670 | C    | O4'-C1' | -6.37 | 1.33        | 1.41     |
| 35  | BB    | 1783 | A    | N3-C4   | -6.37 | 1.31        | 1.34     |
| 35  | BB    | 2362 | C    | C4'-C3' | 6.37  | 1.60        | 1.53     |
| 35  | BB    | 2484 | G    | N9-C8   | -6.37 | 1.33        | 1.37     |
| 1   | AA    | 926  | G    | O4'-C1' | 6.37  | 1.50        | 1.41     |
| 1   | AA    | 1153 | G    | C8-N7   | 6.37  | 1.34        | 1.30     |
| 35  | BB    | 36   | G    | C6-O6   | -6.37 | 1.18        | 1.24     |
| 35  | BB    | 656  | G    | C5-C4   | -6.37 | 1.33        | 1.38     |
| 35  | BB    | 1124 | G    | C6-N1   | 6.37  | 1.44        | 1.39     |
| 35  | BB    | 1371 | G    | C6-N1   | 6.37  | 1.44        | 1.39     |
| 35  | BB    | 1985 | C    | N3-C4   | 6.37  | 1.38        | 1.33     |
| 35  | BB    | 2698 | U    | C2'-C1' | -6.37 | 1.46        | 1.53     |
| 35  | BB    | 353  | C    | C5'-C4' | 6.37  | 1.58        | 1.51     |
| 35  | BB    | 372  | G    | C2'-C1' | -6.37 | 1.46        | 1.53     |
| 35  | BB    | 2247 | A    | C6-N6   | 6.37  | 1.39        | 1.33     |
| 1   | AA    | 155  | A    | C6-N6   | 6.37  | 1.39        | 1.33     |
| 1   | AA    | 888  | G    | C4'-C3' | -6.37 | 1.46        | 1.53     |
| 35  | BB    | 1542 | U    | C2-N3   | 6.37  | 1.42        | 1.37     |
| 35  | BB    | 1603 | A    | P-O5'   | -6.37 | 1.53        | 1.59     |
| 35  | BB    | 2365 | G    | C4'-C3' | -6.37 | 1.46        | 1.53     |
| 35  | BB    | 2685 | G    | C5-C6   | -6.37 | 1.35        | 1.42     |
| 1   | AA    | 668  | G    | C8-N7   | 6.37  | 1.34        | 1.30     |
| 1   | AA    | 1180 | A    | C2'-C1' | -6.37 | 1.46        | 1.53     |
| 1   | AA    | 954  | G    | N3-C4   | -6.37 | 1.30        | 1.35     |
| 35  | BB    | 603  | A    | N7-C5   | -6.37 | 1.35        | 1.39     |
| 35  | BB    | 1925 | C    | P-O5'   | -6.37 | 1.53        | 1.59     |
| 35  | BB    | 2090 | A    | C6-N1   | 6.37  | 1.40        | 1.35     |
| 35  | BB    | 2276 | G    | C2-N2   | 6.37  | 1.41        | 1.34     |
| 35  | BB    | 2853 | C    | N1-C6   | -6.37 | 1.33        | 1.37     |
| 1   | AA    | 351  | G    | N1-C2   | 6.36  | 1.42        | 1.37     |
| 1   | AA    | 504  | C    | C2'-C1' | -6.36 | 1.46        | 1.53     |
| 1   | AA    | 674  | G    | C3'-C2' | -6.36 | 1.45        | 1.52     |
| 1   | AA    | 1004 | A    | C2'-C1' | -6.36 | 1.46        | 1.53     |
| 1   | AA    | 1241 | G    | N7-C5   | 6.36  | 1.43        | 1.39     |
| 1   | AA    | 1496 | C    | C1'-N1  | 6.36  | 1.58        | 1.48     |
| 11  | AK    | 121  | ARG  | CZ-NH1  | 6.36  | 1.41        | 1.33     |
| 35  | BB    | 77   | G    | N1-C2   | 6.36  | 1.42        | 1.37     |
| 35  | BB    | 328  | U    | C4'-C3' | 6.36  | 1.60        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 987  | C    | C4-N4   | 6.36  | 1.39        | 1.33     |
| 35  | BB    | 2014 | A    | C6-N1   | -6.36 | 1.31        | 1.35     |
| 35  | BB    | 2270 | A    | O3'-P   | -6.36 | 1.53        | 1.61     |
| 1   | AA    | 903  | G    | N1-C2   | 6.36  | 1.42        | 1.37     |
| 6   | AF    | 73   | GLU  | CD-OE1  | 6.36  | 1.32        | 1.25     |
| 35  | BB    | 472  | A    | C2'-C1' | -6.36 | 1.46        | 1.53     |
| 35  | BB    | 1690 | A    | C4'-C3' | 6.36  | 1.60        | 1.53     |
| 35  | BB    | 2180 | U    | C2-N3   | 6.36  | 1.42        | 1.37     |
| 1   | AA    | 263  | A    | C6-N6   | 6.36  | 1.39        | 1.33     |
| 35  | BB    | 1537 | G    | N1-C2   | 6.36  | 1.42        | 1.37     |
| 35  | BB    | 2340 | A    | C6-N1   | 6.36  | 1.40        | 1.35     |
| 35  | BB    | 2367 | G    | C8-N7   | -6.36 | 1.27        | 1.30     |
| 1   | AA    | 30   | U    | O4'-C1' | 6.36  | 1.50        | 1.41     |
| 35  | BB    | 1126 | A    | C6-N1   | -6.36 | 1.31        | 1.35     |
| 35  | BB    | 2077 | A    | N7-C5   | -6.36 | 1.35        | 1.39     |
| 35  | BB    | 2228 | G    | C2'-C1' | -6.36 | 1.46        | 1.53     |
| 35  | BB    | 2255 | G    | C5-C4   | 6.36  | 1.42        | 1.38     |
| 35  | BB    | 2289 | G    | C6-N1   | 6.36  | 1.44        | 1.39     |
| 35  | BB    | 2373 | G    | N1-C2   | 6.36  | 1.42        | 1.37     |
| 1   | AA    | 1275 | A    | N3-C4   | -6.36 | 1.31        | 1.34     |
| 1   | AA    | 1504 | G    | N1-C2   | 6.36  | 1.42        | 1.37     |
| 34  | BA    | 69   | G    | N7-C5   | 6.36  | 1.43        | 1.39     |
| 35  | BB    | 396  | G    | N9-C8   | 6.36  | 1.42        | 1.37     |
| 35  | BB    | 1559 | U    | N1-C6   | 6.36  | 1.43        | 1.38     |
| 35  | BB    | 2168 | G    | C5-C6   | -6.36 | 1.35        | 1.42     |
| 35  | BB    | 2295 | C    | C4'-C3' | 6.36  | 1.60        | 1.53     |
| 35  | BB    | 2408 | U    | P-O5'   | 6.36  | 1.66        | 1.59     |
| 35  | BB    | 2503 | A    | N7-C5   | -6.36 | 1.35        | 1.39     |
| 1   | AA    | 1493 | A    | C2-N3   | 6.36  | 1.39        | 1.33     |
| 35  | BB    | 44   | A    | C2'-C1' | -6.36 | 1.46        | 1.53     |
| 35  | BB    | 654  | A    | C8-N7   | -6.36 | 1.27        | 1.31     |
| 35  | BB    | 1061 | U    | C4'-C3' | 6.36  | 1.60        | 1.53     |
| 35  | BB    | 1725 | U    | P-O5'   | -6.36 | 1.53        | 1.59     |
| 1   | AA    | 1167 | A    | N9-C8   | 6.35  | 1.42        | 1.37     |
| 35  | BB    | 237  | C    | C3'-C2' | 6.35  | 1.59        | 1.52     |
| 35  | BB    | 1777 | U    | C2'-C1' | -6.35 | 1.46        | 1.53     |
| 35  | BB    | 2476 | A    | C2-N3   | 6.35  | 1.39        | 1.33     |
| 35  | BB    | 2744 | G    | C2-N3   | 6.35  | 1.37        | 1.32     |
| 35  | BB    | 2846 | G    | C5'-C4' | 6.35  | 1.58        | 1.51     |
| 1   | AA    | 229  | U    | N1-C2   | 6.35  | 1.44        | 1.38     |
| 1   | AA    | 732  | C    | N1-C2   | 6.35  | 1.46        | 1.40     |
| 35  | BB    | 75   | G    | C2-N3   | 6.35  | 1.37        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 862  | G    | C5'-C4' | 6.35  | 1.58        | 1.51     |
| 35  | BB    | 920  | A    | N9-C4   | 6.35  | 1.41        | 1.37     |
| 35  | BB    | 1010 | A    | C6-N1   | 6.35  | 1.40        | 1.35     |
| 35  | BB    | 1719 | G    | C2-N3   | 6.35  | 1.37        | 1.32     |
| 1   | AA    | 928  | G    | N9-C8   | 6.35  | 1.42        | 1.37     |
| 35  | BB    | 589  | U    | C2'-C1' | -6.35 | 1.46        | 1.53     |
| 35  | BB    | 755  | U    | C4-C5   | -6.35 | 1.37        | 1.43     |
| 35  | BB    | 1052 | C    | O4'-C1' | 6.35  | 1.50        | 1.41     |
| 35  | BB    | 1137 | G    | N3-C4   | -6.35 | 1.31        | 1.35     |
| 35  | BB    | 1539 | U    | N1-C2   | 6.35  | 1.44        | 1.38     |
| 35  | BB    | 1708 | C    | C4-N4   | 6.35  | 1.39        | 1.33     |
| 35  | BB    | 1817 | G    | C5'-C4' | 6.35  | 1.58        | 1.51     |
| 35  | BB    | 2025 | C    | C4-N4   | 6.35  | 1.39        | 1.33     |
| 35  | BB    | 2466 | C    | P-O5'   | -6.35 | 1.53        | 1.59     |
| 1   | AA    | 75   | G    | C6-N1   | 6.35  | 1.44        | 1.39     |
| 1   | AA    | 297  | G    | C3'-O3' | 6.35  | 1.51        | 1.42     |
| 1   | AA    | 515  | G    | O4'-C1' | -6.35 | 1.33        | 1.41     |
| 1   | AA    | 1087 | G    | C2-N3   | 6.35  | 1.37        | 1.32     |
| 35  | BB    | 5    | A    | C6-N6   | 6.35  | 1.39        | 1.33     |
| 35  | BB    | 1188 | U    | C2'-C1' | -6.35 | 1.46        | 1.53     |
| 35  | BB    | 2311 | A    | C5-C4   | 6.35  | 1.43        | 1.38     |
| 35  | BB    | 2442 | C    | C5-C6   | 6.35  | 1.39        | 1.34     |
| 35  | BB    | 2694 | G    | N1-C2   | 6.35  | 1.42        | 1.37     |
| 35  | BB    | 2735 | G    | N7-C5   | -6.35 | 1.35        | 1.39     |
| 48  | BO    | 7    | ARG  | NE-CZ   | 6.35  | 1.41        | 1.33     |
| 35  | BB    | 732  | C    | N1-C6   | 6.35  | 1.41        | 1.37     |
| 35  | BB    | 2252 | G    | N7-C5   | -6.35 | 1.35        | 1.39     |
| 26  | B1    | 12   | GLU  | CB-CG   | 6.34  | 1.64        | 1.52     |
| 35  | BB    | 30   | G    | N7-C5   | -6.34 | 1.35        | 1.39     |
| 35  | BB    | 67   | U    | N1-C6   | 6.34  | 1.43        | 1.38     |
| 35  | BB    | 192  | C    | N3-C4   | 6.34  | 1.38        | 1.33     |
| 35  | BB    | 1039 | A    | N7-C5   | -6.34 | 1.35        | 1.39     |
| 35  | BB    | 2253 | G    | C5-C6   | -6.34 | 1.36        | 1.42     |
| 35  | BB    | 2529 | G    | C6-N1   | 6.34  | 1.44        | 1.39     |
| 35  | BB    | 2736 | A    | C6-N6   | 6.34  | 1.39        | 1.33     |
| 1   | AA    | 1507 | A    | C5-C4   | 6.34  | 1.43        | 1.38     |
| 22  | AV    | 76   | A    | C6-N1   | 6.34  | 1.40        | 1.35     |
| 35  | BB    | 684  | G    | C6-N1   | 6.34  | 1.44        | 1.39     |
| 35  | BB    | 1071 | G    | C4'-O4' | -6.34 | 1.37        | 1.45     |
| 35  | BB    | 2806 | C    | C2'-C1' | -6.34 | 1.46        | 1.53     |
| 1   | AA    | 617  | G    | C3'-C2' | -6.34 | 1.45        | 1.52     |
| 1   | AA    | 781  | A    | C6-N6   | 6.34  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 975  | A    | C2-N3   | -6.34 | 1.27        | 1.33     |
| 1   | AA    | 1463 | U    | P-O5'   | -6.34 | 1.53        | 1.59     |
| 35  | BB    | 350  | G    | C5-C4   | -6.34 | 1.33        | 1.38     |
| 35  | BB    | 445  | C    | C5-C6   | -6.34 | 1.29        | 1.34     |
| 35  | BB    | 754  | U    | P-O5'   | -6.34 | 1.53        | 1.59     |
| 35  | BB    | 1407 | G    | N9-C8   | 6.34  | 1.42        | 1.37     |
| 35  | BB    | 2507 | C    | N3-C4   | 6.34  | 1.38        | 1.33     |
| 36  | BC    | 214  | GLY  | CA-C    | -6.34 | 1.41        | 1.51     |
| 1   | AA    | 232  | G    | C8-N7   | 6.34  | 1.34        | 1.30     |
| 1   | AA    | 810  | C    | P-O5'   | -6.34 | 1.53        | 1.59     |
| 1   | AA    | 825  | A    | O5'-C5' | 6.34  | 1.54        | 1.44     |
| 1   | AA    | 1097 | C    | C4'-C3' | -6.34 | 1.46        | 1.53     |
| 1   | AA    | 1333 | A    | C6-N6   | 6.34  | 1.39        | 1.33     |
| 1   | AA    | 1351 | U    | N3-C4   | 6.34  | 1.44        | 1.38     |
| 35  | BB    | 1030 | C    | P-O5'   | -6.34 | 1.53        | 1.59     |
| 35  | BB    | 1535 | A    | C5'-C4' | 6.34  | 1.58        | 1.51     |
| 35  | BB    | 2210 | U    | C4'-C3' | 6.34  | 1.60        | 1.53     |
| 35  | BB    | 2358 | A    | C4'-C3' | 6.34  | 1.60        | 1.53     |
| 1   | AA    | 1416 | G    | N1-C2   | 6.34  | 1.42        | 1.37     |
| 1   | AA    | 151  | A    | N9-C4   | -6.34 | 1.34        | 1.37     |
| 1   | AA    | 619  | U    | O3'-P   | -6.34 | 1.53        | 1.61     |
| 34  | BA    | 58   | A    | N1-C2   | -6.34 | 1.28        | 1.34     |
| 35  | BB    | 135  | U    | C4'-C3' | 6.34  | 1.60        | 1.53     |
| 35  | BB    | 405  | U    | C2-N3   | 6.34  | 1.42        | 1.37     |
| 35  | BB    | 1817 | G    | C2'-C1' | -6.34 | 1.46        | 1.53     |
| 35  | BB    | 2145 | C    | C5'-C4' | 6.34  | 1.58        | 1.51     |
| 35  | BB    | 2716 | C    | C3'-O3' | 6.34  | 1.51        | 1.42     |
| 35  | BB    | 2747 | G    | N9-C8   | 6.34  | 1.42        | 1.37     |
| 35  | BB    | 1633 | G    | C8-N7   | -6.33 | 1.27        | 1.30     |
| 35  | BB    | 2468 | A    | N3-C4   | 6.33  | 1.38        | 1.34     |
| 1   | AA    | 1043 | G    | C4'-O4' | 6.33  | 1.53        | 1.45     |
| 1   | AA    | 1106 | G    | C2'-C1' | -6.33 | 1.46        | 1.53     |
| 1   | AA    | 1332 | A    | C5-C6   | 6.33  | 1.46        | 1.41     |
| 1   | AA    | 1337 | G    | N9-C4   | -6.33 | 1.32        | 1.38     |
| 35  | BB    | 389  | G    | C6-N1   | 6.33  | 1.44        | 1.39     |
| 35  | BB    | 2010 | G    | N7-C5   | -6.33 | 1.35        | 1.39     |
| 35  | BB    | 2439 | A    | N1-C2   | 6.33  | 1.40        | 1.34     |
| 35  | BB    | 2725 | A    | N9-C4   | -6.33 | 1.34        | 1.37     |
| 1   | AA    | 824  | G    | C6-N1   | 6.33  | 1.44        | 1.39     |
| 35  | BB    | 835  | C    | C5'-C4' | 6.33  | 1.58        | 1.51     |
| 35  | BB    | 1044 | C    | C4-N4   | 6.33  | 1.39        | 1.33     |
| 35  | BB    | 1172 | C    | C4-N4   | 6.33  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1244 | A    | N9-C8   | 6.33  | 1.42        | 1.37     |
| 35  | BB    | 1468 | U    | C2-N3   | 6.33  | 1.42        | 1.37     |
| 35  | BB    | 2465 | C    | O3'-P   | -6.33 | 1.53        | 1.61     |
| 34  | BA    | 40   | U    | C5'-C4' | 6.33  | 1.58        | 1.51     |
| 35  | BB    | 684  | G    | N1-C2   | 6.33  | 1.42        | 1.37     |
| 35  | BB    | 1730 | C    | N3-C4   | 6.33  | 1.38        | 1.33     |
| 35  | BB    | 2066 | C    | P-O5'   | -6.33 | 1.53        | 1.59     |
| 35  | BB    | 2615 | U    | C4-O4   | -6.33 | 1.18        | 1.23     |
| 1   | AA    | 94   | G    | C2-N2   | 6.33  | 1.40        | 1.34     |
| 1   | AA    | 663  | A    | C4'-O4' | 6.33  | 1.53        | 1.45     |
| 1   | AA    | 668  | G    | N7-C5   | -6.33 | 1.35        | 1.39     |
| 1   | AA    | 892  | A    | C5-C6   | 6.33  | 1.46        | 1.41     |
| 1   | AA    | 939  | G    | C6-N1   | 6.33  | 1.44        | 1.39     |
| 14  | AN    | 89   | ARG  | CZ-NH2  | 6.33  | 1.41        | 1.33     |
| 35  | BB    | 451  | U    | C2-N3   | 6.33  | 1.42        | 1.37     |
| 35  | BB    | 702  | U    | C2-N3   | 6.33  | 1.42        | 1.37     |
| 35  | BB    | 1813 | G    | C5'-C4' | 6.33  | 1.58        | 1.51     |
| 35  | BB    | 1901 | A    | C8-N7   | -6.33 | 1.27        | 1.31     |
| 35  | BB    | 2321 | U    | C5'-C4' | 6.33  | 1.58        | 1.51     |
| 35  | BB    | 2475 | C    | C4-N4   | 6.33  | 1.39        | 1.33     |
| 35  | BB    | 2576 | G    | C8-N7   | -6.33 | 1.27        | 1.30     |
| 45  | BL    | 130  | GLY  | CA-C    | -6.33 | 1.41        | 1.51     |
| 1   | AA    | 814  | A    | O3'-P   | -6.33 | 1.53        | 1.61     |
| 35  | BB    | 183  | C    | N1-C6   | -6.33 | 1.33        | 1.37     |
| 35  | BB    | 848  | C    | N3-C4   | 6.33  | 1.38        | 1.33     |
| 35  | BB    | 1747 | U    | C2-N3   | 6.33  | 1.42        | 1.37     |
| 1   | AA    | 1508 | A    | N7-C5   | -6.33 | 1.35        | 1.39     |
| 9   | AI    | 25   | GLY  | CA-C    | -6.33 | 1.41        | 1.51     |
| 35  | BB    | 73   | A    | C4'-O4' | -6.33 | 1.37        | 1.45     |
| 35  | BB    | 91   | A    | N9-C4   | -6.33 | 1.34        | 1.37     |
| 35  | BB    | 468  | G    | C2'-C1' | -6.33 | 1.46        | 1.53     |
| 35  | BB    | 789  | A    | C4'-O4' | 6.33  | 1.53        | 1.45     |
| 35  | BB    | 1154 | G    | C3'-C2' | -6.33 | 1.45        | 1.52     |
| 35  | BB    | 2092 | U    | O4'-C1' | 6.33  | 1.49        | 1.41     |
| 35  | BB    | 2874 | C    | C4-N4   | 6.33  | 1.39        | 1.33     |
| 1   | AA    | 859  | G    | C1'-N9  | 6.32  | 1.58        | 1.48     |
| 1   | AA    | 934  | C    | N1-C6   | 6.32  | 1.41        | 1.37     |
| 1   | AA    | 1144 | G    | O4'-C1' | 6.32  | 1.49        | 1.41     |
| 19  | AS    | 33   | TRP  | CD2-CE2 | 6.32  | 1.49        | 1.41     |
| 35  | BB    | 704  | G    | C6-N1   | 6.32  | 1.44        | 1.39     |
| 35  | BB    | 1531 | C    | C2-O2   | 6.32  | 1.30        | 1.24     |
| 35  | BB    | 2386 | A    | C5-C6   | -6.32 | 1.35        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2436 | G    | C3'-C2' | 6.32  | 1.59        | 1.52     |
| 35  | BB    | 2469 | A    | O4'-C1' | -6.32 | 1.33        | 1.41     |
| 35  | BB    | 2873 | A    | C6-N6   | 6.32  | 1.39        | 1.33     |
| 7   | AG    | 49   | LEU  | N-CA    | -6.32 | 1.33        | 1.46     |
| 35  | BB    | 831  | G    | N7-C5   | -6.32 | 1.35        | 1.39     |
| 35  | BB    | 1195 | G    | N7-C5   | -6.32 | 1.35        | 1.39     |
| 1   | AA    | 183  | C    | C4'-C3' | 6.32  | 1.60        | 1.53     |
| 35  | BB    | 651  | G    | C3'-C2' | -6.32 | 1.45        | 1.52     |
| 35  | BB    | 832  | U    | N3-C4   | 6.32  | 1.44        | 1.38     |
| 35  | BB    | 973  | A    | P-O5'   | -6.32 | 1.53        | 1.59     |
| 35  | BB    | 1238 | G    | N1-C2   | 6.32  | 1.42        | 1.37     |
| 35  | BB    | 1637 | A    | N7-C5   | -6.32 | 1.35        | 1.39     |
| 35  | BB    | 1669 | A    | C1'-N9  | 6.32  | 1.58        | 1.48     |
| 35  | BB    | 2336 | A    | P-O5'   | -6.32 | 1.53        | 1.59     |
| 35  | BB    | 2410 | G    | C8-N7   | -6.32 | 1.27        | 1.30     |
| 1   | AA    | 95   | C    | C5'-C4' | 6.32  | 1.58        | 1.51     |
| 35  | BB    | 573  | U    | P-O5'   | -6.32 | 1.53        | 1.59     |
| 35  | BB    | 658  | U    | C4-O4   | -6.32 | 1.18        | 1.23     |
| 35  | BB    | 932  | U    | C4'-C3' | -6.32 | 1.46        | 1.53     |
| 1   | AA    | 656  | G    | C5'-C4' | 6.32  | 1.58        | 1.51     |
| 34  | BA    | 51   | G    | O3'-P   | -6.32 | 1.53        | 1.61     |
| 35  | BB    | 273  | G    | C2-N2   | 6.32  | 1.40        | 1.34     |
| 35  | BB    | 1424 | G    | P-O5'   | -6.32 | 1.53        | 1.59     |
| 35  | BB    | 1596 | A    | C4'-O4' | -6.32 | 1.37        | 1.45     |
| 35  | BB    | 1697 | G    | C2-N2   | 6.32  | 1.40        | 1.34     |
| 35  | BB    | 1904 | G    | C4'-C3' | 6.32  | 1.60        | 1.53     |
| 35  | BB    | 2302 | U    | C2'-C1' | -6.32 | 1.46        | 1.53     |
| 35  | BB    | 2772 | C    | C4'-C3' | -6.32 | 1.46        | 1.53     |
| 35  | BB    | 143  | C    | C4'-C3' | -6.32 | 1.46        | 1.53     |
| 35  | BB    | 1377 | G    | O3'-P   | -6.32 | 1.53        | 1.61     |
| 35  | BB    | 1454 | C    | C3'-C2' | 6.32  | 1.59        | 1.52     |
| 35  | BB    | 1846 | G    | C2-N2   | 6.32  | 1.40        | 1.34     |
| 35  | BB    | 1866 | A    | C4'-C3' | -6.32 | 1.46        | 1.53     |
| 35  | BB    | 2195 | U    | C5'-C4' | 6.32  | 1.58        | 1.51     |
| 35  | BB    | 2481 | G    | C3'-O3' | -6.32 | 1.33        | 1.42     |
| 35  | BB    | 2595 | G    | C5'-C4' | 6.32  | 1.58        | 1.51     |
| 35  | BB    | 360  | U    | C2'-O2' | 6.31  | 1.49        | 1.41     |
| 35  | BB    | 1086 | A    | N9-C8   | -6.31 | 1.32        | 1.37     |
| 35  | BB    | 1891 | G    | N1-C2   | 6.31  | 1.42        | 1.37     |
| 1   | AA    | 445  | G    | N7-C5   | 6.31  | 1.43        | 1.39     |
| 1   | AA    | 773  | G    | N9-C4   | 6.31  | 1.43        | 1.38     |
| 1   | AA    | 1454 | G    | N7-C5   | -6.31 | 1.35        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 278  | A    | N3-C4   | 6.31  | 1.38        | 1.34     |
| 35  | BB    | 382  | A    | C5-C4   | 6.31  | 1.43        | 1.38     |
| 35  | BB    | 1267 | U    | N1-C2   | 6.31  | 1.44        | 1.38     |
| 35  | BB    | 1350 | C    | N3-C4   | 6.31  | 1.38        | 1.33     |
| 35  | BB    | 2025 | C    | C2-O2   | 6.31  | 1.30        | 1.24     |
| 35  | BB    | 2096 | C    | C5-C6   | -6.31 | 1.29        | 1.34     |
| 35  | BB    | 2260 | C    | N1-C6   | 6.31  | 1.41        | 1.37     |
| 35  | BB    | 2711 | A    | C6-N6   | 6.31  | 1.39        | 1.33     |
| 48  | BO    | 95   | SER  | CA-CB   | 6.31  | 1.62        | 1.52     |
| 1   | AA    | 954  | G    | N9-C8   | 6.31  | 1.42        | 1.37     |
| 35  | BB    | 212  | G    | N1-C2   | 6.31  | 1.42        | 1.37     |
| 35  | BB    | 784  | G    | N9-C4   | 6.31  | 1.43        | 1.38     |
| 35  | BB    | 2540 | C    | N3-C4   | 6.31  | 1.38        | 1.33     |
| 23  | AX    | 16   | C    | C5'-C4' | 6.31  | 1.58        | 1.51     |
| 35  | BB    | 431  | U    | C4-C5   | 6.31  | 1.49        | 1.43     |
| 35  | BB    | 701  | G    | C5-C4   | -6.31 | 1.33        | 1.38     |
| 35  | BB    | 829  | A    | N9-C4   | 6.31  | 1.41        | 1.37     |
| 35  | BB    | 1707 | G    | C8-N7   | 6.31  | 1.34        | 1.30     |
| 35  | BB    | 1840 | G    | C2-N3   | 6.31  | 1.37        | 1.32     |
| 35  | BB    | 2841 | C    | C2-N3   | -6.31 | 1.30        | 1.35     |
| 1   | AA    | 316  | C    | C4-N4   | 6.31  | 1.39        | 1.33     |
| 1   | AA    | 1334 | G    | C4'-C3' | 6.31  | 1.60        | 1.53     |
| 35  | BB    | 727  | A    | C2-N3   | 6.31  | 1.39        | 1.33     |
| 35  | BB    | 1194 | A    | C6-N1   | 6.31  | 1.40        | 1.35     |
| 1   | AA    | 663  | A    | C5-C4   | 6.31  | 1.43        | 1.38     |
| 1   | AA    | 684  | U    | C5-C6   | 6.31  | 1.39        | 1.34     |
| 35  | BB    | 9    | G    | N1-C2   | 6.31  | 1.42        | 1.37     |
| 35  | BB    | 682  | G    | C6-N1   | 6.31  | 1.44        | 1.39     |
| 35  | BB    | 757  | G    | C5'-C4' | 6.31  | 1.58        | 1.51     |
| 35  | BB    | 833  | A    | C2-N3   | 6.31  | 1.39        | 1.33     |
| 1   | AA    | 310  | G    | N3-C4   | 6.30  | 1.39        | 1.35     |
| 1   | AA    | 367  | U    | O3'-P   | -6.30 | 1.53        | 1.61     |
| 1   | AA    | 591  | U    | N3-C4   | 6.30  | 1.44        | 1.38     |
| 35  | BB    | 346  | A    | C3'-O3' | 6.30  | 1.50        | 1.42     |
| 35  | BB    | 2732 | G    | O4'-C1' | -6.30 | 1.33        | 1.41     |
| 35  | BB    | 2856 | A    | C2'-C1' | -6.30 | 1.46        | 1.53     |
| 1   | AA    | 215  | C    | N3-C4   | 6.30  | 1.38        | 1.33     |
| 1   | AA    | 341  | C    | O4'-C1' | 6.30  | 1.49        | 1.41     |
| 1   | AA    | 861  | G    | C2-N3   | 6.30  | 1.37        | 1.32     |
| 1   | AA    | 1397 | C    | C4'-C3' | 6.30  | 1.60        | 1.53     |
| 34  | BA    | 29   | A    | C6-N1   | 6.30  | 1.40        | 1.35     |
| 35  | BB    | 772  | C    | N3-C4   | 6.30  | 1.38        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 388  | G    | C3'-C2' | -6.30 | 1.45        | 1.52     |
| 1   | AA    | 395  | C    | C4'-C3' | 6.30  | 1.60        | 1.53     |
| 1   | AA    | 671  | G    | C6-O6   | -6.30 | 1.18        | 1.24     |
| 1   | AA    | 878  | A    | N9-C4   | 6.30  | 1.41        | 1.37     |
| 1   | AA    | 1108 | G    | N1-C2   | 6.30  | 1.42        | 1.37     |
| 1   | AA    | 1288 | A    | C8-N7   | -6.30 | 1.27        | 1.31     |
| 35  | BB    | 577  | G    | C2'-C1' | -6.30 | 1.46        | 1.53     |
| 35  | BB    | 1076 | C    | C4'-O4' | 6.30  | 1.53        | 1.45     |
| 35  | BB    | 1506 | U    | C5-C6   | 6.30  | 1.39        | 1.34     |
| 35  | BB    | 1850 | G    | N1-C2   | 6.30  | 1.42        | 1.37     |
| 35  | BB    | 2886 | A    | C4'-C3' | 6.30  | 1.60        | 1.53     |
| 1   | AA    | 1385 | G    | C5-C4   | 6.30  | 1.42        | 1.38     |
| 35  | BB    | 491  | G    | N1-C2   | 6.30  | 1.42        | 1.37     |
| 35  | BB    | 576  | U    | C2-N3   | 6.30  | 1.42        | 1.37     |
| 35  | BB    | 1753 | G    | C5-C4   | -6.30 | 1.33        | 1.38     |
| 35  | BB    | 1861 | G    | N3-C4   | -6.30 | 1.31        | 1.35     |
| 35  | BB    | 2524 | G    | C5-C6   | -6.30 | 1.36        | 1.42     |
| 35  | BB    | 2602 | A    | N9-C4   | -6.30 | 1.34        | 1.37     |
| 35  | BB    | 2617 | U    | C1'-N1  | 6.30  | 1.58        | 1.48     |
| 1   | AA    | 36   | C    | C4'-C3' | 6.30  | 1.60        | 1.53     |
| 1   | AA    | 357  | G    | N9-C4   | -6.30 | 1.32        | 1.38     |
| 1   | AA    | 939  | G    | O3'-P   | -6.30 | 1.53        | 1.61     |
| 22  | AV    | 2    | G    | N9-C4   | 6.30  | 1.43        | 1.38     |
| 35  | BB    | 1471 | G    | N9-C8   | -6.30 | 1.33        | 1.37     |
| 1   | AA    | 284  | C    | C4-N4   | 6.30  | 1.39        | 1.33     |
| 1   | AA    | 378  | G    | P-O5'   | -6.30 | 1.53        | 1.59     |
| 1   | AA    | 550  | G    | C2-N3   | 6.30  | 1.37        | 1.32     |
| 1   | AA    | 1166 | G    | C2-N3   | 6.30  | 1.37        | 1.32     |
| 1   | AA    | 1448 | C    | C3'-C2' | 6.30  | 1.59        | 1.52     |
| 3   | AC    | 167  | TYR  | CE1-CZ  | 6.30  | 1.46        | 1.38     |
| 34  | BA    | 11   | C    | C2-N3   | -6.30 | 1.30        | 1.35     |
| 35  | BB    | 477  | A    | C2-N3   | 6.30  | 1.39        | 1.33     |
| 35  | BB    | 907  | G    | C8-N7   | 6.30  | 1.34        | 1.30     |
| 35  | BB    | 1736 | U    | N3-C4   | 6.30  | 1.44        | 1.38     |
| 35  | BB    | 1757 | A    | N3-C4   | -6.30 | 1.31        | 1.34     |
| 35  | BB    | 1960 | A    | C3'-O3' | 6.30  | 1.50        | 1.42     |
| 1   | AA    | 60   | A    | C2-N3   | 6.29  | 1.39        | 1.33     |
| 1   | AA    | 1052 | U    | C2'-C1' | -6.29 | 1.46        | 1.53     |
| 1   | AA    | 1254 | A    | O4'-C1' | -6.29 | 1.33        | 1.41     |
| 35  | BB    | 1269 | A    | C6-N6   | 6.29  | 1.39        | 1.33     |
| 35  | BB    | 1276 | A    | N9-C4   | -6.29 | 1.34        | 1.37     |
| 35  | BB    | 2319 | G    | N9-C4   | 6.29  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 192  | A    | C2'-C1' | -6.29 | 1.46        | 1.53     |
| 1   | AA    | 270  | A    | C2'-C1' | -6.29 | 1.46        | 1.53     |
| 1   | AA    | 862  | C    | C4'-C3' | 6.29  | 1.60        | 1.53     |
| 35  | BB    | 316  | C    | N3-C4   | 6.29  | 1.38        | 1.33     |
| 35  | BB    | 945  | A    | C5-C6   | -6.29 | 1.35        | 1.41     |
| 35  | BB    | 2623 | G    | P-O5'   | -6.29 | 1.53        | 1.59     |
| 45  | BL    | 47   | ARG  | CD-NE   | 6.29  | 1.57        | 1.46     |
| 1   | AA    | 156  | C    | C4-N4   | 6.29  | 1.39        | 1.33     |
| 1   | AA    | 329  | A    | C6-N1   | 6.29  | 1.40        | 1.35     |
| 35  | BB    | 81   | G    | C5-C4   | 6.29  | 1.42        | 1.38     |
| 35  | BB    | 402  | A    | C6-N6   | 6.29  | 1.39        | 1.33     |
| 35  | BB    | 678  | C    | N1-C6   | -6.29 | 1.33        | 1.37     |
| 35  | BB    | 712  | G    | C4'-O4' | 6.29  | 1.53        | 1.45     |
| 35  | BB    | 902  | C    | N3-C4   | 6.29  | 1.38        | 1.33     |
| 35  | BB    | 1266 | G    | N9-C4   | 6.29  | 1.43        | 1.38     |
| 35  | BB    | 2165 | C    | C4-N4   | 6.29  | 1.39        | 1.33     |
| 35  | BB    | 2222 | C    | P-O5'   | -6.29 | 1.53        | 1.59     |
| 35  | BB    | 2296 | U    | C5'-C4' | 6.29  | 1.58        | 1.51     |
| 35  | BB    | 2489 | U    | N1-C2   | 6.29  | 1.44        | 1.38     |
| 35  | BB    | 2729 | G    | C6-N1   | 6.29  | 1.44        | 1.39     |
| 1   | AA    | 451  | A    | C6-N1   | 6.29  | 1.40        | 1.35     |
| 1   | AA    | 503  | C    | C5'-C4' | 6.29  | 1.58        | 1.51     |
| 1   | AA    | 766  | A    | P-O5'   | -6.29 | 1.53        | 1.59     |
| 1   | AA    | 331  | G    | O4'-C1' | 6.29  | 1.49        | 1.41     |
| 1   | AA    | 471  | U    | C2'-C1' | -6.29 | 1.46        | 1.53     |
| 1   | AA    | 1390 | U    | C4-C5   | 6.29  | 1.49        | 1.43     |
| 35  | BB    | 1024 | G    | C2-N3   | 6.29  | 1.37        | 1.32     |
| 35  | BB    | 1960 | A    | C2'-C1' | -6.29 | 1.46        | 1.53     |
| 35  | BB    | 2378 | A    | C6-N1   | 6.29  | 1.40        | 1.35     |
| 35  | BB    | 2527 | C    | N3-C4   | 6.29  | 1.38        | 1.33     |
| 34  | BA    | 109  | A    | C8-N7   | -6.29 | 1.27        | 1.31     |
| 35  | BB    | 1966 | A    | N3-C4   | 6.29  | 1.38        | 1.34     |
| 35  | BB    | 2033 | A    | C5-C4   | 6.29  | 1.43        | 1.38     |
| 1   | AA    | 28   | A    | N7-C5   | -6.29 | 1.35        | 1.39     |
| 1   | AA    | 138  | G    | N7-C5   | -6.29 | 1.35        | 1.39     |
| 1   | AA    | 157  | U    | C3'-C2' | -6.29 | 1.45        | 1.52     |
| 1   | AA    | 302  | G    | N3-C4   | -6.29 | 1.31        | 1.35     |
| 1   | AA    | 775  | G    | N7-C5   | -6.29 | 1.35        | 1.39     |
| 1   | AA    | 889  | A    | C5-C4   | 6.29  | 1.43        | 1.38     |
| 1   | AA    | 1229 | A    | C6-N6   | 6.29  | 1.39        | 1.33     |
| 34  | BA    | 99   | A    | N3-C4   | -6.29 | 1.31        | 1.34     |
| 35  | BB    | 1757 | A    | C6-N6   | 6.29  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1938 | A    | N9-C8   | 6.29  | 1.42        | 1.37     |
| 35  | BB    | 2140 | G    | C5'-C4' | 6.29  | 1.58        | 1.51     |
| 1   | AA    | 519  | C    | N3-C4   | 6.28  | 1.38        | 1.33     |
| 1   | AA    | 1220 | G    | N3-C4   | -6.28 | 1.31        | 1.35     |
| 34  | BA    | 100  | G    | C2'-C1' | -6.28 | 1.46        | 1.53     |
| 35  | BB    | 158  | U    | C5'-C4' | -6.28 | 1.43        | 1.51     |
| 35  | BB    | 1106 | G    | C2-N3   | 6.28  | 1.37        | 1.32     |
| 35  | BB    | 2225 | A    | C6-N6   | 6.28  | 1.39        | 1.33     |
| 35  | BB    | 2331 | G    | O3'-P   | -6.28 | 1.53        | 1.61     |
| 35  | BB    | 625  | G    | O3'-P   | -6.28 | 1.53        | 1.61     |
| 35  | BB    | 1195 | G    | O3'-P   | -6.28 | 1.53        | 1.61     |
| 1   | AA    | 1516 | G    | C2-N3   | 6.28  | 1.37        | 1.32     |
| 22  | AV    | 1    | C    | C2-O2   | 6.28  | 1.30        | 1.24     |
| 22  | AV    | 32   | A    | N9-C4   | 6.28  | 1.41        | 1.37     |
| 34  | BA    | 70   | C    | C2-N3   | 6.28  | 1.40        | 1.35     |
| 35  | BB    | 110  | G    | C8-N7   | 6.28  | 1.34        | 1.30     |
| 35  | BB    | 1241 | A    | C4'-O4' | -6.28 | 1.37        | 1.45     |
| 35  | BB    | 2260 | C    | N3-C4   | 6.28  | 1.38        | 1.33     |
| 35  | BB    | 2344 | U    | C4-C5   | 6.28  | 1.49        | 1.43     |
| 35  | BB    | 2885 | G    | C2-N3   | 6.28  | 1.37        | 1.32     |
| 36  | BC    | 202  | ARG  | CD-NE   | 6.28  | 1.57        | 1.46     |
| 1   | AA    | 202  | G    | C4'-O4' | -6.28 | 1.37        | 1.45     |
| 1   | AA    | 491  | G    | N1-C2   | 6.28  | 1.42        | 1.37     |
| 1   | AA    | 1416 | G    | N9-C4   | -6.28 | 1.32        | 1.38     |
| 35  | BB    | 194  | G    | C3'-C2' | 6.28  | 1.59        | 1.52     |
| 35  | BB    | 220  | G    | N9-C4   | -6.28 | 1.32        | 1.38     |
| 35  | BB    | 426  | C    | C2-O2   | 6.28  | 1.30        | 1.24     |
| 35  | BB    | 2341 | G    | C2'-C1' | -6.28 | 1.46        | 1.53     |
| 1   | AA    | 337  | G    | N9-C4   | -6.28 | 1.32        | 1.38     |
| 1   | AA    | 496  | A    | C3'-O3' | 6.28  | 1.50        | 1.42     |
| 1   | AA    | 1150 | A    | C6-N6   | 6.28  | 1.39        | 1.33     |
| 22  | AV    | 34   | G    | C3'-C2' | -6.28 | 1.45        | 1.52     |
| 22  | AV    | 76   | A    | C8-N7   | -6.28 | 1.27        | 1.31     |
| 35  | BB    | 1400 | U    | C4-C5   | 6.28  | 1.49        | 1.43     |
| 35  | BB    | 1584 | U    | C1'-N1  | 6.28  | 1.58        | 1.48     |
| 35  | BB    | 1621 | U    | O3'-P   | -6.28 | 1.53        | 1.61     |
| 35  | BB    | 2070 | A    | P-O5'   | -6.28 | 1.53        | 1.59     |
| 48  | BO    | 111  | ARG  | NE-CZ   | 6.28  | 1.41        | 1.33     |
| 1   | AA    | 931  | C    | C4'-C3' | -6.28 | 1.46        | 1.53     |
| 1   | AA    | 990  | C    | C2'-O2' | -6.28 | 1.33        | 1.41     |
| 1   | AA    | 1487 | G    | N7-C5   | -6.28 | 1.35        | 1.39     |
| 1   | AA    | 1510 | C    | C4-C5   | 6.28  | 1.48        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 137  | U    | C2'-C1' | -6.28 | 1.46        | 1.53     |
| 35  | BB    | 1237 | A    | N3-C4   | 6.28  | 1.38        | 1.34     |
| 1   | AA    | 362  | G    | N7-C5   | -6.27 | 1.35        | 1.39     |
| 35  | BB    | 354  | A    | C4'-O4' | 6.27  | 1.53        | 1.45     |
| 35  | BB    | 2850 | A    | C5-C4   | -6.27 | 1.34        | 1.38     |
| 1   | AA    | 900  | A    | C8-N7   | -6.27 | 1.27        | 1.31     |
| 35  | BB    | 61   | C    | C4-N4   | 6.27  | 1.39        | 1.33     |
| 35  | BB    | 227  | A    | C5'-C4' | 6.27  | 1.58        | 1.51     |
| 35  | BB    | 809  | G    | C8-N7   | -6.27 | 1.27        | 1.30     |
| 35  | BB    | 1033 | U    | C2-N3   | 6.27  | 1.42        | 1.37     |
| 35  | BB    | 2777 | G    | O3'-P   | -6.27 | 1.53        | 1.61     |
| 35  | BB    | 2844 | G    | N1-C2   | 6.27  | 1.42        | 1.37     |
| 43  | BJ    | 69   | ARG  | NE-CZ   | 6.27  | 1.41        | 1.33     |
| 35  | BB    | 176  | A    | N7-C5   | -6.27 | 1.35        | 1.39     |
| 35  | BB    | 665  | U    | C5'-C4' | 6.27  | 1.58        | 1.51     |
| 35  | BB    | 1194 | A    | C8-N7   | -6.27 | 1.27        | 1.31     |
| 35  | BB    | 1472 | C    | O3'-P   | -6.27 | 1.53        | 1.61     |
| 35  | BB    | 1654 | A    | N7-C5   | -6.27 | 1.35        | 1.39     |
| 35  | BB    | 2586 | U    | C2-N3   | 6.27  | 1.42        | 1.37     |
| 35  | BB    | 2718 | G    | N3-C4   | -6.27 | 1.31        | 1.35     |
| 1   | AA    | 703  | G    | C5-C4   | 6.27  | 1.42        | 1.38     |
| 35  | BB    | 299  | A    | N9-C8   | -6.27 | 1.32        | 1.37     |
| 35  | BB    | 482  | A    | C8-N7   | -6.27 | 1.27        | 1.31     |
| 35  | BB    | 799  | G    | N9-C8   | 6.27  | 1.42        | 1.37     |
| 35  | BB    | 1243 | C    | C5-C6   | -6.27 | 1.29        | 1.34     |
| 35  | BB    | 1537 | G    | O3'-P   | -6.27 | 1.53        | 1.61     |
| 35  | BB    | 2069 | G    | O3'-P   | -6.27 | 1.53        | 1.61     |
| 35  | BB    | 2286 | G    | P-O5'   | -6.27 | 1.53        | 1.59     |
| 35  | BB    | 2543 | G    | N9-C8   | 6.27  | 1.42        | 1.37     |
| 35  | BB    | 2817 | U    | C4-C5   | 6.27  | 1.49        | 1.43     |
| 1   | AA    | 635  | A    | C6-N6   | 6.27  | 1.39        | 1.33     |
| 1   | AA    | 1016 | A    | C6-N1   | 6.27  | 1.40        | 1.35     |
| 1   | AA    | 1309 | G    | N9-C8   | 6.27  | 1.42        | 1.37     |
| 1   | AA    | 1386 | G    | C6-O6   | -6.27 | 1.18        | 1.24     |
| 35  | BB    | 225  | C    | O3'-P   | -6.27 | 1.53        | 1.61     |
| 35  | BB    | 2216 | G    | C2-N3   | 6.27  | 1.37        | 1.32     |
| 1   | AA    | 303  | A    | C5-C4   | -6.27 | 1.34        | 1.38     |
| 1   | AA    | 864  | A    | C2-N3   | 6.27  | 1.39        | 1.33     |
| 1   | AA    | 1478 | U    | C2-N3   | 6.27  | 1.42        | 1.37     |
| 35  | BB    | 2150 | C    | O3'-P   | -6.27 | 1.53        | 1.61     |
| 35  | BB    | 2364 | C    | O3'-P   | -6.27 | 1.53        | 1.61     |
| 1   | AA    | 416  | G    | N1-C2   | 6.26  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 20  | AT    | 24   | ARG  | NE-CZ   | 6.26  | 1.41        | 1.33     |
| 35  | BB    | 145  | C    | O3'-P   | 6.26  | 1.68        | 1.61     |
| 35  | BB    | 177  | G    | C2'-C1' | -6.26 | 1.46        | 1.53     |
| 35  | BB    | 959  | A    | C4'-C3' | -6.26 | 1.46        | 1.53     |
| 35  | BB    | 1588 | G    | C8-N7   | 6.26  | 1.34        | 1.30     |
| 35  | BB    | 925  | A    | C5-C6   | -6.26 | 1.35        | 1.41     |
| 35  | BB    | 1862 | G    | P-O5'   | -6.26 | 1.53        | 1.59     |
| 35  | BB    | 2055 | C    | C2-N3   | 6.26  | 1.40        | 1.35     |
| 35  | BB    | 2217 | G    | C2-N2   | -6.26 | 1.28        | 1.34     |
| 35  | BB    | 2422 | C    | N3-C4   | 6.26  | 1.38        | 1.33     |
| 35  | BB    | 2441 | U    | C2-O2   | 6.26  | 1.27        | 1.22     |
| 1   | AA    | 88   | U    | C1'-N1  | 6.26  | 1.58        | 1.48     |
| 35  | BB    | 141  | G    | C4'-C3' | 6.26  | 1.60        | 1.53     |
| 35  | BB    | 2532 | G    | N7-C5   | -6.26 | 1.35        | 1.39     |
| 35  | BB    | 2694 | G    | C2'-C1' | -6.26 | 1.46        | 1.53     |
| 1   | AA    | 116  | A    | N7-C5   | 6.26  | 1.43        | 1.39     |
| 1   | AA    | 221  | C    | C5'-C4' | 6.26  | 1.58        | 1.51     |
| 1   | AA    | 1339 | A    | N9-C8   | -6.26 | 1.32        | 1.37     |
| 1   | AA    | 1375 | A    | C6-N6   | 6.26  | 1.39        | 1.33     |
| 28  | B3    | 16   | ARG  | NE-CZ   | 6.26  | 1.41        | 1.33     |
| 35  | BB    | 626  | A    | P-O5'   | -6.26 | 1.53        | 1.59     |
| 35  | BB    | 839  | U    | N1-C2   | -6.26 | 1.32        | 1.38     |
| 35  | BB    | 1588 | G    | N7-C5   | -6.26 | 1.35        | 1.39     |
| 35  | BB    | 1668 | A    | O4'-C1' | -6.26 | 1.33        | 1.41     |
| 35  | BB    | 2056 | G    | N9-C8   | -6.26 | 1.33        | 1.37     |
| 1   | AA    | 106  | C    | O3'-P   | -6.26 | 1.53        | 1.61     |
| 35  | BB    | 1784 | A    | C6-N6   | 6.26  | 1.39        | 1.33     |
| 35  | BB    | 1221 | C    | C5-C6   | 6.26  | 1.39        | 1.34     |
| 35  | BB    | 1753 | G    | C3'-O3' | 6.26  | 1.50        | 1.42     |
| 35  | BB    | 2587 | A    | C4'-C3' | -6.26 | 1.46        | 1.53     |
| 35  | BB    | 1167 | C    | C4-N4   | 6.25  | 1.39        | 1.33     |
| 35  | BB    | 2590 | A    | C8-N7   | -6.25 | 1.27        | 1.31     |
| 1   | AA    | 593  | U    | C5'-C4' | 6.25  | 1.58        | 1.51     |
| 1   | AA    | 1342 | C    | C2'-C1' | -6.25 | 1.46        | 1.53     |
| 1   | AA    | 1473 | G    | N3-C4   | -6.25 | 1.31        | 1.35     |
| 35  | BB    | 456  | C    | N3-C4   | 6.25  | 1.38        | 1.33     |
| 35  | BB    | 830  | G    | C2-N3   | 6.25  | 1.37        | 1.32     |
| 35  | BB    | 1288 | G    | C8-N7   | 6.25  | 1.34        | 1.30     |
| 35  | BB    | 1466 | U    | C2-N3   | 6.25  | 1.42        | 1.37     |
| 35  | BB    | 1898 | U    | O3'-P   | -6.25 | 1.53        | 1.61     |
| 35  | BB    | 2457 | U    | C2'-C1' | 6.25  | 1.60        | 1.53     |
| 1   | AA    | 241  | G    | N9-C8   | 6.25  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 590  | U    | P-O5'   | -6.25 | 1.53        | 1.59     |
| 1   | AA    | 806  | C    | C2'-C1' | -6.25 | 1.46        | 1.53     |
| 1   | AA    | 898  | G    | C2'-C1' | -6.25 | 1.46        | 1.53     |
| 1   | AA    | 1480 | A    | N9-C8   | -6.25 | 1.32        | 1.37     |
| 35  | BB    | 723  | C    | N3-C4   | 6.25  | 1.38        | 1.33     |
| 35  | BB    | 1470 | A    | C6-N6   | 6.25  | 1.39        | 1.33     |
| 35  | BB    | 1913 | A    | C5-C4   | 6.25  | 1.43        | 1.38     |
| 35  | BB    | 2307 | G    | C2'-C1' | -6.25 | 1.46        | 1.53     |
| 35  | BB    | 2674 | G    | C8-N7   | 6.25  | 1.34        | 1.30     |
| 53  | BT    | 3    | ARG  | NE-CZ   | 6.25  | 1.41        | 1.33     |
| 1   | AA    | 1208 | C    | C3'-O3' | 6.25  | 1.50        | 1.42     |
| 35  | BB    | 664  | G    | C2-N2   | 6.25  | 1.40        | 1.34     |
| 1   | AA    | 537  | G    | C4'-C3' | -6.25 | 1.46        | 1.53     |
| 1   | AA    | 1133 | G    | N9-C8   | 6.25  | 1.42        | 1.37     |
| 35  | BB    | 570  | G    | C4'-O4' | 6.25  | 1.53        | 1.45     |
| 35  | BB    | 1280 | G    | C2-N3   | -6.25 | 1.27        | 1.32     |
| 35  | BB    | 1792 | G    | C2'-C1' | -6.25 | 1.46        | 1.53     |
| 35  | BB    | 1881 | C    | C4'-O4' | -6.25 | 1.37        | 1.45     |
| 35  | BB    | 1899 | A    | C5'-C4' | 6.25  | 1.58        | 1.51     |
| 35  | BB    | 2171 | A    | N9-C8   | -6.25 | 1.32        | 1.37     |
| 35  | BB    | 2748 | A    | C6-N1   | 6.25  | 1.40        | 1.35     |
| 1   | AA    | 326  | G    | C2-N2   | 6.25  | 1.40        | 1.34     |
| 1   | AA    | 691  | G    | C8-N7   | -6.25 | 1.27        | 1.30     |
| 1   | AA    | 1134 | G    | N1-C2   | 6.25  | 1.42        | 1.37     |
| 35  | BB    | 778  | G    | N9-C4   | 6.25  | 1.43        | 1.38     |
| 34  | BA    | 108  | A    | C5-C4   | 6.25  | 1.43        | 1.38     |
| 35  | BB    | 407  | G    | C4'-C3' | 6.25  | 1.60        | 1.53     |
| 1   | AA    | 885  | G    | N7-C5   | -6.24 | 1.35        | 1.39     |
| 35  | BB    | 1572 | A    | N1-C2   | 6.24  | 1.40        | 1.34     |
| 35  | BB    | 1634 | A    | P-O5'   | 6.24  | 1.66        | 1.59     |
| 35  | BB    | 1964 | G    | C5-C4   | 6.24  | 1.42        | 1.38     |
| 35  | BB    | 2284 | A    | N1-C2   | 6.24  | 1.40        | 1.34     |
| 35  | BB    | 2511 | U    | C4-C5   | -6.24 | 1.38        | 1.43     |
| 35  | BB    | 2614 | A    | C4'-O4' | 6.24  | 1.53        | 1.45     |
| 35  | BB    | 390  | U    | C3'-C2' | -6.24 | 1.45        | 1.52     |
| 35  | BB    | 715  | A    | N3-C4   | -6.24 | 1.31        | 1.34     |
| 1   | AA    | 38   | G    | N1-C2   | 6.24  | 1.42        | 1.37     |
| 1   | AA    | 338  | A    | N3-C4   | -6.24 | 1.31        | 1.34     |
| 1   | AA    | 1080 | A    | C8-N7   | 6.24  | 1.35        | 1.31     |
| 1   | AA    | 1437 | A    | C5-C6   | -6.24 | 1.35        | 1.41     |
| 1   | AA    | 1470 | U    | O3'-P   | -6.24 | 1.53        | 1.61     |
| 1   | AA    | 1480 | A    | C6-N6   | 6.24  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1613 | G    | N1-C2   | 6.24  | 1.42        | 1.37     |
| 35  | BB    | 2027 | G    | N9-C8   | -6.24 | 1.33        | 1.37     |
| 34  | BA    | 60   | C    | C4'-C3' | -6.24 | 1.46        | 1.53     |
| 35  | BB    | 299  | A    | C4'-C3' | -6.24 | 1.46        | 1.53     |
| 35  | BB    | 844  | A    | C2'-C1' | -6.24 | 1.46        | 1.53     |
| 35  | BB    | 1901 | A    | C5'-C4' | -6.24 | 1.43        | 1.51     |
| 35  | BB    | 2018 | G    | C8-N7   | -6.24 | 1.27        | 1.30     |
| 35  | BB    | 2249 | U    | C2-N3   | 6.24  | 1.42        | 1.37     |
| 1   | AA    | 1043 | G    | N1-C2   | 6.24  | 1.42        | 1.37     |
| 6   | AF    | 86   | ARG  | CD-NE   | 6.24  | 1.57        | 1.46     |
| 35  | BB    | 110  | G    | C6-N1   | -6.24 | 1.35        | 1.39     |
| 35  | BB    | 209  | C    | C4-C5   | -6.24 | 1.38        | 1.43     |
| 35  | BB    | 2394 | C    | C4'-C3' | 6.24  | 1.60        | 1.53     |
| 1   | AA    | 1357 | A    | C4'-O4' | -6.24 | 1.37        | 1.45     |
| 34  | BA    | 57   | A    | N9-C8   | -6.24 | 1.32        | 1.37     |
| 35  | BB    | 390  | U    | N1-C6   | -6.24 | 1.32        | 1.38     |
| 35  | BB    | 673  | C    | N3-C4   | 6.24  | 1.38        | 1.33     |
| 35  | BB    | 1067 | A    | C5-C4   | 6.24  | 1.43        | 1.38     |
| 35  | BB    | 1645 | G    | C5-C4   | -6.24 | 1.33        | 1.38     |
| 35  | BB    | 2148 | G    | C5-C4   | -6.24 | 1.33        | 1.38     |
| 35  | BB    | 2444 | G    | P-O5'   | -6.24 | 1.53        | 1.59     |
| 1   | AA    | 344  | A    | P-O5'   | -6.23 | 1.53        | 1.59     |
| 1   | AA    | 487  | A    | N9-C8   | -6.23 | 1.32        | 1.37     |
| 35  | BB    | 106  | C    | P-O5'   | -6.23 | 1.53        | 1.59     |
| 35  | BB    | 227  | A    | P-O5'   | -6.23 | 1.53        | 1.59     |
| 35  | BB    | 230  | G    | N9-C8   | 6.23  | 1.42        | 1.37     |
| 35  | BB    | 1987 | A    | N3-C4   | -6.23 | 1.31        | 1.34     |
| 1   | AA    | 958  | A    | N7-C5   | -6.23 | 1.35        | 1.39     |
| 1   | AA    | 1205 | U    | C5-C6   | 6.23  | 1.39        | 1.34     |
| 1   | AA    | 1428 | A    | C5-C6   | -6.23 | 1.35        | 1.41     |
| 35  | BB    | 253  | C    | P-O5'   | -6.23 | 1.53        | 1.59     |
| 35  | BB    | 672  | C    | P-O5'   | -6.23 | 1.53        | 1.59     |
| 35  | BB    | 926  | G    | P-O5'   | -6.23 | 1.53        | 1.59     |
| 35  | BB    | 1731 | G    | C2-N3   | 6.23  | 1.37        | 1.32     |
| 35  | BB    | 1825 | U    | P-O5'   | 6.23  | 1.66        | 1.59     |
| 1   | AA    | 650  | G    | C5-C4   | 6.23  | 1.42        | 1.38     |
| 1   | AA    | 1442 | G    | C8-N7   | 6.23  | 1.34        | 1.30     |
| 1   | AA    | 1525 | G    | N7-C5   | 6.23  | 1.43        | 1.39     |
| 25  | B0    | 10   | ARG  | NE-CZ   | 6.23  | 1.41        | 1.33     |
| 35  | BB    | 1123 | C    | N3-C4   | 6.23  | 1.38        | 1.33     |
| 35  | BB    | 2015 | A    | N9-C8   | 6.23  | 1.42        | 1.37     |
| 35  | BB    | 2400 | G    | C8-N7   | -6.23 | 1.27        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2808 | G    | C5-C4   | 6.23  | 1.42        | 1.38     |
| 1   | AA    | 84   | U    | N1-C2   | 6.23  | 1.44        | 1.38     |
| 1   | AA    | 540  | G    | O3'-P   | -6.23 | 1.53        | 1.61     |
| 1   | AA    | 1025 | U    | C3'-C2' | 6.23  | 1.59        | 1.52     |
| 1   | AA    | 1290 | G    | C2-N3   | 6.23  | 1.37        | 1.32     |
| 1   | AA    | 1511 | G    | N1-C2   | 6.23  | 1.42        | 1.37     |
| 35  | BB    | 254  | G    | C5-C6   | -6.23 | 1.36        | 1.42     |
| 35  | BB    | 1450 | G    | C2-N2   | 6.23  | 1.40        | 1.34     |
| 35  | BB    | 1729 | U    | C2-N3   | 6.23  | 1.42        | 1.37     |
| 35  | BB    | 1896 | G    | N1-C2   | 6.23  | 1.42        | 1.37     |
| 35  | BB    | 1982 | U    | O4'-C1' | 6.23  | 1.49        | 1.41     |
| 35  | BB    | 2153 | C    | C2'-C1' | -6.23 | 1.46        | 1.53     |
| 1   | AA    | 270  | A    | N3-C4   | -6.23 | 1.31        | 1.34     |
| 1   | AA    | 923  | A    | C6-N6   | 6.23  | 1.39        | 1.33     |
| 35  | BB    | 677  | A    | N7-C5   | -6.23 | 1.35        | 1.39     |
| 35  | BB    | 960  | A    | C8-N7   | -6.23 | 1.27        | 1.31     |
| 1   | AA    | 1128 | C    | C2-N3   | 6.22  | 1.40        | 1.35     |
| 22  | AV    | 5    | A    | C2-N3   | 6.22  | 1.39        | 1.33     |
| 35  | BB    | 120  | U    | N1-C6   | 6.22  | 1.43        | 1.38     |
| 35  | BB    | 192  | C    | N1-C6   | 6.22  | 1.40        | 1.37     |
| 35  | BB    | 391  | A    | C5-C4   | -6.22 | 1.34        | 1.38     |
| 35  | BB    | 491  | G    | C6-N1   | 6.22  | 1.44        | 1.39     |
| 35  | BB    | 605  | G    | C3'-C2' | 6.22  | 1.59        | 1.52     |
| 35  | BB    | 993  | G    | C5'-C4' | -6.22 | 1.43        | 1.51     |
| 35  | BB    | 1109 | C    | C5'-C4' | 6.22  | 1.58        | 1.51     |
| 35  | BB    | 1830 | C    | C5-C6   | -6.22 | 1.29        | 1.34     |
| 35  | BB    | 1892 | C    | C2'-C1' | -6.22 | 1.46        | 1.53     |
| 1   | AA    | 1278 | G    | N3-C4   | 6.22  | 1.39        | 1.35     |
| 4   | AD    | 3    | TYR  | CG-CD1  | 6.22  | 1.47        | 1.39     |
| 35  | BB    | 747  | U    | C1'-N1  | 6.22  | 1.58        | 1.48     |
| 35  | BB    | 972  | A    | P-O5'   | -6.22 | 1.53        | 1.59     |
| 35  | BB    | 2117 | A    | N3-C4   | 6.22  | 1.38        | 1.34     |
| 1   | AA    | 1316 | G    | O3'-P   | -6.22 | 1.53        | 1.61     |
| 1   | AA    | 1491 | G    | C5'-C4' | 6.22  | 1.58        | 1.51     |
| 35  | BB    | 2149 | U    | C2'-C1' | -6.22 | 1.46        | 1.53     |
| 1   | AA    | 518  | C    | P-O5'   | -6.22 | 1.53        | 1.59     |
| 1   | AA    | 872  | A    | N7-C5   | -6.22 | 1.35        | 1.39     |
| 1   | AA    | 1098 | C    | N1-C6   | 6.22  | 1.40        | 1.37     |
| 2   | AB    | 21   | TYR  | CG-CD2  | 6.22  | 1.47        | 1.39     |
| 35  | BB    | 484  | C    | C2'-C1' | -6.22 | 1.46        | 1.53     |
| 35  | BB    | 1334 | G    | C2'-C1' | -6.22 | 1.46        | 1.53     |
| 35  | BB    | 2217 | G    | N1-C2   | 6.22  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 396  | C    | N3-C4   | 6.22  | 1.38        | 1.33     |
| 7   | AG    | 52   | ARG  | CZ-NH2  | 6.22  | 1.41        | 1.33     |
| 34  | BA    | 56   | G    | P-O5'   | 6.22  | 1.66        | 1.59     |
| 35  | BB    | 21   | A    | C5-C4   | -6.22 | 1.34        | 1.38     |
| 35  | BB    | 237  | C    | C2-O2   | -6.22 | 1.18        | 1.24     |
| 35  | BB    | 1272 | A    | C6-N6   | 6.22  | 1.39        | 1.33     |
| 1   | AA    | 339  | C    | C2-N3   | 6.22  | 1.40        | 1.35     |
| 1   | AA    | 822  | U    | N1-C2   | 6.22  | 1.44        | 1.38     |
| 1   | AA    | 872  | A    | C8-N7   | -6.22 | 1.27        | 1.31     |
| 1   | AA    | 1091 | U    | O3'-P   | -6.22 | 1.53        | 1.61     |
| 35  | BB    | 700  | G    | N1-C2   | 6.22  | 1.42        | 1.37     |
| 35  | BB    | 977  | G    | C3'-C2' | 6.22  | 1.59        | 1.52     |
| 35  | BB    | 1845 | G    | C8-N7   | 6.22  | 1.34        | 1.30     |
| 35  | BB    | 2252 | G    | P-O5'   | -6.22 | 1.53        | 1.59     |
| 35  | BB    | 2410 | G    | N9-C4   | 6.22  | 1.43        | 1.38     |
| 35  | BB    | 2791 | G    | N1-C2   | 6.22  | 1.42        | 1.37     |
| 1   | AA    | 487  | A    | C5'-C4' | 6.21  | 1.58        | 1.51     |
| 1   | AA    | 753  | A    | N7-C5   | -6.21 | 1.35        | 1.39     |
| 1   | AA    | 1016 | A    | C3'-C2' | 6.21  | 1.59        | 1.52     |
| 35  | BB    | 333  | G    | C6-O6   | -6.21 | 1.18        | 1.24     |
| 35  | BB    | 849  | A    | C4'-O4' | -6.21 | 1.37        | 1.45     |
| 35  | BB    | 1435 | G    | C3'-O3' | 6.21  | 1.50        | 1.42     |
| 35  | BB    | 1676 | A    | C2'-C1' | -6.21 | 1.46        | 1.53     |
| 35  | BB    | 1839 | G    | C2-N3   | 6.21  | 1.37        | 1.32     |
| 35  | BB    | 1858 | A    | C4'-C3' | 6.21  | 1.59        | 1.53     |
| 35  | BB    | 1863 | G    | C4'-C3' | -6.21 | 1.46        | 1.53     |
| 35  | BB    | 2484 | G    | C2'-C1' | -6.21 | 1.46        | 1.53     |
| 35  | BB    | 2869 | G    | C5'-C4' | 6.21  | 1.58        | 1.51     |
| 1   | AA    | 582  | C    | N3-C4   | 6.21  | 1.38        | 1.33     |
| 35  | BB    | 1092 | C    | C3'-C2' | 6.21  | 1.59        | 1.52     |
| 35  | BB    | 1210 | G    | C3'-C2' | -6.21 | 1.46        | 1.52     |
| 35  | BB    | 1856 | U    | C5'-C4' | 6.21  | 1.58        | 1.51     |
| 35  | BB    | 2316 | G    | N7-C5   | 6.21  | 1.43        | 1.39     |
| 35  | BB    | 2739 | U    | C5'-C4' | 6.21  | 1.58        | 1.51     |
| 1   | AA    | 320  | A    | C6-N6   | 6.21  | 1.39        | 1.33     |
| 1   | AA    | 488  | C    | C2'-C1' | -6.21 | 1.46        | 1.53     |
| 1   | AA    | 1143 | G    | O4'-C1' | 6.21  | 1.49        | 1.41     |
| 35  | BB    | 24   | G    | C6-N1   | 6.21  | 1.43        | 1.39     |
| 35  | BB    | 1010 | A    | C2'-C1' | -6.21 | 1.46        | 1.53     |
| 35  | BB    | 2043 | C    | O3'-P   | -6.21 | 1.53        | 1.61     |
| 35  | BB    | 2127 | G    | N7-C5   | -6.21 | 1.35        | 1.39     |
| 1   | AA    | 1342 | C    | C3'-C2' | -6.21 | 1.46        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1437 | A    | O3'-P   | -6.21 | 1.53        | 1.61     |
| 1   | AA    | 1480 | A    | C2'-C1' | -6.21 | 1.46        | 1.53     |
| 35  | BB    | 586  | A    | C3'-O3' | 6.21  | 1.50        | 1.42     |
| 1   | AA    | 856  | C    | C5'-C4' | 6.21  | 1.58        | 1.51     |
| 1   | AA    | 1256 | A    | N7-C5   | 6.21  | 1.43        | 1.39     |
| 1   | AA    | 1275 | A    | C6-N1   | 6.21  | 1.39        | 1.35     |
| 1   | AA    | 1461 | G    | C2'-C1' | -6.21 | 1.46        | 1.53     |
| 1   | AA    | 1513 | A    | P-O5'   | -6.21 | 1.53        | 1.59     |
| 35  | BB    | 805  | G    | C8-N7   | 6.21  | 1.34        | 1.30     |
| 35  | BB    | 1051 | G    | N9-C8   | 6.21  | 1.42        | 1.37     |
| 35  | BB    | 1288 | G    | C5-C6   | -6.21 | 1.36        | 1.42     |
| 35  | BB    | 2209 | G    | N9-C4   | -6.21 | 1.32        | 1.38     |
| 35  | BB    | 2591 | C    | N3-C4   | 6.21  | 1.38        | 1.33     |
| 35  | BB    | 2729 | G    | N9-C8   | 6.21  | 1.42        | 1.37     |
| 1   | AA    | 356  | A    | N7-C5   | -6.21 | 1.35        | 1.39     |
| 1   | AA    | 381  | C    | C2-N3   | -6.21 | 1.30        | 1.35     |
| 1   | AA    | 959  | A    | O3'-P   | -6.21 | 1.53        | 1.61     |
| 1   | AA    | 1310 | G    | O3'-P   | -6.21 | 1.53        | 1.61     |
| 1   | AA    | 1501 | C    | C4-C5   | -6.21 | 1.38        | 1.43     |
| 35  | BB    | 400  | G    | N9-C8   | 6.21  | 1.42        | 1.37     |
| 35  | BB    | 467  | G    | P-O5'   | -6.21 | 1.53        | 1.59     |
| 35  | BB    | 640  | C    | C3'-C2' | -6.21 | 1.46        | 1.52     |
| 35  | BB    | 928  | A    | C4'-C3' | 6.21  | 1.59        | 1.53     |
| 35  | BB    | 1083 | U    | N1-C2   | -6.21 | 1.32        | 1.38     |
| 35  | BB    | 2399 | G    | C5-C4   | -6.21 | 1.34        | 1.38     |
| 1   | AA    | 904  | U    | N1-C2   | -6.21 | 1.32        | 1.38     |
| 35  | BB    | 57   | C    | O4'-C1' | 6.21  | 1.49        | 1.41     |
| 35  | BB    | 939  | G    | N9-C4   | -6.21 | 1.32        | 1.38     |
| 35  | BB    | 2403 | C    | C4-N4   | 6.21  | 1.39        | 1.33     |
| 1   | AA    | 112  | G    | N1-C2   | 6.20  | 1.42        | 1.37     |
| 1   | AA    | 366  | A    | C5-C4   | -6.20 | 1.34        | 1.38     |
| 1   | AA    | 902  | G    | C5-C6   | 6.20  | 1.48        | 1.42     |
| 1   | AA    | 1230 | C    | C4-N4   | 6.20  | 1.39        | 1.33     |
| 35  | BB    | 399  | U    | C4'-O4' | -6.20 | 1.37        | 1.45     |
| 35  | BB    | 518  | G    | N3-C4   | -6.20 | 1.31        | 1.35     |
| 35  | BB    | 670  | A    | N3-C4   | -6.20 | 1.31        | 1.34     |
| 35  | BB    | 1416 | G    | N7-C5   | -6.20 | 1.35        | 1.39     |
| 35  | BB    | 1835 | G    | N1-C2   | 6.20  | 1.42        | 1.37     |
| 35  | BB    | 2107 | G    | N7-C5   | -6.20 | 1.35        | 1.39     |
| 35  | BB    | 2456 | C    | C4-N4   | 6.20  | 1.39        | 1.33     |
| 35  | BB    | 2689 | U    | N3-C4   | 6.20  | 1.44        | 1.38     |
| 35  | BB    | 2717 | C    | C2'-C1' | -6.20 | 1.46        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 155  | A    | C6-N1   | 6.20  | 1.39        | 1.35     |
| 10  | AJ    | 62   | ARG  | CD-NE   | 6.20  | 1.56        | 1.46     |
| 34  | BA    | 9    | G    | N9-C4   | -6.20 | 1.32        | 1.38     |
| 35  | BB    | 815  | C    | N1-C6   | 6.20  | 1.40        | 1.37     |
| 48  | BO    | 9    | ARG  | CZ-NH1  | 6.20  | 1.41        | 1.33     |
| 34  | BA    | 23   | G    | C2-N2   | 6.20  | 1.40        | 1.34     |
| 35  | BB    | 146  | A    | C6-N1   | 6.20  | 1.39        | 1.35     |
| 35  | BB    | 174  | U    | N3-C4   | 6.20  | 1.44        | 1.38     |
| 35  | BB    | 608  | A    | O3'-P   | -6.20 | 1.53        | 1.61     |
| 35  | BB    | 1251 | C    | C4'-C3' | 6.20  | 1.59        | 1.53     |
| 1   | AA    | 975  | A    | N3-C4   | -6.20 | 1.31        | 1.34     |
| 1   | AA    | 1213 | A    | C4'-C3' | -6.20 | 1.46        | 1.53     |
| 35  | BB    | 30   | G    | C2-N3   | 6.20  | 1.37        | 1.32     |
| 35  | BB    | 331  | C    | C4-N4   | 6.20  | 1.39        | 1.33     |
| 35  | BB    | 1835 | G    | C5-C6   | -6.20 | 1.36        | 1.42     |
| 35  | BB    | 1947 | C    | C4'-O4' | 6.20  | 1.53        | 1.45     |
| 35  | BB    | 2023 | C    | P-O5'   | -6.20 | 1.53        | 1.59     |
| 1   | AA    | 559  | A    | C2'-C1' | -6.20 | 1.46        | 1.53     |
| 1   | AA    | 646  | G    | N9-C4   | -6.20 | 1.32        | 1.38     |
| 10  | AJ    | 41   | PRO  | CA-CB   | 6.20  | 1.66        | 1.53     |
| 35  | BB    | 252  | G    | C5'-C4' | -6.20 | 1.44        | 1.51     |
| 35  | BB    | 1703 | G    | C2-N3   | 6.20  | 1.37        | 1.32     |
| 35  | BB    | 1800 | C    | C2'-C1' | -6.20 | 1.46        | 1.53     |
| 35  | BB    | 382  | A    | C2'-C1' | -6.20 | 1.46        | 1.53     |
| 35  | BB    | 695  | G    | C5-C4   | -6.20 | 1.34        | 1.38     |
| 35  | BB    | 891  | G    | N9-C8   | -6.20 | 1.33        | 1.37     |
| 35  | BB    | 1122 | G    | N9-C4   | 6.20  | 1.43        | 1.38     |
| 35  | BB    | 2631 | G    | C2-N3   | 6.20  | 1.37        | 1.32     |
| 35  | BB    | 2900 | A    | N9-C8   | 6.20  | 1.42        | 1.37     |
| 1   | AA    | 303  | A    | O3'-P   | -6.19 | 1.53        | 1.61     |
| 35  | BB    | 1353 | A    | C5-C4   | 6.19  | 1.43        | 1.38     |
| 35  | BB    | 1375 | U    | C5'-C4' | 6.19  | 1.58        | 1.51     |
| 1   | AA    | 1039 | G    | N9-C8   | -6.19 | 1.33        | 1.37     |
| 34  | BA    | 51   | G    | N9-C4   | 6.19  | 1.43        | 1.38     |
| 34  | BA    | 72   | G    | C5-C4   | 6.19  | 1.42        | 1.38     |
| 35  | BB    | 21   | A    | N7-C5   | -6.19 | 1.35        | 1.39     |
| 35  | BB    | 882  | G    | C4'-C3' | -6.19 | 1.46        | 1.53     |
| 35  | BB    | 1973 | G    | N9-C8   | 6.19  | 1.42        | 1.37     |
| 35  | BB    | 2341 | G    | N1-C2   | 6.19  | 1.42        | 1.37     |
| 35  | BB    | 2681 | C    | C3'-O3' | 6.19  | 1.50        | 1.42     |
| 1   | AA    | 1449 | C    | C4-C5   | 6.19  | 1.48        | 1.43     |
| 35  | BB    | 847  | U    | O3'-P   | -6.19 | 1.53        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 972  | A    | O4'-C1' | -6.19 | 1.33        | 1.41     |
| 35  | BB    | 997  | G    | C5-C4   | 6.19  | 1.42        | 1.38     |
| 35  | BB    | 2062 | A    | C4'-C3' | 6.19  | 1.59        | 1.53     |
| 35  | BB    | 2687 | U    | O3'-P   | -6.19 | 1.53        | 1.61     |
| 35  | BB    | 2894 | G    | N7-C5   | -6.19 | 1.35        | 1.39     |
| 1   | AA    | 399  | G    | C6-N1   | 6.19  | 1.43        | 1.39     |
| 1   | AA    | 449  | G    | C4'-C3' | 6.19  | 1.59        | 1.53     |
| 1   | AA    | 561  | U    | C5'-C4' | 6.19  | 1.58        | 1.51     |
| 1   | AA    | 1259 | C    | C5-C6   | 6.19  | 1.39        | 1.34     |
| 1   | AA    | 53   | A    | N9-C8   | -6.19 | 1.32        | 1.37     |
| 1   | AA    | 368  | U    | C4-C5   | 6.19  | 1.49        | 1.43     |
| 35  | BB    | 269  | C    | O3'-P   | -6.19 | 1.53        | 1.61     |
| 35  | BB    | 694  | U    | C4-C5   | 6.19  | 1.49        | 1.43     |
| 35  | BB    | 1917 | U    | C2-N3   | 6.19  | 1.42        | 1.37     |
| 35  | BB    | 1970 | A    | N9-C4   | -6.19 | 1.34        | 1.37     |
| 35  | BB    | 2652 | C    | C4-N4   | 6.19  | 1.39        | 1.33     |
| 35  | BB    | 2729 | G    | N3-C4   | -6.19 | 1.31        | 1.35     |
| 35  | BB    | 2804 | U    | N3-C4   | 6.19  | 1.44        | 1.38     |
| 1   | AA    | 1122 | U    | N3-C4   | 6.19  | 1.44        | 1.38     |
| 35  | BB    | 7    | G    | C8-N7   | -6.19 | 1.27        | 1.30     |
| 35  | BB    | 997  | G    | C4'-C3' | -6.19 | 1.46        | 1.53     |
| 1   | AA    | 590  | U    | C4'-C3' | -6.18 | 1.46        | 1.53     |
| 1   | AA    | 622  | A    | C6-N1   | 6.18  | 1.39        | 1.35     |
| 1   | AA    | 1286 | U    | C2-N3   | 6.18  | 1.42        | 1.37     |
| 35  | BB    | 176  | A    | C8-N7   | -6.18 | 1.27        | 1.31     |
| 35  | BB    | 442  | G    | N9-C8   | -6.18 | 1.33        | 1.37     |
| 35  | BB    | 926  | G    | C2-N2   | -6.18 | 1.28        | 1.34     |
| 35  | BB    | 1176 | U    | C5'-C4' | 6.18  | 1.58        | 1.51     |
| 35  | BB    | 1978 | A    | C2'-C1' | -6.18 | 1.46        | 1.53     |
| 1   | AA    | 596  | A    | N9-C8   | 6.18  | 1.42        | 1.37     |
| 1   | AA    | 801  | U    | O3'-P   | -6.18 | 1.53        | 1.61     |
| 1   | AA    | 1271 | A    | P-O5'   | -6.18 | 1.53        | 1.59     |
| 1   | AA    | 1319 | A    | C8-N7   | -6.18 | 1.27        | 1.31     |
| 35  | BB    | 855  | G    | O3'-P   | -6.18 | 1.53        | 1.61     |
| 35  | BB    | 1696 | G    | O3'-P   | -6.18 | 1.53        | 1.61     |
| 35  | BB    | 1838 | C    | C2'-C1' | -6.18 | 1.46        | 1.53     |
| 35  | BB    | 2057 | G    | N3-C4   | -6.18 | 1.31        | 1.35     |
| 35  | BB    | 2716 | C    | C4-N4   | 6.18  | 1.39        | 1.33     |
| 1   | AA    | 108  | G    | P-O5'   | 6.18  | 1.66        | 1.59     |
| 1   | AA    | 445  | G    | C8-N7   | -6.18 | 1.27        | 1.30     |
| 35  | BB    | 1592 | C    | C5'-C4' | 6.18  | 1.58        | 1.51     |
| 35  | BB    | 2120 | G    | O3'-P   | -6.18 | 1.53        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 389  | A    | C4'-C3' | -6.18 | 1.46        | 1.53     |
| 1   | AA    | 465  | A    | N7-C5   | -6.18 | 1.35        | 1.39     |
| 1   | AA    | 1323 | G    | C2-N3   | 6.18  | 1.37        | 1.32     |
| 35  | BB    | 261  | G    | C8-N7   | -6.18 | 1.27        | 1.30     |
| 35  | BB    | 477  | A    | C1'-N9  | -6.18 | 1.38        | 1.46     |
| 35  | BB    | 535  | G    | C4'-C3' | -6.18 | 1.46        | 1.53     |
| 35  | BB    | 664  | G    | C3'-C2' | 6.18  | 1.59        | 1.52     |
| 35  | BB    | 1022 | G    | C6-N1   | -6.18 | 1.35        | 1.39     |
| 35  | BB    | 1425 | G    | N7-C5   | -6.18 | 1.35        | 1.39     |
| 35  | BB    | 1452 | G    | N1-C2   | 6.18  | 1.42        | 1.37     |
| 35  | BB    | 1732 | C    | O3'-P   | -6.18 | 1.53        | 1.61     |
| 35  | BB    | 1975 | G    | N7-C5   | -6.18 | 1.35        | 1.39     |
| 8   | AH    | 44   | PHE  | CG-CD2  | 6.18  | 1.48        | 1.38     |
| 35  | BB    | 158  | U    | P-O5'   | -6.18 | 1.53        | 1.59     |
| 35  | BB    | 247  | G    | C4'-C3' | -6.18 | 1.46        | 1.53     |
| 35  | BB    | 1347 | A    | C2'-C1' | -6.18 | 1.46        | 1.53     |
| 35  | BB    | 1869 | G    | O3'-P   | -6.18 | 1.53        | 1.61     |
| 35  | BB    | 2742 | G    | N7-C5   | 6.18  | 1.43        | 1.39     |
| 1   | AA    | 456  | A    | C5-C4   | 6.18  | 1.43        | 1.38     |
| 1   | AA    | 1151 | A    | C5-C6   | 6.18  | 1.46        | 1.41     |
| 1   | AA    | 1241 | G    | C8-N7   | 6.18  | 1.34        | 1.30     |
| 34  | BA    | 62   | C    | C4-N4   | 6.18  | 1.39        | 1.33     |
| 35  | BB    | 1015 | U    | C2-N3   | 6.18  | 1.42        | 1.37     |
| 35  | BB    | 1246 | A    | C6-N1   | 6.18  | 1.39        | 1.35     |
| 35  | BB    | 1563 | U    | C4-C5   | -6.18 | 1.38        | 1.43     |
| 35  | BB    | 2112 | G    | C2-N2   | 6.18  | 1.40        | 1.34     |
| 35  | BB    | 2236 | U    | C4-C5   | 6.18  | 1.49        | 1.43     |
| 35  | BB    | 2287 | A    | N9-C4   | -6.18 | 1.34        | 1.37     |
| 35  | BB    | 2454 | G    | N1-C2   | 6.18  | 1.42        | 1.37     |
| 1   | AA    | 199  | A    | C4'-C3' | -6.17 | 1.46        | 1.53     |
| 1   | AA    | 411  | A    | N3-C4   | -6.17 | 1.31        | 1.34     |
| 1   | AA    | 1350 | A    | C5-C4   | 6.17  | 1.43        | 1.38     |
| 34  | BA    | 79   | G    | N9-C4   | 6.17  | 1.42        | 1.38     |
| 35  | BB    | 23   | G    | C5'-C4' | 6.17  | 1.58        | 1.51     |
| 35  | BB    | 98   | G    | C6-N1   | 6.17  | 1.43        | 1.39     |
| 35  | BB    | 530  | G    | C2-N3   | 6.17  | 1.37        | 1.32     |
| 35  | BB    | 659  | G    | C2-N2   | 6.17  | 1.40        | 1.34     |
| 35  | BB    | 984  | A    | N9-C8   | 6.17  | 1.42        | 1.37     |
| 35  | BB    | 1679 | A    | C6-N6   | 6.17  | 1.38        | 1.33     |
| 35  | BB    | 1843 | C    | C2-N3   | 6.17  | 1.40        | 1.35     |
| 35  | BB    | 1891 | G    | C6-N1   | -6.17 | 1.35        | 1.39     |
| 35  | BB    | 2418 | A    | N7-C5   | -6.17 | 1.35        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2700 | A    | C5-C6   | -6.17 | 1.35        | 1.41     |
| 35  | BB    | 2744 | G    | O4'-C1' | -6.17 | 1.33        | 1.41     |
| 1   | AA    | 550  | G    | C6-O6   | -6.17 | 1.18        | 1.24     |
| 34  | BA    | 2    | G    | N7-C5   | -6.17 | 1.35        | 1.39     |
| 35  | BB    | 2404 | U    | N3-C4   | 6.17  | 1.44        | 1.38     |
| 1   | AA    | 926  | G    | N3-C4   | -6.17 | 1.31        | 1.35     |
| 1   | AA    | 1185 | G    | O3'-P   | -6.17 | 1.53        | 1.61     |
| 1   | AA    | 1243 | C    | C2-N3   | 6.17  | 1.40        | 1.35     |
| 1   | AA    | 1472 | U    | C5'-C4' | 6.17  | 1.58        | 1.51     |
| 35  | BB    | 32   | C    | C2'-C1' | -6.17 | 1.46        | 1.53     |
| 35  | BB    | 2885 | G    | C3'-C2' | -6.17 | 1.46        | 1.52     |
| 1   | AA    | 1233 | G    | C6-N1   | 6.17  | 1.43        | 1.39     |
| 34  | BA    | 61   | G    | C3'-C2' | -6.17 | 1.46        | 1.52     |
| 35  | BB    | 1668 | A    | C3'-C2' | -6.17 | 1.46        | 1.52     |
| 35  | BB    | 2308 | G    | N9-C4   | -6.17 | 1.33        | 1.38     |
| 35  | BB    | 2408 | U    | C3'-C2' | 6.17  | 1.59        | 1.52     |
| 35  | BB    | 2519 | U    | O4'-C1' | -6.17 | 1.33        | 1.41     |
| 35  | BB    | 2693 | G    | C6-N1   | 6.17  | 1.43        | 1.39     |
| 1   | AA    | 912  | C    | O3'-P   | -6.17 | 1.53        | 1.61     |
| 35  | BB    | 598  | U    | C4'-C3' | 6.17  | 1.59        | 1.53     |
| 35  | BB    | 2136 | G    | C4'-C3' | 6.17  | 1.59        | 1.53     |
| 35  | BB    | 2138 | G    | C2-N3   | 6.17  | 1.37        | 1.32     |
| 35  | BB    | 2675 | A    | N9-C4   | -6.17 | 1.34        | 1.37     |
| 35  | BB    | 2882 | A    | C6-N1   | -6.17 | 1.31        | 1.35     |
| 43  | BJ    | 35   | ARG  | NE-CZ   | 6.17  | 1.41        | 1.33     |
| 1   | AA    | 580  | C    | O3'-P   | -6.17 | 1.53        | 1.61     |
| 1   | AA    | 998  | C    | C5'-C4' | 6.17  | 1.58        | 1.51     |
| 1   | AA    | 1020 | G    | C6-N1   | 6.17  | 1.43        | 1.39     |
| 35  | BB    | 388  | G    | C2-N3   | 6.17  | 1.37        | 1.32     |
| 35  | BB    | 397  | U    | C2-N3   | 6.17  | 1.42        | 1.37     |
| 35  | BB    | 789  | A    | C6-N6   | 6.17  | 1.38        | 1.33     |
| 35  | BB    | 997  | G    | N3-C4   | -6.17 | 1.31        | 1.35     |
| 35  | BB    | 1048 | A    | N7-C5   | -6.17 | 1.35        | 1.39     |
| 1   | AA    | 964  | A    | C6-N6   | 6.17  | 1.38        | 1.33     |
| 35  | BB    | 72   | U    | C2'-C1' | -6.17 | 1.46        | 1.53     |
| 35  | BB    | 851  | C    | N1-C6   | 6.17  | 1.40        | 1.37     |
| 35  | BB    | 1059 | G    | N3-C4   | -6.17 | 1.31        | 1.35     |
| 35  | BB    | 284  | U    | C4-C5   | 6.16  | 1.49        | 1.43     |
| 35  | BB    | 2263 | C    | C2-O2   | 6.16  | 1.29        | 1.24     |
| 35  | BB    | 2497 | A    | N7-C5   | -6.16 | 1.35        | 1.39     |
| 1   | AA    | 66   | A    | N1-C2   | -6.16 | 1.28        | 1.34     |
| 1   | AA    | 1112 | C    | N1-C2   | 6.16  | 1.46        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1297 | G    | N9-C4   | 6.16  | 1.42        | 1.38     |
| 35  | BB    | 42   | A    | C6-N1   | 6.16  | 1.39        | 1.35     |
| 35  | BB    | 1448 | G    | C4'-C3' | -6.16 | 1.46        | 1.53     |
| 1   | AA    | 230  | G    | C2-N2   | 6.16  | 1.40        | 1.34     |
| 1   | AA    | 653  | U    | O3'-P   | -6.16 | 1.53        | 1.61     |
| 1   | AA    | 687  | A    | C4'-C3' | 6.16  | 1.59        | 1.53     |
| 1   | AA    | 761  | G    | O3'-P   | 6.16  | 1.68        | 1.61     |
| 1   | AA    | 1279 | G    | C5-C4   | 6.16  | 1.42        | 1.38     |
| 35  | BB    | 115  | C    | N1-C6   | -6.16 | 1.33        | 1.37     |
| 35  | BB    | 241  | A    | N7-C5   | -6.16 | 1.35        | 1.39     |
| 35  | BB    | 1566 | A    | C6-N1   | 6.16  | 1.39        | 1.35     |
| 35  | BB    | 1951 | U    | C3'-C2' | -6.16 | 1.46        | 1.52     |
| 35  | BB    | 2899 | A    | N7-C5   | -6.16 | 1.35        | 1.39     |
| 1   | AA    | 1018 | G    | N1-C2   | 6.16  | 1.42        | 1.37     |
| 1   | AA    | 1058 | G    | N9-C8   | 6.16  | 1.42        | 1.37     |
| 35  | BB    | 370  | G    | N7-C5   | -6.16 | 1.35        | 1.39     |
| 35  | BB    | 1216 | G    | C2-N2   | 6.16  | 1.40        | 1.34     |
| 35  | BB    | 1978 | A    | C2'-O2' | -6.16 | 1.33        | 1.41     |
| 35  | BB    | 2776 | A    | N7-C5   | -6.16 | 1.35        | 1.39     |
| 35  | BB    | 2901 | C    | N1-C6   | -6.16 | 1.33        | 1.37     |
| 51  | BR    | 9    | GLY  | CA-C    | -6.16 | 1.42        | 1.51     |
| 1   | AA    | 547  | A    | N9-C4   | -6.16 | 1.34        | 1.37     |
| 1   | AA    | 759  | A    | N7-C5   | -6.16 | 1.35        | 1.39     |
| 35  | BB    | 1928 | A    | O3'-P   | -6.16 | 1.53        | 1.61     |
| 35  | BB    | 2808 | G    | C4'-O4' | -6.16 | 1.37        | 1.45     |
| 1   | AA    | 392  | C    | P-O5'   | -6.16 | 1.53        | 1.59     |
| 35  | BB    | 1478 | G    | N1-C2   | 6.16  | 1.42        | 1.37     |
| 35  | BB    | 2041 | U    | C1'-N1  | 6.16  | 1.57        | 1.48     |
| 35  | BB    | 2410 | G    | C2'-C1' | -6.16 | 1.46        | 1.53     |
| 35  | BB    | 2508 | G    | C8-N7   | -6.16 | 1.27        | 1.30     |
| 35  | BB    | 2683 | C    | N3-C4   | 6.16  | 1.38        | 1.33     |
| 35  | BB    | 2895 | G    | N3-C4   | 6.16  | 1.39        | 1.35     |
| 34  | BA    | 49   | C    | P-O5'   | -6.15 | 1.53        | 1.59     |
| 35  | BB    | 1001 | A    | P-O5'   | -6.15 | 1.53        | 1.59     |
| 1   | AA    | 241  | G    | C5-C6   | -6.15 | 1.36        | 1.42     |
| 35  | BB    | 220  | G    | C5-C4   | -6.15 | 1.34        | 1.38     |
| 35  | BB    | 1212 | G    | C2-N2   | 6.15  | 1.40        | 1.34     |
| 35  | BB    | 1514 | G    | O3'-P   | -6.15 | 1.53        | 1.61     |
| 35  | BB    | 1949 | G    | N1-C2   | 6.15  | 1.42        | 1.37     |
| 35  | BB    | 2181 | U    | C5'-C4' | 6.15  | 1.58        | 1.51     |
| 35  | BB    | 2216 | G    | N1-C2   | 6.15  | 1.42        | 1.37     |
| 35  | BB    | 2504 | U    | P-O5'   | -6.15 | 1.53        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2745 | C    | N1-C2   | 6.15  | 1.46        | 1.40     |
| 35  | BB    | 2747 | G    | C4'-C3' | 6.15  | 1.59        | 1.53     |
| 1   | AA    | 383  | A    | N9-C4   | 6.15  | 1.41        | 1.37     |
| 1   | AA    | 1440 | U    | N1-C2   | 6.15  | 1.44        | 1.38     |
| 1   | AA    | 1472 | U    | N1-C2   | 6.15  | 1.44        | 1.38     |
| 35  | BB    | 147  | C    | C4-N4   | 6.15  | 1.39        | 1.33     |
| 35  | BB    | 384  | A    | C4'-O4' | 6.15  | 1.53        | 1.45     |
| 35  | BB    | 674  | G    | N3-C4   | -6.15 | 1.31        | 1.35     |
| 35  | BB    | 955  | U    | C4-C5   | 6.15  | 1.49        | 1.43     |
| 35  | BB    | 1098 | A    | N3-C4   | 6.15  | 1.38        | 1.34     |
| 35  | BB    | 1671 | U    | P-O5'   | -6.15 | 1.53        | 1.59     |
| 37  | BD    | 117  | GLY  | N-CA    | -6.15 | 1.36        | 1.46     |
| 35  | BB    | 1080 | A    | C6-N6   | 6.15  | 1.38        | 1.33     |
| 35  | BB    | 1126 | A    | C5-C4   | -6.15 | 1.34        | 1.38     |
| 35  | BB    | 2395 | C    | N3-C4   | 6.15  | 1.38        | 1.33     |
| 7   | AG    | 101  | ARG  | NE-CZ   | 6.15  | 1.41        | 1.33     |
| 34  | BA    | 5    | U    | P-O5'   | -6.15 | 1.53        | 1.59     |
| 35  | BB    | 779  | U    | C2-N3   | 6.15  | 1.42        | 1.37     |
| 35  | BB    | 1633 | G    | C2-N3   | 6.15  | 1.37        | 1.32     |
| 35  | BB    | 1740 | G    | C2-N2   | 6.15  | 1.40        | 1.34     |
| 35  | BB    | 2888 | C    | N1-C6   | 6.15  | 1.40        | 1.37     |
| 1   | AA    | 162  | A    | N3-C4   | -6.15 | 1.31        | 1.34     |
| 1   | AA    | 989  | U    | C5'-C4' | 6.15  | 1.58        | 1.51     |
| 1   | AA    | 1270 | G    | N3-C4   | -6.15 | 1.31        | 1.35     |
| 12  | AL    | 82   | ARG  | CZ-NH1  | 6.15  | 1.41        | 1.33     |
| 35  | BB    | 115  | C    | N3-C4   | 6.15  | 1.38        | 1.33     |
| 35  | BB    | 1560 | G    | C2-N3   | 6.15  | 1.37        | 1.32     |
| 1   | AA    | 818  | G    | C2-N2   | 6.14  | 1.40        | 1.34     |
| 1   | AA    | 1167 | A    | C3'-O3' | 6.14  | 1.50        | 1.42     |
| 12  | AL    | 30   | ARG  | NE-CZ   | 6.14  | 1.41        | 1.33     |
| 35  | BB    | 257  | C    | N1-C6   | 6.14  | 1.40        | 1.37     |
| 35  | BB    | 309  | A    | C4'-C3' | -6.14 | 1.46        | 1.53     |
| 35  | BB    | 420  | C    | O3'-P   | -6.14 | 1.53        | 1.61     |
| 35  | BB    | 429  | A    | P-O5'   | -6.14 | 1.53        | 1.59     |
| 35  | BB    | 1346 | G    | C8-N7   | -6.14 | 1.27        | 1.30     |
| 35  | BB    | 1446 | C    | C2'-C1' | -6.14 | 1.46        | 1.53     |
| 35  | BB    | 1797 | G    | P-O5'   | -6.14 | 1.53        | 1.59     |
| 35  | BB    | 1963 | U    | C2-N3   | 6.14  | 1.42        | 1.37     |
| 35  | BB    | 2136 | G    | N1-C2   | 6.14  | 1.42        | 1.37     |
| 35  | BB    | 2830 | C    | C5-C6   | -6.14 | 1.29        | 1.34     |
| 1   | AA    | 299  | G    | N7-C5   | -6.14 | 1.35        | 1.39     |
| 1   | AA    | 481  | G    | C6-N1   | 6.14  | 1.43        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34  | BA    | 35   | C    | C4-N4   | 6.14  | 1.39        | 1.33     |
| 35  | BB    | 144  | A    | C6-N1   | 6.14  | 1.39        | 1.35     |
| 35  | BB    | 658  | U    | C2-N3   | 6.14  | 1.42        | 1.37     |
| 35  | BB    | 1711 | A    | C6-N1   | 6.14  | 1.39        | 1.35     |
| 35  | BB    | 2333 | A    | C4'-C3' | -6.14 | 1.46        | 1.53     |
| 35  | BB    | 2726 | A    | C6-N6   | 6.14  | 1.38        | 1.33     |
| 1   | AA    | 1459 | G    | C5'-C4' | 6.14  | 1.58        | 1.51     |
| 35  | BB    | 2034 | U    | C4-C5   | 6.14  | 1.49        | 1.43     |
| 35  | BB    | 2337 | G    | O3'-P   | -6.14 | 1.53        | 1.61     |
| 35  | BB    | 2555 | U    | C5'-C4' | 6.14  | 1.58        | 1.51     |
| 1   | AA    | 13   | U    | N1-C6   | 6.14  | 1.43        | 1.38     |
| 1   | AA    | 60   | A    | C5-C6   | -6.14 | 1.35        | 1.41     |
| 1   | AA    | 236  | A    | C2-N3   | 6.14  | 1.39        | 1.33     |
| 1   | AA    | 483  | C    | N1-C2   | -6.14 | 1.34        | 1.40     |
| 1   | AA    | 1459 | G    | C2'-C1' | -6.14 | 1.46        | 1.53     |
| 34  | BA    | 61   | G    | N7-C5   | -6.14 | 1.35        | 1.39     |
| 35  | BB    | 64   | A    | C2'-C1' | -6.14 | 1.46        | 1.53     |
| 35  | BB    | 155  | A    | N7-C5   | -6.14 | 1.35        | 1.39     |
| 35  | BB    | 1332 | G    | C2-N3   | 6.14  | 1.37        | 1.32     |
| 35  | BB    | 1457 | U    | C1'-N1  | 6.14  | 1.57        | 1.48     |
| 35  | BB    | 1530 | G    | C5'-C4' | 6.14  | 1.58        | 1.51     |
| 35  | BB    | 2804 | U    | O4'-C1' | 6.14  | 1.49        | 1.41     |
| 35  | BB    | 2171 | A    | N7-C5   | -6.14 | 1.35        | 1.39     |
| 1   | AA    | 1091 | U    | N1-C2   | 6.14  | 1.44        | 1.38     |
| 12  | AL    | 68   | GLY  | CA-C    | -6.14 | 1.42        | 1.51     |
| 35  | BB    | 212  | G    | C8-N7   | -6.14 | 1.27        | 1.30     |
| 35  | BB    | 1654 | A    | N9-C8   | 6.14  | 1.42        | 1.37     |
| 35  | BB    | 2621 | G    | N1-C2   | 6.14  | 1.42        | 1.37     |
| 11  | AK    | 127  | ARG  | CZ-NH2  | 6.13  | 1.41        | 1.33     |
| 34  | BA    | 79   | G    | C5-C6   | -6.13 | 1.36        | 1.42     |
| 35  | BB    | 518  | G    | C2-N3   | 6.13  | 1.37        | 1.32     |
| 35  | BB    | 2140 | G    | C6-N1   | 6.13  | 1.43        | 1.39     |
| 35  | BB    | 2570 | G    | N7-C5   | 6.13  | 1.43        | 1.39     |
| 1   | AA    | 541  | G    | C5-C6   | -6.13 | 1.36        | 1.42     |
| 34  | BA    | 54   | G    | N7-C5   | -6.13 | 1.35        | 1.39     |
| 35  | BB    | 234  | U    | O3'-P   | -6.13 | 1.53        | 1.61     |
| 35  | BB    | 730  | A    | C4'-C3' | 6.13  | 1.59        | 1.53     |
| 35  | BB    | 1063 | G    | N7-C5   | 6.13  | 1.43        | 1.39     |
| 35  | BB    | 1286 | A    | N9-C4   | -6.13 | 1.34        | 1.37     |
| 1   | AA    | 362  | G    | N9-C4   | -6.13 | 1.33        | 1.38     |
| 1   | AA    | 782  | A    | C5'-C4' | 6.13  | 1.58        | 1.51     |
| 1   | AA    | 1067 | A    | C1'-N9  | -6.13 | 1.38        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 265  | A    | N9-C4   | -6.13 | 1.34        | 1.37     |
| 35  | BB    | 1021 | A    | N7-C5   | -6.13 | 1.35        | 1.39     |
| 35  | BB    | 1316 | U    | C5'-C4' | 6.13  | 1.58        | 1.51     |
| 35  | BB    | 1924 | C    | C2'-C1' | -6.13 | 1.46        | 1.53     |
| 35  | BB    | 2113 | U    | P-O5'   | -6.13 | 1.53        | 1.59     |
| 35  | BB    | 2514 | U    | N3-C4   | 6.13  | 1.44        | 1.38     |
| 37  | BD    | 124  | ARG  | CZ-NH2  | 6.13  | 1.41        | 1.33     |
| 1   | AA    | 819  | A    | C6-N6   | 6.13  | 1.38        | 1.33     |
| 1   | AA    | 1104 | G    | N7-C5   | -6.13 | 1.35        | 1.39     |
| 35  | BB    | 486  | C    | C3'-O3' | 6.13  | 1.50        | 1.42     |
| 35  | BB    | 1104 | C    | C4-C5   | -6.13 | 1.38        | 1.43     |
| 35  | BB    | 1335 | C    | O3'-P   | -6.13 | 1.53        | 1.61     |
| 35  | BB    | 2336 | A    | N7-C5   | -6.13 | 1.35        | 1.39     |
| 1   | AA    | 1258 | G    | N1-C2   | 6.13  | 1.42        | 1.37     |
| 34  | BA    | 95   | U    | O3'-P   | -6.13 | 1.53        | 1.61     |
| 35  | BB    | 37   | C    | C2'-C1' | -6.13 | 1.46        | 1.53     |
| 35  | BB    | 154  | U    | C4'-C3' | -6.13 | 1.46        | 1.53     |
| 35  | BB    | 428  | A    | O4'-C1' | 6.13  | 1.49        | 1.41     |
| 35  | BB    | 1589 | U    | N3-C4   | 6.13  | 1.44        | 1.38     |
| 35  | BB    | 1801 | A    | C6-N6   | 6.13  | 1.38        | 1.33     |
| 35  | BB    | 2379 | G    | N3-C4   | -6.13 | 1.31        | 1.35     |
| 1   | AA    | 300  | A    | N9-C4   | -6.13 | 1.34        | 1.37     |
| 1   | AA    | 415  | A    | C2'-C1' | -6.13 | 1.46        | 1.53     |
| 1   | AA    | 451  | A    | N9-C4   | 6.13  | 1.41        | 1.37     |
| 1   | AA    | 625  | U    | O3'-P   | -6.13 | 1.53        | 1.61     |
| 1   | AA    | 853  | C    | C3'-C2' | 6.13  | 1.59        | 1.52     |
| 1   | AA    | 1068 | G    | N7-C5   | -6.13 | 1.35        | 1.39     |
| 5   | AE    | 28   | ARG  | CZ-NH2  | 6.13  | 1.41        | 1.33     |
| 35  | BB    | 915  | C    | C4-C5   | -6.13 | 1.38        | 1.43     |
| 35  | BB    | 1080 | A    | C5'-C4' | 6.13  | 1.58        | 1.51     |
| 35  | BB    | 1569 | A    | C4'-O4' | -6.13 | 1.37        | 1.45     |
| 35  | BB    | 1718 | G    | C8-N7   | -6.13 | 1.27        | 1.30     |
| 35  | BB    | 2458 | G    | C2-N3   | -6.13 | 1.27        | 1.32     |
| 35  | BB    | 2894 | G    | C5'-C4' | 6.13  | 1.58        | 1.51     |
| 1   | AA    | 1333 | A    | C4'-O4' | -6.12 | 1.37        | 1.45     |
| 35  | BB    | 319  | G    | C3'-O3' | 6.12  | 1.50        | 1.42     |
| 35  | BB    | 491  | G    | O4'-C1' | -6.12 | 1.33        | 1.41     |
| 1   | AA    | 592  | G    | N7-C5   | -6.12 | 1.35        | 1.39     |
| 1   | AA    | 1004 | A    | C5-C4   | 6.12  | 1.43        | 1.38     |
| 1   | AA    | 1419 | G    | C8-N7   | -6.12 | 1.27        | 1.30     |
| 34  | BA    | 61   | G    | N1-C2   | 6.12  | 1.42        | 1.37     |
| 35  | BB    | 368  | A    | C3'-C2' | 6.12  | 1.59        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1089 | A    | C6-N1   | -6.12 | 1.31        | 1.35     |
| 35  | BB    | 2160 | C    | N3-C4   | 6.12  | 1.38        | 1.33     |
| 35  | BB    | 2286 | G    | C2-N3   | 6.12  | 1.37        | 1.32     |
| 35  | BB    | 2682 | A    | N7-C5   | -6.12 | 1.35        | 1.39     |
| 1   | AA    | 498  | A    | C8-N7   | -6.12 | 1.27        | 1.31     |
| 1   | AA    | 515  | G    | C2'-C1' | -6.12 | 1.46        | 1.53     |
| 1   | AA    | 527  | G    | C6-N1   | 6.12  | 1.43        | 1.39     |
| 1   | AA    | 940  | C    | C2'-O2' | 6.12  | 1.49        | 1.41     |
| 34  | BA    | 106  | G    | C4'-O4' | 6.12  | 1.53        | 1.45     |
| 35  | BB    | 69   | C    | C3'-O3' | 6.12  | 1.50        | 1.42     |
| 35  | BB    | 763  | G    | C2-N2   | 6.12  | 1.40        | 1.34     |
| 35  | BB    | 888  | C    | N1-C6   | 6.12  | 1.40        | 1.37     |
| 35  | BB    | 1451 | C    | C4-N4   | 6.12  | 1.39        | 1.33     |
| 35  | BB    | 1603 | A    | C5-C4   | 6.12  | 1.43        | 1.38     |
| 35  | BB    | 2454 | G    | N9-C8   | 6.12  | 1.42        | 1.37     |
| 1   | AA    | 1153 | G    | N3-C4   | 6.12  | 1.39        | 1.35     |
| 35  | BB    | 401  | A    | N9-C4   | -6.12 | 1.34        | 1.37     |
| 35  | BB    | 1785 | A    | O3'-P   | -6.12 | 1.53        | 1.61     |
| 1   | AA    | 511  | C    | C4'-C3' | -6.12 | 1.46        | 1.53     |
| 1   | AA    | 763  | G    | C8-N7   | 6.12  | 1.34        | 1.30     |
| 1   | AA    | 804  | U    | C2'-C1' | -6.12 | 1.46        | 1.53     |
| 1   | AA    | 830  | G    | C5'-C4' | 6.12  | 1.58        | 1.51     |
| 35  | BB    | 1525 | A    | C6-N6   | 6.12  | 1.38        | 1.33     |
| 35  | BB    | 2529 | G    | C8-N7   | -6.12 | 1.27        | 1.30     |
| 1   | AA    | 502  | A    | P-O5'   | -6.12 | 1.53        | 1.59     |
| 1   | AA    | 1190 | G    | P-O5'   | -6.12 | 1.53        | 1.59     |
| 35  | BB    | 960  | A    | O3'-P   | -6.12 | 1.53        | 1.61     |
| 35  | BB    | 1176 | U    | N1-C6   | -6.12 | 1.32        | 1.38     |
| 35  | BB    | 1772 | A    | C4'-C3' | -6.12 | 1.46        | 1.53     |
| 35  | BB    | 1997 | C    | O3'-P   | -6.12 | 1.53        | 1.61     |
| 35  | BB    | 2233 | U    | C4-C5   | 6.12  | 1.49        | 1.43     |
| 35  | BB    | 2844 | G    | O4'-C1' | 6.12  | 1.49        | 1.41     |
| 1   | AA    | 208  | U    | N3-C4   | 6.12  | 1.44        | 1.38     |
| 1   | AA    | 281  | G    | C2-N3   | 6.12  | 1.37        | 1.32     |
| 3   | AC    | 202  | PHE  | CG-CD2  | 6.12  | 1.48        | 1.38     |
| 35  | BB    | 800  | A    | N3-C4   | -6.12 | 1.31        | 1.34     |
| 35  | BB    | 1056 | G    | N3-C4   | -6.12 | 1.31        | 1.35     |
| 35  | BB    | 1654 | A    | P-O5'   | -6.12 | 1.53        | 1.59     |
| 35  | BB    | 2098 | U    | C4-C5   | 6.12  | 1.49        | 1.43     |
| 35  | BB    | 2474 | U    | N3-C4   | 6.12  | 1.44        | 1.38     |
| 1   | AA    | 753  | A    | C5'-C4' | 6.11  | 1.58        | 1.51     |
| 1   | AA    | 1120 | C    | N3-C4   | 6.11  | 1.38        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12  | AL    | 85   | ARG  | NE-CZ   | 6.11  | 1.41        | 1.33     |
| 35  | BB    | 222  | A    | N9-C4   | -6.11 | 1.34        | 1.37     |
| 35  | BB    | 527  | C    | N3-C4   | 6.11  | 1.38        | 1.33     |
| 35  | BB    | 1218 | G    | N1-C2   | 6.11  | 1.42        | 1.37     |
| 35  | BB    | 1479 | G    | C5-C4   | -6.11 | 1.34        | 1.38     |
| 35  | BB    | 2186 | G    | C8-N7   | -6.11 | 1.27        | 1.30     |
| 49  | BP    | 88   | ARG  | CZ-NH1  | 6.11  | 1.41        | 1.33     |
| 1   | AA    | 657  | U    | C2'-C1' | -6.11 | 1.46        | 1.53     |
| 1   | AA    | 1162 | C    | C2'-C1' | -6.11 | 1.46        | 1.53     |
| 35  | BB    | 1233 | C    | N1-C2   | -6.11 | 1.34        | 1.40     |
| 1   | AA    | 788  | U    | P-O5'   | -6.11 | 1.53        | 1.59     |
| 1   | AA    | 1510 | C    | C2-N3   | 6.11  | 1.40        | 1.35     |
| 9   | AI    | 5    | TYR  | CE2-CZ  | 6.11  | 1.46        | 1.38     |
| 35  | BB    | 598  | U    | C5-C6   | -6.11 | 1.28        | 1.34     |
| 35  | BB    | 1228 | G    | C2'-C1' | -6.11 | 1.46        | 1.53     |
| 35  | BB    | 2040 | G    | C3'-C2' | -6.11 | 1.46        | 1.52     |
| 35  | BB    | 2890 | G    | N7-C5   | -6.11 | 1.35        | 1.39     |
| 45  | BL    | 69   | ARG  | CZ-NH1  | 6.11  | 1.41        | 1.33     |
| 51  | BR    | 67   | GLY  | CA-C    | -6.11 | 1.42        | 1.51     |
| 1   | AA    | 805  | C    | C4'-O4' | 6.11  | 1.53        | 1.45     |
| 1   | AA    | 1011 | C    | C4'-O4' | -6.11 | 1.37        | 1.45     |
| 28  | B3    | 47   | TYR  | CG-CD2  | 6.11  | 1.47        | 1.39     |
| 35  | BB    | 513  | A    | O4'-C1' | -6.11 | 1.33        | 1.41     |
| 35  | BB    | 1159 | U    | O4'-C1' | 6.11  | 1.49        | 1.41     |
| 35  | BB    | 2012 | G    | C6-N1   | 6.11  | 1.43        | 1.39     |
| 35  | BB    | 2307 | G    | O3'-P   | -6.11 | 1.53        | 1.61     |
| 1   | AA    | 600  | A    | N7-C5   | -6.11 | 1.35        | 1.39     |
| 1   | AA    | 834  | U    | C2'-C1' | 6.11  | 1.60        | 1.53     |
| 35  | BB    | 438  | G    | C8-N7   | 6.11  | 1.34        | 1.30     |
| 35  | BB    | 954  | G    | P-O5'   | -6.11 | 1.53        | 1.59     |
| 35  | BB    | 2775 | G    | N9-C8   | 6.11  | 1.42        | 1.37     |
| 35  | BB    | 1054 | A    | N7-C5   | -6.11 | 1.35        | 1.39     |
| 35  | BB    | 1425 | G    | N1-C2   | 6.11  | 1.42        | 1.37     |
| 35  | BB    | 1460 | U    | C4-O4   | -6.11 | 1.18        | 1.23     |
| 35  | BB    | 96   | C    | C4'-C3' | -6.10 | 1.46        | 1.53     |
| 35  | BB    | 1103 | A    | N1-C2   | 6.10  | 1.39        | 1.34     |
| 35  | BB    | 1628 | G    | N3-C4   | 6.10  | 1.39        | 1.35     |
| 35  | BB    | 1813 | G    | O3'-P   | -6.10 | 1.53        | 1.61     |
| 35  | BB    | 1885 | A    | C2-N3   | 6.10  | 1.39        | 1.33     |
| 35  | BB    | 1992 | G    | N3-C4   | -6.10 | 1.31        | 1.35     |
| 35  | BB    | 2319 | G    | C4'-C3' | -6.10 | 1.46        | 1.53     |
| 35  | BB    | 2642 | G    | C6-O6   | -6.10 | 1.18        | 1.24     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1024 | G    | N7-C5   | -6.10 | 1.35        | 1.39     |
| 34  | BA    | 13   | G    | N9-C4   | -6.10 | 1.33        | 1.38     |
| 35  | BB    | 1321 | A    | C2'-C1' | -6.10 | 1.46        | 1.53     |
| 35  | BB    | 1476 | U    | C2'-C1' | -6.10 | 1.46        | 1.53     |
| 35  | BB    | 1569 | A    | C8-N7   | -6.10 | 1.27        | 1.31     |
| 35  | BB    | 1493 | C    | C5'-C4' | 6.10  | 1.58        | 1.51     |
| 35  | BB    | 2110 | G    | N7-C5   | -6.10 | 1.35        | 1.39     |
| 1   | AA    | 41   | G    | C5'-C4' | 6.10  | 1.58        | 1.51     |
| 1   | AA    | 1096 | C    | P-O5'   | -6.10 | 1.53        | 1.59     |
| 1   | AA    | 1172 | C    | O4'-C1' | -6.10 | 1.33        | 1.41     |
| 1   | AA    | 1269 | A    | O3'-P   | -6.10 | 1.53        | 1.61     |
| 35  | BB    | 430  | A    | N9-C4   | -6.10 | 1.34        | 1.37     |
| 35  | BB    | 1090 | A    | N1-C2   | 6.10  | 1.39        | 1.34     |
| 35  | BB    | 2587 | A    | N1-C2   | 6.10  | 1.39        | 1.34     |
| 50  | BQ    | 27   | ARG  | NE-CZ   | 6.10  | 1.41        | 1.33     |
| 1   | AA    | 78   | A    | C3'-O3' | 6.10  | 1.50        | 1.42     |
| 1   | AA    | 366  | A    | C6-N6   | 6.10  | 1.38        | 1.33     |
| 1   | AA    | 1075 | U    | O4'-C1' | 6.10  | 1.49        | 1.41     |
| 1   | AA    | 1463 | U    | N3-C4   | 6.10  | 1.44        | 1.38     |
| 35  | BB    | 1191 | G    | N3-C4   | -6.10 | 1.31        | 1.35     |
| 35  | BB    | 1646 | C    | N1-C6   | -6.10 | 1.33        | 1.37     |
| 35  | BB    | 2012 | G    | C2-N2   | 6.10  | 1.40        | 1.34     |
| 35  | BB    | 2240 | U    | C2'-C1' | -6.10 | 1.46        | 1.53     |
| 35  | BB    | 2523 | G    | P-O5'   | -6.10 | 1.53        | 1.59     |
| 35  | BB    | 2645 | G    | N9-C4   | 6.10  | 1.42        | 1.38     |
| 43  | BJ    | 27   | ARG  | CZ-NH2  | 6.10  | 1.41        | 1.33     |
| 1   | AA    | 234  | C    | C4'-O4' | 6.10  | 1.53        | 1.45     |
| 34  | BA    | 76   | G    | C5-C4   | 6.10  | 1.42        | 1.38     |
| 35  | BB    | 1547 | C    | C2'-C1' | -6.10 | 1.46        | 1.53     |
| 35  | BB    | 1573 | G    | O3'-P   | -6.09 | 1.53        | 1.61     |
| 35  | BB    | 1585 | C    | N3-C4   | 6.09  | 1.38        | 1.33     |
| 35  | BB    | 2007 | U    | N1-C2   | 6.09  | 1.44        | 1.38     |
| 35  | BB    | 2337 | G    | N3-C4   | 6.09  | 1.39        | 1.35     |
| 35  | BB    | 2691 | C    | C3'-C2' | -6.09 | 1.46        | 1.52     |
| 1   | AA    | 270  | A    | C6-N1   | 6.09  | 1.39        | 1.35     |
| 1   | AA    | 389  | A    | C6-N6   | 6.09  | 1.38        | 1.33     |
| 1   | AA    | 799  | G    | N3-C4   | -6.09 | 1.31        | 1.35     |
| 1   | AA    | 909  | A    | C4'-C3' | 6.09  | 1.59        | 1.53     |
| 1   | AA    | 944  | G    | P-O5'   | -6.09 | 1.53        | 1.59     |
| 1   | AA    | 1059 | C    | C3'-C2' | -6.09 | 1.46        | 1.52     |
| 35  | BB    | 494  | G    | N9-C8   | -6.09 | 1.33        | 1.37     |
| 1   | AA    | 1397 | C    | C2-N3   | 6.09  | 1.40        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 438  | G    | C4'-C3' | 6.09  | 1.59        | 1.53     |
| 35  | BB    | 1812 | U    | N3-C4   | 6.09  | 1.44        | 1.38     |
| 35  | BB    | 2887 | A    | C8-N7   | -6.09 | 1.27        | 1.31     |
| 1   | AA    | 190  | A    | P-O5'   | 6.09  | 1.65        | 1.59     |
| 35  | BB    | 821  | A    | C5'-C4' | 6.09  | 1.58        | 1.51     |
| 35  | BB    | 1319 | C    | C4-N4   | 6.09  | 1.39        | 1.33     |
| 35  | BB    | 2248 | C    | N3-C4   | 6.09  | 1.38        | 1.33     |
| 1   | AA    | 211  | G    | C5-C4   | 6.09  | 1.42        | 1.38     |
| 1   | AA    | 586  | C    | P-O5'   | -6.09 | 1.53        | 1.59     |
| 20  | AT    | 14   | GLU  | CG-CD   | 6.09  | 1.61        | 1.51     |
| 35  | BB    | 1109 | C    | P-O5'   | -6.09 | 1.53        | 1.59     |
| 35  | BB    | 1269 | A    | N9-C8   | 6.09  | 1.42        | 1.37     |
| 1   | AA    | 574  | A    | P-O5'   | -6.09 | 1.53        | 1.59     |
| 1   | AA    | 657  | U    | C4-O4   | -6.09 | 1.18        | 1.23     |
| 1   | AA    | 673  | A    | N9-C8   | -6.09 | 1.32        | 1.37     |
| 1   | AA    | 918  | A    | C4'-O4' | -6.09 | 1.37        | 1.45     |
| 1   | AA    | 1010 | U    | P-O5'   | -6.09 | 1.53        | 1.59     |
| 1   | AA    | 1268 | G    | N9-C4   | 6.09  | 1.42        | 1.38     |
| 35  | BB    | 1171 | G    | C2'-C1' | -6.09 | 1.46        | 1.53     |
| 35  | BB    | 1244 | A    | C8-N7   | -6.09 | 1.27        | 1.31     |
| 35  | BB    | 2211 | A    | N1-C2   | 6.09  | 1.39        | 1.34     |
| 36  | BC    | 101  | ARG  | NE-CZ   | 6.09  | 1.41        | 1.33     |
| 1   | AA    | 707  | U    | N3-C4   | 6.08  | 1.44        | 1.38     |
| 1   | AA    | 1163 | A    | C2-N3   | 6.08  | 1.39        | 1.33     |
| 35  | BB    | 272  | A    | N9-C4   | -6.08 | 1.34        | 1.37     |
| 35  | BB    | 316  | C    | C4-N4   | 6.08  | 1.39        | 1.33     |
| 1   | AA    | 1124 | G    | N3-C4   | 6.08  | 1.39        | 1.35     |
| 35  | BB    | 39   | G    | C6-N1   | 6.08  | 1.43        | 1.39     |
| 35  | BB    | 1234 | U    | C2-N3   | 6.08  | 1.42        | 1.37     |
| 35  | BB    | 1408 | G    | C1'-N9  | -6.08 | 1.38        | 1.46     |
| 35  | BB    | 2273 | A    | C4'-C3' | 6.08  | 1.59        | 1.53     |
| 35  | BB    | 2299 | U    | C2-N3   | 6.08  | 1.42        | 1.37     |
| 35  | BB    | 2653 | U    | N3-C4   | 6.08  | 1.44        | 1.38     |
| 1   | AA    | 534  | U    | C5'-C4' | 6.08  | 1.58        | 1.51     |
| 1   | AA    | 970  | C    | C5'-C4' | 6.08  | 1.58        | 1.51     |
| 1   | AA    | 1099 | G    | C5-C6   | 6.08  | 1.48        | 1.42     |
| 1   | AA    | 1149 | C    | N3-C4   | 6.08  | 1.38        | 1.33     |
| 1   | AA    | 1379 | G    | C5'-C4' | 6.08  | 1.58        | 1.51     |
| 35  | BB    | 143  | C    | C5-C6   | 6.08  | 1.39        | 1.34     |
| 35  | BB    | 997  | G    | C5'-C4' | 6.08  | 1.58        | 1.51     |
| 35  | BB    | 1162 | G    | C2-N3   | 6.08  | 1.37        | 1.32     |
| 35  | BB    | 1949 | G    | C5-C6   | -6.08 | 1.36        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2887 | A    | N9-C4   | 6.08  | 1.41        | 1.37     |
| 1   | AA    | 685  | G    | C8-N7   | -6.08 | 1.27        | 1.30     |
| 35  | BB    | 342  | A    | C6-N6   | 6.08  | 1.38        | 1.33     |
| 35  | BB    | 439  | A    | N7-C5   | -6.08 | 1.35        | 1.39     |
| 35  | BB    | 1197 | G    | C3'-C2' | -6.08 | 1.46        | 1.52     |
| 35  | BB    | 2180 | U    | C3'-C2' | 6.08  | 1.59        | 1.52     |
| 1   | AA    | 76   | G    | N9-C8   | 6.08  | 1.42        | 1.37     |
| 34  | BA    | 95   | U    | C4-C5   | 6.08  | 1.49        | 1.43     |
| 35  | BB    | 1276 | A    | C5-C4   | 6.08  | 1.43        | 1.38     |
| 35  | BB    | 1982 | U    | C5'-C4' | 6.08  | 1.58        | 1.51     |
| 35  | BB    | 2491 | U    | C5-C6   | -6.08 | 1.28        | 1.34     |
| 52  | BS    | 84   | ARG  | CZ-NH2  | 6.08  | 1.41        | 1.33     |
| 1   | AA    | 357  | G    | N3-C4   | 6.08  | 1.39        | 1.35     |
| 1   | AA    | 391  | G    | C5-C4   | 6.08  | 1.42        | 1.38     |
| 35  | BB    | 803  | U    | C4'-C3' | 6.08  | 1.59        | 1.53     |
| 35  | BB    | 1059 | G    | C8-N7   | 6.08  | 1.34        | 1.30     |
| 35  | BB    | 1157 | G    | C2-N3   | 6.08  | 1.37        | 1.32     |
| 35  | BB    | 2012 | G    | C8-N7   | 6.08  | 1.34        | 1.30     |
| 36  | BC    | 68   | ARG  | CD-NE   | 6.08  | 1.56        | 1.46     |
| 1   | AA    | 1072 | G    | P-O5'   | -6.08 | 1.53        | 1.59     |
| 1   | AA    | 1102 | A    | C4'-O4' | -6.08 | 1.37        | 1.45     |
| 35  | BB    | 1765 | U    | C2-N3   | 6.08  | 1.42        | 1.37     |
| 35  | BB    | 1807 | G    | C2-N3   | 6.08  | 1.37        | 1.32     |
| 35  | BB    | 2092 | U    | C5'-C4' | 6.08  | 1.58        | 1.51     |
| 35  | BB    | 2397 | G    | N9-C4   | 6.08  | 1.42        | 1.38     |
| 1   | AA    | 254  | G    | C5-C4   | 6.07  | 1.42        | 1.38     |
| 1   | AA    | 336  | A    | N7-C5   | -6.07 | 1.35        | 1.39     |
| 1   | AA    | 789  | U    | C3'-O3' | 6.07  | 1.50        | 1.42     |
| 4   | AD    | 13   | ARG  | CD-NE   | 6.07  | 1.56        | 1.46     |
| 31  | B6    | 12   | ARG  | NE-CZ   | 6.07  | 1.41        | 1.33     |
| 35  | BB    | 380  | G    | C6-N1   | 6.07  | 1.43        | 1.39     |
| 35  | BB    | 1597 | A    | C4'-C3' | 6.07  | 1.59        | 1.53     |
| 35  | BB    | 1719 | G    | N1-C2   | 6.07  | 1.42        | 1.37     |
| 35  | BB    | 2232 | C    | N1-C6   | 6.07  | 1.40        | 1.37     |
| 35  | BB    | 2358 | A    | N3-C4   | -6.07 | 1.31        | 1.34     |
| 35  | BB    | 2695 | U    | P-O5'   | -6.07 | 1.53        | 1.59     |
| 1   | AA    | 135  | C    | C4-C5   | -6.07 | 1.38        | 1.43     |
| 1   | AA    | 702  | A    | N9-C4   | 6.07  | 1.41        | 1.37     |
| 35  | BB    | 878  | A    | C4'-O4' | 6.07  | 1.53        | 1.45     |
| 35  | BB    | 1375 | U    | C4-C5   | 6.07  | 1.49        | 1.43     |
| 35  | BB    | 2284 | A    | C2'-C1' | -6.07 | 1.46        | 1.53     |
| 1   | AA    | 179  | A    | N9-C4   | -6.07 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1225 | A    | C5-C4   | 6.07  | 1.43        | 1.38     |
| 7   | AG    | 78   | ARG  | CD-NE   | 6.07  | 1.56        | 1.46     |
| 35  | BB    | 525  | U    | C5-C6   | 6.07  | 1.39        | 1.34     |
| 35  | BB    | 1011 | G    | C2-N3   | -6.07 | 1.27        | 1.32     |
| 35  | BB    | 1608 | A    | C2'-C1' | -6.07 | 1.46        | 1.53     |
| 35  | BB    | 1973 | G    | C2-N3   | 6.07  | 1.37        | 1.32     |
| 35  | BB    | 2188 | U    | C1'-N1  | 6.07  | 1.57        | 1.48     |
| 35  | BB    | 2660 | A    | C6-N1   | 6.07  | 1.39        | 1.35     |
| 1   | AA    | 405  | U    | C2-N3   | 6.07  | 1.42        | 1.37     |
| 1   | AA    | 538  | G    | C3'-C2' | -6.07 | 1.46        | 1.52     |
| 1   | AA    | 854  | U    | C4'-C3' | -6.07 | 1.46        | 1.53     |
| 1   | AA    | 145  | G    | C2-N2   | 6.07  | 1.40        | 1.34     |
| 1   | AA    | 628  | G    | N3-C4   | -6.07 | 1.31        | 1.35     |
| 1   | AA    | 1006 | G    | N9-C8   | -6.07 | 1.33        | 1.37     |
| 1   | AA    | 1048 | G    | C5-C4   | 6.07  | 1.42        | 1.38     |
| 1   | AA    | 1051 | C    | O4'-C1' | 6.07  | 1.49        | 1.41     |
| 1   | AA    | 1131 | G    | C6-N1   | 6.07  | 1.43        | 1.39     |
| 1   | AA    | 273  | U    | C2-O2   | 6.07  | 1.27        | 1.22     |
| 1   | AA    | 423  | G    | C4'-C3' | 6.07  | 1.59        | 1.53     |
| 1   | AA    | 1021 | A    | C8-N7   | -6.07 | 1.27        | 1.31     |
| 1   | AA    | 1127 | G    | C2'-C1' | -6.07 | 1.46        | 1.53     |
| 1   | AA    | 1240 | U    | N3-C4   | 6.07  | 1.44        | 1.38     |
| 35  | BB    | 942  | G    | C4'-C3' | 6.07  | 1.59        | 1.53     |
| 35  | BB    | 1103 | A    | O3'-P   | -6.07 | 1.53        | 1.61     |
| 35  | BB    | 1938 | A    | C5'-C4' | 6.07  | 1.58        | 1.51     |
| 35  | BB    | 2482 | A    | C2'-C1' | -6.07 | 1.46        | 1.53     |
| 35  | BB    | 2892 | G    | C5-C4   | 6.07  | 1.42        | 1.38     |
| 37  | BD    | 124  | ARG  | NE-CZ   | 6.07  | 1.41        | 1.33     |
| 1   | AA    | 284  | C    | P-O5'   | -6.06 | 1.53        | 1.59     |
| 1   | AA    | 854  | U    | C5'-C4' | 6.06  | 1.58        | 1.51     |
| 1   | AA    | 1191 | A    | P-O5'   | -6.06 | 1.53        | 1.59     |
| 1   | AA    | 1530 | G    | C6-N1   | 6.06  | 1.43        | 1.39     |
| 34  | BA    | 64   | G    | N9-C8   | 6.06  | 1.42        | 1.37     |
| 35  | BB    | 284  | U    | N1-C2   | -6.06 | 1.33        | 1.38     |
| 1   | AA    | 23   | C    | C2'-C1' | -6.06 | 1.46        | 1.53     |
| 1   | AA    | 786  | G    | N7-C5   | -6.06 | 1.35        | 1.39     |
| 1   | AA    | 1368 | A    | C8-N7   | -6.06 | 1.27        | 1.31     |
| 35  | BB    | 152  | A    | P-O5'   | -6.06 | 1.53        | 1.59     |
| 35  | BB    | 582  | A    | O3'-P   | -6.06 | 1.53        | 1.61     |
| 35  | BB    | 2242 | G    | C2'-C1' | -6.06 | 1.46        | 1.53     |
| 35  | BB    | 42   | A    | N1-C2   | -6.06 | 1.28        | 1.34     |
| 35  | BB    | 1375 | U    | N1-C6   | 6.06  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1403 | A    | N3-C4   | -6.06 | 1.31        | 1.34     |
| 35  | BB    | 2388 | A    | P-O5'   | -6.06 | 1.53        | 1.59     |
| 35  | BB    | 2608 | G    | N7-C5   | -6.06 | 1.35        | 1.39     |
| 1   | AA    | 283  | U    | O4'-C1' | -6.06 | 1.33        | 1.41     |
| 1   | AA    | 293  | G    | N9-C8   | 6.06  | 1.42        | 1.37     |
| 1   | AA    | 745  | G    | C8-N7   | -6.06 | 1.27        | 1.30     |
| 1   | AA    | 906  | A    | O3'-P   | -6.06 | 1.53        | 1.61     |
| 1   | AA    | 1421 | G    | P-O5'   | -6.06 | 1.53        | 1.59     |
| 2   | AB    | 55   | GLU  | CD-OE2  | 6.06  | 1.32        | 1.25     |
| 35  | BB    | 296  | U    | N3-C4   | 6.06  | 1.44        | 1.38     |
| 35  | BB    | 1659 | G    | C2'-O2' | 6.06  | 1.49        | 1.41     |
| 35  | BB    | 1700 | A    | C6-N6   | 6.06  | 1.38        | 1.33     |
| 35  | BB    | 2573 | C    | C2'-C1' | -6.06 | 1.46        | 1.53     |
| 1   | AA    | 1101 | A    | N7-C5   | -6.06 | 1.35        | 1.39     |
| 35  | BB    | 443  | A    | C8-N7   | 6.06  | 1.35        | 1.31     |
| 35  | BB    | 730  | A    | C6-N1   | 6.06  | 1.39        | 1.35     |
| 35  | BB    | 733  | G    | C4'-O4' | 6.06  | 1.53        | 1.45     |
| 35  | BB    | 1108 | U    | C2'-C1' | -6.06 | 1.46        | 1.53     |
| 35  | BB    | 1358 | G    | C2-N3   | 6.06  | 1.37        | 1.32     |
| 35  | BB    | 1739 | A    | N3-C4   | 6.06  | 1.38        | 1.34     |
| 35  | BB    | 1743 | G    | C2-N2   | 6.06  | 1.40        | 1.34     |
| 35  | BB    | 2068 | U    | N3-C4   | 6.06  | 1.44        | 1.38     |
| 35  | BB    | 550  | C    | C4'-C3' | -6.06 | 1.46        | 1.53     |
| 35  | BB    | 868  | U    | C2'-C1' | -6.06 | 1.46        | 1.53     |
| 35  | BB    | 1292 | G    | N1-C2   | 6.06  | 1.42        | 1.37     |
| 35  | BB    | 2100 | G    | C8-N7   | 6.06  | 1.34        | 1.30     |
| 1   | AA    | 850  | U    | C4-C5   | 6.05  | 1.49        | 1.43     |
| 1   | AA    | 1185 | G    | C6-O6   | -6.05 | 1.18        | 1.24     |
| 1   | AA    | 1321 | U    | C4'-O4' | -6.05 | 1.37        | 1.45     |
| 1   | AA    | 1514 | G    | C8-N7   | -6.05 | 1.27        | 1.30     |
| 34  | BA    | 71   | C    | C4-N4   | 6.05  | 1.39        | 1.33     |
| 35  | BB    | 43   | G    | C6-N1   | 6.05  | 1.43        | 1.39     |
| 35  | BB    | 352  | A    | C6-N6   | 6.05  | 1.38        | 1.33     |
| 35  | BB    | 388  | G    | N1-C2   | 6.05  | 1.42        | 1.37     |
| 35  | BB    | 913  | U    | C4'-C3' | 6.05  | 1.59        | 1.53     |
| 35  | BB    | 973  | A    | C5-C6   | -6.05 | 1.35        | 1.41     |
| 35  | BB    | 1006 | C    | N1-C2   | -6.05 | 1.34        | 1.40     |
| 35  | BB    | 1306 | C    | N3-C4   | 6.05  | 1.38        | 1.33     |
| 35  | BB    | 2614 | A    | C6-N6   | 6.05  | 1.38        | 1.33     |
| 35  | BB    | 474  | G    | N9-C8   | -6.05 | 1.33        | 1.37     |
| 35  | BB    | 526  | A    | C5'-C4' | 6.05  | 1.58        | 1.51     |
| 35  | BB    | 1498 | C    | C2-N3   | 6.05  | 1.40        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1748 | C    | C5-C6   | 6.05  | 1.39        | 1.34     |
| 35  | BB    | 2259 | U    | C3'-O3' | 6.05  | 1.50        | 1.42     |
| 1   | AA    | 116  | A    | N9-C8   | 6.05  | 1.42        | 1.37     |
| 1   | AA    | 367  | U    | C4-C5   | 6.05  | 1.49        | 1.43     |
| 1   | AA    | 495  | A    | C4'-O4' | 6.05  | 1.53        | 1.45     |
| 1   | AA    | 768  | A    | C2'-C1' | -6.05 | 1.46        | 1.53     |
| 1   | AA    | 1046 | A    | O3'-P   | -6.05 | 1.53        | 1.61     |
| 35  | BB    | 14   | A    | C4'-C3' | 6.05  | 1.59        | 1.53     |
| 35  | BB    | 180  | G    | C2-N3   | 6.05  | 1.37        | 1.32     |
| 35  | BB    | 559  | G    | P-O5'   | -6.05 | 1.53        | 1.59     |
| 35  | BB    | 699  | A    | P-O5'   | -6.05 | 1.53        | 1.59     |
| 35  | BB    | 1187 | G    | P-O5'   | 6.05  | 1.65        | 1.59     |
| 35  | BB    | 1938 | A    | C6-N6   | 6.05  | 1.38        | 1.33     |
| 35  | BB    | 2087 | G    | C4'-O4' | 6.05  | 1.53        | 1.45     |
| 35  | BB    | 2369 | A    | C2'-C1' | -6.05 | 1.46        | 1.53     |
| 35  | BB    | 2852 | G    | C5-C4   | 6.05  | 1.42        | 1.38     |
| 1   | AA    | 354  | G    | C6-N1   | 6.05  | 1.43        | 1.39     |
| 1   | AA    | 630  | A    | C6-N6   | 6.05  | 1.38        | 1.33     |
| 1   | AA    | 705  | G    | C6-O6   | -6.05 | 1.18        | 1.24     |
| 1   | AA    | 1155 | A    | P-O5'   | -6.05 | 1.53        | 1.59     |
| 35  | BB    | 525  | U    | C4-C5   | 6.05  | 1.49        | 1.43     |
| 35  | BB    | 720  | U    | P-O5'   | -6.05 | 1.53        | 1.59     |
| 35  | BB    | 1151 | A    | C8-N7   | 6.05  | 1.35        | 1.31     |
| 35  | BB    | 1415 | U    | N1-C6   | 6.05  | 1.43        | 1.38     |
| 35  | BB    | 1603 | A    | C8-N7   | 6.05  | 1.35        | 1.31     |
| 35  | BB    | 2040 | G    | P-O5'   | -6.05 | 1.53        | 1.59     |
| 35  | BB    | 2050 | C    | C4'-C3' | -6.05 | 1.46        | 1.53     |
| 35  | BB    | 2088 | A    | C2'-C1' | -6.05 | 1.46        | 1.53     |
| 1   | AA    | 259  | G    | N1-C2   | 6.05  | 1.42        | 1.37     |
| 35  | BB    | 207  | A    | N3-C4   | -6.05 | 1.31        | 1.34     |
| 1   | AA    | 611  | C    | N1-C6   | -6.05 | 1.33        | 1.37     |
| 1   | AA    | 986  | U    | O3'-P   | -6.05 | 1.53        | 1.61     |
| 35  | BB    | 1133 | A    | C4'-O4' | -6.05 | 1.37        | 1.45     |
| 35  | BB    | 1143 | A    | C6-N1   | 6.05  | 1.39        | 1.35     |
| 35  | BB    | 1317 | G    | N1-C2   | 6.05  | 1.42        | 1.37     |
| 35  | BB    | 1549 | A    | C4'-C3' | -6.05 | 1.46        | 1.53     |
| 1   | AA    | 890  | G    | C2'-C1' | -6.04 | 1.46        | 1.53     |
| 1   | AA    | 1465 | A    | N9-C8   | 6.04  | 1.42        | 1.37     |
| 35  | BB    | 163  | C    | O4'-C1' | 6.04  | 1.49        | 1.41     |
| 35  | BB    | 216  | A    | N7-C5   | -6.04 | 1.35        | 1.39     |
| 1   | AA    | 710  | G    | N9-C8   | -6.04 | 1.33        | 1.37     |
| 1   | AA    | 1028 | C    | C4'-C3' | 6.04  | 1.59        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1035 | A    | C8-N7   | -6.04 | 1.27        | 1.31     |
| 1   | AA    | 1174 | G    | N1-C2   | 6.04  | 1.42        | 1.37     |
| 1   | AA    | 1306 | A    | C2-N3   | 6.04  | 1.39        | 1.33     |
| 35  | BB    | 1045 | C    | C5-C6   | -6.04 | 1.29        | 1.34     |
| 35  | BB    | 1834 | U    | C2'-C1' | 6.04  | 1.59        | 1.53     |
| 35  | BB    | 1927 | A    | C2'-C1' | -6.04 | 1.46        | 1.53     |
| 35  | BB    | 2011 | U    | C5'-C4' | 6.04  | 1.58        | 1.51     |
| 35  | BB    | 2499 | C    | C5'-C4' | 6.04  | 1.58        | 1.51     |
| 1   | AA    | 719  | C    | C4-N4   | 6.04  | 1.39        | 1.33     |
| 35  | BB    | 300  | A    | N9-C4   | -6.04 | 1.34        | 1.37     |
| 35  | BB    | 1399 | C    | N1-C6   | -6.04 | 1.33        | 1.37     |
| 43  | BJ    | 81   | ILE  | C-N     | 6.04  | 1.44        | 1.33     |
| 1   | AA    | 280  | C    | C2'-C1' | 6.04  | 1.59        | 1.53     |
| 1   | AA    | 967  | C    | C2-N3   | 6.04  | 1.40        | 1.35     |
| 2   | AB    | 212  | TYR  | CZ-OH   | 6.04  | 1.48        | 1.37     |
| 35  | BB    | 897  | C    | C2-N3   | 6.04  | 1.40        | 1.35     |
| 35  | BB    | 1109 | C    | C4-N4   | 6.04  | 1.39        | 1.33     |
| 35  | BB    | 2837 | A    | N9-C4   | 6.04  | 1.41        | 1.37     |
| 1   | AA    | 1113 | C    | C4'-O4' | 6.04  | 1.53        | 1.45     |
| 1   | AA    | 1146 | A    | N9-C8   | -6.04 | 1.32        | 1.37     |
| 1   | AA    | 1191 | A    | C6-N6   | 6.04  | 1.38        | 1.33     |
| 1   | AA    | 1246 | A    | N7-C5   | -6.04 | 1.35        | 1.39     |
| 34  | BA    | 41   | G    | C5-C6   | -6.04 | 1.36        | 1.42     |
| 35  | BB    | 578  | G    | C5'-C4' | 6.04  | 1.58        | 1.51     |
| 35  | BB    | 614  | A    | C5-C6   | -6.04 | 1.35        | 1.41     |
| 35  | BB    | 655  | A    | N7-C5   | -6.04 | 1.35        | 1.39     |
| 35  | BB    | 933  | A    | C6-N1   | 6.04  | 1.39        | 1.35     |
| 35  | BB    | 1176 | U    | C3'-C2' | 6.04  | 1.59        | 1.52     |
| 35  | BB    | 1269 | A    | C5'-C4' | 6.04  | 1.58        | 1.51     |
| 35  | BB    | 1648 | U    | N3-C4   | 6.04  | 1.43        | 1.38     |
| 35  | BB    | 2089 | C    | C5-C6   | -6.04 | 1.29        | 1.34     |
| 35  | BB    | 2135 | A    | C6-N6   | 6.04  | 1.38        | 1.33     |
| 35  | BB    | 2625 | G    | N1-C2   | 6.04  | 1.42        | 1.37     |
| 1   | AA    | 1201 | A    | C6-N1   | 6.04  | 1.39        | 1.35     |
| 35  | BB    | 308  | G    | N1-C2   | 6.04  | 1.42        | 1.37     |
| 35  | BB    | 1235 | G    | C2-N2   | 6.04  | 1.40        | 1.34     |
| 35  | BB    | 1361 | G    | C8-N7   | 6.04  | 1.34        | 1.30     |
| 35  | BB    | 1695 | G    | N9-C8   | -6.04 | 1.33        | 1.37     |
| 35  | BB    | 2764 | A    | C3'-C2' | 6.04  | 1.59        | 1.52     |
| 1   | AA    | 159  | G    | C2-N2   | 6.04  | 1.40        | 1.34     |
| 1   | AA    | 730  | G    | N9-C8   | -6.04 | 1.33        | 1.37     |
| 1   | AA    | 1013 | G    | N3-C4   | -6.04 | 1.31        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1534 | A    | C6-N6   | 6.04  | 1.38        | 1.33     |
| 35  | BB    | 722  | A    | C3'-O3' | 6.04  | 1.50        | 1.42     |
| 35  | BB    | 1170 | C    | C1'-N1  | 6.04  | 1.57        | 1.48     |
| 35  | BB    | 1330 | C    | C4-C5   | 6.04  | 1.47        | 1.43     |
| 35  | BB    | 1824 | G    | C2-N2   | 6.04  | 1.40        | 1.34     |
| 1   | AA    | 187  | G    | C5'-C4' | 6.03  | 1.58        | 1.51     |
| 1   | AA    | 467  | U    | P-O5'   | -6.03 | 1.53        | 1.59     |
| 1   | AA    | 1268 | G    | C2-N3   | 6.03  | 1.37        | 1.32     |
| 1   | AA    | 1465 | A    | O3'-P   | -6.03 | 1.53        | 1.61     |
| 34  | BA    | 99   | A    | N9-C4   | -6.03 | 1.34        | 1.37     |
| 35  | BB    | 1293 | C    | P-O5'   | -6.03 | 1.53        | 1.59     |
| 35  | BB    | 1317 | G    | P-O5'   | -6.03 | 1.53        | 1.59     |
| 35  | BB    | 2007 | U    | O4'-C1' | 6.03  | 1.49        | 1.41     |
| 35  | BB    | 2718 | G    | C2-N3   | 6.03  | 1.37        | 1.32     |
| 1   | AA    | 155  | A    | N7-C5   | -6.03 | 1.35        | 1.39     |
| 1   | AA    | 1082 | A    | C6-N1   | 6.03  | 1.39        | 1.35     |
| 35  | BB    | 770  | G    | C2-N2   | 6.03  | 1.40        | 1.34     |
| 35  | BB    | 1829 | A    | C2'-C1' | -6.03 | 1.46        | 1.53     |
| 35  | BB    | 2114 | A    | O3'-P   | -6.03 | 1.53        | 1.61     |
| 35  | BB    | 2370 | G    | C5-C4   | 6.03  | 1.42        | 1.38     |
| 35  | BB    | 2538 | C    | N3-C4   | 6.03  | 1.38        | 1.33     |
| 34  | BA    | 64   | G    | C8-N7   | -6.03 | 1.27        | 1.30     |
| 35  | BB    | 543  | G    | C5-C4   | 6.03  | 1.42        | 1.38     |
| 35  | BB    | 650  | C    | C3'-C2' | 6.03  | 1.59        | 1.52     |
| 35  | BB    | 1139 | G    | C5'-C4' | 6.03  | 1.58        | 1.51     |
| 35  | BB    | 1232 | G    | C8-N7   | -6.03 | 1.27        | 1.30     |
| 35  | BB    | 1845 | G    | P-O5'   | -6.03 | 1.53        | 1.59     |
| 35  | BB    | 2003 | A    | P-O5'   | -6.03 | 1.53        | 1.59     |
| 35  | BB    | 2481 | G    | C2-N3   | 6.03  | 1.37        | 1.32     |
| 52  | BS    | 92   | ARG  | CD-NE   | 6.03  | 1.56        | 1.46     |
| 30  | B5    | 49   | GLY  | N-CA    | 6.03  | 1.55        | 1.46     |
| 35  | BB    | 357  | C    | N1-C6   | 6.03  | 1.40        | 1.37     |
| 35  | BB    | 504  | A    | N9-C4   | 6.03  | 1.41        | 1.37     |
| 35  | BB    | 566  | U    | C5-C6   | 6.03  | 1.39        | 1.34     |
| 35  | BB    | 948  | C    | C5-C6   | -6.03 | 1.29        | 1.34     |
| 35  | BB    | 1689 | A    | N1-C2   | -6.03 | 1.28        | 1.34     |
| 35  | BB    | 2441 | U    | C2'-C1' | 6.03  | 1.59        | 1.53     |
| 1   | AA    | 466  | A    | C2'-C1' | -6.03 | 1.46        | 1.53     |
| 1   | AA    | 900  | A    | N7-C5   | -6.03 | 1.35        | 1.39     |
| 35  | BB    | 1142 | A    | C2-N3   | -6.03 | 1.28        | 1.33     |
| 35  | BB    | 1946 | U    | C5'-C4' | 6.03  | 1.58        | 1.51     |
| 35  | BB    | 1966 | A    | C6-N1   | 6.03  | 1.39        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2276 | G    | C8-N7   | -6.03 | 1.27        | 1.30     |
| 1   | AA    | 785  | G    | C2-N3   | 6.03  | 1.37        | 1.32     |
| 34  | BA    | 73   | A    | C5-C4   | -6.03 | 1.34        | 1.38     |
| 35  | BB    | 1679 | A    | C3'-C2' | 6.03  | 1.59        | 1.52     |
| 1   | AA    | 330  | C    | C3'-C2' | 6.02  | 1.59        | 1.52     |
| 1   | AA    | 882  | C    | C4-C5   | 6.02  | 1.47        | 1.43     |
| 1   | AA    | 1191 | A    | N9-C4   | -6.02 | 1.34        | 1.37     |
| 34  | BA    | 94   | A    | C8-N7   | -6.02 | 1.27        | 1.31     |
| 35  | BB    | 976  | G    | O3'-P   | -6.02 | 1.53        | 1.61     |
| 1   | AA    | 10   | A    | C2'-C1' | -6.02 | 1.46        | 1.53     |
| 11  | AK    | 54   | SER  | CA-CB   | 6.02  | 1.61        | 1.52     |
| 35  | BB    | 251  | A    | N3-C4   | 6.02  | 1.38        | 1.34     |
| 35  | BB    | 901  | C    | C4-N4   | 6.02  | 1.39        | 1.33     |
| 35  | BB    | 1149 | G    | C5-C4   | 6.02  | 1.42        | 1.38     |
| 35  | BB    | 1376 | C    | N3-C4   | 6.02  | 1.38        | 1.33     |
| 35  | BB    | 1579 | A    | C6-N1   | 6.02  | 1.39        | 1.35     |
| 35  | BB    | 1784 | A    | N3-C4   | -6.02 | 1.31        | 1.34     |
| 35  | BB    | 2146 | C    | C4-N4   | 6.02  | 1.39        | 1.33     |
| 35  | BB    | 2540 | C    | N1-C6   | 6.02  | 1.40        | 1.37     |
| 35  | BB    | 2800 | A    | C5-C4   | -6.02 | 1.34        | 1.38     |
| 35  | BB    | 33   | C    | C5'-C4' | 6.02  | 1.58        | 1.51     |
| 35  | BB    | 355  | U    | C5-C6   | 6.02  | 1.39        | 1.34     |
| 35  | BB    | 1839 | G    | C4'-C3' | -6.02 | 1.46        | 1.53     |
| 1   | AA    | 1382 | C    | N1-C6   | 6.02  | 1.40        | 1.37     |
| 35  | BB    | 1623 | G    | C6-N1   | 6.02  | 1.43        | 1.39     |
| 35  | BB    | 2262 | U    | C2-N3   | 6.02  | 1.42        | 1.37     |
| 35  | BB    | 626  | A    | N1-C2   | -6.02 | 1.28        | 1.34     |
| 35  | BB    | 1285 | A    | N9-C8   | 6.02  | 1.42        | 1.37     |
| 35  | BB    | 1880 | U    | N1-C2   | -6.02 | 1.33        | 1.38     |
| 35  | BB    | 2174 | C    | N1-C6   | 6.02  | 1.40        | 1.37     |
| 35  | BB    | 2252 | G    | C2-N3   | 6.02  | 1.37        | 1.32     |
| 1   | AA    | 254  | G    | C3'-O3' | 6.02  | 1.50        | 1.42     |
| 1   | AA    | 1288 | A    | C6-N6   | 6.02  | 1.38        | 1.33     |
| 35  | BB    | 666  | A    | C2-N3   | 6.02  | 1.39        | 1.33     |
| 35  | BB    | 2384 | U    | C4-O4   | 6.02  | 1.28        | 1.23     |
| 35  | BB    | 2672 | U    | C2'-C1' | -6.02 | 1.46        | 1.53     |
| 1   | AA    | 247  | G    | C6-N1   | -6.01 | 1.35        | 1.39     |
| 1   | AA    | 1030 | U    | N3-C4   | 6.01  | 1.43        | 1.38     |
| 35  | BB    | 395  | U    | C2-N3   | 6.01  | 1.42        | 1.37     |
| 35  | BB    | 1080 | A    | N9-C4   | 6.01  | 1.41        | 1.37     |
| 35  | BB    | 1642 | G    | C2'-O2' | 6.01  | 1.49        | 1.41     |
| 35  | BB    | 1657 | U    | N1-C6   | -6.01 | 1.32        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1949 | G    | C2-N3   | 6.01  | 1.37        | 1.32     |
| 35  | BB    | 2128 | G    | N3-C4   | 6.01  | 1.39        | 1.35     |
| 35  | BB    | 745  | G    | N3-C4   | -6.01 | 1.31        | 1.35     |
| 35  | BB    | 1084 | A    | N7-C5   | -6.01 | 1.35        | 1.39     |
| 1   | AA    | 680  | C    | N1-C6   | 6.01  | 1.40        | 1.37     |
| 1   | AA    | 984  | C    | O4'-C1' | 6.01  | 1.49        | 1.41     |
| 35  | BB    | 250  | G    | C8-N7   | -6.01 | 1.27        | 1.30     |
| 35  | BB    | 306  | U    | C2'-C1' | -6.01 | 1.46        | 1.53     |
| 35  | BB    | 813  | U    | C2'-C1' | -6.01 | 1.46        | 1.53     |
| 35  | BB    | 1130 | U    | N1-C2   | -6.01 | 1.33        | 1.38     |
| 35  | BB    | 1231 | U    | C4'-C3' | -6.01 | 1.46        | 1.53     |
| 35  | BB    | 1353 | A    | O3'-P   | -6.01 | 1.53        | 1.61     |
| 35  | BB    | 2270 | A    | C5-C4   | 6.01  | 1.43        | 1.38     |
| 1   | AA    | 438  | U    | O4'-C1' | -6.01 | 1.33        | 1.41     |
| 1   | AA    | 510  | A    | C6-N1   | 6.01  | 1.39        | 1.35     |
| 1   | AA    | 818  | G    | O3'-P   | -6.01 | 1.53        | 1.61     |
| 35  | BB    | 278  | A    | N9-C4   | 6.01  | 1.41        | 1.37     |
| 35  | BB    | 892  | A    | N7-C5   | -6.01 | 1.35        | 1.39     |
| 35  | BB    | 2435 | A    | C1'-N9  | -6.01 | 1.38        | 1.46     |
| 35  | BB    | 385  | C    | N1-C6   | 6.01  | 1.40        | 1.37     |
| 35  | BB    | 538  | A    | C2'-C1' | -6.01 | 1.46        | 1.53     |
| 35  | BB    | 1401 | G    | N9-C4   | 6.01  | 1.42        | 1.38     |
| 1   | AA    | 274  | A    | C6-N1   | 6.01  | 1.39        | 1.35     |
| 1   | AA    | 1432 | G    | C6-N1   | -6.01 | 1.35        | 1.39     |
| 14  | AN    | 8    | ARG  | NE-CZ   | 6.01  | 1.40        | 1.33     |
| 35  | BB    | 228  | C    | C4'-C3' | 6.01  | 1.59        | 1.53     |
| 35  | BB    | 866  | A    | C8-N7   | 6.01  | 1.35        | 1.31     |
| 35  | BB    | 1351 | C    | C2'-C1' | -6.01 | 1.46        | 1.53     |
| 35  | BB    | 2223 | G    | P-O5'   | -6.01 | 1.53        | 1.59     |
| 35  | BB    | 2311 | A    | N7-C5   | 6.01  | 1.42        | 1.39     |
| 35  | BB    | 2662 | A    | C2'-C1' | -6.01 | 1.46        | 1.53     |
| 1   | AA    | 226  | G    | N9-C8   | -6.00 | 1.33        | 1.37     |
| 1   | AA    | 1459 | G    | C2-N3   | 6.00  | 1.37        | 1.32     |
| 35  | BB    | 303  | G    | C2-N2   | 6.00  | 1.40        | 1.34     |
| 35  | BB    | 721  | A    | O4'-C1' | -6.00 | 1.33        | 1.41     |
| 35  | BB    | 1310 | G    | C5'-C4' | 6.00  | 1.58        | 1.51     |
| 35  | BB    | 1717 | A    | C6-N6   | 6.00  | 1.38        | 1.33     |
| 35  | BB    | 2562 | U    | N1-C2   | 6.00  | 1.44        | 1.38     |
| 35  | BB    | 2708 | G    | N9-C8   | 6.00  | 1.42        | 1.37     |
| 40  | BG    | 151  | ARG  | NE-CZ   | 6.00  | 1.40        | 1.33     |
| 35  | BB    | 608  | A    | N9-C4   | 6.00  | 1.41        | 1.37     |
| 35  | BB    | 1689 | A    | C6-N1   | 6.00  | 1.39        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1773 | A    | C2'-C1' | -6.00 | 1.46        | 1.53     |
| 35  | BB    | 2498 | C    | N1-C6   | -6.00 | 1.33        | 1.37     |
| 1   | AA    | 13   | U    | C3'-C2' | 6.00  | 1.59        | 1.52     |
| 1   | AA    | 147  | G    | C4'-C3' | 6.00  | 1.59        | 1.53     |
| 1   | AA    | 400  | C    | C2'-C1' | -6.00 | 1.46        | 1.53     |
| 1   | AA    | 603  | U    | N1-C6   | 6.00  | 1.43        | 1.38     |
| 35  | BB    | 433  | C    | N3-C4   | 6.00  | 1.38        | 1.33     |
| 35  | BB    | 825  | A    | C4'-C3' | 6.00  | 1.59        | 1.53     |
| 35  | BB    | 838  | C    | N1-C6   | -6.00 | 1.33        | 1.37     |
| 35  | BB    | 877  | A    | N9-C8   | 6.00  | 1.42        | 1.37     |
| 35  | BB    | 1372 | U    | N3-C4   | -6.00 | 1.33        | 1.38     |
| 35  | BB    | 1423 | G    | N1-C2   | 6.00  | 1.42        | 1.37     |
| 35  | BB    | 1466 | U    | N3-C4   | 6.00  | 1.43        | 1.38     |
| 35  | BB    | 1638 | C    | O3'-P   | -6.00 | 1.53        | 1.61     |
| 35  | BB    | 2458 | G    | C5-C4   | 6.00  | 1.42        | 1.38     |
| 35  | BB    | 2557 | G    | C8-N7   | 6.00  | 1.34        | 1.30     |
| 35  | BB    | 2620 | C    | C2-N3   | -6.00 | 1.30        | 1.35     |
| 52  | BS    | 108  | SER  | CA-CB   | 6.00  | 1.61        | 1.52     |
| 1   | AA    | 392  | C    | C4-N4   | 6.00  | 1.39        | 1.33     |
| 1   | AA    | 872  | A    | C2'-C1' | -6.00 | 1.46        | 1.53     |
| 35  | BB    | 2189 | U    | P-O5'   | -6.00 | 1.53        | 1.59     |
| 1   | AA    | 18   | C    | P-O5'   | -6.00 | 1.53        | 1.59     |
| 1   | AA    | 388  | G    | C8-N7   | 6.00  | 1.34        | 1.30     |
| 1   | AA    | 535  | A    | N9-C8   | 6.00  | 1.42        | 1.37     |
| 1   | AA    | 1102 | A    | C6-N1   | 6.00  | 1.39        | 1.35     |
| 34  | BA    | 50   | A    | N7-C5   | -6.00 | 1.35        | 1.39     |
| 35  | BB    | 503  | A    | C2'-C1' | -6.00 | 1.46        | 1.53     |
| 35  | BB    | 738  | G    | C2'-C1' | -6.00 | 1.46        | 1.53     |
| 1   | AA    | 350  | G    | O3'-P   | -6.00 | 1.53        | 1.61     |
| 34  | BA    | 81   | G    | C6-N1   | -6.00 | 1.35        | 1.39     |
| 35  | BB    | 33   | C    | C2-N3   | 6.00  | 1.40        | 1.35     |
| 35  | BB    | 477  | A    | C5-C4   | 6.00  | 1.43        | 1.38     |
| 35  | BB    | 654  | A    | C6-N1   | 6.00  | 1.39        | 1.35     |
| 35  | BB    | 799  | G    | C3'-C2' | -6.00 | 1.46        | 1.52     |
| 35  | BB    | 805  | G    | C2-N3   | 6.00  | 1.37        | 1.32     |
| 35  | BB    | 1359 | A    | N1-C2   | -6.00 | 1.28        | 1.34     |
| 35  | BB    | 1800 | C    | C2-O2   | 6.00  | 1.29        | 1.24     |
| 35  | BB    | 2254 | C    | C4-N4   | 6.00  | 1.39        | 1.33     |
| 35  | BB    | 2632 | A    | C6-N6   | 6.00  | 1.38        | 1.33     |
| 16  | AP    | 68   | SER  | CA-CB   | 6.00  | 1.61        | 1.52     |
| 35  | BB    | 1508 | A    | C5-C4   | 6.00  | 1.43        | 1.38     |
| 35  | BB    | 1780 | A    | C6-N1   | 6.00  | 1.39        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1848 | A    | N7-C5   | -6.00 | 1.35        | 1.39     |
| 1   | AA    | 920  | U    | C2'-C1' | -5.99 | 1.46        | 1.53     |
| 1   | AA    | 1523 | G    | C8-N7   | -5.99 | 1.27        | 1.30     |
| 35  | BB    | 107  | G    | N3-C4   | -5.99 | 1.31        | 1.35     |
| 35  | BB    | 320  | A    | C2'-C1' | -5.99 | 1.46        | 1.53     |
| 35  | BB    | 438  | G    | C5-C4   | 5.99  | 1.42        | 1.38     |
| 35  | BB    | 441  | U    | C4-O4   | -5.99 | 1.18        | 1.23     |
| 35  | BB    | 449  | A    | N7-C5   | -5.99 | 1.35        | 1.39     |
| 35  | BB    | 965  | C    | C3'-C2' | -5.99 | 1.46        | 1.52     |
| 35  | BB    | 1212 | G    | O3'-P   | -5.99 | 1.53        | 1.61     |
| 35  | BB    | 1692 | U    | C2-O2   | 5.99  | 1.27        | 1.22     |
| 35  | BB    | 2119 | A    | N1-C2   | 5.99  | 1.39        | 1.34     |
| 35  | BB    | 2516 | A    | C2'-C1' | -5.99 | 1.46        | 1.53     |
| 1   | AA    | 1019 | A    | C6-N1   | 5.99  | 1.39        | 1.35     |
| 35  | BB    | 1433 | A    | C8-N7   | -5.99 | 1.27        | 1.31     |
| 35  | BB    | 1666 | G    | O3'-P   | -5.99 | 1.53        | 1.61     |
| 35  | BB    | 1965 | C    | O3'-P   | -5.99 | 1.53        | 1.61     |
| 35  | BB    | 2099 | U    | N3-C4   | 5.99  | 1.43        | 1.38     |
| 1   | AA    | 807  | A    | C4'-C3' | 5.99  | 1.59        | 1.53     |
| 1   | AA    | 995  | C    | C4-C5   | -5.99 | 1.38        | 1.43     |
| 1   | AA    | 1001 | C    | N1-C6   | 5.99  | 1.40        | 1.37     |
| 1   | AA    | 1047 | G    | C2'-C1' | -5.99 | 1.46        | 1.53     |
| 35  | BB    | 1230 | A    | C2'-C1' | -5.99 | 1.46        | 1.53     |
| 35  | BB    | 1364 | G    | C2-N2   | 5.99  | 1.40        | 1.34     |
| 35  | BB    | 1548 | A    | C5-C4   | -5.99 | 1.34        | 1.38     |
| 35  | BB    | 1776 | G    | C5-C4   | 5.99  | 1.42        | 1.38     |
| 1   | AA    | 719  | C    | C2'-C1' | -5.99 | 1.46        | 1.53     |
| 1   | AA    | 1169 | A    | N9-C4   | -5.99 | 1.34        | 1.37     |
| 2   | AB    | 107  | ARG  | CD-NE   | 5.99  | 1.56        | 1.46     |
| 34  | BA    | 99   | A    | N7-C5   | -5.99 | 1.35        | 1.39     |
| 35  | BB    | 279  | A    | C4'-C3' | 5.99  | 1.59        | 1.53     |
| 35  | BB    | 439  | A    | C6-N6   | 5.99  | 1.38        | 1.33     |
| 35  | BB    | 943  | A    | C6-N6   | 5.99  | 1.38        | 1.33     |
| 35  | BB    | 1505 | A    | N3-C4   | -5.99 | 1.31        | 1.34     |
| 35  | BB    | 2159 | G    | N9-C4   | 5.99  | 1.42        | 1.38     |
| 35  | BB    | 2848 | G    | N3-C4   | 5.99  | 1.39        | 1.35     |
| 35  | BB    | 135  | U    | C2'-C1' | 5.99  | 1.59        | 1.53     |
| 35  | BB    | 138  | U    | N1-C6   | -5.99 | 1.32        | 1.38     |
| 35  | BB    | 195  | A    | C5-C4   | -5.99 | 1.34        | 1.38     |
| 35  | BB    | 884  | U    | P-O5'   | -5.99 | 1.53        | 1.59     |
| 35  | BB    | 1845 | G    | C5-C6   | -5.99 | 1.36        | 1.42     |
| 35  | BB    | 2308 | G    | N9-C8   | 5.99  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2360 | G    | C2-N3   | 5.99  | 1.37        | 1.32     |
| 35  | BB    | 2530 | A    | C6-N1   | 5.99  | 1.39        | 1.35     |
| 35  | BB    | 2678 | C    | C5'-C4' | 5.99  | 1.58        | 1.51     |
| 46  | BM    | 44   | ARG  | NE-CZ   | 5.99  | 1.40        | 1.33     |
| 1   | AA    | 743  | A    | N9-C8   | 5.99  | 1.42        | 1.37     |
| 1   | AA    | 799  | G    | C6-O6   | -5.99 | 1.18        | 1.24     |
| 1   | AA    | 872  | A    | C2-N3   | 5.99  | 1.39        | 1.33     |
| 1   | AA    | 1517 | G    | N3-C4   | -5.99 | 1.31        | 1.35     |
| 35  | BB    | 449  | A    | N3-C4   | -5.99 | 1.31        | 1.34     |
| 35  | BB    | 861  | A    | C4'-C3' | -5.99 | 1.46        | 1.52     |
| 35  | BB    | 1150 | C    | N1-C6   | 5.99  | 1.40        | 1.37     |
| 35  | BB    | 1468 | U    | N3-C4   | 5.99  | 1.43        | 1.38     |
| 35  | BB    | 1581 | G    | N1-C2   | 5.99  | 1.42        | 1.37     |
| 35  | BB    | 2270 | A    | C4'-C3' | -5.99 | 1.46        | 1.52     |
| 35  | BB    | 2411 | A    | N7-C5   | -5.99 | 1.35        | 1.39     |
| 35  | BB    | 2679 | A    | C8-N7   | -5.99 | 1.27        | 1.31     |
| 35  | BB    | 2861 | U    | C5-C6   | -5.99 | 1.28        | 1.34     |
| 1   | AA    | 1211 | U    | C2-N3   | 5.98  | 1.42        | 1.37     |
| 35  | BB    | 1483 | G    | C2-N2   | 5.98  | 1.40        | 1.34     |
| 35  | BB    | 2335 | A    | C3'-C2' | -5.98 | 1.46        | 1.52     |
| 1   | AA    | 216  | U    | C3'-C2' | -5.98 | 1.46        | 1.52     |
| 1   | AA    | 381  | C    | O3'-P   | -5.98 | 1.53        | 1.61     |
| 1   | AA    | 508  | U    | C2'-C1' | -5.98 | 1.46        | 1.53     |
| 5   | AE    | 92   | ARG  | CD-NE   | 5.98  | 1.56        | 1.46     |
| 34  | BA    | 36   | C    | N1-C2   | 5.98  | 1.46        | 1.40     |
| 35  | BB    | 642  | U    | N3-C4   | 5.98  | 1.43        | 1.38     |
| 35  | BB    | 1219 | U    | C4-O4   | 5.98  | 1.28        | 1.23     |
| 35  | BB    | 1734 | G    | C6-N1   | 5.98  | 1.43        | 1.39     |
| 1   | AA    | 81   | A    | N7-C5   | -5.98 | 1.35        | 1.39     |
| 1   | AA    | 200  | G    | C8-N7   | 5.98  | 1.34        | 1.30     |
| 35  | BB    | 54   | G    | C2-N2   | 5.98  | 1.40        | 1.34     |
| 35  | BB    | 1638 | C    | O4'-C1' | 5.98  | 1.49        | 1.41     |
| 1   | AA    | 174  | A    | N9-C4   | -5.98 | 1.34        | 1.37     |
| 1   | AA    | 249  | U    | N3-C4   | 5.98  | 1.43        | 1.38     |
| 35  | BB    | 425  | G    | N1-C2   | 5.98  | 1.42        | 1.37     |
| 35  | BB    | 1436 | G    | N9-C4   | 5.98  | 1.42        | 1.38     |
| 35  | BB    | 1989 | G    | C3'-O3' | 5.98  | 1.50        | 1.42     |
| 1   | AA    | 105  | G    | C5-C4   | -5.98 | 1.34        | 1.38     |
| 1   | AA    | 117  | G    | C5-C4   | -5.98 | 1.34        | 1.38     |
| 1   | AA    | 782  | A    | P-O5'   | -5.98 | 1.53        | 1.59     |
| 12  | AL    | 35   | ARG  | NE-CZ   | 5.98  | 1.40        | 1.33     |
| 35  | BB    | 1334 | G    | N7-C5   | -5.98 | 1.35        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1858 | A    | N1-C2   | 5.98  | 1.39        | 1.34     |
| 35  | BB    | 2437 | G    | C2'-C1' | -5.98 | 1.46        | 1.53     |
| 35  | BB    | 77   | G    | C5'-C4' | 5.98  | 1.58        | 1.51     |
| 35  | BB    | 1625 | C    | C4-N4   | 5.98  | 1.39        | 1.33     |
| 35  | BB    | 2353 | G    | N3-C4   | -5.98 | 1.31        | 1.35     |
| 35  | BB    | 2542 | A    | C6-N1   | 5.98  | 1.39        | 1.35     |
| 1   | AA    | 46   | G    | O3'-P   | -5.97 | 1.53        | 1.61     |
| 1   | AA    | 128  | G    | O3'-P   | -5.97 | 1.53        | 1.61     |
| 1   | AA    | 180  | U    | C3'-O3' | 5.97  | 1.50        | 1.42     |
| 1   | AA    | 882  | C    | P-O5'   | 5.97  | 1.65        | 1.59     |
| 1   | AA    | 1074 | G    | C6-N1   | -5.97 | 1.35        | 1.39     |
| 1   | AA    | 1138 | G    | C6-O6   | -5.97 | 1.18        | 1.24     |
| 1   | AA    | 1357 | A    | C5-C6   | -5.97 | 1.35        | 1.41     |
| 35  | BB    | 1418 | G    | C4'-C3' | 5.97  | 1.59        | 1.53     |
| 35  | BB    | 1482 | G    | N1-C2   | 5.97  | 1.42        | 1.37     |
| 35  | BB    | 1957 | C    | C2-N3   | -5.97 | 1.30        | 1.35     |
| 35  | BB    | 2256 | G    | O4'-C1' | 5.97  | 1.49        | 1.41     |
| 1   | AA    | 152  | A    | N7-C5   | -5.97 | 1.35        | 1.39     |
| 1   | AA    | 734  | G    | N3-C4   | -5.97 | 1.31        | 1.35     |
| 1   | AA    | 769  | G    | C2-N2   | 5.97  | 1.40        | 1.34     |
| 1   | AA    | 931  | C    | N1-C6   | 5.97  | 1.40        | 1.37     |
| 1   | AA    | 973  | G    | N1-C2   | 5.97  | 1.42        | 1.37     |
| 1   | AA    | 1189 | U    | C4'-O4' | -5.97 | 1.37        | 1.45     |
| 35  | BB    | 627  | A    | N9-C4   | -5.97 | 1.34        | 1.37     |
| 35  | BB    | 1277 | G    | C2'-C1' | -5.97 | 1.46        | 1.53     |
| 35  | BB    | 1796 | U    | N1-C6   | -5.97 | 1.32        | 1.38     |
| 35  | BB    | 1972 | G    | C6-N1   | 5.97  | 1.43        | 1.39     |
| 35  | BB    | 2638 | G    | N1-C2   | 5.97  | 1.42        | 1.37     |
| 35  | BB    | 411  | G    | N9-C8   | -5.97 | 1.33        | 1.37     |
| 35  | BB    | 1346 | G    | P-O5'   | -5.97 | 1.53        | 1.59     |
| 35  | BB    | 2827 | C    | C4-C5   | 5.97  | 1.47        | 1.43     |
| 1   | AA    | 99   | C    | N3-C4   | 5.97  | 1.38        | 1.33     |
| 1   | AA    | 381  | C    | C4'-C3' | 5.97  | 1.59        | 1.53     |
| 1   | AA    | 469  | C    | P-O5'   | -5.97 | 1.53        | 1.59     |
| 1   | AA    | 547  | A    | N3-C4   | -5.97 | 1.31        | 1.34     |
| 1   | AA    | 1176 | A    | C3'-O3' | 5.97  | 1.50        | 1.42     |
| 1   | AA    | 1333 | A    | C5'-C4' | 5.97  | 1.58        | 1.51     |
| 1   | AA    | 1359 | C    | P-O5'   | -5.97 | 1.53        | 1.59     |
| 35  | BB    | 485  | C    | N3-C4   | 5.97  | 1.38        | 1.33     |
| 35  | BB    | 1410 | G    | P-O5'   | -5.97 | 1.53        | 1.59     |
| 35  | BB    | 1632 | A    | N1-C2   | -5.97 | 1.28        | 1.34     |
| 35  | BB    | 1737 | G    | N9-C8   | 5.97  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2392 | A    | N7-C5   | -5.97 | 1.35        | 1.39     |
| 1   | AA    | 967  | C    | C2'-C1' | 5.97  | 1.59        | 1.53     |
| 35  | BB    | 261  | G    | C4'-C3' | -5.97 | 1.46        | 1.52     |
| 35  | BB    | 930  | G    | N9-C4   | -5.97 | 1.33        | 1.38     |
| 35  | BB    | 958  | U    | C4-C5   | 5.97  | 1.49        | 1.43     |
| 35  | BB    | 1112 | G    | O3'-P   | -5.97 | 1.53        | 1.61     |
| 1   | AA    | 639  | G    | N3-C4   | -5.97 | 1.31        | 1.35     |
| 1   | AA    | 652  | U    | C2'-C1' | -5.97 | 1.46        | 1.53     |
| 1   | AA    | 856  | C    | C2'-C1' | -5.97 | 1.46        | 1.53     |
| 35  | BB    | 929  | U    | C2'-C1' | -5.97 | 1.46        | 1.53     |
| 35  | BB    | 960  | A    | N7-C5   | -5.97 | 1.35        | 1.39     |
| 35  | BB    | 1119 | U    | C3'-O3' | 5.97  | 1.50        | 1.42     |
| 35  | BB    | 2286 | G    | N7-C5   | 5.97  | 1.42        | 1.39     |
| 35  | BB    | 2773 | C    | N1-C6   | -5.97 | 1.33        | 1.37     |
| 44  | BK    | 64   | ARG  | NE-CZ   | 5.97  | 1.40        | 1.33     |
| 1   | AA    | 127  | G    | C3'-O3' | 5.96  | 1.50        | 1.42     |
| 1   | AA    | 326  | G    | C4'-C3' | -5.96 | 1.46        | 1.52     |
| 1   | AA    | 417  | G    | C2-N2   | 5.96  | 1.40        | 1.34     |
| 1   | AA    | 1417 | G    | N1-C2   | 5.96  | 1.42        | 1.37     |
| 35  | BB    | 2153 | C    | P-O5'   | -5.96 | 1.53        | 1.59     |
| 35  | BB    | 2692 | G    | C2-N2   | 5.96  | 1.40        | 1.34     |
| 1   | AA    | 1052 | U    | N3-C4   | 5.96  | 1.43        | 1.38     |
| 35  | BB    | 1385 | A    | N1-C2   | -5.96 | 1.28        | 1.34     |
| 35  | BB    | 1418 | G    | C2-N3   | 5.96  | 1.37        | 1.32     |
| 35  | BB    | 2025 | C    | C2'-C1' | -5.96 | 1.46        | 1.53     |
| 35  | BB    | 2483 | C    | C3'-O3' | -5.96 | 1.33        | 1.42     |
| 35  | BB    | 2898 | U    | C2-N3   | 5.96  | 1.42        | 1.37     |
| 1   | AA    | 110  | C    | N3-C4   | 5.96  | 1.38        | 1.33     |
| 1   | AA    | 485  | U    | C2-N3   | 5.96  | 1.42        | 1.37     |
| 1   | AA    | 654  | G    | C5'-C4' | 5.96  | 1.58        | 1.51     |
| 1   | AA    | 1012 | A    | C3'-O3' | 5.96  | 1.50        | 1.42     |
| 1   | AA    | 1468 | A    | O3'-P   | -5.96 | 1.53        | 1.61     |
| 35  | BB    | 288  | U    | C3'-C2' | 5.96  | 1.59        | 1.52     |
| 35  | BB    | 1471 | G    | C1'-N9  | -5.96 | 1.38        | 1.46     |
| 35  | BB    | 1692 | U    | C5'-C4' | 5.96  | 1.58        | 1.51     |
| 35  | BB    | 1767 | G    | C4'-O4' | 5.96  | 1.53        | 1.45     |
| 35  | BB    | 2146 | C    | C1'-N1  | 5.96  | 1.57        | 1.48     |
| 35  | BB    | 2416 | C    | O4'-C1' | -5.96 | 1.33        | 1.41     |
| 1   | AA    | 889  | A    | C5'-C4' | 5.96  | 1.58        | 1.51     |
| 1   | AA    | 1349 | A    | C3'-C2' | -5.96 | 1.46        | 1.52     |
| 35  | BB    | 1550 | C    | N1-C6   | 5.96  | 1.40        | 1.37     |
| 35  | BB    | 1846 | G    | C5-C4   | -5.96 | 1.34        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 309  | A    | C5-C4   | 5.96  | 1.43        | 1.38     |
| 1   | AA    | 466  | A    | C6-N6   | 5.96  | 1.38        | 1.33     |
| 1   | AA    | 703  | G    | C8-N7   | 5.96  | 1.34        | 1.30     |
| 1   | AA    | 718  | A    | P-O5'   | -5.96 | 1.53        | 1.59     |
| 1   | AA    | 1282 | C    | C4-C5   | 5.96  | 1.47        | 1.43     |
| 34  | BA    | 17   | C    | C3'-C2' | 5.96  | 1.59        | 1.52     |
| 35  | BB    | 298  | G    | C3'-O3' | 5.96  | 1.50        | 1.42     |
| 35  | BB    | 842  | U    | O3'-P   | -5.96 | 1.53        | 1.61     |
| 35  | BB    | 1543 | G    | C2-N2   | 5.96  | 1.40        | 1.34     |
| 35  | BB    | 1853 | A    | C6-N6   | 5.96  | 1.38        | 1.33     |
| 35  | BB    | 2058 | A    | C3'-C2' | 5.96  | 1.59        | 1.52     |
| 35  | BB    | 2261 | C    | C4-N4   | 5.96  | 1.39        | 1.33     |
| 35  | BB    | 2677 | G    | C2-N3   | 5.96  | 1.37        | 1.32     |
| 1   | AA    | 821  | G    | C5-C4   | 5.96  | 1.42        | 1.38     |
| 1   | AA    | 1513 | A    | C8-N7   | 5.96  | 1.35        | 1.31     |
| 35  | BB    | 53   | A    | C5-C6   | -5.96 | 1.35        | 1.41     |
| 35  | BB    | 544  | C    | C4-C5   | 5.96  | 1.47        | 1.43     |
| 35  | BB    | 913  | U    | C4'-O4' | 5.96  | 1.53        | 1.45     |
| 35  | BB    | 1639 | C    | N1-C6   | 5.96  | 1.40        | 1.37     |
| 35  | BB    | 2214 | C    | C4-C5   | 5.96  | 1.47        | 1.43     |
| 35  | BB    | 2553 | G    | N9-C8   | -5.96 | 1.33        | 1.37     |
| 1   | AA    | 528  | C    | C2'-C1' | -5.96 | 1.46        | 1.53     |
| 22  | AV    | 5    | A    | N1-C2   | -5.96 | 1.28        | 1.34     |
| 35  | BB    | 967  | U    | P-O5'   | -5.96 | 1.53        | 1.59     |
| 35  | BB    | 2770 | G    | C6-O6   | 5.96  | 1.29        | 1.24     |
| 1   | AA    | 420  | U    | P-O5'   | 5.95  | 1.65        | 1.59     |
| 7   | AG    | 84   | TYR  | CE1-CZ  | 5.95  | 1.46        | 1.38     |
| 34  | BA    | 86   | G    | C6-N1   | 5.95  | 1.43        | 1.39     |
| 35  | BB    | 333  | G    | C4'-C3' | 5.95  | 1.59        | 1.53     |
| 35  | BB    | 473  | G    | N7-C5   | -5.95 | 1.35        | 1.39     |
| 35  | BB    | 531  | C    | N1-C2   | 5.95  | 1.46        | 1.40     |
| 35  | BB    | 1282 | U    | P-O5'   | -5.95 | 1.53        | 1.59     |
| 35  | BB    | 1617 | C    | C1'-N1  | 5.95  | 1.57        | 1.48     |
| 1   | AA    | 778  | G    | C6-N1   | 5.95  | 1.43        | 1.39     |
| 1   | AA    | 1022 | A    | P-O5'   | -5.95 | 1.53        | 1.59     |
| 1   | AA    | 1186 | G    | C2'-C1' | 5.95  | 1.59        | 1.53     |
| 35  | BB    | 1007 | C    | C2'-C1' | -5.95 | 1.46        | 1.53     |
| 35  | BB    | 1255 | U    | C4'-C3' | 5.95  | 1.59        | 1.53     |
| 35  | BB    | 2160 | C    | N1-C2   | -5.95 | 1.34        | 1.40     |
| 1   | AA    | 364  | A    | N7-C5   | -5.95 | 1.35        | 1.39     |
| 1   | AA    | 786  | G    | N9-C4   | 5.95  | 1.42        | 1.38     |
| 1   | AA    | 969  | A    | C2'-C1' | -5.95 | 1.46        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 971  | G    | C6-O6   | -5.95 | 1.18        | 1.24     |
| 35  | BB    | 1533 | C    | N1-C6   | 5.95  | 1.40        | 1.37     |
| 35  | BB    | 1941 | C    | C3'-C2' | -5.95 | 1.46        | 1.52     |
| 35  | BB    | 2428 | G    | N1-C2   | 5.95  | 1.42        | 1.37     |
| 35  | BB    | 2844 | G    | P-O5'   | -5.95 | 1.53        | 1.59     |
| 1   | AA    | 831  | A    | C5-C4   | 5.95  | 1.43        | 1.38     |
| 1   | AA    | 908  | A    | C6-N1   | 5.95  | 1.39        | 1.35     |
| 21  | AU    | 46   | ARG  | NE-CZ   | 5.95  | 1.40        | 1.33     |
| 35  | BB    | 327  | G    | C2'-C1' | -5.95 | 1.46        | 1.53     |
| 35  | BB    | 574  | A    | N9-C8   | -5.95 | 1.32        | 1.37     |
| 35  | BB    | 2134 | A    | N7-C5   | 5.95  | 1.42        | 1.39     |
| 1   | AA    | 8    | A    | C2'-C1' | -5.95 | 1.46        | 1.53     |
| 35  | BB    | 1448 | G    | C5'-C4' | 5.95  | 1.58        | 1.51     |
| 35  | BB    | 1689 | A    | C5-C4   | 5.95  | 1.43        | 1.38     |
| 35  | BB    | 1799 | G    | N3-C4   | -5.95 | 1.31        | 1.35     |
| 35  | BB    | 2054 | A    | C5-C6   | -5.95 | 1.35        | 1.41     |
| 35  | BB    | 784  | G    | N9-C8   | -5.94 | 1.33        | 1.37     |
| 45  | BL    | 11   | GLY  | CA-C    | -5.94 | 1.42        | 1.51     |
| 47  | BN    | 64   | ARG  | CZ-NH2  | 5.94  | 1.40        | 1.33     |
| 1   | AA    | 38   | G    | C5'-C4' | 5.94  | 1.58        | 1.51     |
| 1   | AA    | 435  | A    | O3'-P   | 5.94  | 1.68        | 1.61     |
| 1   | AA    | 825  | A    | N7-C5   | -5.94 | 1.35        | 1.39     |
| 1   | AA    | 1013 | G    | C5-C6   | -5.94 | 1.36        | 1.42     |
| 1   | AA    | 1433 | A    | N1-C2   | 5.94  | 1.39        | 1.34     |
| 35  | BB    | 679  | C    | O3'-P   | 5.94  | 1.68        | 1.61     |
| 35  | BB    | 968  | C    | C4'-C3' | 5.94  | 1.59        | 1.53     |
| 35  | BB    | 1215 | G    | C2-N3   | 5.94  | 1.37        | 1.32     |
| 35  | BB    | 1419 | A    | N9-C4   | -5.94 | 1.34        | 1.37     |
| 35  | BB    | 1723 | G    | C5'-C4' | 5.94  | 1.58        | 1.51     |
| 35  | BB    | 2016 | U    | C5'-C4' | -5.94 | 1.44        | 1.51     |
| 35  | BB    | 2451 | A    | C8-N7   | -5.94 | 1.27        | 1.31     |
| 35  | BB    | 2753 | A    | P-O5'   | -5.94 | 1.53        | 1.59     |
| 1   | AA    | 123  | U    | O3'-P   | -5.94 | 1.54        | 1.61     |
| 1   | AA    | 424  | G    | C5-C6   | 5.94  | 1.48        | 1.42     |
| 1   | AA    | 575  | G    | C5-C4   | -5.94 | 1.34        | 1.38     |
| 1   | AA    | 871  | U    | C3'-C2' | -5.94 | 1.46        | 1.52     |
| 1   | AA    | 977  | A    | P-O5'   | -5.94 | 1.53        | 1.59     |
| 9   | AI    | 40   | ARG  | CD-NE   | 5.94  | 1.56        | 1.46     |
| 34  | BA    | 4    | C    | C4-C5   | 5.94  | 1.47        | 1.43     |
| 35  | BB    | 535  | G    | C2'-C1' | -5.94 | 1.46        | 1.53     |
| 35  | BB    | 1781 | U    | C4-C5   | 5.94  | 1.48        | 1.43     |
| 35  | BB    | 1979 | U    | C2-N3   | 5.94  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2151 | U    | C2-N3   | 5.94  | 1.42        | 1.37     |
| 35  | BB    | 370  | G    | O3'-P   | -5.94 | 1.54        | 1.61     |
| 35  | BB    | 776  | G    | N9-C8   | -5.94 | 1.33        | 1.37     |
| 35  | BB    | 1080 | A    | C4'-O4' | 5.94  | 1.53        | 1.45     |
| 35  | BB    | 1201 | U    | C4-O4   | -5.94 | 1.18        | 1.23     |
| 1   | AA    | 281  | G    | C5'-C4' | 5.94  | 1.58        | 1.51     |
| 1   | AA    | 477  | C    | C4-N4   | 5.94  | 1.39        | 1.33     |
| 1   | AA    | 681  | A    | C5-C6   | 5.94  | 1.46        | 1.41     |
| 1   | AA    | 815  | A    | C5'-C4' | 5.94  | 1.58        | 1.51     |
| 1   | AA    | 1126 | U    | C4-O4   | 5.94  | 1.28        | 1.23     |
| 1   | AA    | 1200 | C    | C3'-O3' | 5.94  | 1.50        | 1.42     |
| 1   | AA    | 1267 | C    | C5'-C4' | 5.94  | 1.58        | 1.51     |
| 35  | BB    | 285  | G    | C1'-N9  | -5.94 | 1.38        | 1.46     |
| 35  | BB    | 569  | U    | C3'-O3' | 5.94  | 1.50        | 1.42     |
| 35  | BB    | 601  | C    | C4-N4   | 5.94  | 1.39        | 1.33     |
| 35  | BB    | 603  | A    | C1'-N9  | 5.94  | 1.57        | 1.48     |
| 35  | BB    | 612  | G    | O3'-P   | -5.94 | 1.54        | 1.61     |
| 35  | BB    | 1635 | A    | O3'-P   | -5.94 | 1.54        | 1.61     |
| 35  | BB    | 1776 | G    | C2'-C1' | -5.94 | 1.46        | 1.53     |
| 35  | BB    | 2562 | U    | C4'-O4' | -5.94 | 1.37        | 1.45     |
| 1   | AA    | 755  | G    | C3'-C2' | -5.94 | 1.46        | 1.52     |
| 1   | AA    | 985  | C    | C2-N3   | 5.94  | 1.40        | 1.35     |
| 1   | AA    | 1270 | G    | N9-C8   | 5.94  | 1.42        | 1.37     |
| 35  | BB    | 572  | A    | C6-N1   | 5.94  | 1.39        | 1.35     |
| 35  | BB    | 1055 | G    | N1-C2   | 5.94  | 1.42        | 1.37     |
| 1   | AA    | 247  | G    | N1-C2   | 5.93  | 1.42        | 1.37     |
| 1   | AA    | 343  | U    | C4-C5   | 5.93  | 1.48        | 1.43     |
| 1   | AA    | 1404 | C    | C2'-O2' | -5.93 | 1.33        | 1.41     |
| 1   | AA    | 1525 | G    | N1-C2   | 5.93  | 1.42        | 1.37     |
| 35  | BB    | 945  | A    | C2-N3   | 5.93  | 1.38        | 1.33     |
| 35  | BB    | 1371 | G    | C8-N7   | 5.93  | 1.34        | 1.30     |
| 35  | BB    | 1503 | A    | O3'-P   | -5.93 | 1.54        | 1.61     |
| 35  | BB    | 2276 | G    | O3'-P   | -5.93 | 1.54        | 1.61     |
| 35  | BB    | 2693 | G    | N9-C4   | -5.93 | 1.33        | 1.38     |
| 35  | BB    | 2801 | G    | C3'-C2' | 5.93  | 1.59        | 1.52     |
| 1   | AA    | 159  | G    | O5'-C5' | 5.93  | 1.53        | 1.44     |
| 1   | AA    | 717  | U    | C3'-O3' | 5.93  | 1.50        | 1.42     |
| 1   | AA    | 1443 | C    | C3'-C2' | 5.93  | 1.59        | 1.52     |
| 23  | AX    | 19   | A    | C5'-C4' | 5.93  | 1.58        | 1.51     |
| 35  | BB    | 440  | C    | C4-C5   | -5.93 | 1.38        | 1.43     |
| 35  | BB    | 831  | G    | N1-C2   | 5.93  | 1.42        | 1.37     |
| 35  | BB    | 851  | C    | N3-C4   | 5.93  | 1.38        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 976  | G    | N9-C8   | 5.93  | 1.42        | 1.37     |
| 35  | BB    | 983  | A    | N9-C4   | -5.93 | 1.34        | 1.37     |
| 35  | BB    | 1813 | G    | C5-C4   | -5.93 | 1.34        | 1.38     |
| 51  | BR    | 92   | TRP  | CE3-CZ3 | 5.93  | 1.48        | 1.38     |
| 1   | AA    | 153  | C    | N3-C4   | 5.93  | 1.38        | 1.33     |
| 1   | AA    | 840  | C    | C4-N4   | 5.93  | 1.39        | 1.33     |
| 1   | AA    | 1398 | A    | C6-N6   | 5.93  | 1.38        | 1.33     |
| 5   | AE    | 53   | ARG  | CZ-NH1  | 5.93  | 1.40        | 1.33     |
| 9   | AI    | 11   | ARG  | CZ-NH1  | 5.93  | 1.40        | 1.33     |
| 35  | BB    | 359  | G    | C3'-C2' | -5.93 | 1.46        | 1.52     |
| 40  | BG    | 93   | TYR  | CG-CD2  | 5.93  | 1.46        | 1.39     |
| 1   | AA    | 569  | C    | C4'-C3' | -5.93 | 1.46        | 1.52     |
| 1   | AA    | 794  | A    | C3'-C2' | -5.93 | 1.46        | 1.52     |
| 1   | AA    | 932  | C    | N1-C6   | 5.93  | 1.40        | 1.37     |
| 34  | BA    | 25   | U    | N1-C6   | 5.93  | 1.43        | 1.38     |
| 35  | BB    | 1392 | A    | N7-C5   | -5.93 | 1.35        | 1.39     |
| 35  | BB    | 1758 | U    | N3-C4   | 5.93  | 1.43        | 1.38     |
| 35  | BB    | 2854 | G    | N7-C5   | -5.93 | 1.35        | 1.39     |
| 1   | AA    | 567  | G    | P-O5'   | -5.93 | 1.53        | 1.59     |
| 1   | AA    | 621  | A    | C5-C6   | 5.93  | 1.46        | 1.41     |
| 35  | BB    | 713  | G    | C2-N2   | -5.93 | 1.28        | 1.34     |
| 35  | BB    | 1179 | G    | C8-N7   | -5.93 | 1.27        | 1.30     |
| 35  | BB    | 1424 | G    | C6-N1   | -5.93 | 1.35        | 1.39     |
| 35  | BB    | 1487 | U    | C2-N3   | 5.93  | 1.41        | 1.37     |
| 35  | BB    | 1797 | G    | O3'-P   | -5.93 | 1.54        | 1.61     |
| 35  | BB    | 1820 | U    | C5-C6   | 5.93  | 1.39        | 1.34     |
| 35  | BB    | 1893 | C    | N3-C4   | 5.93  | 1.38        | 1.33     |
| 39  | BF    | 113  | PHE  | CE2-CZ  | 5.93  | 1.48        | 1.37     |
| 1   | AA    | 410  | G    | P-O5'   | -5.93 | 1.53        | 1.59     |
| 1   | AA    | 446  | G    | C8-N7   | -5.93 | 1.27        | 1.30     |
| 1   | AA    | 977  | A    | N3-C4   | 5.93  | 1.38        | 1.34     |
| 1   | AA    | 1482 | G    | C8-N7   | -5.93 | 1.27        | 1.30     |
| 35  | BB    | 214  | G    | P-O5'   | -5.93 | 1.53        | 1.59     |
| 35  | BB    | 2524 | G    | N3-C4   | 5.93  | 1.39        | 1.35     |
| 1   | AA    | 225  | C    | C2-N3   | 5.92  | 1.40        | 1.35     |
| 1   | AA    | 665  | A    | C4'-C3' | -5.92 | 1.46        | 1.52     |
| 1   | AA    | 682  | G    | O4'-C1' | -5.92 | 1.33        | 1.41     |
| 1   | AA    | 1096 | C    | N1-C2   | -5.92 | 1.34        | 1.40     |
| 1   | AA    | 1232 | U    | C2'-C1' | -5.92 | 1.46        | 1.53     |
| 1   | AA    | 1360 | A    | C8-N7   | -5.92 | 1.27        | 1.31     |
| 35  | BB    | 797  | G    | C5-C4   | 5.92  | 1.42        | 1.38     |
| 35  | BB    | 998  | C    | C2-N3   | 5.92  | 1.40        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1015 | U    | C4'-O4' | 5.92  | 1.53        | 1.45     |
| 35  | BB    | 1162 | G    | C8-N7   | -5.92 | 1.27        | 1.30     |
| 35  | BB    | 1428 | C    | C4-C5   | 5.92  | 1.47        | 1.43     |
| 35  | BB    | 2864 | G    | C6-N1   | 5.92  | 1.43        | 1.39     |
| 1   | AA    | 241  | G    | C2-N3   | 5.92  | 1.37        | 1.32     |
| 1   | AA    | 246  | A    | C8-N7   | 5.92  | 1.35        | 1.31     |
| 1   | AA    | 306  | A    | O3'-P   | -5.92 | 1.54        | 1.61     |
| 35  | BB    | 51   | G    | C1'-N9  | -5.92 | 1.38        | 1.46     |
| 35  | BB    | 1057 | A    | C3'-O3' | 5.92  | 1.50        | 1.42     |
| 35  | BB    | 1193 | G    | C8-N7   | 5.92  | 1.34        | 1.30     |
| 35  | BB    | 1345 | C    | C4-C5   | 5.92  | 1.47        | 1.43     |
| 35  | BB    | 1354 | A    | C8-N7   | -5.92 | 1.27        | 1.31     |
| 1   | AA    | 124  | C    | N3-C4   | 5.92  | 1.38        | 1.33     |
| 1   | AA    | 572  | A    | C6-N6   | 5.92  | 1.38        | 1.33     |
| 1   | AA    | 1281 | C    | N3-C4   | 5.92  | 1.38        | 1.33     |
| 35  | BB    | 2042 | A    | C6-N1   | 5.92  | 1.39        | 1.35     |
| 1   | AA    | 1026 | G    | N9-C8   | 5.92  | 1.42        | 1.37     |
| 1   | AA    | 1050 | G    | C3'-O3' | 5.92  | 1.50        | 1.42     |
| 2   | AB    | 207  | ARG  | CD-NE   | 5.92  | 1.56        | 1.46     |
| 35  | BB    | 30   | G    | N3-C4   | -5.92 | 1.31        | 1.35     |
| 35  | BB    | 1259 | G    | N1-C2   | 5.92  | 1.42        | 1.37     |
| 35  | BB    | 2252 | G    | C2-N2   | 5.92  | 1.40        | 1.34     |
| 51  | BR    | 21   | ARG  | NE-CZ   | 5.92  | 1.40        | 1.33     |
| 1   | AA    | 1004 | A    | C4'-C3' | 5.92  | 1.59        | 1.53     |
| 1   | AA    | 1392 | G    | O3'-P   | -5.92 | 1.54        | 1.61     |
| 34  | BA    | 84   | G    | C6-N1   | -5.92 | 1.35        | 1.39     |
| 35  | BB    | 117  | G    | C2-N3   | 5.92  | 1.37        | 1.32     |
| 35  | BB    | 236  | C    | N3-C4   | 5.92  | 1.38        | 1.33     |
| 35  | BB    | 376  | G    | C6-N1   | 5.92  | 1.43        | 1.39     |
| 35  | BB    | 2323 | G    | C3'-C2' | -5.92 | 1.46        | 1.52     |
| 35  | BB    | 2388 | A    | C5-C4   | 5.92  | 1.42        | 1.38     |
| 35  | BB    | 2628 | C    | N3-C4   | 5.92  | 1.38        | 1.33     |
| 35  | BB    | 2733 | A    | N3-C4   | 5.92  | 1.38        | 1.34     |
| 35  | BB    | 2855 | C    | N3-C4   | 5.92  | 1.38        | 1.33     |
| 1   | AA    | 524  | G    | C4'-C3' | 5.92  | 1.59        | 1.53     |
| 1   | AA    | 651  | C    | N3-C4   | 5.92  | 1.38        | 1.33     |
| 1   | AA    | 1102 | A    | N7-C5   | -5.92 | 1.35        | 1.39     |
| 1   | AA    | 1138 | G    | C6-N1   | 5.92  | 1.43        | 1.39     |
| 35  | BB    | 112  | U    | C4-C5   | 5.92  | 1.48        | 1.43     |
| 35  | BB    | 503  | A    | C5'-C4' | 5.92  | 1.58        | 1.51     |
| 35  | BB    | 615  | U    | C5'-C4' | 5.92  | 1.58        | 1.51     |
| 35  | BB    | 680  | C    | C5'-C4' | 5.92  | 1.58        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1114 | C    | C2-O2   | 5.92  | 1.29        | 1.24     |
| 35  | BB    | 1177 | G    | C2'-C1' | -5.92 | 1.46        | 1.53     |
| 35  | BB    | 1298 | C    | N3-C4   | 5.92  | 1.38        | 1.33     |
| 35  | BB    | 1341 | G    | N7-C5   | -5.92 | 1.35        | 1.39     |
| 35  | BB    | 1444 | G    | C4'-C3' | -5.92 | 1.46        | 1.52     |
| 35  | BB    | 2267 | A    | O4'-C1' | 5.92  | 1.49        | 1.41     |
| 35  | BB    | 2902 | C    | C5-C6   | -5.92 | 1.29        | 1.34     |
| 35  | BB    | 1    | G    | C2'-C1' | -5.92 | 1.46        | 1.53     |
| 35  | BB    | 1438 | U    | C2-N3   | 5.92  | 1.41        | 1.37     |
| 35  | BB    | 1496 | A    | C6-N6   | 5.92  | 1.38        | 1.33     |
| 35  | BB    | 1558 | C    | O3'-P   | -5.92 | 1.54        | 1.61     |
| 35  | BB    | 2476 | A    | N9-C4   | -5.92 | 1.34        | 1.37     |
| 1   | AA    | 191  | G    | C2-N3   | 5.91  | 1.37        | 1.32     |
| 1   | AA    | 607  | A    | N9-C4   | -5.91 | 1.34        | 1.37     |
| 1   | AA    | 1109 | C    | C4'-O4' | -5.91 | 1.37        | 1.45     |
| 34  | BA    | 60   | C    | P-O5'   | -5.91 | 1.53        | 1.59     |
| 35  | BB    | 418  | C    | N3-C4   | 5.91  | 1.38        | 1.33     |
| 35  | BB    | 638  | G    | N9-C4   | -5.91 | 1.33        | 1.38     |
| 35  | BB    | 1129 | A    | C4'-C3' | 5.91  | 1.59        | 1.53     |
| 35  | BB    | 1664 | A    | N9-C4   | 5.91  | 1.41        | 1.37     |
| 35  | BB    | 1850 | G    | O3'-P   | 5.91  | 1.68        | 1.61     |
| 35  | BB    | 2065 | C    | C4'-C3' | 5.91  | 1.59        | 1.53     |
| 35  | BB    | 2443 | C    | C2-O2   | -5.91 | 1.19        | 1.24     |
| 35  | BB    | 424  | G    | N1-C2   | 5.91  | 1.42        | 1.37     |
| 35  | BB    | 452  | G    | C6-N1   | 5.91  | 1.43        | 1.39     |
| 35  | BB    | 2777 | G    | C3'-O3' | 5.91  | 1.50        | 1.42     |
| 1   | AA    | 533  | A    | C8-N7   | -5.91 | 1.27        | 1.31     |
| 1   | AA    | 1039 | G    | N3-C4   | 5.91  | 1.39        | 1.35     |
| 35  | BB    | 522  | A    | C6-N6   | 5.91  | 1.38        | 1.33     |
| 35  | BB    | 757  | G    | N7-C5   | -5.91 | 1.35        | 1.39     |
| 35  | BB    | 2408 | U    | N1-C6   | 5.91  | 1.43        | 1.38     |
| 1   | AA    | 102  | G    | C5-C4   | -5.91 | 1.34        | 1.38     |
| 1   | AA    | 520  | A    | P-O5'   | -5.91 | 1.53        | 1.59     |
| 1   | AA    | 892  | A    | C3'-C2' | -5.91 | 1.46        | 1.52     |
| 1   | AA    | 1463 | U    | C2'-C1' | -5.91 | 1.46        | 1.53     |
| 34  | BA    | 102  | G    | N7-C5   | 5.91  | 1.42        | 1.39     |
| 35  | BB    | 187  | G    | N7-C5   | 5.91  | 1.42        | 1.39     |
| 35  | BB    | 1137 | G    | C2-N2   | -5.91 | 1.28        | 1.34     |
| 35  | BB    | 1289 | C    | N3-C4   | 5.91  | 1.38        | 1.33     |
| 35  | BB    | 1766 | G    | N3-C4   | -5.91 | 1.31        | 1.35     |
| 35  | BB    | 2196 | C    | C2-N3   | 5.91  | 1.40        | 1.35     |
| 1   | AA    | 21   | G    | N7-C5   | -5.91 | 1.35        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 174  | A    | C6-N6   | 5.91  | 1.38        | 1.33     |
| 1   | AA    | 232  | G    | C2-N3   | 5.91  | 1.37        | 1.32     |
| 1   | AA    | 264  | C    | O4'-C1' | 5.91  | 1.49        | 1.41     |
| 1   | AA    | 474  | G    | O3'-P   | -5.91 | 1.54        | 1.61     |
| 35  | BB    | 1941 | C    | O3'-P   | -5.91 | 1.54        | 1.61     |
| 1   | AA    | 765  | G    | C5-C4   | 5.91  | 1.42        | 1.38     |
| 1   | AA    | 1329 | A    | C6-N1   | 5.91  | 1.39        | 1.35     |
| 3   | AC    | 168  | ARG  | CZ-NH2  | 5.91  | 1.40        | 1.33     |
| 35  | BB    | 16   | C    | N3-C4   | 5.91  | 1.38        | 1.33     |
| 35  | BB    | 862  | G    | N7-C5   | -5.91 | 1.35        | 1.39     |
| 35  | BB    | 873  | C    | O4'-C1' | -5.91 | 1.33        | 1.41     |
| 35  | BB    | 955  | U    | N3-C4   | 5.91  | 1.43        | 1.38     |
| 35  | BB    | 1164 | C    | C4'-O4' | 5.91  | 1.53        | 1.45     |
| 35  | BB    | 2487 | G    | C2-N3   | 5.91  | 1.37        | 1.32     |
| 35  | BB    | 2612 | C    | N1-C6   | 5.91  | 1.40        | 1.37     |
| 35  | BB    | 2886 | A    | N9-C4   | 5.91  | 1.41        | 1.37     |
| 54  | BU    | 95   | PHE  | CG-CD1  | 5.91  | 1.47        | 1.38     |
| 1   | AA    | 153  | C    | C3'-C2' | -5.90 | 1.46        | 1.52     |
| 1   | AA    | 723  | U    | O3'-P   | -5.90 | 1.54        | 1.61     |
| 1   | AA    | 1106 | G    | N7-C5   | 5.90  | 1.42        | 1.39     |
| 34  | BA    | 78   | A    | C5'-C4' | 5.90  | 1.58        | 1.51     |
| 35  | BB    | 2482 | A    | C6-N6   | 5.90  | 1.38        | 1.33     |
| 35  | BB    | 2783 | U    | P-O5'   | -5.90 | 1.53        | 1.59     |
| 35  | BB    | 806  | C    | C4-C5   | 5.90  | 1.47        | 1.43     |
| 35  | BB    | 1480 | C    | O4'-C1' | 5.90  | 1.49        | 1.41     |
| 35  | BB    | 1932 | A    | N9-C4   | 5.90  | 1.41        | 1.37     |
| 35  | BB    | 2301 | C    | N3-C4   | 5.90  | 1.38        | 1.33     |
| 1   | AA    | 457  | G    | N3-C4   | -5.90 | 1.31        | 1.35     |
| 1   | AA    | 1252 | A    | N7-C5   | -5.90 | 1.35        | 1.39     |
| 6   | AF    | 25   | TYR  | CG-CD2  | 5.90  | 1.46        | 1.39     |
| 35  | BB    | 213  | A    | C2'-C1' | -5.90 | 1.46        | 1.53     |
| 35  | BB    | 216  | A    | C2'-C1' | -5.90 | 1.46        | 1.53     |
| 35  | BB    | 348  | A    | N1-C2   | 5.90  | 1.39        | 1.34     |
| 35  | BB    | 1068 | G    | N7-C5   | 5.90  | 1.42        | 1.39     |
| 35  | BB    | 1512 | C    | C2'-C1' | 5.90  | 1.59        | 1.53     |
| 35  | BB    | 1695 | G    | C2'-C1' | -5.90 | 1.46        | 1.53     |
| 35  | BB    | 2601 | C    | C3'-C2' | -5.90 | 1.46        | 1.52     |
| 35  | BB    | 2694 | G    | N7-C5   | -5.90 | 1.35        | 1.39     |
| 35  | BB    | 2781 | A    | C4'-C3' | 5.90  | 1.59        | 1.53     |
| 35  | BB    | 2882 | A    | C2'-C1' | -5.90 | 1.46        | 1.53     |
| 1   | AA    | 1335 | U    | N3-C4   | 5.90  | 1.43        | 1.38     |
| 35  | BB    | 40   | U    | C5'-C4' | 5.90  | 1.58        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 846  | U    | N3-C4   | 5.90  | 1.43        | 1.38     |
| 35  | BB    | 1103 | A    | O4'-C1' | -5.90 | 1.33        | 1.41     |
| 1   | AA    | 380  | G    | C6-N1   | 5.90  | 1.43        | 1.39     |
| 34  | BA    | 34   | A    | C6-N6   | 5.90  | 1.38        | 1.33     |
| 35  | BB    | 104  | A    | C4'-O4' | 5.90  | 1.53        | 1.45     |
| 35  | BB    | 372  | G    | O3'-P   | -5.90 | 1.54        | 1.61     |
| 35  | BB    | 744  | U    | C3'-C2' | -5.90 | 1.46        | 1.52     |
| 35  | BB    | 1083 | U    | C2'-C1' | -5.90 | 1.46        | 1.53     |
| 35  | BB    | 1282 | U    | C2'-C1' | -5.90 | 1.46        | 1.53     |
| 35  | BB    | 1665 | A    | N9-C4   | 5.90  | 1.41        | 1.37     |
| 35  | BB    | 1677 | A    | C4'-O4' | -5.90 | 1.37        | 1.45     |
| 35  | BB    | 1843 | C    | N1-C6   | 5.90  | 1.40        | 1.37     |
| 35  | BB    | 2011 | U    | O3'-P   | -5.90 | 1.54        | 1.61     |
| 1   | AA    | 1133 | G    | P-O5'   | 5.90  | 1.65        | 1.59     |
| 34  | BA    | 52   | A    | N7-C5   | -5.90 | 1.35        | 1.39     |
| 35  | BB    | 1823 | G    | C3'-O3' | 5.90  | 1.50        | 1.42     |
| 34  | BA    | 56   | G    | O3'-P   | -5.89 | 1.54        | 1.61     |
| 35  | BB    | 636  | G    | C8-N7   | -5.89 | 1.27        | 1.30     |
| 35  | BB    | 1282 | U    | C4-C5   | 5.89  | 1.48        | 1.43     |
| 35  | BB    | 1560 | G    | N1-C2   | 5.89  | 1.42        | 1.37     |
| 35  | BB    | 1700 | A    | C6-N1   | 5.89  | 1.39        | 1.35     |
| 35  | BB    | 1839 | G    | N1-C2   | 5.89  | 1.42        | 1.37     |
| 35  | BB    | 1870 | C    | C4-C5   | 5.89  | 1.47        | 1.43     |
| 35  | BB    | 2499 | C    | N1-C6   | -5.89 | 1.33        | 1.37     |
| 1   | AA    | 1322 | C    | C5'-C4' | 5.89  | 1.58        | 1.51     |
| 35  | BB    | 418  | C    | N1-C6   | 5.89  | 1.40        | 1.37     |
| 35  | BB    | 453  | A    | N9-C8   | -5.89 | 1.33        | 1.37     |
| 35  | BB    | 767  | U    | C2'-O2' | 5.89  | 1.49        | 1.41     |
| 35  | BB    | 872  | U    | C1'-N1  | 5.89  | 1.57        | 1.48     |
| 35  | BB    | 1490 | A    | O3'-P   | -5.89 | 1.54        | 1.61     |
| 55  | BW    | 11   | GLU  | CD-OE1  | 5.89  | 1.32        | 1.25     |
| 35  | BB    | 41   | C    | N3-C4   | 5.89  | 1.38        | 1.33     |
| 35  | BB    | 903  | C    | C4-C5   | 5.89  | 1.47        | 1.43     |
| 35  | BB    | 1423 | G    | C3'-C2' | -5.89 | 1.46        | 1.52     |
| 1   | AA    | 88   | U    | N1-C6   | -5.89 | 1.32        | 1.38     |
| 1   | AA    | 399  | G    | C2-N3   | 5.89  | 1.37        | 1.32     |
| 1   | AA    | 1078 | U    | N3-C4   | 5.89  | 1.43        | 1.38     |
| 35  | BB    | 207  | A    | C5'-C4' | 5.89  | 1.58        | 1.51     |
| 35  | BB    | 1830 | C    | P-O5'   | -5.89 | 1.53        | 1.59     |
| 35  | BB    | 2331 | G    | C2-N3   | 5.89  | 1.37        | 1.32     |
| 1   | AA    | 131  | A    | N9-C4   | 5.89  | 1.41        | 1.37     |
| 1   | AA    | 560  | A    | N9-C4   | 5.89  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 831  | A    | C4'-C3' | 5.89  | 1.59        | 1.53     |
| 1   | AA    | 1129 | C    | O3'-P   | -5.89 | 1.54        | 1.61     |
| 34  | BA    | 50   | A    | C2'-C1' | -5.89 | 1.46        | 1.53     |
| 35  | BB    | 804  | A    | N9-C8   | 5.89  | 1.42        | 1.37     |
| 35  | BB    | 2049 | G    | C8-N7   | 5.89  | 1.34        | 1.30     |
| 1   | AA    | 21   | G    | C8-N7   | -5.89 | 1.27        | 1.30     |
| 1   | AA    | 305  | G    | C5-C4   | 5.89  | 1.42        | 1.38     |
| 1   | AA    | 810  | C    | N3-C4   | 5.89  | 1.38        | 1.33     |
| 1   | AA    | 905  | U    | N1-C6   | 5.89  | 1.43        | 1.38     |
| 1   | AA    | 1350 | A    | N9-C8   | 5.89  | 1.42        | 1.37     |
| 35  | BB    | 651  | G    | O3'-P   | -5.89 | 1.54        | 1.61     |
| 35  | BB    | 881  | G    | C2-N3   | 5.89  | 1.37        | 1.32     |
| 35  | BB    | 938  | G    | C6-O6   | -5.89 | 1.18        | 1.24     |
| 35  | BB    | 2141 | G    | N3-C4   | -5.89 | 1.31        | 1.35     |
| 35  | BB    | 2585 | U    | N3-C4   | 5.89  | 1.43        | 1.38     |
| 1   | AA    | 149  | A    | N1-C2   | 5.88  | 1.39        | 1.34     |
| 1   | AA    | 927  | G    | C5-C6   | -5.88 | 1.36        | 1.42     |
| 35  | BB    | 379  | G    | C2-N3   | 5.88  | 1.37        | 1.32     |
| 35  | BB    | 2374 | C    | C4-N4   | 5.88  | 1.39        | 1.33     |
| 35  | BB    | 2463 | C    | C2'-C1' | -5.88 | 1.46        | 1.53     |
| 1   | AA    | 352  | C    | C5'-C4' | 5.88  | 1.58        | 1.51     |
| 1   | AA    | 845  | A    | N7-C5   | -5.88 | 1.35        | 1.39     |
| 1   | AA    | 1211 | U    | C4'-O4' | -5.88 | 1.38        | 1.45     |
| 35  | BB    | 58   | G    | C4'-O4' | -5.88 | 1.38        | 1.45     |
| 35  | BB    | 1026 | G    | N9-C8   | 5.88  | 1.42        | 1.37     |
| 1   | AA    | 456  | A    | N7-C5   | -5.88 | 1.35        | 1.39     |
| 1   | AA    | 1507 | A    | C6-N1   | 5.88  | 1.39        | 1.35     |
| 5   | AE    | 126  | ALA  | CA-CB   | 5.88  | 1.64        | 1.52     |
| 35  | BB    | 242  | G    | C8-N7   | -5.88 | 1.27        | 1.30     |
| 35  | BB    | 834  | G    | N9-C8   | 5.88  | 1.42        | 1.37     |
| 35  | BB    | 1096 | A    | C6-N1   | 5.88  | 1.39        | 1.35     |
| 35  | BB    | 2320 | U    | N3-C4   | 5.88  | 1.43        | 1.38     |
| 1   | AA    | 1028 | C    | C4-N4   | 5.88  | 1.39        | 1.33     |
| 35  | BB    | 1674 | G    | C8-N7   | -5.88 | 1.27        | 1.30     |
| 35  | BB    | 2295 | C    | C4-N4   | 5.88  | 1.39        | 1.33     |
| 35  | BB    | 2644 | G    | C2-N3   | 5.88  | 1.37        | 1.32     |
| 35  | BB    | 2709 | G    | N9-C8   | 5.88  | 1.42        | 1.37     |
| 1   | AA    | 162  | A    | C2'-C1' | -5.88 | 1.46        | 1.53     |
| 1   | AA    | 1169 | A    | C6-N6   | 5.88  | 1.38        | 1.33     |
| 1   | AA    | 1451 | U    | C4'-C3' | -5.88 | 1.46        | 1.52     |
| 35  | BB    | 126  | A    | O3'-P   | -5.88 | 1.54        | 1.61     |
| 35  | BB    | 201  | C    | N3-C4   | 5.88  | 1.38        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 310  | A    | C6-N1   | 5.88  | 1.39        | 1.35     |
| 35  | BB    | 402  | A    | N1-C2   | 5.88  | 1.39        | 1.34     |
| 35  | BB    | 435  | C    | O3'-P   | -5.88 | 1.54        | 1.61     |
| 35  | BB    | 711  | G    | N1-C2   | 5.88  | 1.42        | 1.37     |
| 35  | BB    | 1193 | G    | N1-C2   | 5.88  | 1.42        | 1.37     |
| 35  | BB    | 1825 | U    | N1-C6   | -5.88 | 1.32        | 1.38     |
| 35  | BB    | 2422 | C    | P-O5'   | -5.88 | 1.53        | 1.59     |
| 39  | BF    | 147  | ARG  | CA-CB   | 5.88  | 1.66        | 1.53     |
| 1   | AA    | 318  | G    | O4'-C1' | 5.88  | 1.49        | 1.41     |
| 1   | AA    | 401  | C    | N3-C4   | 5.88  | 1.38        | 1.33     |
| 1   | AA    | 1181 | G    | C5'-C4' | 5.88  | 1.58        | 1.51     |
| 1   | AA    | 1192 | C    | C2'-C1' | -5.88 | 1.46        | 1.53     |
| 35  | BB    | 287  | G    | N9-C8   | 5.88  | 1.42        | 1.37     |
| 35  | BB    | 1210 | G    | N1-C2   | 5.88  | 1.42        | 1.37     |
| 35  | BB    | 1254 | A    | C8-N7   | -5.88 | 1.27        | 1.31     |
| 35  | BB    | 1269 | A    | N3-C4   | -5.88 | 1.31        | 1.34     |
| 35  | BB    | 2207 | C    | C5'-C4' | 5.88  | 1.58        | 1.51     |
| 35  | BB    | 2233 | U    | C1'-N1  | 5.88  | 1.57        | 1.48     |
| 35  | BB    | 2298 | A    | C5'-C4' | 5.88  | 1.58        | 1.51     |
| 35  | BB    | 2399 | G    | C4'-C3' | 5.88  | 1.59        | 1.53     |
| 35  | BB    | 2768 | U    | C1'-N1  | 5.88  | 1.57        | 1.48     |
| 1   | AA    | 1037 | C    | C3'-O3' | 5.88  | 1.50        | 1.42     |
| 31  | B6    | 14   | ARG  | NE-CZ   | 5.88  | 1.40        | 1.33     |
| 35  | BB    | 287  | G    | O3'-P   | -5.88 | 1.54        | 1.61     |
| 35  | BB    | 1292 | G    | N3-C4   | -5.88 | 1.31        | 1.35     |
| 35  | BB    | 1342 | A    | N3-C4   | -5.88 | 1.31        | 1.34     |
| 35  | BB    | 2063 | C    | N1-C6   | -5.88 | 1.33        | 1.37     |
| 51  | BR    | 88   | GLY  | N-CA    | -5.88 | 1.37        | 1.46     |
| 1   | AA    | 769  | G    | N3-C4   | -5.87 | 1.31        | 1.35     |
| 7   | AG    | 138  | GLU  | CG-CD   | -5.87 | 1.43        | 1.51     |
| 34  | BA    | 41   | G    | C5'-C4' | 5.87  | 1.58        | 1.51     |
| 35  | BB    | 251  | A    | C8-N7   | 5.87  | 1.35        | 1.31     |
| 35  | BB    | 585  | G    | N3-C4   | -5.87 | 1.31        | 1.35     |
| 35  | BB    | 831  | G    | C3'-O3' | 5.87  | 1.50        | 1.42     |
| 35  | BB    | 1085 | A    | N9-C8   | -5.87 | 1.33        | 1.37     |
| 35  | BB    | 1192 | G    | C5-C6   | -5.87 | 1.36        | 1.42     |
| 35  | BB    | 1329 | U    | C3'-O3' | 5.87  | 1.50        | 1.42     |
| 1   | AA    | 321  | A    | N9-C8   | 5.87  | 1.42        | 1.37     |
| 1   | AA    | 539  | A    | N7-C5   | -5.87 | 1.35        | 1.39     |
| 1   | AA    | 1064 | G    | N9-C8   | 5.87  | 1.42        | 1.37     |
| 7   | AG    | 91   | ARG  | CZ-NH1  | 5.87  | 1.40        | 1.33     |
| 12  | AL    | 116  | TYR  | C-N     | 5.87  | 1.43        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 76   | C    | C2-N3   | 5.87  | 1.40        | 1.35     |
| 35  | BB    | 787  | C    | C4-C5   | 5.87  | 1.47        | 1.43     |
| 35  | BB    | 885  | C    | O3'-P   | -5.87 | 1.54        | 1.61     |
| 35  | BB    | 1670 | C    | C4'-C3' | -5.87 | 1.46        | 1.52     |
| 35  | BB    | 1982 | U    | C4'-O4' | -5.87 | 1.38        | 1.45     |
| 35  | BB    | 2130 | U    | N3-C4   | 5.87  | 1.43        | 1.38     |
| 35  | BB    | 2529 | G    | C6-O6   | -5.87 | 1.18        | 1.24     |
| 35  | BB    | 2896 | C    | C5-C6   | -5.87 | 1.29        | 1.34     |
| 38  | BE    | 79   | ARG  | NE-CZ   | 5.87  | 1.40        | 1.33     |
| 39  | BF    | 127  | TYR  | CG-CD1  | 5.87  | 1.46        | 1.39     |
| 53  | BT    | 80   | TRP  | CE3-CZ3 | 5.87  | 1.48        | 1.38     |
| 35  | BB    | 1222 | U    | N1-C2   | 5.87  | 1.43        | 1.38     |
| 35  | BB    | 1256 | G    | C2-N2   | 5.87  | 1.40        | 1.34     |
| 35  | BB    | 1417 | C    | N1-C2   | -5.87 | 1.34        | 1.40     |
| 35  | BB    | 2084 | C    | C4-N4   | 5.87  | 1.39        | 1.33     |
| 35  | BB    | 2551 | C    | P-O5'   | -5.87 | 1.53        | 1.59     |
| 35  | BB    | 2614 | A    | C5-C4   | -5.87 | 1.34        | 1.38     |
| 35  | BB    | 2711 | A    | C6-N1   | 5.87  | 1.39        | 1.35     |
| 35  | BB    | 2773 | C    | N3-C4   | 5.87  | 1.38        | 1.33     |
| 1   | AA    | 257  | G    | C2-N3   | 5.87  | 1.37        | 1.32     |
| 1   | AA    | 1239 | A    | N1-C2   | -5.87 | 1.29        | 1.34     |
| 1   | AA    | 1309 | G    | N7-C5   | -5.87 | 1.35        | 1.39     |
| 4   | AD    | 80   | ARG  | CZ-NH1  | 5.87  | 1.40        | 1.33     |
| 35  | BB    | 112  | U    | C4'-C3' | 5.87  | 1.59        | 1.53     |
| 35  | BB    | 114  | U    | O3'-P   | -5.87 | 1.54        | 1.61     |
| 35  | BB    | 257  | C    | N3-C4   | 5.87  | 1.38        | 1.33     |
| 35  | BB    | 494  | G    | N9-C4   | 5.87  | 1.42        | 1.38     |
| 35  | BB    | 767  | U    | C2'-C1' | -5.87 | 1.46        | 1.53     |
| 35  | BB    | 1096 | A    | N1-C2   | 5.87  | 1.39        | 1.34     |
| 35  | BB    | 1227 | G    | P-O5'   | -5.87 | 1.53        | 1.59     |
| 35  | BB    | 1268 | A    | N9-C8   | -5.87 | 1.33        | 1.37     |
| 35  | BB    | 1503 | A    | C3'-C2' | -5.87 | 1.46        | 1.52     |
| 35  | BB    | 1856 | U    | C2'-C1' | -5.87 | 1.46        | 1.53     |
| 35  | BB    | 1905 | C    | C2'-C1' | -5.87 | 1.46        | 1.53     |
| 35  | BB    | 2276 | G    | C2'-C1' | -5.87 | 1.46        | 1.53     |
| 35  | BB    | 2337 | G    | C2-N3   | 5.87  | 1.37        | 1.32     |
| 35  | BB    | 2383 | G    | C2'-C1' | -5.87 | 1.46        | 1.53     |
| 35  | BB    | 2532 | G    | N9-C4   | -5.87 | 1.33        | 1.38     |
| 1   | AA    | 1188 | A    | N7-C5   | -5.87 | 1.35        | 1.39     |
| 34  | BA    | 79   | G    | C8-N7   | -5.87 | 1.27        | 1.30     |
| 35  | BB    | 389  | G    | C5-C4   | -5.87 | 1.34        | 1.38     |
| 35  | BB    | 492  | A    | C6-N6   | 5.87  | 1.38        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2165 | C    | N3-C4   | 5.87  | 1.38        | 1.33     |
| 1   | AA    | 36   | C    | O3'-P   | -5.87 | 1.54        | 1.61     |
| 1   | AA    | 248  | C    | O3'-P   | -5.87 | 1.54        | 1.61     |
| 1   | AA    | 984  | C    | C2'-C1' | -5.87 | 1.46        | 1.53     |
| 34  | BA    | 105  | G    | C5-C4   | -5.87 | 1.34        | 1.38     |
| 35  | BB    | 1134 | A    | C6-N6   | 5.87  | 1.38        | 1.33     |
| 35  | BB    | 1408 | G    | C5-C6   | -5.87 | 1.36        | 1.42     |
| 35  | BB    | 1673 | G    | N7-C5   | -5.87 | 1.35        | 1.39     |
| 35  | BB    | 1989 | G    | C5-C6   | -5.87 | 1.36        | 1.42     |
| 35  | BB    | 2110 | G    | C5'-C4' | 5.87  | 1.58        | 1.51     |
| 35  | BB    | 2177 | C    | C4-C5   | 5.87  | 1.47        | 1.43     |
| 35  | BB    | 2331 | G    | N7-C5   | -5.87 | 1.35        | 1.39     |
| 1   | AA    | 168  | G    | C6-N1   | 5.86  | 1.43        | 1.39     |
| 1   | AA    | 433  | G    | C4'-O4' | -5.86 | 1.38        | 1.45     |
| 1   | AA    | 651  | C    | C2-O2   | -5.86 | 1.19        | 1.24     |
| 34  | BA    | 16   | G    | P-O5'   | -5.86 | 1.53        | 1.59     |
| 35  | BB    | 865  | C    | C2'-C1' | -5.86 | 1.47        | 1.53     |
| 35  | BB    | 2164 | C    | C4-N4   | 5.86  | 1.39        | 1.33     |
| 35  | BB    | 2266 | A    | N3-C4   | -5.86 | 1.31        | 1.34     |
| 35  | BB    | 2666 | C    | C2'-C1' | -5.86 | 1.46        | 1.53     |
| 1   | AA    | 315  | A    | C8-N7   | 5.86  | 1.35        | 1.31     |
| 1   | AA    | 650  | G    | C2'-C1' | -5.86 | 1.47        | 1.53     |
| 1   | AA    | 1039 | G    | C2-N2   | -5.86 | 1.28        | 1.34     |
| 35  | BB    | 421  | C    | C2'-C1' | -5.86 | 1.47        | 1.53     |
| 35  | BB    | 510  | C    | C2-O2   | 5.86  | 1.29        | 1.24     |
| 1   | AA    | 781  | A    | C4'-C3' | -5.86 | 1.46        | 1.52     |
| 1   | AA    | 819  | A    | C4'-C3' | 5.86  | 1.59        | 1.53     |
| 1   | AA    | 1092 | A    | N1-C2   | 5.86  | 1.39        | 1.34     |
| 35  | BB    | 36   | G    | O3'-P   | -5.86 | 1.54        | 1.61     |
| 35  | BB    | 86   | G    | C5-C4   | -5.86 | 1.34        | 1.38     |
| 35  | BB    | 149  | A    | N3-C4   | 5.86  | 1.38        | 1.34     |
| 35  | BB    | 862  | G    | N9-C4   | 5.86  | 1.42        | 1.38     |
| 35  | BB    | 1076 | C    | C4-N4   | 5.86  | 1.39        | 1.33     |
| 35  | BB    | 2058 | A    | N9-C4   | -5.86 | 1.34        | 1.37     |
| 1   | AA    | 141  | G    | N7-C5   | -5.86 | 1.35        | 1.39     |
| 1   | AA    | 179  | A    | C6-N6   | 5.86  | 1.38        | 1.33     |
| 35  | BB    | 1203 | U    | N3-C4   | 5.86  | 1.43        | 1.38     |
| 38  | BE    | 88   | ARG  | NE-CZ   | 5.86  | 1.40        | 1.33     |
| 1   | AA    | 141  | G    | N3-C4   | 5.86  | 1.39        | 1.35     |
| 1   | AA    | 239  | U    | N1-C6   | 5.86  | 1.43        | 1.38     |
| 1   | AA    | 483  | C    | N3-C4   | 5.86  | 1.38        | 1.33     |
| 4   | AD    | 181  | PHE  | CG-CD1  | 5.86  | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 56   | A    | C2'-C1' | -5.86 | 1.47        | 1.53     |
| 35  | BB    | 77   | G    | N9-C4   | -5.86 | 1.33        | 1.38     |
| 35  | BB    | 85   | G    | C5-C4   | 5.86  | 1.42        | 1.38     |
| 35  | BB    | 676  | A    | C6-N1   | -5.86 | 1.31        | 1.35     |
| 35  | BB    | 1086 | A    | N7-C5   | -5.86 | 1.35        | 1.39     |
| 35  | BB    | 1165 | A    | N9-C4   | -5.86 | 1.34        | 1.37     |
| 35  | BB    | 1387 | A    | N7-C5   | -5.86 | 1.35        | 1.39     |
| 35  | BB    | 2862 | G    | C5-C4   | 5.86  | 1.42        | 1.38     |
| 1   | AA    | 1099 | G    | N7-C5   | -5.86 | 1.35        | 1.39     |
| 1   | AA    | 1282 | C    | N1-C6   | 5.86  | 1.40        | 1.37     |
| 34  | BA    | 64   | G    | N1-C2   | 5.86  | 1.42        | 1.37     |
| 35  | BB    | 2244 | U    | N1-C2   | -5.86 | 1.33        | 1.38     |
| 1   | AA    | 72   | A    | C8-N7   | -5.85 | 1.27        | 1.31     |
| 1   | AA    | 458  | U    | C2-O2   | 5.85  | 1.27        | 1.22     |
| 1   | AA    | 1134 | G    | C2-N2   | 5.85  | 1.40        | 1.34     |
| 13  | AM    | 2    | ARG  | CD-NE   | 5.85  | 1.56        | 1.46     |
| 35  | BB    | 809  | G    | C2-N3   | -5.85 | 1.28        | 1.32     |
| 35  | BB    | 1134 | A    | C3'-O3' | 5.85  | 1.50        | 1.42     |
| 35  | BB    | 1278 | C    | C4'-O4' | -5.85 | 1.38        | 1.45     |
| 35  | BB    | 2261 | C    | C2'-C1' | -5.85 | 1.47        | 1.53     |
| 1   | AA    | 812  | G    | C2-N3   | 5.85  | 1.37        | 1.32     |
| 7   | AG    | 43   | TYR  | CD2-CE2 | 5.85  | 1.48        | 1.39     |
| 15  | AO    | 52   | ARG  | CZ-NH2  | 5.85  | 1.40        | 1.33     |
| 35  | BB    | 546  | U    | N1-C2   | 5.85  | 1.43        | 1.38     |
| 35  | BB    | 1445 | G    | N7-C5   | -5.85 | 1.35        | 1.39     |
| 35  | BB    | 1447 | C    | N3-C4   | 5.85  | 1.38        | 1.33     |
| 35  | BB    | 1643 | G    | C6-N1   | -5.85 | 1.35        | 1.39     |
| 35  | BB    | 2087 | G    | O3'-P   | -5.85 | 1.54        | 1.61     |
| 35  | BB    | 2242 | G    | C2-N2   | 5.85  | 1.40        | 1.34     |
| 35  | BB    | 2640 | G    | N7-C5   | -5.85 | 1.35        | 1.39     |
| 1   | AA    | 145  | G    | N3-C4   | -5.85 | 1.31        | 1.35     |
| 1   | AA    | 282  | A    | P-O5'   | -5.85 | 1.53        | 1.59     |
| 1   | AA    | 552  | U    | O3'-P   | -5.85 | 1.54        | 1.61     |
| 1   | AA    | 823  | C    | C2-N3   | 5.85  | 1.40        | 1.35     |
| 1   | AA    | 882  | C    | C3'-C2' | 5.85  | 1.59        | 1.52     |
| 1   | AA    | 1312 | G    | C2-N3   | -5.85 | 1.28        | 1.32     |
| 33  | B8    | 36   | ARG  | NE-CZ   | 5.85  | 1.40        | 1.33     |
| 35  | BB    | 88   | G    | N9-C8   | -5.85 | 1.33        | 1.37     |
| 35  | BB    | 501  | A    | N3-C4   | -5.85 | 1.31        | 1.34     |
| 35  | BB    | 691  | C    | N3-C4   | 5.85  | 1.38        | 1.33     |
| 35  | BB    | 953  | G    | C2-N3   | 5.85  | 1.37        | 1.32     |
| 35  | BB    | 1311 | G    | C2-N2   | 5.85  | 1.40        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1993 | U    | N1-C2   | 5.85  | 1.43        | 1.38     |
| 1   | AA    | 436  | C    | P-O5'   | -5.85 | 1.53        | 1.59     |
| 1   | AA    | 769  | G    | C5-C6   | -5.85 | 1.36        | 1.42     |
| 1   | AA    | 845  | A    | N3-C4   | -5.85 | 1.31        | 1.34     |
| 15  | AO    | 62   | ARG  | CZ-NH2  | 5.85  | 1.40        | 1.33     |
| 28  | B3    | 15   | ARG  | CD-NE   | 5.85  | 1.56        | 1.46     |
| 35  | BB    | 310  | A    | N7-C5   | -5.85 | 1.35        | 1.39     |
| 35  | BB    | 340  | A    | N9-C4   | 5.85  | 1.41        | 1.37     |
| 35  | BB    | 726  | G    | N9-C8   | -5.85 | 1.33        | 1.37     |
| 35  | BB    | 1333 | G    | C5-C4   | -5.85 | 1.34        | 1.38     |
| 35  | BB    | 1367 | A    | N7-C5   | -5.85 | 1.35        | 1.39     |
| 35  | BB    | 2475 | C    | N1-C6   | 5.85  | 1.40        | 1.37     |
| 35  | BB    | 2634 | A    | C5-C6   | -5.85 | 1.35        | 1.41     |
| 39  | BF    | 132  | ARG  | CZ-NH2  | 5.85  | 1.40        | 1.33     |
| 1   | AA    | 219  | U    | C4'-O4' | -5.85 | 1.38        | 1.45     |
| 1   | AA    | 643  | C    | P-O5'   | 5.85  | 1.65        | 1.59     |
| 1   | AA    | 1174 | G    | C3'-O3' | 5.85  | 1.50        | 1.42     |
| 1   | AA    | 1408 | A    | O3'-P   | -5.85 | 1.54        | 1.61     |
| 22  | AV    | 5    | A    | C5-C6   | 5.85  | 1.46        | 1.41     |
| 35  | BB    | 461  | C    | C4-N4   | 5.85  | 1.39        | 1.33     |
| 35  | BB    | 1343 | G    | C2-N3   | 5.85  | 1.37        | 1.32     |
| 35  | BB    | 1888 | G    | O4'-C1' | 5.85  | 1.49        | 1.41     |
| 35  | BB    | 2253 | G    | N7-C5   | 5.85  | 1.42        | 1.39     |
| 35  | BB    | 2665 | A    | C5-C6   | 5.85  | 1.46        | 1.41     |
| 1   | AA    | 219  | U    | N3-C4   | 5.85  | 1.43        | 1.38     |
| 1   | AA    | 368  | U    | O4'-C1' | -5.85 | 1.34        | 1.41     |
| 1   | AA    | 506  | G    | P-O5'   | -5.85 | 1.53        | 1.59     |
| 35  | BB    | 1715 | G    | C5'-C4' | 5.85  | 1.58        | 1.51     |
| 35  | BB    | 1782 | U    | C1'-N1  | 5.85  | 1.57        | 1.48     |
| 35  | BB    | 2351 | G    | P-O5'   | -5.85 | 1.53        | 1.59     |
| 1   | AA    | 64   | G    | C5'-C4' | 5.84  | 1.58        | 1.51     |
| 1   | AA    | 521  | G    | N7-C5   | 5.84  | 1.42        | 1.39     |
| 1   | AA    | 697  | U    | N3-C4   | 5.84  | 1.43        | 1.38     |
| 1   | AA    | 815  | A    | N1-C2   | -5.84 | 1.29        | 1.34     |
| 1   | AA    | 1008 | U    | N3-C4   | 5.84  | 1.43        | 1.38     |
| 34  | BA    | 99   | A    | C6-N6   | 5.84  | 1.38        | 1.33     |
| 35  | BB    | 1228 | G    | C6-N1   | 5.84  | 1.43        | 1.39     |
| 35  | BB    | 1515 | A    | C8-N7   | -5.84 | 1.27        | 1.31     |
| 35  | BB    | 1949 | G    | C1'-N9  | 5.84  | 1.57        | 1.48     |
| 35  | BB    | 2001 | C    | C4-N4   | 5.84  | 1.39        | 1.33     |
| 35  | BB    | 2842 | G    | C5-C4   | -5.84 | 1.34        | 1.38     |
| 1   | AA    | 292  | G    | C6-N1   | 5.84  | 1.43        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 529  | A    | C3'-C2' | 5.84  | 1.59        | 1.52     |
| 35  | BB    | 2206 | C    | C2'-C1' | -5.84 | 1.47        | 1.53     |
| 35  | BB    | 2222 | C    | C2-N3   | 5.84  | 1.40        | 1.35     |
| 1   | AA    | 384  | G    | N7-C5   | -5.84 | 1.35        | 1.39     |
| 35  | BB    | 862  | G    | C2'-C1' | -5.84 | 1.47        | 1.53     |
| 35  | BB    | 1319 | C    | N1-C6   | 5.84  | 1.40        | 1.37     |
| 35  | BB    | 1338 | G    | C8-N7   | -5.84 | 1.27        | 1.30     |
| 35  | BB    | 2029 | G    | C2'-C1' | -5.84 | 1.47        | 1.53     |
| 35  | BB    | 2445 | G    | C2-N3   | 5.84  | 1.37        | 1.32     |
| 1   | AA    | 122  | G    | N3-C4   | 5.84  | 1.39        | 1.35     |
| 1   | AA    | 365  | U    | C1'-N1  | 5.84  | 1.57        | 1.48     |
| 1   | AA    | 466  | A    | C4'-C3' | 5.84  | 1.59        | 1.53     |
| 1   | AA    | 688  | G    | N9-C8   | -5.84 | 1.33        | 1.37     |
| 1   | AA    | 991  | U    | C3'-O3' | 5.84  | 1.50        | 1.42     |
| 1   | AA    | 1085 | U    | C2'-C1' | -5.84 | 1.47        | 1.53     |
| 1   | AA    | 1407 | C    | C5'-C4' | 5.84  | 1.58        | 1.51     |
| 1   | AA    | 1413 | A    | N9-C8   | -5.84 | 1.33        | 1.37     |
| 35  | BB    | 56   | A    | N3-C4   | 5.84  | 1.38        | 1.34     |
| 35  | BB    | 1147 | A    | C2'-O2' | 5.84  | 1.49        | 1.41     |
| 35  | BB    | 2567 | G    | C2-N3   | 5.84  | 1.37        | 1.32     |
| 1   | AA    | 307  | C    | C2-N3   | 5.84  | 1.40        | 1.35     |
| 34  | BA    | 23   | G    | C5-C4   | -5.84 | 1.34        | 1.38     |
| 35  | BB    | 118  | A    | C2'-C1' | -5.84 | 1.47        | 1.53     |
| 35  | BB    | 849  | A    | P-O5'   | -5.84 | 1.53        | 1.59     |
| 35  | BB    | 1877 | A    | C5-C6   | -5.84 | 1.35        | 1.41     |
| 1   | AA    | 884  | U    | P-O5'   | -5.84 | 1.53        | 1.59     |
| 1   | AA    | 1490 | U    | N1-C6   | -5.84 | 1.32        | 1.38     |
| 3   | AC    | 167  | TYR  | CA-CB   | 5.84  | 1.66        | 1.53     |
| 35  | BB    | 237  | C    | C2'-C1' | -5.84 | 1.47        | 1.53     |
| 35  | BB    | 530  | G    | N1-C2   | 5.84  | 1.42        | 1.37     |
| 35  | BB    | 1217 | U    | N1-C2   | -5.84 | 1.33        | 1.38     |
| 35  | BB    | 2232 | C    | C4-C5   | 5.84  | 1.47        | 1.43     |
| 35  | BB    | 2334 | U    | N3-C4   | 5.84  | 1.43        | 1.38     |
| 1   | AA    | 618  | C    | N3-C4   | 5.83  | 1.38        | 1.33     |
| 1   | AA    | 697  | U    | C4-C5   | -5.83 | 1.38        | 1.43     |
| 1   | AA    | 259  | G    | C3'-C2' | -5.83 | 1.46        | 1.52     |
| 1   | AA    | 916  | U    | C2-N3   | 5.83  | 1.41        | 1.37     |
| 1   | AA    | 1094 | G    | C2'-C1' | -5.83 | 1.47        | 1.53     |
| 1   | AA    | 1100 | C    | P-O5'   | -5.83 | 1.53        | 1.59     |
| 35  | BB    | 595  | C    | C4'-C3' | -5.83 | 1.46        | 1.52     |
| 35  | BB    | 922  | C    | C5-C6   | 5.83  | 1.39        | 1.34     |
| 35  | BB    | 1120 | G    | C6-N1   | 5.83  | 1.43        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1161 | C    | N1-C6   | 5.83  | 1.40        | 1.37     |
| 35  | BB    | 1261 | C    | C4-N4   | 5.83  | 1.39        | 1.33     |
| 35  | BB    | 2278 | A    | C5-C6   | -5.83 | 1.35        | 1.41     |
| 35  | BB    | 2630 | G    | C8-N7   | -5.83 | 1.27        | 1.30     |
| 35  | BB    | 2837 | A    | O3'-P   | 5.83  | 1.68        | 1.61     |
| 1   | AA    | 538  | G    | C2-N3   | 5.83  | 1.37        | 1.32     |
| 1   | AA    | 835  | U    | C2'-C1' | -5.83 | 1.47        | 1.53     |
| 1   | AA    | 846  | G    | N1-C2   | 5.83  | 1.42        | 1.37     |
| 1   | AA    | 1004 | A    | C6-N1   | 5.83  | 1.39        | 1.35     |
| 1   | AA    | 1421 | G    | O3'-P   | -5.83 | 1.54        | 1.61     |
| 34  | BA    | 8    | C    | C4-C5   | -5.83 | 1.38        | 1.43     |
| 35  | BB    | 115  | C    | C5'-C4' | 5.83  | 1.58        | 1.51     |
| 35  | BB    | 122  | G    | C3'-O3' | 5.83  | 1.50        | 1.42     |
| 35  | BB    | 684  | G    | P-O5'   | 5.83  | 1.65        | 1.59     |
| 35  | BB    | 1232 | G    | C6-O6   | 5.83  | 1.29        | 1.24     |
| 35  | BB    | 1271 | G    | C5-C4   | 5.83  | 1.42        | 1.38     |
| 35  | BB    | 1369 | G    | N1-C2   | 5.83  | 1.42        | 1.37     |
| 35  | BB    | 1411 | U    | C4-O4   | -5.83 | 1.19        | 1.23     |
| 35  | BB    | 1465 | G    | C6-N1   | 5.83  | 1.43        | 1.39     |
| 35  | BB    | 1506 | U    | C2-N3   | 5.83  | 1.41        | 1.37     |
| 35  | BB    | 1665 | A    | C1'-N9  | -5.83 | 1.38        | 1.46     |
| 35  | BB    | 1677 | A    | C8-N7   | -5.83 | 1.27        | 1.31     |
| 35  | BB    | 2144 | G    | C6-N1   | 5.83  | 1.43        | 1.39     |
| 35  | BB    | 2598 | A    | O3'-P   | -5.83 | 1.54        | 1.61     |
| 1   | AA    | 35   | G    | P-O5'   | -5.83 | 1.53        | 1.59     |
| 1   | AA    | 1126 | U    | N1-C2   | 5.83  | 1.43        | 1.38     |
| 1   | AA    | 1169 | A    | N9-C8   | 5.83  | 1.42        | 1.37     |
| 35  | BB    | 123  | G    | C2-N3   | 5.83  | 1.37        | 1.32     |
| 35  | BB    | 408  | G    | C2-N3   | 5.83  | 1.37        | 1.32     |
| 35  | BB    | 829  | A    | C1'-N9  | -5.83 | 1.38        | 1.46     |
| 35  | BB    | 1127 | A    | N3-C4   | -5.83 | 1.31        | 1.34     |
| 35  | BB    | 2319 | G    | C2-N2   | 5.83  | 1.40        | 1.34     |
| 35  | BB    | 2432 | A    | C6-N6   | 5.83  | 1.38        | 1.33     |
| 35  | BB    | 2495 | G    | N9-C8   | 5.83  | 1.42        | 1.37     |
| 1   | AA    | 493  | A    | C6-N6   | 5.83  | 1.38        | 1.33     |
| 35  | BB    | 585  | G    | C6-N1   | 5.83  | 1.43        | 1.39     |
| 35  | BB    | 954  | G    | N3-C4   | -5.83 | 1.31        | 1.35     |
| 35  | BB    | 1046 | A    | C8-N7   | 5.83  | 1.35        | 1.31     |
| 35  | BB    | 1681 | G    | N3-C4   | 5.83  | 1.39        | 1.35     |
| 35  | BB    | 1708 | C    | C5'-C4' | 5.83  | 1.58        | 1.51     |
| 35  | BB    | 1828 | G    | N3-C4   | -5.83 | 1.31        | 1.35     |
| 35  | BB    | 2200 | C    | C4-N4   | 5.83  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2337 | G    | C5-C4   | 5.83  | 1.42        | 1.38     |
| 35  | BB    | 2676 | C    | C3'-O3' | 5.83  | 1.50        | 1.42     |
| 35  | BB    | 2682 | A    | N9-C8   | -5.83 | 1.33        | 1.37     |
| 35  | BB    | 2753 | A    | C2-N3   | 5.83  | 1.38        | 1.33     |
| 1   | AA    | 655  | A    | C6-N6   | 5.83  | 1.38        | 1.33     |
| 1   | AA    | 685  | G    | N9-C8   | -5.83 | 1.33        | 1.37     |
| 34  | BA    | 20   | G    | N1-C2   | 5.83  | 1.42        | 1.37     |
| 34  | BA    | 109  | A    | C3'-C2' | 5.83  | 1.59        | 1.52     |
| 35  | BB    | 307  | G    | C8-N7   | 5.83  | 1.34        | 1.30     |
| 35  | BB    | 654  | A    | N3-C4   | -5.83 | 1.31        | 1.34     |
| 35  | BB    | 1737 | G    | C2'-C1' | -5.83 | 1.47        | 1.53     |
| 36  | BC    | 181  | ARG  | NE-CZ   | 5.83  | 1.40        | 1.33     |
| 1   | AA    | 340  | U    | O3'-P   | -5.83 | 1.54        | 1.61     |
| 1   | AA    | 717  | U    | O3'-P   | -5.83 | 1.54        | 1.61     |
| 35  | BB    | 481  | G    | C5-C4   | -5.83 | 1.34        | 1.38     |
| 35  | BB    | 1616 | A    | C6-N6   | 5.83  | 1.38        | 1.33     |
| 35  | BB    | 1945 | G    | N1-C2   | 5.83  | 1.42        | 1.37     |
| 35  | BB    | 2223 | G    | C5-C6   | -5.83 | 1.36        | 1.42     |
| 35  | BB    | 2276 | G    | C2-N3   | 5.83  | 1.37        | 1.32     |
| 35  | BB    | 2654 | A    | N9-C4   | -5.83 | 1.34        | 1.37     |
| 1   | AA    | 336  | A    | C5'-C4' | 5.82  | 1.58        | 1.51     |
| 1   | AA    | 337  | G    | C5-C4   | -5.82 | 1.34        | 1.38     |
| 35  | BB    | 544  | C    | P-O5'   | 5.82  | 1.65        | 1.59     |
| 35  | BB    | 597  | G    | N1-C2   | 5.82  | 1.42        | 1.37     |
| 35  | BB    | 660  | C    | C5'-C4' | 5.82  | 1.58        | 1.51     |
| 35  | BB    | 1354 | A    | C2'-O2' | -5.82 | 1.34        | 1.41     |
| 35  | BB    | 1415 | U    | C1'-N1  | 5.82  | 1.57        | 1.48     |
| 35  | BB    | 1582 | C    | N1-C6   | 5.82  | 1.40        | 1.37     |
| 35  | BB    | 1624 | U    | C5-C6   | -5.82 | 1.28        | 1.34     |
| 35  | BB    | 2566 | A    | C5-C4   | -5.82 | 1.34        | 1.38     |
| 35  | BB    | 2850 | A    | P-O5'   | -5.82 | 1.53        | 1.59     |
| 1   | AA    | 290  | C    | P-O5'   | -5.82 | 1.53        | 1.59     |
| 35  | BB    | 1804 | C    | N3-C4   | 5.82  | 1.38        | 1.33     |
| 35  | BB    | 1884 | G    | C2'-C1' | -5.82 | 1.47        | 1.53     |
| 35  | BB    | 2795 | C    | C4'-O4' | 5.82  | 1.53        | 1.45     |
| 1   | AA    | 38   | G    | O3'-P   | -5.82 | 1.54        | 1.61     |
| 1   | AA    | 489  | C    | C2'-C1' | -5.82 | 1.47        | 1.53     |
| 1   | AA    | 523  | A    | N3-C4   | -5.82 | 1.31        | 1.34     |
| 1   | AA    | 1171 | A    | N7-C5   | -5.82 | 1.35        | 1.39     |
| 1   | AA    | 1275 | A    | N9-C4   | -5.82 | 1.34        | 1.37     |
| 1   | AA    | 1518 | A    | N9-C8   | -5.82 | 1.33        | 1.37     |
| 2   | AB    | 221  | ARG  | CZ-NH1  | 5.82  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34  | BA    | 35   | C    | N1-C6   | 5.82  | 1.40        | 1.37     |
| 34  | BA    | 114  | C    | C2-O2   | 5.82  | 1.29        | 1.24     |
| 35  | BB    | 214  | G    | N1-C2   | 5.82  | 1.42        | 1.37     |
| 35  | BB    | 501  | A    | C6-N6   | 5.82  | 1.38        | 1.33     |
| 35  | BB    | 1241 | A    | C6-N6   | 5.82  | 1.38        | 1.33     |
| 35  | BB    | 1826 | G    | C3'-O3' | 5.82  | 1.50        | 1.42     |
| 35  | BB    | 2229 | U    | C4'-C3' | 5.82  | 1.59        | 1.53     |
| 35  | BB    | 2315 | G    | N9-C4   | -5.82 | 1.33        | 1.38     |
| 35  | BB    | 2445 | G    | N3-C4   | 5.82  | 1.39        | 1.35     |
| 35  | BB    | 2752 | C    | C4-N4   | 5.82  | 1.39        | 1.33     |
| 1   | AA    | 225  | C    | C4-N4   | 5.82  | 1.39        | 1.33     |
| 1   | AA    | 1001 | C    | P-O5'   | -5.82 | 1.53        | 1.59     |
| 35  | BB    | 745  | G    | C2-N3   | 5.82  | 1.37        | 1.32     |
| 35  | BB    | 1451 | C    | C2-N3   | 5.82  | 1.40        | 1.35     |
| 35  | BB    | 2780 | G    | C5-C4   | 5.82  | 1.42        | 1.38     |
| 1   | AA    | 357  | G    | C2-N3   | 5.82  | 1.37        | 1.32     |
| 1   | AA    | 1490 | U    | C5-C6   | 5.82  | 1.39        | 1.34     |
| 35  | BB    | 291  | G    | N1-C2   | 5.82  | 1.42        | 1.37     |
| 35  | BB    | 738  | G    | P-O5'   | -5.82 | 1.53        | 1.59     |
| 35  | BB    | 1668 | A    | C8-N7   | -5.82 | 1.27        | 1.31     |
| 35  | BB    | 1873 | G    | C5-C6   | -5.82 | 1.36        | 1.42     |
| 35  | BB    | 2623 | G    | N3-C4   | -5.82 | 1.31        | 1.35     |
| 35  | BB    | 2838 | G    | C2-N3   | 5.82  | 1.37        | 1.32     |
| 41  | BH    | 45   | GLU  | CD-OE1  | 5.82  | 1.32        | 1.25     |
| 1   | AA    | 182  | A    | N9-C4   | -5.82 | 1.34        | 1.37     |
| 1   | AA    | 292  | G    | C2'-C1' | -5.82 | 1.47        | 1.53     |
| 1   | AA    | 371  | A    | C8-N7   | 5.82  | 1.35        | 1.31     |
| 1   | AA    | 832  | G    | N9-C4   | -5.82 | 1.33        | 1.38     |
| 35  | BB    | 1235 | G    | C5-C4   | 5.82  | 1.42        | 1.38     |
| 35  | BB    | 1565 | C    | C5-C6   | -5.82 | 1.29        | 1.34     |
| 35  | BB    | 2549 | G    | N9-C4   | -5.82 | 1.33        | 1.38     |
| 50  | BQ    | 2    | ARG  | CZ-NH2  | 5.82  | 1.40        | 1.33     |
| 1   | AA    | 113  | G    | N3-C4   | -5.81 | 1.31        | 1.35     |
| 1   | AA    | 547  | A    | C4'-C3' | -5.81 | 1.46        | 1.52     |
| 1   | AA    | 895  | G    | C5-C6   | -5.81 | 1.36        | 1.42     |
| 1   | AA    | 908  | A    | C6-N6   | 5.81  | 1.38        | 1.33     |
| 35  | BB    | 114  | U    | C4-C5   | 5.81  | 1.48        | 1.43     |
| 1   | AA    | 211  | G    | C6-O6   | 5.81  | 1.29        | 1.24     |
| 35  | BB    | 1109 | C    | C2'-C1' | -5.81 | 1.47        | 1.53     |
| 35  | BB    | 1167 | C    | C2-N3   | -5.81 | 1.31        | 1.35     |
| 35  | BB    | 2226 | C    | C2'-C1' | -5.81 | 1.47        | 1.53     |
| 35  | BB    | 2279 | G    | C8-N7   | 5.81  | 1.34        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2830 | C    | C4-N4   | 5.81  | 1.39        | 1.33     |
| 35  | BB    | 2893 | A    | C5-C6   | -5.81 | 1.35        | 1.41     |
| 1   | AA    | 171  | A    | N7-C5   | -5.81 | 1.35        | 1.39     |
| 35  | BB    | 2288 | A    | C6-N6   | 5.81  | 1.38        | 1.33     |
| 1   | AA    | 18   | C    | N3-C4   | 5.81  | 1.38        | 1.33     |
| 1   | AA    | 280  | C    | C5-C6   | 5.81  | 1.39        | 1.34     |
| 1   | AA    | 1276 | G    | N3-C4   | -5.81 | 1.31        | 1.35     |
| 34  | BA    | 53   | A    | C3'-O3' | 5.81  | 1.50        | 1.42     |
| 35  | BB    | 235  | U    | C2-N3   | 5.81  | 1.41        | 1.37     |
| 35  | BB    | 494  | G    | C3'-O3' | 5.81  | 1.50        | 1.42     |
| 35  | BB    | 1356 | G    | C6-O6   | 5.81  | 1.29        | 1.24     |
| 35  | BB    | 1784 | A    | N9-C8   | -5.81 | 1.33        | 1.37     |
| 35  | BB    | 2335 | A    | C6-N6   | 5.81  | 1.38        | 1.33     |
| 35  | BB    | 2393 | U    | N1-C2   | 5.81  | 1.43        | 1.38     |
| 35  | BB    | 2880 | C    | C4'-C3' | 5.81  | 1.59        | 1.53     |
| 1   | AA    | 158  | G    | C2'-C1' | -5.81 | 1.47        | 1.53     |
| 1   | AA    | 407  | U    | N1-C2   | 5.81  | 1.43        | 1.38     |
| 35  | BB    | 240  | C    | N3-C4   | 5.81  | 1.38        | 1.33     |
| 35  | BB    | 279  | A    | C8-N7   | -5.81 | 1.27        | 1.31     |
| 35  | BB    | 443  | A    | C4'-O4' | -5.81 | 1.38        | 1.45     |
| 35  | BB    | 1928 | A    | P-O5'   | -5.81 | 1.53        | 1.59     |
| 35  | BB    | 2610 | C    | C2'-C1' | -5.81 | 1.47        | 1.53     |
| 1   | AA    | 364  | A    | N9-C4   | 5.81  | 1.41        | 1.37     |
| 1   | AA    | 734  | G    | N9-C8   | -5.81 | 1.33        | 1.37     |
| 35  | BB    | 60   | G    | C8-N7   | 5.81  | 1.34        | 1.30     |
| 35  | BB    | 1296 | G    | C8-N7   | 5.81  | 1.34        | 1.30     |
| 35  | BB    | 1378 | A    | C4'-O4' | 5.81  | 1.53        | 1.45     |
| 35  | BB    | 1556 | C    | N3-C4   | 5.81  | 1.38        | 1.33     |
| 35  | BB    | 1865 | U    | O3'-P   | -5.81 | 1.54        | 1.61     |
| 35  | BB    | 2640 | G    | N3-C4   | 5.81  | 1.39        | 1.35     |
| 1   | AA    | 269  | C    | C4-C5   | 5.80  | 1.47        | 1.43     |
| 1   | AA    | 544  | G    | C6-N1   | 5.80  | 1.43        | 1.39     |
| 1   | AA    | 549  | C    | C2-N3   | 5.80  | 1.40        | 1.35     |
| 1   | AA    | 691  | G    | C2'-C1' | -5.80 | 1.47        | 1.53     |
| 1   | AA    | 849  | G    | O3'-P   | -5.80 | 1.54        | 1.61     |
| 1   | AA    | 1109 | C    | C4-N4   | 5.80  | 1.39        | 1.33     |
| 1   | AA    | 1156 | G    | C2-N3   | 5.80  | 1.37        | 1.32     |
| 1   | AA    | 1449 | C    | C2-N3   | 5.80  | 1.40        | 1.35     |
| 34  | BA    | 69   | G    | C2-N2   | 5.80  | 1.40        | 1.34     |
| 35  | BB    | 1035 | U    | C1'-N1  | 5.80  | 1.57        | 1.48     |
| 35  | BB    | 1856 | U    | C2-N3   | 5.80  | 1.41        | 1.37     |
| 7   | AG    | 91   | ARG  | NE-CZ   | 5.80  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 569  | U    | C4-O4   | -5.80 | 1.19        | 1.23     |
| 35  | BB    | 917  | A    | C3'-O3' | 5.80  | 1.50        | 1.42     |
| 35  | BB    | 2541 | A    | O3'-P   | -5.80 | 1.54        | 1.61     |
| 35  | BB    | 2875 | C    | N1-C2   | 5.80  | 1.46        | 1.40     |
| 1   | AA    | 300  | A    | C8-N7   | -5.80 | 1.27        | 1.31     |
| 1   | AA    | 369  | G    | N9-C8   | 5.80  | 1.42        | 1.37     |
| 1   | AA    | 959  | A    | C6-N1   | 5.80  | 1.39        | 1.35     |
| 35  | BB    | 1328 | A    | C4'-C3' | 5.80  | 1.59        | 1.53     |
| 35  | BB    | 1463 | C    | N3-C4   | 5.80  | 1.38        | 1.33     |
| 35  | BB    | 1670 | C    | C4-N4   | 5.80  | 1.39        | 1.33     |
| 35  | BB    | 1985 | C    | P-O5'   | -5.80 | 1.53        | 1.59     |
| 1   | AA    | 564  | C    | C4'-O4' | 5.80  | 1.53        | 1.45     |
| 34  | BA    | 15   | A    | N3-C4   | 5.80  | 1.38        | 1.34     |
| 35  | BB    | 549  | G    | C2'-C1' | -5.80 | 1.47        | 1.53     |
| 35  | BB    | 647  | G    | C2'-O2' | 5.80  | 1.49        | 1.41     |
| 35  | BB    | 802  | A    | P-O5'   | -5.80 | 1.53        | 1.59     |
| 35  | BB    | 1386 | C    | C3'-C2' | 5.80  | 1.59        | 1.52     |
| 35  | BB    | 2008 | C    | C4-C5   | 5.80  | 1.47        | 1.43     |
| 35  | BB    | 2169 | A    | N3-C4   | 5.80  | 1.38        | 1.34     |
| 35  | BB    | 2500 | U    | P-O5'   | -5.80 | 1.53        | 1.59     |
| 35  | BB    | 2831 | G    | N9-C8   | -5.80 | 1.33        | 1.37     |
| 37  | BD    | 77   | ARG  | CZ-NH2  | 5.80  | 1.40        | 1.33     |
| 1   | AA    | 625  | U    | C2-N3   | 5.80  | 1.41        | 1.37     |
| 1   | AA    | 748  | G    | N9-C8   | 5.80  | 1.42        | 1.37     |
| 1   | AA    | 1370 | G    | C3'-O3' | 5.80  | 1.50        | 1.42     |
| 35  | BB    | 1036 | G    | N7-C5   | -5.80 | 1.35        | 1.39     |
| 35  | BB    | 1791 | A    | O3'-P   | -5.80 | 1.54        | 1.61     |
| 35  | BB    | 2342 | C    | N3-C4   | 5.80  | 1.38        | 1.33     |
| 1   | AA    | 103  | U    | C5-C6   | -5.80 | 1.28        | 1.34     |
| 1   | AA    | 105  | G    | P-O5'   | -5.80 | 1.53        | 1.59     |
| 1   | AA    | 922  | G    | C8-N7   | -5.80 | 1.27        | 1.30     |
| 1   | AA    | 1202 | U    | O4'-C1' | 5.80  | 1.49        | 1.41     |
| 35  | BB    | 642  | U    | O3'-P   | -5.80 | 1.54        | 1.61     |
| 35  | BB    | 924  | G    | O3'-P   | -5.80 | 1.54        | 1.61     |
| 35  | BB    | 1669 | A    | N3-C4   | 5.80  | 1.38        | 1.34     |
| 35  | BB    | 1916 | A    | C6-N1   | 5.80  | 1.39        | 1.35     |
| 35  | BB    | 2077 | A    | C2'-O2' | 5.80  | 1.49        | 1.41     |
| 35  | BB    | 2478 | A    | C5-C4   | 5.80  | 1.42        | 1.38     |
| 35  | BB    | 2822 | G    | C5'-C4' | 5.80  | 1.58        | 1.51     |
| 1   | AA    | 1272 | G    | C5-C4   | 5.79  | 1.42        | 1.38     |
| 35  | BB    | 106  | C    | C2'-C1' | -5.79 | 1.47        | 1.53     |
| 35  | BB    | 1464 | G    | N3-C4   | 5.79  | 1.39        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 517  | G    | P-O5'   | -5.79 | 1.53        | 1.59     |
| 1   | AA    | 575  | G    | N9-C8   | -5.79 | 1.33        | 1.37     |
| 1   | AA    | 1320 | C    | C1'-N1  | 5.79  | 1.57        | 1.48     |
| 1   | AA    | 1342 | C    | C1'-N1  | 5.79  | 1.57        | 1.48     |
| 34  | BA    | 17   | C    | C5-C6   | 5.79  | 1.39        | 1.34     |
| 35  | BB    | 85   | G    | C5'-C4' | 5.79  | 1.58        | 1.51     |
| 35  | BB    | 238  | C    | C5-C6   | 5.79  | 1.39        | 1.34     |
| 35  | BB    | 465  | G    | O3'-P   | -5.79 | 1.54        | 1.61     |
| 35  | BB    | 493  | G    | C2'-C1' | -5.79 | 1.47        | 1.53     |
| 35  | BB    | 704  | G    | C3'-O3' | 5.79  | 1.50        | 1.42     |
| 35  | BB    | 750  | A    | C6-N6   | 5.79  | 1.38        | 1.33     |
| 35  | BB    | 880  | G    | C3'-C2' | -5.79 | 1.46        | 1.52     |
| 35  | BB    | 1929 | G    | C5'-C4' | 5.79  | 1.58        | 1.51     |
| 1   | AA    | 275  | G    | C2-N3   | 5.79  | 1.37        | 1.32     |
| 1   | AA    | 822  | U    | N3-C4   | 5.79  | 1.43        | 1.38     |
| 1   | AA    | 1286 | U    | C4-O4   | 5.79  | 1.28        | 1.23     |
| 1   | AA    | 1346 | A    | N3-C4   | 5.79  | 1.38        | 1.34     |
| 35  | BB    | 126  | A    | C2'-C1' | -5.79 | 1.47        | 1.53     |
| 35  | BB    | 592  | A    | C3'-O3' | 5.79  | 1.50        | 1.42     |
| 35  | BB    | 719  | C    | C5'-C4' | 5.79  | 1.58        | 1.51     |
| 35  | BB    | 889  | C    | N3-C4   | 5.79  | 1.38        | 1.33     |
| 35  | BB    | 1327 | A    | N9-C4   | 5.79  | 1.41        | 1.37     |
| 35  | BB    | 1436 | G    | C2-N3   | 5.79  | 1.37        | 1.32     |
| 35  | BB    | 2588 | G    | C2'-C1' | -5.79 | 1.47        | 1.53     |
| 35  | BB    | 2664 | G    | C2'-C1' | -5.79 | 1.47        | 1.53     |
| 35  | BB    | 2870 | C    | C4-C5   | 5.79  | 1.47        | 1.43     |
| 38  | BE    | 114  | ARG  | CZ-NH2  | 5.79  | 1.40        | 1.33     |
| 1   | AA    | 1154 | G    | O4'-C1' | -5.79 | 1.34        | 1.41     |
| 1   | AA    | 288  | A    | C3'-C2' | -5.79 | 1.46        | 1.52     |
| 4   | AD    | 43   | ARG  | CZ-NH1  | 5.79  | 1.40        | 1.33     |
| 4   | AD    | 134  | TYR  | CB-CG   | 5.79  | 1.60        | 1.51     |
| 35  | BB    | 820  | A    | N9-C8   | -5.79 | 1.33        | 1.37     |
| 35  | BB    | 1582 | C    | C3'-C2' | -5.79 | 1.46        | 1.52     |
| 35  | BB    | 1601 | G    | C8-N7   | -5.79 | 1.27        | 1.30     |
| 35  | BB    | 2343 | U    | N1-C2   | 5.79  | 1.43        | 1.38     |
| 35  | BB    | 2358 | A    | C5-C6   | 5.79  | 1.46        | 1.41     |
| 35  | BB    | 2762 | C    | C4-C5   | 5.79  | 1.47        | 1.43     |
| 1   | AA    | 954  | G    | C5-C4   | 5.79  | 1.42        | 1.38     |
| 1   | AA    | 1207 | G    | N9-C4   | 5.79  | 1.42        | 1.38     |
| 35  | BB    | 2831 | G    | N3-C4   | -5.79 | 1.31        | 1.35     |
| 1   | AA    | 602  | A    | O4'-C1' | 5.79  | 1.49        | 1.41     |
| 1   | AA    | 757  | U    | N3-C4   | 5.79  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | AV    | 70   | C    | O3'-P   | 5.79  | 1.68        | 1.61     |
| 34  | BA    | 83   | G    | C6-N1   | -5.79 | 1.35        | 1.39     |
| 35  | BB    | 543  | G    | O3'-P   | -5.79 | 1.54        | 1.61     |
| 35  | BB    | 613  | A    | C2'-C1' | -5.79 | 1.47        | 1.53     |
| 35  | BB    | 1782 | U    | C5'-C4' | 5.79  | 1.58        | 1.51     |
| 35  | BB    | 1788 | C    | C4-C5   | 5.79  | 1.47        | 1.43     |
| 35  | BB    | 2682 | A    | C6-N1   | 5.79  | 1.39        | 1.35     |
| 1   | AA    | 550  | G    | O4'-C1' | 5.78  | 1.49        | 1.41     |
| 1   | AA    | 806  | C    | C3'-C2' | -5.78 | 1.46        | 1.52     |
| 1   | AA    | 1057 | G    | C5-C4   | 5.78  | 1.42        | 1.38     |
| 1   | AA    | 1120 | C    | N1-C2   | -5.78 | 1.34        | 1.40     |
| 1   | AA    | 1281 | C    | N1-C6   | 5.78  | 1.40        | 1.37     |
| 1   | AA    | 1498 | U    | N3-C4   | 5.78  | 1.43        | 1.38     |
| 35  | BB    | 18   | U    | C2-N3   | 5.78  | 1.41        | 1.37     |
| 35  | BB    | 156  | A    | C4'-C3' | -5.78 | 1.46        | 1.52     |
| 35  | BB    | 733  | G    | C8-N7   | -5.78 | 1.27        | 1.30     |
| 35  | BB    | 897  | C    | N1-C6   | 5.78  | 1.40        | 1.37     |
| 35  | BB    | 1438 | U    | P-O5'   | -5.78 | 1.53        | 1.59     |
| 35  | BB    | 1591 | A    | N7-C5   | -5.78 | 1.35        | 1.39     |
| 35  | BB    | 2878 | U    | O3'-P   | -5.78 | 1.54        | 1.61     |
| 1   | AA    | 65   | A    | N9-C4   | -5.78 | 1.34        | 1.37     |
| 1   | AA    | 481  | G    | N9-C4   | -5.78 | 1.33        | 1.38     |
| 3   | AC    | 71   | ARG  | CZ-NH2  | 5.78  | 1.40        | 1.33     |
| 35  | BB    | 27   | G    | O4'-C1' | -5.78 | 1.34        | 1.41     |
| 35  | BB    | 2715 | C    | P-O5'   | -5.78 | 1.53        | 1.59     |
| 1   | AA    | 191  | G    | C5-C4   | -5.78 | 1.34        | 1.38     |
| 1   | AA    | 388  | G    | N1-C2   | 5.78  | 1.42        | 1.37     |
| 1   | AA    | 1052 | U    | C4-O4   | -5.78 | 1.19        | 1.23     |
| 1   | AA    | 1071 | C    | N3-C4   | 5.78  | 1.38        | 1.33     |
| 16  | AP    | 14   | ARG  | CZ-NH1  | 5.78  | 1.40        | 1.33     |
| 28  | B3    | 39   | ARG  | CZ-NH1  | 5.78  | 1.40        | 1.33     |
| 35  | BB    | 122  | G    | C3'-C2' | -5.78 | 1.46        | 1.52     |
| 35  | BB    | 553  | G    | N9-C8   | 5.78  | 1.41        | 1.37     |
| 35  | BB    | 2567 | G    | C2'-C1' | -5.78 | 1.47        | 1.53     |
| 1   | AA    | 935  | A    | C5-C6   | 5.78  | 1.46        | 1.41     |
| 8   | AH    | 16   | GLY  | CA-C    | -5.78 | 1.42        | 1.51     |
| 35  | BB    | 78   | U    | C4-C5   | 5.78  | 1.48        | 1.43     |
| 35  | BB    | 1181 | U    | C4-C5   | -5.78 | 1.38        | 1.43     |
| 35  | BB    | 1711 | A    | C6-N6   | 5.78  | 1.38        | 1.33     |
| 1   | AA    | 203  | G    | C3'-C2' | 5.78  | 1.59        | 1.52     |
| 1   | AA    | 315  | A    | N7-C5   | 5.78  | 1.42        | 1.39     |
| 1   | AA    | 637  | C    | C4'-C3' | 5.78  | 1.59        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1425 | U    | C2-N3   | 5.78  | 1.41        | 1.37     |
| 9   | AI    | 5    | TYR  | CG-CD2  | 5.78  | 1.46        | 1.39     |
| 35  | BB    | 187  | G    | C8-N7   | 5.78  | 1.34        | 1.30     |
| 35  | BB    | 477  | A    | C8-N7   | -5.78 | 1.27        | 1.31     |
| 35  | BB    | 602  | A    | C5-C6   | -5.78 | 1.35        | 1.41     |
| 35  | BB    | 651  | G    | C6-N1   | 5.78  | 1.43        | 1.39     |
| 35  | BB    | 656  | G    | C2-N3   | 5.78  | 1.37        | 1.32     |
| 35  | BB    | 960  | A    | N3-C4   | 5.78  | 1.38        | 1.34     |
| 35  | BB    | 2231 | U    | C2-O2   | 5.78  | 1.27        | 1.22     |
| 35  | BB    | 2327 | A    | C5-C4   | -5.78 | 1.34        | 1.38     |
| 35  | BB    | 2569 | G    | C3'-O3' | 5.78  | 1.50        | 1.42     |
| 1   | AA    | 117  | G    | C5-C6   | -5.78 | 1.36        | 1.42     |
| 1   | AA    | 135  | C    | O3'-P   | -5.78 | 1.54        | 1.61     |
| 22  | AV    | 2    | G    | C4'-C3' | -5.78 | 1.46        | 1.52     |
| 35  | BB    | 270  | A    | C6-N1   | -5.78 | 1.31        | 1.35     |
| 35  | BB    | 360  | U    | C5'-C4' | 5.78  | 1.58        | 1.51     |
| 35  | BB    | 1195 | G    | N9-C4   | -5.78 | 1.33        | 1.38     |
| 35  | BB    | 1380 | G    | C5-C4   | 5.78  | 1.42        | 1.38     |
| 35  | BB    | 1449 | G    | N7-C5   | -5.78 | 1.35        | 1.39     |
| 35  | BB    | 1773 | A    | C5-C4   | 5.78  | 1.42        | 1.38     |
| 35  | BB    | 2226 | C    | C4-C5   | 5.78  | 1.47        | 1.43     |
| 55  | BW    | 55   | GLU  | CD-OE2  | -5.78 | 1.19        | 1.25     |
| 35  | BB    | 232  | G    | C2-N3   | 5.77  | 1.37        | 1.32     |
| 35  | BB    | 856  | G    | O3'-P   | -5.77 | 1.54        | 1.61     |
| 35  | BB    | 989  | G    | C2-N3   | 5.77  | 1.37        | 1.32     |
| 35  | BB    | 2783 | U    | N1-C6   | -5.77 | 1.32        | 1.38     |
| 1   | AA    | 369  | G    | C2-N2   | 5.77  | 1.40        | 1.34     |
| 1   | AA    | 401  | C    | C2'-C1' | -5.77 | 1.47        | 1.53     |
| 1   | AA    | 1298 | U    | C4'-O4' | 5.77  | 1.53        | 1.45     |
| 3   | AC    | 52   | SER  | CA-CB   | 5.77  | 1.61        | 1.52     |
| 35  | BB    | 336  | C    | N3-C4   | 5.77  | 1.38        | 1.33     |
| 35  | BB    | 636  | G    | C2-N2   | 5.77  | 1.40        | 1.34     |
| 35  | BB    | 685  | A    | C2'-C1' | -5.77 | 1.47        | 1.53     |
| 35  | BB    | 918  | A    | C8-N7   | 5.77  | 1.35        | 1.31     |
| 35  | BB    | 1666 | G    | C4'-O4' | 5.77  | 1.53        | 1.45     |
| 1   | AA    | 254  | G    | C6-O6   | -5.77 | 1.19        | 1.24     |
| 1   | AA    | 484  | G    | C5-C6   | 5.77  | 1.48        | 1.42     |
| 1   | AA    | 1082 | A    | N3-C4   | -5.77 | 1.31        | 1.34     |
| 1   | AA    | 1252 | A    | P-O5'   | -5.77 | 1.53        | 1.59     |
| 1   | AA    | 1383 | C    | C4-N4   | 5.77  | 1.39        | 1.33     |
| 34  | BA    | 68   | C    | C4-C5   | 5.77  | 1.47        | 1.43     |
| 35  | BB    | 1246 | A    | C5-C6   | 5.77  | 1.46        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1560 | G    | N3-C4   | -5.77 | 1.31        | 1.35     |
| 35  | BB    | 2309 | A    | O3'-P   | -5.77 | 1.54        | 1.61     |
| 35  | BB    | 2716 | C    | O3'-P   | -5.77 | 1.54        | 1.61     |
| 35  | BB    | 2722 | G    | P-O5'   | -5.77 | 1.53        | 1.59     |
| 1   | AA    | 206  | C    | N1-C6   | 5.77  | 1.40        | 1.37     |
| 1   | AA    | 1171 | A    | N3-C4   | -5.77 | 1.31        | 1.34     |
| 35  | BB    | 25   | U    | N1-C6   | -5.77 | 1.32        | 1.38     |
| 35  | BB    | 114  | U    | C2-N3   | 5.77  | 1.41        | 1.37     |
| 35  | BB    | 170  | U    | N3-C4   | 5.77  | 1.43        | 1.38     |
| 35  | BB    | 1493 | C    | C3'-C2' | -5.77 | 1.46        | 1.52     |
| 35  | BB    | 1692 | U    | C2'-C1' | -5.77 | 1.47        | 1.53     |
| 35  | BB    | 2201 | G    | C8-N7   | 5.77  | 1.34        | 1.30     |
| 35  | BB    | 2238 | G    | N9-C4   | -5.77 | 1.33        | 1.38     |
| 35  | BB    | 2392 | A    | C6-N1   | 5.77  | 1.39        | 1.35     |
| 1   | AA    | 164  | G    | C5-C4   | 5.77  | 1.42        | 1.38     |
| 1   | AA    | 261  | U    | C5-C6   | 5.77  | 1.39        | 1.34     |
| 1   | AA    | 553  | A    | N3-C4   | 5.77  | 1.38        | 1.34     |
| 1   | AA    | 587  | G    | C2-N2   | 5.77  | 1.40        | 1.34     |
| 1   | AA    | 1515 | G    | N3-C4   | -5.77 | 1.31        | 1.35     |
| 34  | BA    | 26   | C    | C4-C5   | 5.77  | 1.47        | 1.43     |
| 35  | BB    | 829  | A    | C8-N7   | -5.77 | 1.27        | 1.31     |
| 35  | BB    | 913  | U    | N1-C6   | 5.77  | 1.43        | 1.38     |
| 35  | BB    | 1125 | G    | C5'-C4' | 5.77  | 1.58        | 1.51     |
| 35  | BB    | 1818 | U    | O4'-C1' | 5.77  | 1.49        | 1.41     |
| 35  | BB    | 2234 | G    | O3'-P   | -5.77 | 1.54        | 1.61     |
| 35  | BB    | 2451 | A    | C6-N6   | 5.77  | 1.38        | 1.33     |
| 35  | BB    | 2718 | G    | C5-C6   | -5.77 | 1.36        | 1.42     |
| 1   | AA    | 92   | U    | O3'-P   | -5.77 | 1.54        | 1.61     |
| 1   | AA    | 431  | A    | P-O5'   | -5.77 | 1.53        | 1.59     |
| 1   | AA    | 1497 | G    | C5'-C4' | 5.77  | 1.58        | 1.51     |
| 1   | AA    | 1511 | G    | C6-N1   | 5.77  | 1.43        | 1.39     |
| 35  | BB    | 1914 | C    | C5'-C4' | 5.77  | 1.58        | 1.51     |
| 1   | AA    | 1227 | A    | C6-N6   | 5.76  | 1.38        | 1.33     |
| 1   | AA    | 1272 | G    | N9-C8   | 5.76  | 1.41        | 1.37     |
| 1   | AA    | 1405 | G    | N3-C4   | -5.76 | 1.31        | 1.35     |
| 35  | BB    | 93   | G    | C8-N7   | 5.76  | 1.34        | 1.30     |
| 35  | BB    | 486  | C    | P-O5'   | -5.76 | 1.53        | 1.59     |
| 35  | BB    | 1879 | C    | P-O5'   | -5.76 | 1.53        | 1.59     |
| 1   | AA    | 61   | G    | N9-C8   | 5.76  | 1.41        | 1.37     |
| 35  | BB    | 2716 | C    | C2-N3   | 5.76  | 1.40        | 1.35     |
| 1   | AA    | 361  | G    | C2-N3   | 5.76  | 1.37        | 1.32     |
| 1   | AA    | 936  | C    | N1-C6   | 5.76  | 1.40        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1042 | A    | N9-C4   | 5.76  | 1.41        | 1.37     |
| 1   | AA    | 1314 | C    | N1-C6   | -5.76 | 1.33        | 1.37     |
| 1   | AA    | 1501 | C    | N3-C4   | 5.76  | 1.38        | 1.33     |
| 34  | BA    | 82   | U    | P-O5'   | -5.76 | 1.53        | 1.59     |
| 35  | BB    | 414  | C    | P-O5'   | -5.76 | 1.53        | 1.59     |
| 35  | BB    | 613  | A    | N9-C4   | 5.76  | 1.41        | 1.37     |
| 35  | BB    | 628  | G    | N9-C8   | -5.76 | 1.33        | 1.37     |
| 35  | BB    | 697  | G    | O3'-P   | -5.76 | 1.54        | 1.61     |
| 35  | BB    | 729  | G    | C1'-N9  | 5.76  | 1.57        | 1.48     |
| 35  | BB    | 1313 | U    | C2-N3   | 5.76  | 1.41        | 1.37     |
| 35  | BB    | 1559 | U    | O3'-P   | -5.76 | 1.54        | 1.61     |
| 35  | BB    | 1992 | G    | C3'-C2' | -5.76 | 1.46        | 1.52     |
| 35  | BB    | 2084 | C    | C2'-C1' | -5.76 | 1.47        | 1.53     |
| 35  | BB    | 2784 | U    | N3-C4   | 5.76  | 1.43        | 1.38     |
| 1   | AA    | 262  | A    | N7-C5   | -5.76 | 1.35        | 1.39     |
| 1   | AA    | 397  | A    | N9-C8   | -5.76 | 1.33        | 1.37     |
| 1   | AA    | 1435 | G    | C6-N1   | 5.76  | 1.43        | 1.39     |
| 1   | AA    | 1488 | G    | C2'-C1' | -5.76 | 1.47        | 1.53     |
| 1   | AA    | 1500 | A    | N9-C4   | -5.76 | 1.34        | 1.37     |
| 35  | BB    | 1439 | A    | C4'-O4' | -5.76 | 1.38        | 1.45     |
| 35  | BB    | 1608 | A    | N1-C2   | 5.76  | 1.39        | 1.34     |
| 35  | BB    | 1791 | A    | N7-C5   | -5.76 | 1.35        | 1.39     |
| 35  | BB    | 1984 | G    | C2-N3   | 5.76  | 1.37        | 1.32     |
| 35  | BB    | 2535 | G    | C4'-O4' | -5.76 | 1.38        | 1.45     |
| 47  | BN    | 118  | ARG  | CZ-NH1  | 5.76  | 1.40        | 1.33     |
| 34  | BA    | 118  | C    | N3-C4   | 5.76  | 1.38        | 1.33     |
| 35  | BB    | 365  | U    | C2-N3   | 5.76  | 1.41        | 1.37     |
| 35  | BB    | 475  | C    | P-O5'   | -5.76 | 1.53        | 1.59     |
| 35  | BB    | 605  | G    | C8-N7   | 5.76  | 1.34        | 1.30     |
| 35  | BB    | 770  | G    | O4'-C1' | -5.76 | 1.34        | 1.41     |
| 35  | BB    | 1099 | G    | P-O5'   | -5.76 | 1.53        | 1.59     |
| 35  | BB    | 1265 | A    | N3-C4   | -5.76 | 1.31        | 1.34     |
| 35  | BB    | 1614 | A    | C3'-C2' | 5.76  | 1.59        | 1.52     |
| 35  | BB    | 1850 | G    | C6-N1   | -5.76 | 1.35        | 1.39     |
| 35  | BB    | 2026 | U    | P-O5'   | -5.76 | 1.53        | 1.59     |
| 35  | BB    | 2205 | A    | N9-C4   | 5.76  | 1.41        | 1.37     |
| 1   | AA    | 538  | G    | P-O5'   | -5.76 | 1.53        | 1.59     |
| 1   | AA    | 607  | A    | C4'-O4' | -5.76 | 1.38        | 1.45     |
| 1   | AA    | 758  | C    | C5'-C4' | 5.76  | 1.58        | 1.51     |
| 1   | AA    | 989  | U    | C4'-C3' | -5.76 | 1.46        | 1.52     |
| 35  | BB    | 862  | G    | C2-N3   | 5.76  | 1.37        | 1.32     |
| 35  | BB    | 1671 | U    | C4-O4   | -5.76 | 1.19        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1764 | C    | C1'-N1  | 5.76  | 1.57        | 1.48     |
| 35  | BB    | 1948 | G    | N1-C2   | 5.76  | 1.42        | 1.37     |
| 35  | BB    | 2463 | C    | C4-C5   | 5.76  | 1.47        | 1.43     |
| 35  | BB    | 469  | G    | C2-N3   | 5.75  | 1.37        | 1.32     |
| 35  | BB    | 1043 | C    | C4-N4   | 5.75  | 1.39        | 1.33     |
| 35  | BB    | 1071 | G    | N1-C2   | 5.75  | 1.42        | 1.37     |
| 35  | BB    | 1461 | C    | C2-N3   | -5.75 | 1.31        | 1.35     |
| 35  | BB    | 1811 | G    | P-O5'   | -5.75 | 1.53        | 1.59     |
| 35  | BB    | 2632 | A    | C4'-C3' | -5.75 | 1.46        | 1.52     |
| 1   | AA    | 68   | G    | C2'-C1' | -5.75 | 1.47        | 1.53     |
| 1   | AA    | 460  | A    | C5-C6   | -5.75 | 1.35        | 1.41     |
| 1   | AA    | 690  | G    | C6-N1   | 5.75  | 1.43        | 1.39     |
| 1   | AA    | 924  | C    | C4-C5   | 5.75  | 1.47        | 1.43     |
| 35  | BB    | 271  | G    | C5-C4   | 5.75  | 1.42        | 1.38     |
| 35  | BB    | 551  | G    | O4'-C1' | 5.75  | 1.49        | 1.41     |
| 35  | BB    | 1062 | G    | C5'-C4' | 5.75  | 1.58        | 1.51     |
| 35  | BB    | 2218 | G    | C5-C6   | -5.75 | 1.36        | 1.42     |
| 1   | AA    | 398  | U    | C4-C5   | 5.75  | 1.48        | 1.43     |
| 1   | AA    | 914  | A    | C6-N6   | 5.75  | 1.38        | 1.33     |
| 34  | BA    | 69   | G    | C2-N3   | 5.75  | 1.37        | 1.32     |
| 35  | BB    | 260  | G    | C2-N2   | 5.75  | 1.40        | 1.34     |
| 35  | BB    | 1065 | U    | C5'-C4' | 5.75  | 1.58        | 1.51     |
| 35  | BB    | 1852 | U    | C4-C5   | 5.75  | 1.48        | 1.43     |
| 35  | BB    | 2016 | U    | N1-C2   | 5.75  | 1.43        | 1.38     |
| 35  | BB    | 2092 | U    | O3'-P   | -5.75 | 1.54        | 1.61     |
| 35  | BB    | 2142 | A    | C5-C6   | -5.75 | 1.35        | 1.41     |
| 35  | BB    | 2190 | G    | N9-C8   | 5.75  | 1.41        | 1.37     |
| 35  | BB    | 2271 | G    | N7-C5   | -5.75 | 1.35        | 1.39     |
| 35  | BB    | 2865 | U    | C4-C5   | 5.75  | 1.48        | 1.43     |
| 35  | BB    | 2867 | G    | O3'-P   | 5.75  | 1.68        | 1.61     |
| 40  | BG    | 109  | SER  | CA-CB   | 5.75  | 1.61        | 1.52     |
| 35  | BB    | 1927 | A    | N9-C4   | -5.75 | 1.34        | 1.37     |
| 35  | BB    | 2096 | C    | C4'-C3' | 5.75  | 1.59        | 1.53     |
| 35  | BB    | 2817 | U    | O3'-P   | -5.75 | 1.54        | 1.61     |
| 1   | AA    | 578  | C    | N3-C4   | 5.75  | 1.38        | 1.33     |
| 34  | BA    | 100  | G    | N1-C2   | 5.75  | 1.42        | 1.37     |
| 35  | BB    | 256  | A    | C2'-C1' | -5.75 | 1.47        | 1.53     |
| 35  | BB    | 473  | G    | C5-C6   | -5.75 | 1.36        | 1.42     |
| 35  | BB    | 882  | G    | O3'-P   | -5.75 | 1.54        | 1.61     |
| 35  | BB    | 1047 | G    | C3'-C2' | -5.75 | 1.46        | 1.52     |
| 35  | BB    | 1359 | A    | C5-C6   | -5.75 | 1.35        | 1.41     |
| 35  | BB    | 1381 | G    | P-O5'   | -5.75 | 1.54        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2868 | A    | C6-N6   | 5.75  | 1.38        | 1.33     |
| 1   | AA    | 407  | U    | O3'-P   | -5.75 | 1.54        | 1.61     |
| 1   | AA    | 978  | A    | N7-C5   | -5.75 | 1.35        | 1.39     |
| 1   | AA    | 1474 | U    | C1'-N1  | 5.75  | 1.57        | 1.48     |
| 35  | BB    | 25   | U    | C4-O4   | -5.75 | 1.19        | 1.23     |
| 35  | BB    | 1253 | A    | C3'-C2' | -5.75 | 1.46        | 1.52     |
| 35  | BB    | 1422 | G    | N9-C4   | -5.75 | 1.33        | 1.38     |
| 35  | BB    | 2753 | A    | C8-N7   | 5.75  | 1.35        | 1.31     |
| 35  | BB    | 2727 | A    | C6-N1   | 5.75  | 1.39        | 1.35     |
| 38  | BE    | 79   | ARG  | CZ-NH1  | 5.75  | 1.40        | 1.33     |
| 40  | BG    | 34   | ARG  | CZ-NH2  | 5.75  | 1.40        | 1.33     |
| 1   | AA    | 301  | G    | C2'-C1' | -5.74 | 1.47        | 1.53     |
| 1   | AA    | 360  | G    | N9-C8   | -5.74 | 1.33        | 1.37     |
| 1   | AA    | 376  | G    | C2-N3   | 5.74  | 1.37        | 1.32     |
| 1   | AA    | 877  | G    | C2'-C1' | -5.74 | 1.47        | 1.53     |
| 1   | AA    | 1069 | C    | C4'-C3' | 5.74  | 1.59        | 1.53     |
| 2   | AB    | 73   | ARG  | CZ-NH2  | 5.74  | 1.40        | 1.33     |
| 34  | BA    | 54   | G    | N1-C2   | 5.74  | 1.42        | 1.37     |
| 35  | BB    | 74   | A    | P-O5'   | -5.74 | 1.54        | 1.59     |
| 35  | BB    | 358  | U    | O3'-P   | -5.74 | 1.54        | 1.61     |
| 35  | BB    | 479  | A    | N7-C5   | -5.74 | 1.35        | 1.39     |
| 35  | BB    | 553  | G    | C2-N3   | 5.74  | 1.37        | 1.32     |
| 35  | BB    | 1831 | G    | N1-C2   | 5.74  | 1.42        | 1.37     |
| 35  | BB    | 1929 | G    | N9-C8   | 5.74  | 1.41        | 1.37     |
| 35  | BB    | 2272 | U    | C2-N3   | 5.74  | 1.41        | 1.37     |
| 35  | BB    | 2340 | A    | C3'-O3' | 5.74  | 1.50        | 1.42     |
| 35  | BB    | 2471 | A    | C6-N1   | 5.74  | 1.39        | 1.35     |
| 35  | BB    | 2498 | C    | N3-C4   | 5.74  | 1.38        | 1.33     |
| 35  | BB    | 2617 | U    | P-O5'   | -5.74 | 1.54        | 1.59     |
| 1   | AA    | 270  | A    | C2-N3   | 5.74  | 1.38        | 1.33     |
| 1   | AA    | 883  | C    | N3-C4   | 5.74  | 1.38        | 1.33     |
| 1   | AA    | 1340 | A    | C2'-C1' | -5.74 | 1.47        | 1.53     |
| 35  | BB    | 1652 | A    | N9-C8   | 5.74  | 1.42        | 1.37     |
| 1   | AA    | 1000 | A    | N7-C5   | -5.74 | 1.35        | 1.39     |
| 22  | AV    | 4    | C    | C4'-C3' | 5.74  | 1.59        | 1.53     |
| 35  | BB    | 56   | A    | C6-N6   | 5.74  | 1.38        | 1.33     |
| 35  | BB    | 919  | U    | N1-C6   | 5.74  | 1.43        | 1.38     |
| 35  | BB    | 1347 | A    | N7-C5   | -5.74 | 1.35        | 1.39     |
| 1   | AA    | 944  | G    | C2-N3   | 5.74  | 1.37        | 1.32     |
| 1   | AA    | 1221 | G    | N7-C5   | -5.74 | 1.35        | 1.39     |
| 34  | BA    | 2    | G    | C5-C6   | -5.74 | 1.36        | 1.42     |
| 35  | BB    | 71   | A    | O3'-P   | -5.74 | 1.54        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1380 | G    | C5-C6   | -5.74 | 1.36        | 1.42     |
| 35  | BB    | 1509 | A    | N9-C4   | 5.74  | 1.41        | 1.37     |
| 35  | BB    | 1588 | G    | N9-C8   | -5.74 | 1.33        | 1.37     |
| 35  | BB    | 2101 | A    | N9-C4   | -5.74 | 1.34        | 1.37     |
| 35  | BB    | 2115 | G    | C2-N3   | 5.74  | 1.37        | 1.32     |
| 35  | BB    | 2141 | G    | C2-N2   | 5.74  | 1.40        | 1.34     |
| 35  | BB    | 2534 | A    | N7-C5   | -5.74 | 1.35        | 1.39     |
| 35  | BB    | 2827 | C    | C4-N4   | 5.74  | 1.39        | 1.33     |
| 1   | AA    | 728  | A    | N7-C5   | -5.74 | 1.35        | 1.39     |
| 1   | AA    | 1060 | U    | C3'-O3' | -5.74 | 1.34        | 1.42     |
| 7   | AG    | 94   | ARG  | CZ-NH1  | 5.74  | 1.40        | 1.33     |
| 35  | BB    | 88   | G    | C4'-C3' | -5.74 | 1.46        | 1.52     |
| 35  | BB    | 179  | C    | C4-C5   | -5.74 | 1.38        | 1.43     |
| 35  | BB    | 450  | G    | C8-N7   | -5.74 | 1.27        | 1.30     |
| 35  | BB    | 1462 | C    | C2'-C1' | -5.74 | 1.47        | 1.53     |
| 35  | BB    | 1954 | G    | N3-C4   | 5.74  | 1.39        | 1.35     |
| 1   | AA    | 147  | G    | C8-N7   | -5.74 | 1.27        | 1.30     |
| 1   | AA    | 1221 | G    | C3'-O3' | 5.74  | 1.50        | 1.42     |
| 35  | BB    | 488  | G    | C2-N3   | 5.74  | 1.37        | 1.32     |
| 35  | BB    | 784  | G    | C8-N7   | 5.74  | 1.34        | 1.30     |
| 35  | BB    | 1271 | G    | C2-N2   | 5.74  | 1.40        | 1.34     |
| 35  | BB    | 1593 | A    | C5-C6   | -5.74 | 1.35        | 1.41     |
| 35  | BB    | 2261 | C    | N1-C6   | 5.74  | 1.40        | 1.37     |
| 35  | BB    | 2300 | C    | N1-C6   | 5.74  | 1.40        | 1.37     |
| 35  | BB    | 2458 | G    | C6-O6   | -5.74 | 1.19        | 1.24     |
| 1   | AA    | 1086 | U    | C1'-N1  | 5.73  | 1.57        | 1.48     |
| 35  | BB    | 763  | G    | N9-C4   | 5.73  | 1.42        | 1.38     |
| 1   | AA    | 505  | G    | C1'-N9  | -5.73 | 1.38        | 1.46     |
| 1   | AA    | 767  | A    | N3-C4   | -5.73 | 1.31        | 1.34     |
| 35  | BB    | 90   | U    | C5-C6   | 5.73  | 1.39        | 1.34     |
| 35  | BB    | 380  | G    | C3'-C2' | -5.73 | 1.46        | 1.52     |
| 35  | BB    | 1057 | A    | C3'-C2' | 5.73  | 1.59        | 1.52     |
| 35  | BB    | 2119 | A    | C8-N7   | 5.73  | 1.35        | 1.31     |
| 35  | BB    | 2234 | G    | N3-C4   | 5.73  | 1.39        | 1.35     |
| 35  | BB    | 2570 | G    | N3-C4   | -5.73 | 1.31        | 1.35     |
| 1   | AA    | 28   | A    | P-O5'   | -5.73 | 1.54        | 1.59     |
| 35  | BB    | 663  | G    | C2'-C1' | -5.73 | 1.47        | 1.53     |
| 35  | BB    | 1078 | U    | O4'-C1' | 5.73  | 1.49        | 1.41     |
| 35  | BB    | 1082 | U    | C4-O4   | 5.73  | 1.28        | 1.23     |
| 35  | BB    | 1419 | A    | C2'-C1' | -5.73 | 1.47        | 1.53     |
| 35  | BB    | 1964 | G    | C8-N7   | 5.73  | 1.34        | 1.30     |
| 35  | BB    | 2522 | U    | O3'-P   | -5.73 | 1.54        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 949  | A    | C5-C6   | -5.73 | 1.35        | 1.41     |
| 1   | AA    | 1179 | A    | N1-C2   | -5.73 | 1.29        | 1.34     |
| 1   | AA    | 1309 | G    | P-O5'   | -5.73 | 1.54        | 1.59     |
| 35  | BB    | 294  | A    | N3-C4   | -5.73 | 1.31        | 1.34     |
| 35  | BB    | 1331 | G    | C6-N1   | 5.73  | 1.43        | 1.39     |
| 1   | AA    | 206  | C    | C4'-O4' | 5.73  | 1.52        | 1.45     |
| 1   | AA    | 339  | C    | N1-C6   | -5.73 | 1.33        | 1.37     |
| 1   | AA    | 867  | G    | C4'-C3' | 5.73  | 1.59        | 1.53     |
| 1   | AA    | 946  | A    | N3-C4   | -5.73 | 1.31        | 1.34     |
| 1   | AA    | 949  | A    | C2'-C1' | -5.73 | 1.47        | 1.53     |
| 1   | AA    | 977  | A    | C3'-O3' | 5.73  | 1.50        | 1.42     |
| 1   | AA    | 1106 | G    | C5-C4   | 5.73  | 1.42        | 1.38     |
| 18  | AR    | 62   | ARG  | CD-NE   | 5.73  | 1.56        | 1.46     |
| 35  | BB    | 125  | A    | C6-N6   | 5.73  | 1.38        | 1.33     |
| 35  | BB    | 1125 | G    | C2-N2   | 5.73  | 1.40        | 1.34     |
| 35  | BB    | 1493 | C    | N1-C6   | 5.73  | 1.40        | 1.37     |
| 35  | BB    | 2141 | G    | N9-C4   | -5.73 | 1.33        | 1.38     |
| 35  | BB    | 2889 | C    | C4-N4   | 5.73  | 1.39        | 1.33     |
| 1   | AA    | 8    | A    | C8-N7   | -5.73 | 1.27        | 1.31     |
| 35  | BB    | 895  | U    | N3-C4   | 5.73  | 1.43        | 1.38     |
| 35  | BB    | 1362 | C    | N3-C4   | 5.73  | 1.38        | 1.33     |
| 35  | BB    | 2400 | G    | P-O5'   | -5.73 | 1.54        | 1.59     |
| 35  | BB    | 2843 | G    | N1-C2   | 5.73  | 1.42        | 1.37     |
| 1   | AA    | 1254 | A    | C1'-N9  | 5.72  | 1.57        | 1.48     |
| 7   | AG    | 145  | GLU  | CD-OE2  | 5.72  | 1.31        | 1.25     |
| 35  | BB    | 134  | G    | C2'-C1' | -5.72 | 1.47        | 1.53     |
| 35  | BB    | 173  | A    | N7-C5   | -5.72 | 1.35        | 1.39     |
| 35  | BB    | 1038 | G    | N7-C5   | -5.72 | 1.35        | 1.39     |
| 35  | BB    | 1530 | G    | N3-C4   | -5.72 | 1.31        | 1.35     |
| 35  | BB    | 1797 | G    | N3-C4   | -5.72 | 1.31        | 1.35     |
| 35  | BB    | 2359 | C    | C5'-C4' | 5.72  | 1.58        | 1.51     |
| 35  | BB    | 2761 | A    | C6-N6   | 5.72  | 1.38        | 1.33     |
| 37  | BD    | 82   | PHE  | CG-CD2  | 5.72  | 1.47        | 1.38     |
| 1   | AA    | 171  | A    | C4'-O4' | 5.72  | 1.52        | 1.45     |
| 1   | AA    | 454  | G    | O3'-P   | -5.72 | 1.54        | 1.61     |
| 1   | AA    | 725  | G    | C2'-C1' | -5.72 | 1.47        | 1.53     |
| 1   | AA    | 797  | C    | O4'-C1' | 5.72  | 1.49        | 1.41     |
| 1   | AA    | 1057 | G    | C6-N1   | -5.72 | 1.35        | 1.39     |
| 35  | BB    | 245  | G    | P-O5'   | -5.72 | 1.54        | 1.59     |
| 35  | BB    | 601  | C    | C1'-N1  | 5.72  | 1.57        | 1.48     |
| 35  | BB    | 778  | G    | N1-C2   | 5.72  | 1.42        | 1.37     |
| 35  | BB    | 2525 | G    | C3'-C2' | 5.72  | 1.59        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 585  | G    | C4'-C3' | -5.72 | 1.46        | 1.52     |
| 35  | BB    | 2264 | C    | C4'-C3' | 5.72  | 1.59        | 1.53     |
| 35  | BB    | 2416 | C    | P-O5'   | -5.72 | 1.54        | 1.59     |
| 1   | AA    | 646  | G    | C2-N3   | 5.72  | 1.37        | 1.32     |
| 1   | AA    | 925  | G    | C2'-C1' | -5.72 | 1.47        | 1.53     |
| 15  | AO    | 88   | ARG  | NE-CZ   | 5.72  | 1.40        | 1.33     |
| 35  | BB    | 379  | G    | C5'-C4' | 5.72  | 1.58        | 1.51     |
| 35  | BB    | 742  | A    | C2'-C1' | -5.72 | 1.47        | 1.53     |
| 35  | BB    | 1344 | U    | C5'-C4' | 5.72  | 1.58        | 1.51     |
| 35  | BB    | 1641 | A    | C4'-C3' | -5.72 | 1.46        | 1.52     |
| 35  | BB    | 1981 | A    | C2-N3   | 5.72  | 1.38        | 1.33     |
| 35  | BB    | 2272 | U    | N1-C2   | 5.72  | 1.43        | 1.38     |
| 35  | BB    | 2537 | U    | N1-C2   | 5.72  | 1.43        | 1.38     |
| 35  | BB    | 2622 | U    | C4'-O4' | -5.72 | 1.38        | 1.45     |
| 35  | BB    | 2899 | A    | C8-N7   | -5.72 | 1.27        | 1.31     |
| 1   | AA    | 925  | G    | C2-N3   | 5.72  | 1.37        | 1.32     |
| 35  | BB    | 910  | A    | N9-C4   | -5.72 | 1.34        | 1.37     |
| 35  | BB    | 1167 | C    | C4-C5   | -5.72 | 1.38        | 1.43     |
| 35  | BB    | 2765 | A    | N9-C4   | -5.72 | 1.34        | 1.37     |
| 35  | BB    | 2851 | A    | C6-N1   | 5.72  | 1.39        | 1.35     |
| 1   | AA    | 99   | C    | C4'-C3' | 5.72  | 1.59        | 1.53     |
| 1   | AA    | 100  | G    | N1-C2   | 5.72  | 1.42        | 1.37     |
| 1   | AA    | 123  | U    | C5'-C4' | 5.72  | 1.58        | 1.51     |
| 1   | AA    | 144  | G    | C2-N3   | 5.72  | 1.37        | 1.32     |
| 1   | AA    | 384  | G    | C3'-C2' | -5.72 | 1.46        | 1.52     |
| 1   | AA    | 784  | A    | C4'-C3' | 5.72  | 1.59        | 1.53     |
| 1   | AA    | 800  | G    | C8-N7   | 5.72  | 1.34        | 1.30     |
| 1   | AA    | 1458 | G    | C5-C6   | -5.72 | 1.36        | 1.42     |
| 35  | BB    | 90   | U    | C4'-C3' | 5.72  | 1.59        | 1.53     |
| 35  | BB    | 124  | G    | N7-C5   | -5.72 | 1.35        | 1.39     |
| 35  | BB    | 178  | G    | N1-C2   | 5.72  | 1.42        | 1.37     |
| 35  | BB    | 1103 | A    | P-O5'   | -5.72 | 1.54        | 1.59     |
| 35  | BB    | 1473 | G    | N3-C4   | -5.72 | 1.31        | 1.35     |
| 35  | BB    | 1962 | C    | C4-C5   | 5.72  | 1.47        | 1.43     |
| 35  | BB    | 2800 | A    | C6-N1   | 5.72  | 1.39        | 1.35     |
| 1   | AA    | 856  | C    | C4-C5   | 5.71  | 1.47        | 1.43     |
| 1   | AA    | 1370 | G    | C4'-O4' | 5.71  | 1.52        | 1.45     |
| 35  | BB    | 808  | G    | C2-N2   | 5.71  | 1.40        | 1.34     |
| 35  | BB    | 846  | U    | C4'-O4' | 5.71  | 1.52        | 1.45     |
| 35  | BB    | 1418 | G    | C5-C4   | 5.71  | 1.42        | 1.38     |
| 35  | BB    | 1436 | G    | C4'-C3' | -5.71 | 1.46        | 1.52     |
| 35  | BB    | 1652 | A    | N3-C4   | -5.71 | 1.31        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1832 | C    | C3'-C2' | 5.71  | 1.59        | 1.52     |
| 35  | BB    | 2184 | A    | O3'-P   | -5.71 | 1.54        | 1.61     |
| 35  | BB    | 2720 | U    | C2'-C1' | -5.71 | 1.47        | 1.53     |
| 35  | BB    | 2871 | U    | P-O5'   | -5.71 | 1.54        | 1.59     |
| 35  | BB    | 2880 | C    | C2'-C1' | -5.71 | 1.47        | 1.53     |
| 1   | AA    | 403  | C    | N1-C6   | -5.71 | 1.33        | 1.37     |
| 35  | BB    | 285  | G    | N7-C5   | -5.71 | 1.35        | 1.39     |
| 35  | BB    | 618  | G    | N1-C2   | 5.71  | 1.42        | 1.37     |
| 35  | BB    | 823  | C    | C5'-C4' | 5.71  | 1.58        | 1.51     |
| 35  | BB    | 1078 | U    | C1'-N1  | 5.71  | 1.57        | 1.48     |
| 35  | BB    | 1515 | A    | P-O5'   | -5.71 | 1.54        | 1.59     |
| 35  | BB    | 2396 | G    | N7-C5   | -5.71 | 1.35        | 1.39     |
| 1   | AA    | 58   | C    | C5'-C4' | 5.71  | 1.58        | 1.51     |
| 1   | AA    | 102  | G    | N3-C4   | 5.71  | 1.39        | 1.35     |
| 1   | AA    | 739  | C    | N3-C4   | 5.71  | 1.38        | 1.33     |
| 1   | AA    | 946  | A    | C3'-C2' | 5.71  | 1.59        | 1.52     |
| 13  | AM    | 89   | ARG  | CD-NE   | 5.71  | 1.56        | 1.46     |
| 34  | BA    | 75   | G    | C2-N2   | 5.71  | 1.40        | 1.34     |
| 34  | BA    | 96   | G    | N3-C4   | 5.71  | 1.39        | 1.35     |
| 35  | BB    | 1207 | C    | C2'-C1' | -5.71 | 1.47        | 1.53     |
| 35  | BB    | 1291 | C    | P-O5'   | -5.71 | 1.54        | 1.59     |
| 35  | BB    | 1619 | G    | O4'-C1' | 5.71  | 1.49        | 1.41     |
| 35  | BB    | 2163 | A    | N1-C2   | 5.71  | 1.39        | 1.34     |
| 35  | BB    | 2362 | C    | N1-C6   | 5.71  | 1.40        | 1.37     |
| 35  | BB    | 2479 | U    | C5'-C4' | 5.71  | 1.58        | 1.51     |
| 35  | BB    | 2521 | C    | C2'-C1' | -5.71 | 1.47        | 1.53     |
| 35  | BB    | 2666 | C    | O4'-C1' | -5.71 | 1.34        | 1.41     |
| 1   | AA    | 27   | G    | P-O5'   | -5.71 | 1.54        | 1.59     |
| 1   | AA    | 539  | A    | C6-N1   | 5.71  | 1.39        | 1.35     |
| 1   | AA    | 654  | G    | O3'-P   | -5.71 | 1.54        | 1.61     |
| 1   | AA    | 1396 | A    | C6-N6   | 5.71  | 1.38        | 1.33     |
| 1   | AA    | 146  | G    | O4'-C1' | 5.71  | 1.49        | 1.41     |
| 1   | AA    | 1169 | A    | N3-C4   | -5.71 | 1.31        | 1.34     |
| 1   | AA    | 1403 | C    | C2-N3   | -5.71 | 1.31        | 1.35     |
| 9   | AI    | 116  | GLY  | N-CA    | -5.71 | 1.37        | 1.46     |
| 22  | AV    | 7    | G    | P-O5'   | -5.71 | 1.54        | 1.59     |
| 35  | BB    | 308  | G    | N3-C4   | 5.71  | 1.39        | 1.35     |
| 35  | BB    | 832  | U    | O4'-C1' | 5.71  | 1.49        | 1.41     |
| 35  | BB    | 1643 | G    | C2-N3   | 5.71  | 1.37        | 1.32     |
| 35  | BB    | 2255 | G    | C3'-C2' | -5.71 | 1.46        | 1.52     |
| 35  | BB    | 2360 | G    | C8-N7   | -5.71 | 1.27        | 1.30     |
| 48  | BO    | 100  | HIS  | C-N     | 5.71  | 1.43        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 167  | A    | C2'-C1' | -5.71 | 1.47        | 1.53     |
| 1   | AA    | 177  | G    | C2'-C1' | -5.71 | 1.47        | 1.53     |
| 1   | AA    | 202  | G    | C3'-C2' | 5.71  | 1.59        | 1.52     |
| 1   | AA    | 336  | A    | C3'-C2' | -5.71 | 1.46        | 1.52     |
| 1   | AA    | 731  | G    | C2-N3   | -5.71 | 1.28        | 1.32     |
| 1   | AA    | 882  | C    | N1-C6   | 5.71  | 1.40        | 1.37     |
| 1   | AA    | 1152 | A    | N1-C2   | 5.71  | 1.39        | 1.34     |
| 1   | AA    | 1243 | C    | C4-C5   | 5.71  | 1.47        | 1.43     |
| 1   | AA    | 1276 | G    | N1-C2   | 5.71  | 1.42        | 1.37     |
| 34  | BA    | 59   | A    | N9-C4   | 5.71  | 1.41        | 1.37     |
| 35  | BB    | 1787 | A    | C2-N3   | 5.71  | 1.38        | 1.33     |
| 35  | BB    | 1813 | G    | C2-N3   | 5.71  | 1.37        | 1.32     |
| 35  | BB    | 2102 | G    | C5'-C4' | 5.71  | 1.58        | 1.51     |
| 35  | BB    | 2354 | C    | C4-N4   | 5.71  | 1.39        | 1.33     |
| 35  | BB    | 2379 | G    | C3'-O3' | 5.71  | 1.50        | 1.42     |
| 35  | BB    | 2702 | G    | C2-N3   | 5.71  | 1.37        | 1.32     |
| 34  | BA    | 97   | C    | N1-C6   | 5.71  | 1.40        | 1.37     |
| 35  | BB    | 1180 | U    | C2-O2   | 5.71  | 1.27        | 1.22     |
| 35  | BB    | 1229 | C    | C2-N3   | 5.71  | 1.40        | 1.35     |
| 35  | BB    | 1233 | C    | C3'-O3' | 5.71  | 1.50        | 1.42     |
| 35  | BB    | 1307 | A    | N3-C4   | -5.71 | 1.31        | 1.34     |
| 35  | BB    | 1338 | G    | O3'-P   | -5.71 | 1.54        | 1.61     |
| 35  | BB    | 2235 | G    | C2-N2   | 5.71  | 1.40        | 1.34     |
| 35  | BB    | 2377 | A    | C6-N1   | 5.71  | 1.39        | 1.35     |
| 1   | AA    | 984  | C    | C4-N4   | 5.70  | 1.39        | 1.33     |
| 1   | AA    | 1385 | G    | C4'-C3' | 5.70  | 1.59        | 1.53     |
| 35  | BB    | 328  | U    | C4-C5   | 5.70  | 1.48        | 1.43     |
| 35  | BB    | 1056 | G    | C5'-C4' | -5.70 | 1.44        | 1.51     |
| 35  | BB    | 1456 | G    | N1-C2   | 5.70  | 1.42        | 1.37     |
| 35  | BB    | 1488 | C    | N3-C4   | 5.70  | 1.38        | 1.33     |
| 35  | BB    | 2079 | U    | N1-C2   | -5.70 | 1.33        | 1.38     |
| 35  | BB    | 2106 | U    | C3'-C2' | -5.70 | 1.46        | 1.52     |
| 35  | BB    | 2136 | G    | N9-C8   | 5.70  | 1.41        | 1.37     |
| 35  | BB    | 2186 | G    | C1'-N9  | 5.70  | 1.57        | 1.48     |
| 35  | BB    | 2477 | U    | P-O5'   | -5.70 | 1.54        | 1.59     |
| 35  | BB    | 2555 | U    | N3-C4   | 5.70  | 1.43        | 1.38     |
| 35  | BB    | 2842 | G    | C3'-C2' | 5.70  | 1.59        | 1.52     |
| 1   | AA    | 311  | C    | C2-N3   | -5.70 | 1.31        | 1.35     |
| 1   | AA    | 1502 | A    | C2'-C1' | -5.70 | 1.47        | 1.53     |
| 35  | BB    | 1157 | G    | C4'-O4' | 5.70  | 1.52        | 1.45     |
| 35  | BB    | 1411 | U    | C5'-C4' | 5.70  | 1.58        | 1.51     |
| 35  | BB    | 1634 | A    | C6-N1   | 5.70  | 1.39        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2086 | U    | O3'-P   | -5.70 | 1.54        | 1.61     |
| 1   | AA    | 65   | A    | C4'-C3' | 5.70  | 1.59        | 1.53     |
| 1   | AA    | 355  | C    | C3'-C2' | -5.70 | 1.46        | 1.52     |
| 1   | AA    | 564  | C    | C2-N3   | 5.70  | 1.40        | 1.35     |
| 1   | AA    | 1125 | U    | C5'-C4' | 5.70  | 1.58        | 1.51     |
| 34  | BA    | 22   | U    | N1-C2   | 5.70  | 1.43        | 1.38     |
| 35  | BB    | 271  | G    | N1-C2   | 5.70  | 1.42        | 1.37     |
| 35  | BB    | 301  | G    | N7-C5   | -5.70 | 1.35        | 1.39     |
| 35  | BB    | 1036 | G    | C2'-C1' | -5.70 | 1.47        | 1.53     |
| 35  | BB    | 1496 | A    | N3-C4   | 5.70  | 1.38        | 1.34     |
| 35  | BB    | 1680 | U    | N1-C2   | 5.70  | 1.43        | 1.38     |
| 35  | BB    | 2542 | A    | C2-N3   | 5.70  | 1.38        | 1.33     |
| 1   | AA    | 396  | C    | C4-N4   | 5.70  | 1.39        | 1.33     |
| 34  | BA    | 97   | C    | C2-N3   | 5.70  | 1.40        | 1.35     |
| 35  | BB    | 720  | U    | C4-C5   | 5.70  | 1.48        | 1.43     |
| 35  | BB    | 1530 | G    | C2'-C1' | -5.70 | 1.47        | 1.53     |
| 35  | BB    | 2759 | G    | N9-C4   | 5.70  | 1.42        | 1.38     |
| 35  | BB    | 2783 | U    | N3-C4   | 5.70  | 1.43        | 1.38     |
| 45  | BL    | 41   | ARG  | CD-NE   | 5.70  | 1.56        | 1.46     |
| 1   | AA    | 288  | A    | C5'-C4' | 5.70  | 1.58        | 1.51     |
| 1   | AA    | 661  | G    | C4'-O4' | -5.70 | 1.38        | 1.45     |
| 1   | AA    | 806  | C    | C5-C6   | -5.70 | 1.29        | 1.34     |
| 1   | AA    | 1430 | A    | C5-C4   | 5.70  | 1.42        | 1.38     |
| 1   | AA    | 92   | U    | C3'-C2' | 5.70  | 1.59        | 1.52     |
| 1   | AA    | 726  | C    | C3'-C2' | 5.70  | 1.59        | 1.52     |
| 1   | AA    | 801  | U    | C2-N3   | 5.70  | 1.41        | 1.37     |
| 35  | BB    | 226  | A    | C2'-C1' | -5.70 | 1.47        | 1.53     |
| 35  | BB    | 1086 | A    | C2-N3   | 5.70  | 1.38        | 1.33     |
| 35  | BB    | 1204 | A    | N3-C4   | 5.70  | 1.38        | 1.34     |
| 35  | BB    | 1643 | G    | C5-C4   | 5.70  | 1.42        | 1.38     |
| 35  | BB    | 2694 | G    | N9-C4   | -5.70 | 1.33        | 1.38     |
| 35  | BB    | 2865 | U    | O3'-P   | -5.70 | 1.54        | 1.61     |
| 40  | BG    | 152  | ARG  | CD-NE   | 5.70  | 1.56        | 1.46     |
| 1   | AA    | 1219 | A    | P-O5'   | -5.69 | 1.54        | 1.59     |
| 35  | BB    | 150  | U    | C2'-C1' | -5.69 | 1.47        | 1.53     |
| 35  | BB    | 2482 | A    | O4'-C1' | 5.69  | 1.49        | 1.41     |
| 35  | BB    | 2516 | A    | C2-N3   | -5.69 | 1.28        | 1.33     |
| 1   | AA    | 113  | G    | C2-N3   | 5.69  | 1.37        | 1.32     |
| 1   | AA    | 530  | G    | N3-C4   | -5.69 | 1.31        | 1.35     |
| 1   | AA    | 801  | U    | N1-C6   | 5.69  | 1.43        | 1.38     |
| 1   | AA    | 940  | C    | C4'-O4' | -5.69 | 1.38        | 1.45     |
| 34  | BA    | 25   | U    | C2-N3   | 5.69  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 173  | A    | C6-N6   | 5.69  | 1.38        | 1.33     |
| 35  | BB    | 382  | A    | C8-N7   | 5.69  | 1.35        | 1.31     |
| 35  | BB    | 1201 | U    | C4-C5   | 5.69  | 1.48        | 1.43     |
| 35  | BB    | 1279 | G    | C2-N2   | 5.69  | 1.40        | 1.34     |
| 35  | BB    | 1897 | G    | C2-N2   | 5.69  | 1.40        | 1.34     |
| 35  | BB    | 2071 | A    | C6-N6   | 5.69  | 1.38        | 1.33     |
| 35  | BB    | 2177 | C    | P-O5'   | 5.69  | 1.65        | 1.59     |
| 35  | BB    | 2461 | A    | N1-C2   | 5.69  | 1.39        | 1.34     |
| 35  | BB    | 2716 | C    | C2'-C1' | -5.69 | 1.47        | 1.53     |
| 35  | BB    | 2778 | A    | C2-N3   | 5.69  | 1.38        | 1.33     |
| 1   | AA    | 108  | G    | C5-C4   | -5.69 | 1.34        | 1.38     |
| 1   | AA    | 689  | C    | O3'-P   | -5.69 | 1.54        | 1.61     |
| 1   | AA    | 1331 | G    | N7-C5   | -5.69 | 1.35        | 1.39     |
| 35  | BB    | 165  | A    | N9-C4   | -5.69 | 1.34        | 1.37     |
| 35  | BB    | 566  | U    | P-O5'   | -5.69 | 1.54        | 1.59     |
| 35  | BB    | 1604 | C    | O3'-P   | -5.69 | 1.54        | 1.61     |
| 35  | BB    | 1768 | C    | P-O5'   | -5.69 | 1.54        | 1.59     |
| 35  | BB    | 2028 | U    | P-O5'   | -5.69 | 1.54        | 1.59     |
| 1   | AA    | 138  | G    | C3'-O3' | 5.69  | 1.50        | 1.42     |
| 1   | AA    | 1244 | G    | N9-C8   | 5.69  | 1.41        | 1.37     |
| 1   | AA    | 1311 | A    | C6-N6   | 5.69  | 1.38        | 1.33     |
| 1   | AA    | 1521 | C    | C2-N3   | 5.69  | 1.40        | 1.35     |
| 35  | BB    | 1773 | A    | C4'-O4' | -5.69 | 1.38        | 1.45     |
| 35  | BB    | 2885 | G    | N9-C8   | 5.69  | 1.41        | 1.37     |
| 1   | AA    | 309  | A    | C4'-C3' | 5.69  | 1.59        | 1.53     |
| 1   | AA    | 352  | C    | C5-C6   | 5.69  | 1.39        | 1.34     |
| 1   | AA    | 499  | A    | C6-N6   | 5.69  | 1.38        | 1.33     |
| 1   | AA    | 778  | G    | N9-C8   | 5.69  | 1.41        | 1.37     |
| 1   | AA    | 996  | A    | C2'-C1' | -5.69 | 1.47        | 1.53     |
| 35  | BB    | 847  | U    | C2'-O2' | -5.69 | 1.34        | 1.41     |
| 35  | BB    | 1051 | G    | O4'-C1' | 5.69  | 1.49        | 1.41     |
| 35  | BB    | 2038 | G    | N9-C8   | 5.69  | 1.41        | 1.37     |
| 35  | BB    | 2731 | G    | C4'-C3' | 5.69  | 1.59        | 1.53     |
| 35  | BB    | 2875 | C    | C2-O2   | -5.69 | 1.19        | 1.24     |
| 35  | BB    | 900  | A    | C5-C6   | -5.69 | 1.35        | 1.41     |
| 35  | BB    | 1511 | G    | N1-C2   | 5.69  | 1.42        | 1.37     |
| 35  | BB    | 1900 | A    | C6-N1   | 5.69  | 1.39        | 1.35     |
| 35  | BB    | 2312 | U    | N1-C2   | 5.69  | 1.43        | 1.38     |
| 35  | BB    | 2847 | U    | C4-O4   | 5.69  | 1.28        | 1.23     |
| 1   | AA    | 300  | A    | P-O5'   | -5.68 | 1.54        | 1.59     |
| 1   | AA    | 1176 | A    | C3'-C2' | -5.68 | 1.46        | 1.52     |
| 1   | AA    | 1516 | G    | O3'-P   | -5.68 | 1.54        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2    | G    | P-O5'   | 5.68  | 1.65        | 1.59     |
| 35  | BB    | 244  | A    | N9-C8   | 5.68  | 1.42        | 1.37     |
| 35  | BB    | 1384 | A    | C6-N1   | 5.68  | 1.39        | 1.35     |
| 35  | BB    | 1456 | G    | C8-N7   | 5.68  | 1.34        | 1.30     |
| 35  | BB    | 1572 | A    | O3'-P   | -5.68 | 1.54        | 1.61     |
| 35  | BB    | 1728 | C    | C2-O2   | 5.68  | 1.29        | 1.24     |
| 35  | BB    | 2388 | A    | C2-N3   | 5.68  | 1.38        | 1.33     |
| 1   | AA    | 136  | C    | N1-C2   | 5.68  | 1.45        | 1.40     |
| 1   | AA    | 761  | G    | C8-N7   | -5.68 | 1.27        | 1.30     |
| 1   | AA    | 942  | G    | N9-C8   | 5.68  | 1.41        | 1.37     |
| 1   | AA    | 1004 | A    | C5'-C4' | 5.68  | 1.58        | 1.51     |
| 1   | AA    | 1474 | U    | C4-C5   | 5.68  | 1.48        | 1.43     |
| 35  | BB    | 712  | G    | O4'-C1' | -5.68 | 1.34        | 1.41     |
| 35  | BB    | 1537 | G    | N9-C4   | 5.68  | 1.42        | 1.38     |
| 35  | BB    | 1651 | G    | N7-C5   | -5.68 | 1.35        | 1.39     |
| 35  | BB    | 1821 | A    | C2'-O2' | -5.68 | 1.34        | 1.41     |
| 35  | BB    | 2072 | C    | N1-C2   | 5.68  | 1.45        | 1.40     |
| 35  | BB    | 2594 | C    | C4-N4   | 5.68  | 1.39        | 1.33     |
| 35  | BB    | 2780 | G    | C6-N1   | 5.68  | 1.43        | 1.39     |
| 5   | AE    | 44   | ARG  | CZ-NH1  | 5.68  | 1.40        | 1.33     |
| 35  | BB    | 581  | C    | N3-C4   | 5.68  | 1.38        | 1.33     |
| 35  | BB    | 1530 | G    | O3'-P   | -5.68 | 1.54        | 1.61     |
| 35  | BB    | 1868 | C    | C5'-C4' | 5.68  | 1.58        | 1.51     |
| 1   | AA    | 749  | A    | C8-N7   | -5.68 | 1.27        | 1.31     |
| 1   | AA    | 880  | C    | C2'-C1' | -5.68 | 1.47        | 1.53     |
| 1   | AA    | 897  | C    | N1-C2   | 5.68  | 1.45        | 1.40     |
| 1   | AA    | 1202 | U    | C3'-C2' | 5.68  | 1.59        | 1.52     |
| 35  | BB    | 537  | G    | N9-C8   | -5.68 | 1.33        | 1.37     |
| 35  | BB    | 1513 | U    | C1'-N1  | 5.68  | 1.57        | 1.48     |
| 35  | BB    | 2002 | G    | C5-C6   | -5.68 | 1.36        | 1.42     |
| 35  | BB    | 2013 | A    | N9-C8   | -5.68 | 1.33        | 1.37     |
| 35  | BB    | 2274 | A    | N9-C4   | -5.68 | 1.34        | 1.37     |
| 1   | AA    | 476  | U    | N3-C4   | 5.68  | 1.43        | 1.38     |
| 1   | AA    | 783  | C    | C2'-C1' | -5.68 | 1.47        | 1.53     |
| 35  | BB    | 520  | G    | O3'-P   | -5.68 | 1.54        | 1.61     |
| 35  | BB    | 1012 | U    | N1-C6   | -5.68 | 1.32        | 1.38     |
| 35  | BB    | 1888 | G    | P-O5'   | -5.68 | 1.54        | 1.59     |
| 1   | AA    | 389  | A    | C1'-N9  | 5.68  | 1.57        | 1.48     |
| 1   | AA    | 535  | A    | C1'-N9  | -5.68 | 1.39        | 1.46     |
| 1   | AA    | 574  | A    | C4'-C3' | 5.68  | 1.59        | 1.53     |
| 1   | AA    | 1307 | U    | O3'-P   | -5.68 | 1.54        | 1.61     |
| 16  | AP    | 51   | ARG  | CD-NE   | 5.68  | 1.56        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 573  | U    | C5'-C4' | 5.68  | 1.58        | 1.51     |
| 35  | BB    | 648  | G    | C8-N7   | -5.68 | 1.27        | 1.30     |
| 35  | BB    | 983  | A    | N3-C4   | -5.68 | 1.31        | 1.34     |
| 35  | BB    | 1479 | G    | C5-C6   | -5.68 | 1.36        | 1.42     |
| 35  | BB    | 1735 | A    | C8-N7   | -5.68 | 1.27        | 1.31     |
| 35  | BB    | 2120 | G    | N9-C4   | -5.68 | 1.33        | 1.38     |
| 35  | BB    | 2196 | C    | C2-O2   | 5.68  | 1.29        | 1.24     |
| 35  | BB    | 2665 | A    | N3-C4   | 5.68  | 1.38        | 1.34     |
| 35  | BB    | 2868 | A    | C3'-O3' | 5.68  | 1.50        | 1.42     |
| 1   | AA    | 361  | G    | C1'-N9  | 5.67  | 1.57        | 1.48     |
| 1   | AA    | 614  | C    | C4-N4   | 5.67  | 1.39        | 1.33     |
| 1   | AA    | 892  | A    | N7-C5   | -5.67 | 1.35        | 1.39     |
| 2   | AB    | 20   | ARG  | CD-NE   | 5.67  | 1.56        | 1.46     |
| 35  | BB    | 245  | G    | C2-N3   | 5.67  | 1.37        | 1.32     |
| 35  | BB    | 664  | G    | C2'-C1' | -5.67 | 1.47        | 1.53     |
| 35  | BB    | 1655 | A    | O3'-P   | -5.67 | 1.54        | 1.61     |
| 35  | BB    | 2118 | U    | C5'-C4' | 5.67  | 1.58        | 1.51     |
| 35  | BB    | 2357 | G    | C2-N3   | 5.67  | 1.37        | 1.32     |
| 35  | BB    | 2857 | G    | N9-C8   | 5.67  | 1.41        | 1.37     |
| 41  | BH    | 25   | TYR  | CE2-CZ  | 5.67  | 1.46        | 1.38     |
| 44  | BK    | 1    | MET  | CA-CB   | 5.67  | 1.66        | 1.53     |
| 35  | BB    | 1414 | C    | C2-O2   | 5.67  | 1.29        | 1.24     |
| 35  | BB    | 1567 | G    | C2'-C1' | -5.67 | 1.47        | 1.53     |
| 35  | BB    | 1569 | A    | C5-C6   | -5.67 | 1.35        | 1.41     |
| 35  | BB    | 153  | U    | N1-C2   | 5.67  | 1.43        | 1.38     |
| 35  | BB    | 2210 | U    | C5'-C4' | -5.67 | 1.44        | 1.51     |
| 35  | BB    | 2654 | A    | N9-C8   | -5.67 | 1.33        | 1.37     |
| 1   | AA    | 139  | A    | C2-N3   | -5.67 | 1.28        | 1.33     |
| 1   | AA    | 424  | G    | C2'-C1' | -5.67 | 1.47        | 1.53     |
| 35  | BB    | 631  | A    | C2'-C1' | 5.67  | 1.59        | 1.53     |
| 35  | BB    | 1341 | G    | P-O5'   | -5.67 | 1.54        | 1.59     |
| 35  | BB    | 2256 | G    | P-O5'   | 5.67  | 1.65        | 1.59     |
| 1   | AA    | 39   | G    | C6-O6   | -5.67 | 1.19        | 1.24     |
| 1   | AA    | 536  | C    | O3'-P   | -5.67 | 1.54        | 1.61     |
| 1   | AA    | 1060 | U    | C4-O4   | -5.67 | 1.19        | 1.23     |
| 35  | BB    | 145  | C    | C2-N3   | 5.67  | 1.40        | 1.35     |
| 35  | BB    | 275  | C    | C5-C6   | 5.67  | 1.38        | 1.34     |
| 35  | BB    | 522  | A    | C6-N1   | 5.67  | 1.39        | 1.35     |
| 35  | BB    | 527  | C    | C2'-C1' | -5.67 | 1.47        | 1.53     |
| 35  | BB    | 618  | G    | C5-C4   | -5.67 | 1.34        | 1.38     |
| 35  | BB    | 2468 | A    | C2'-C1' | -5.67 | 1.47        | 1.53     |
| 1   | AA    | 198  | G    | C4'-C3' | 5.67  | 1.59        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 569  | C    | N3-C4   | 5.67  | 1.38        | 1.33     |
| 1   | AA    | 878  | A    | C6-N1   | 5.67  | 1.39        | 1.35     |
| 3   | AC    | 39   | ARG  | NE-CZ   | 5.67  | 1.40        | 1.33     |
| 35  | BB    | 1788 | C    | C4'-C3' | 5.67  | 1.59        | 1.53     |
| 35  | BB    | 1981 | A    | N9-C4   | -5.67 | 1.34        | 1.37     |
| 35  | BB    | 2626 | C    | C4-C5   | 5.67  | 1.47        | 1.43     |
| 1   | AA    | 782  | A    | C6-N1   | 5.67  | 1.39        | 1.35     |
| 1   | AA    | 1097 | C    | C4-N4   | 5.67  | 1.39        | 1.33     |
| 35  | BB    | 366  | C    | P-O5'   | -5.66 | 1.54        | 1.59     |
| 35  | BB    | 1304 | A    | C4'-O4' | -5.66 | 1.38        | 1.45     |
| 35  | BB    | 1566 | A    | C4'-O4' | -5.66 | 1.38        | 1.45     |
| 35  | BB    | 1863 | G    | C2'-C1' | -5.66 | 1.47        | 1.53     |
| 35  | BB    | 1985 | C    | C3'-C2' | -5.66 | 1.46        | 1.52     |
| 35  | BB    | 2172 | U    | C3'-O3' | 5.66  | 1.50        | 1.42     |
| 35  | BB    | 2559 | C    | O3'-P   | -5.66 | 1.54        | 1.61     |
| 35  | BB    | 2803 | G    | P-O5'   | -5.66 | 1.54        | 1.59     |
| 35  | BB    | 2811 | G    | C6-O6   | 5.66  | 1.29        | 1.24     |
| 1   | AA    | 140  | U    | C4'-O4' | 5.66  | 1.52        | 1.45     |
| 1   | AA    | 503  | C    | O4'-C1' | 5.66  | 1.49        | 1.41     |
| 1   | AA    | 737  | C    | O4'-C1' | 5.66  | 1.49        | 1.41     |
| 1   | AA    | 1072 | G    | C2'-C1' | -5.66 | 1.47        | 1.53     |
| 1   | AA    | 1493 | A    | C1'-N9  | 5.66  | 1.57        | 1.48     |
| 35  | BB    | 689  | A    | C2-N3   | 5.66  | 1.38        | 1.33     |
| 35  | BB    | 1230 | A    | C5-C4   | -5.66 | 1.34        | 1.38     |
| 35  | BB    | 1761 | C    | O4'-C1' | -5.66 | 1.34        | 1.41     |
| 35  | BB    | 2296 | U    | C4'-C3' | 5.66  | 1.59        | 1.53     |
| 35  | BB    | 2751 | G    | C2-N2   | 5.66  | 1.40        | 1.34     |
| 1   | AA    | 394  | G    | C4'-C3' | -5.66 | 1.46        | 1.52     |
| 1   | AA    | 573  | A    | N9-C4   | 5.66  | 1.41        | 1.37     |
| 1   | AA    | 850  | U    | C4'-C3' | 5.66  | 1.59        | 1.53     |
| 1   | AA    | 886  | G    | C8-N7   | 5.66  | 1.34        | 1.30     |
| 1   | AA    | 1088 | G    | C8-N7   | -5.66 | 1.27        | 1.30     |
| 12  | AL    | 85   | ARG  | CD-NE   | 5.66  | 1.56        | 1.46     |
| 35  | BB    | 218  | A    | C5-C6   | -5.66 | 1.35        | 1.41     |
| 35  | BB    | 802  | A    | C5'-C4' | 5.66  | 1.58        | 1.51     |
| 35  | BB    | 2279 | G    | C3'-C2' | -5.66 | 1.46        | 1.52     |
| 35  | BB    | 2823 | A    | N7-C5   | -5.66 | 1.35        | 1.39     |
| 1   | AA    | 345  | C    | C2-N3   | -5.66 | 1.31        | 1.35     |
| 1   | AA    | 369  | G    | C2-N3   | 5.66  | 1.37        | 1.32     |
| 1   | AA    | 615  | G    | N9-C8   | -5.66 | 1.33        | 1.37     |
| 1   | AA    | 656  | G    | C8-N7   | 5.66  | 1.34        | 1.30     |
| 1   | AA    | 1322 | C    | C4-N4   | 5.66  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | AD    | 12   | ARG  | CD-NE   | 5.66  | 1.56        | 1.46     |
| 35  | BB    | 213  | A    | C5-C4   | 5.66  | 1.42        | 1.38     |
| 35  | BB    | 2363 | G    | C3'-C2' | 5.66  | 1.59        | 1.52     |
| 35  | BB    | 2465 | C    | C5-C6   | -5.66 | 1.29        | 1.34     |
| 35  | BB    | 2737 | G    | N7-C5   | -5.66 | 1.35        | 1.39     |
| 39  | BF    | 111  | ARG  | CZ-NH2  | 5.66  | 1.40        | 1.33     |
| 43  | BJ    | 75   | TYR  | N-CA    | -5.66 | 1.35        | 1.46     |
| 1   | AA    | 387  | U    | O3'-P   | -5.66 | 1.54        | 1.61     |
| 1   | AA    | 724  | G    | C5'-C4' | -5.66 | 1.44        | 1.51     |
| 35  | BB    | 1151 | A    | C4'-O4' | -5.66 | 1.38        | 1.45     |
| 1   | AA    | 541  | G    | N3-C4   | 5.66  | 1.39        | 1.35     |
| 35  | BB    | 340  | A    | P-O5'   | -5.66 | 1.54        | 1.59     |
| 35  | BB    | 593  | U    | C4-C5   | 5.66  | 1.48        | 1.43     |
| 35  | BB    | 1047 | G    | C5-C6   | -5.66 | 1.36        | 1.42     |
| 35  | BB    | 1139 | G    | N3-C4   | -5.66 | 1.31        | 1.35     |
| 35  | BB    | 1216 | G    | C8-N7   | -5.66 | 1.27        | 1.30     |
| 35  | BB    | 1483 | G    | C5-C4   | -5.66 | 1.34        | 1.38     |
| 35  | BB    | 1777 | U    | C3'-O3' | 5.66  | 1.50        | 1.42     |
| 35  | BB    | 2039 | U    | P-O5'   | -5.66 | 1.54        | 1.59     |
| 43  | BJ    | 37   | ARG  | NE-CZ   | 5.66  | 1.40        | 1.33     |
| 1   | AA    | 611  | C    | O3'-P   | -5.65 | 1.54        | 1.61     |
| 35  | BB    | 311  | A    | O3'-P   | -5.65 | 1.54        | 1.61     |
| 35  | BB    | 561  | G    | C5'-C4' | 5.65  | 1.58        | 1.51     |
| 35  | BB    | 1959 | G    | C2'-C1' | -5.65 | 1.47        | 1.53     |
| 1   | AA    | 1371 | G    | C2-N2   | 5.65  | 1.40        | 1.34     |
| 14  | AN    | 25   | GLU  | CD-OE2  | 5.65  | 1.31        | 1.25     |
| 35  | BB    | 1257 | C    | C2'-O2' | -5.65 | 1.34        | 1.41     |
| 35  | BB    | 1649 | G    | C2-N2   | 5.65  | 1.40        | 1.34     |
| 35  | BB    | 1822 | C    | C2-O2   | 5.65  | 1.29        | 1.24     |
| 35  | BB    | 2183 | A    | C6-N6   | 5.65  | 1.38        | 1.33     |
| 35  | BB    | 2565 | A    | C6-N6   | 5.65  | 1.38        | 1.33     |
| 50  | BQ    | 10   | ARG  | NE-CZ   | 5.65  | 1.40        | 1.33     |
| 1   | AA    | 367  | U    | C4'-C3' | -5.65 | 1.46        | 1.52     |
| 1   | AA    | 413  | G    | C6-N1   | 5.65  | 1.43        | 1.39     |
| 1   | AA    | 947  | G    | N9-C4   | -5.65 | 1.33        | 1.38     |
| 1   | AA    | 1197 | A    | C5-C6   | -5.65 | 1.35        | 1.41     |
| 35  | BB    | 674  | G    | C6-N1   | 5.65  | 1.43        | 1.39     |
| 35  | BB    | 1410 | G    | N7-C5   | -5.65 | 1.35        | 1.39     |
| 35  | BB    | 2201 | G    | C2-N3   | 5.65  | 1.37        | 1.32     |
| 35  | BB    | 2486 | C    | C4-C5   | -5.65 | 1.38        | 1.43     |
| 1   | AA    | 82   | G    | C2'-C1' | -5.65 | 1.47        | 1.53     |
| 35  | BB    | 1124 | G    | C8-N7   | 5.65  | 1.34        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1327 | A    | C5-C4   | -5.65 | 1.34        | 1.38     |
| 1   | AA    | 40   | C    | C5-C6   | -5.65 | 1.29        | 1.34     |
| 1   | AA    | 153  | C    | O3'-P   | 5.65  | 1.68        | 1.61     |
| 1   | AA    | 417  | G    | C2'-C1' | 5.65  | 1.59        | 1.53     |
| 1   | AA    | 514  | C    | N1-C6   | 5.65  | 1.40        | 1.37     |
| 1   | AA    | 540  | G    | C2-N3   | 5.65  | 1.37        | 1.32     |
| 1   | AA    | 917  | G    | O3'-P   | -5.65 | 1.54        | 1.61     |
| 1   | AA    | 1328 | C    | O3'-P   | -5.65 | 1.54        | 1.61     |
| 35  | BB    | 354  | A    | N9-C4   | -5.65 | 1.34        | 1.37     |
| 44  | BK    | 17   | ARG  | CZ-NH2  | 5.65  | 1.40        | 1.33     |
| 1   | AA    | 890  | G    | C4'-O4' | -5.65 | 1.38        | 1.45     |
| 25  | B0    | 14   | GLY  | CA-C    | -5.65 | 1.42        | 1.51     |
| 35  | BB    | 137  | U    | C2-N3   | 5.65  | 1.41        | 1.37     |
| 35  | BB    | 1085 | A    | O3'-P   | -5.65 | 1.54        | 1.61     |
| 35  | BB    | 1480 | C    | C5'-C4' | 5.65  | 1.58        | 1.51     |
| 35  | BB    | 1516 | G    | C5-C4   | 5.65  | 1.42        | 1.38     |
| 35  | BB    | 2539 | C    | O4'-C1' | -5.65 | 1.34        | 1.41     |
| 1   | AA    | 84   | U    | C2'-C1' | 5.64  | 1.59        | 1.53     |
| 1   | AA    | 724  | G    | N3-C4   | -5.64 | 1.31        | 1.35     |
| 1   | AA    | 1481 | U    | N1-C6   | -5.64 | 1.32        | 1.38     |
| 35  | BB    | 367  | G    | C2'-C1' | -5.64 | 1.47        | 1.53     |
| 35  | BB    | 1162 | G    | C2-N2   | 5.64  | 1.40        | 1.34     |
| 35  | BB    | 1507 | C    | C1'-N1  | 5.64  | 1.57        | 1.48     |
| 35  | BB    | 1814 | G    | C4'-O4' | 5.64  | 1.52        | 1.45     |
| 35  | BB    | 1866 | A    | O4'-C1' | 5.64  | 1.49        | 1.41     |
| 35  | BB    | 1975 | G    | C2'-C1' | -5.64 | 1.47        | 1.53     |
| 35  | BB    | 2029 | G    | N9-C4   | -5.64 | 1.33        | 1.38     |
| 35  | BB    | 2366 | A    | C6-N1   | -5.64 | 1.31        | 1.35     |
| 35  | BB    | 2703 | C    | C1'-N1  | 5.64  | 1.57        | 1.48     |
| 1   | AA    | 422  | C    | N3-C4   | 5.64  | 1.38        | 1.33     |
| 1   | AA    | 847  | G    | C8-N7   | -5.64 | 1.27        | 1.30     |
| 30  | B5    | 134  | ARG  | CD-NE   | 5.64  | 1.56        | 1.46     |
| 35  | BB    | 175  | G    | N3-C4   | -5.64 | 1.31        | 1.35     |
| 35  | BB    | 455  | C    | C2-N3   | 5.64  | 1.40        | 1.35     |
| 35  | BB    | 1168 | G    | C4'-C3' | 5.64  | 1.59        | 1.53     |
| 35  | BB    | 2804 | U    | C5'-C4' | 5.64  | 1.58        | 1.51     |
| 1   | AA    | 1157 | A    | C2'-C1' | -5.64 | 1.47        | 1.53     |
| 35  | BB    | 899  | A    | P-O5'   | -5.64 | 1.54        | 1.59     |
| 35  | BB    | 2153 | C    | O3'-P   | -5.64 | 1.54        | 1.61     |
| 35  | BB    | 2660 | A    | O4'-C1' | 5.64  | 1.49        | 1.41     |
| 1   | AA    | 154  | U    | N1-C2   | -5.64 | 1.33        | 1.38     |
| 1   | AA    | 363  | A    | C3'-C2' | -5.64 | 1.46        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 477  | C    | C2'-C1' | -5.64 | 1.47        | 1.53     |
| 35  | BB    | 848  | C    | C2-N3   | 5.64  | 1.40        | 1.35     |
| 35  | BB    | 1130 | U    | O3'-P   | -5.64 | 1.54        | 1.61     |
| 35  | BB    | 1733 | G    | N1-C2   | 5.64  | 1.42        | 1.37     |
| 35  | BB    | 1987 | A    | C6-N6   | 5.64  | 1.38        | 1.33     |
| 35  | BB    | 2157 | G    | C5-C6   | -5.64 | 1.36        | 1.42     |
| 35  | BB    | 2159 | G    | C2'-C1' | 5.64  | 1.59        | 1.53     |
| 35  | BB    | 2371 | G    | N3-C4   | -5.64 | 1.31        | 1.35     |
| 35  | BB    | 2375 | G    | C8-N7   | -5.64 | 1.27        | 1.30     |
| 35  | BB    | 2863 | C    | C4-N4   | 5.64  | 1.39        | 1.33     |
| 1   | AA    | 316  | C    | O4'-C1' | 5.64  | 1.49        | 1.41     |
| 35  | BB    | 124  | G    | C8-N7   | -5.64 | 1.27        | 1.30     |
| 35  | BB    | 374  | A    | O4'-C1' | -5.64 | 1.34        | 1.41     |
| 35  | BB    | 1179 | G    | C2-N3   | 5.64  | 1.37        | 1.32     |
| 1   | AA    | 588  | G    | C2-N3   | 5.64  | 1.37        | 1.32     |
| 1   | AA    | 991  | U    | N1-C2   | 5.64  | 1.43        | 1.38     |
| 1   | AA    | 1479 | C    | N1-C6   | -5.64 | 1.33        | 1.37     |
| 34  | BA    | 102  | G    | C2'-C1' | -5.64 | 1.47        | 1.53     |
| 35  | BB    | 33   | C    | O4'-C1' | 5.64  | 1.49        | 1.41     |
| 35  | BB    | 449  | A    | C2'-C1' | -5.64 | 1.47        | 1.53     |
| 35  | BB    | 1051 | G    | C2'-C1' | -5.64 | 1.47        | 1.53     |
| 35  | BB    | 1901 | A    | N3-C4   | -5.64 | 1.31        | 1.34     |
| 35  | BB    | 2046 | G    | N3-C4   | -5.64 | 1.31        | 1.35     |
| 35  | BB    | 2485 | G    | C6-N1   | 5.64  | 1.43        | 1.39     |
| 1   | AA    | 6    | G    | P-O5'   | -5.63 | 1.54        | 1.59     |
| 1   | AA    | 1013 | G    | C4'-O4' | -5.63 | 1.38        | 1.45     |
| 1   | AA    | 1032 | G    | N9-C8   | -5.63 | 1.33        | 1.37     |
| 1   | AA    | 1257 | A    | O3'-P   | -5.63 | 1.54        | 1.61     |
| 35  | BB    | 340  | A    | C8-N7   | -5.63 | 1.27        | 1.31     |
| 35  | BB    | 544  | C    | C2-N3   | 5.63  | 1.40        | 1.35     |
| 35  | BB    | 816  | C    | C3'-C2' | -5.63 | 1.46        | 1.52     |
| 35  | BB    | 859  | G    | N7-C5   | -5.63 | 1.35        | 1.39     |
| 35  | BB    | 1276 | A    | N7-C5   | -5.63 | 1.35        | 1.39     |
| 35  | BB    | 1567 | G    | C2-N2   | -5.63 | 1.28        | 1.34     |
| 35  | BB    | 1817 | G    | C1'-N9  | 5.63  | 1.57        | 1.48     |
| 35  | BB    | 1957 | C    | C4-N4   | 5.63  | 1.39        | 1.33     |
| 35  | BB    | 2003 | A    | C2-N3   | 5.63  | 1.38        | 1.33     |
| 35  | BB    | 2194 | U    | C2-O2   | 5.63  | 1.27        | 1.22     |
| 35  | BB    | 195  | A    | N3-C4   | -5.63 | 1.31        | 1.34     |
| 35  | BB    | 892  | A    | C3'-C2' | 5.63  | 1.59        | 1.52     |
| 35  | BB    | 1446 | C    | N1-C6   | -5.63 | 1.33        | 1.37     |
| 35  | BB    | 2369 | A    | C6-N1   | 5.63  | 1.39        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 147  | G    | C2-N2   | 5.63  | 1.40        | 1.34     |
| 1   | AA    | 328  | C    | C4'-O4' | 5.63  | 1.52        | 1.45     |
| 1   | AA    | 840  | C    | O3'-P   | -5.63 | 1.54        | 1.61     |
| 1   | AA    | 949  | A    | N3-C4   | 5.63  | 1.38        | 1.34     |
| 1   | AA    | 1318 | A    | C6-N6   | 5.63  | 1.38        | 1.33     |
| 35  | BB    | 167  | A    | C8-N7   | -5.63 | 1.27        | 1.31     |
| 35  | BB    | 542  | C    | C4-N4   | 5.63  | 1.39        | 1.33     |
| 35  | BB    | 928  | A    | C8-N7   | 5.63  | 1.35        | 1.31     |
| 35  | BB    | 1059 | G    | O3'-P   | -5.63 | 1.54        | 1.61     |
| 35  | BB    | 1146 | C    | N3-C4   | 5.63  | 1.37        | 1.33     |
| 35  | BB    | 1321 | A    | C3'-C2' | 5.63  | 1.59        | 1.52     |
| 35  | BB    | 1986 | C    | N3-C4   | 5.63  | 1.37        | 1.33     |
| 35  | BB    | 2268 | A    | N7-C5   | -5.63 | 1.35        | 1.39     |
| 35  | BB    | 2316 | G    | C2-N3   | 5.63  | 1.37        | 1.32     |
| 1   | AA    | 149  | A    | N7-C5   | -5.63 | 1.35        | 1.39     |
| 1   | AA    | 210  | C    | N1-C6   | -5.63 | 1.33        | 1.37     |
| 35  | BB    | 334  | C    | P-O5'   | -5.63 | 1.54        | 1.59     |
| 35  | BB    | 443  | A    | C6-N1   | 5.63  | 1.39        | 1.35     |
| 35  | BB    | 1917 | U    | C4'-O4' | 5.63  | 1.52        | 1.45     |
| 1   | AA    | 323  | U    | C1'-N1  | 5.63  | 1.57        | 1.48     |
| 1   | AA    | 449  | G    | C5-C4   | -5.63 | 1.34        | 1.38     |
| 1   | AA    | 559  | A    | C5'-C4' | -5.63 | 1.44        | 1.51     |
| 1   | AA    | 975  | A    | O3'-P   | -5.63 | 1.54        | 1.61     |
| 1   | AA    | 1076 | U    | C2-N3   | -5.63 | 1.33        | 1.37     |
| 1   | AA    | 1100 | C    | C2-O2   | -5.63 | 1.19        | 1.24     |
| 1   | AA    | 1159 | U    | C5'-C4' | 5.63  | 1.58        | 1.51     |
| 1   | AA    | 1490 | U    | N1-C2   | -5.63 | 1.33        | 1.38     |
| 17  | AQ    | 26   | ARG  | CZ-NH1  | 5.63  | 1.40        | 1.33     |
| 35  | BB    | 855  | G    | N3-C4   | -5.63 | 1.31        | 1.35     |
| 35  | BB    | 1126 | A    | N9-C8   | 5.63  | 1.42        | 1.37     |
| 35  | BB    | 2456 | C    | C5-C6   | -5.63 | 1.29        | 1.34     |
| 35  | BB    | 2668 | G    | N3-C4   | -5.63 | 1.31        | 1.35     |
| 1   | AA    | 1056 | U    | N1-C2   | 5.63  | 1.43        | 1.38     |
| 1   | AA    | 1065 | U    | C5'-C4' | 5.63  | 1.58        | 1.51     |
| 35  | BB    | 630  | G    | O3'-P   | -5.63 | 1.54        | 1.61     |
| 35  | BB    | 974  | G    | C2-N3   | 5.63  | 1.37        | 1.32     |
| 35  | BB    | 1020 | A    | C5'-C4' | 5.63  | 1.58        | 1.51     |
| 35  | BB    | 1491 | G    | N9-C4   | 5.63  | 1.42        | 1.38     |
| 35  | BB    | 1867 | G    | N9-C8   | 5.63  | 1.41        | 1.37     |
| 35  | BB    | 1874 | C    | C5'-C4' | 5.63  | 1.58        | 1.51     |
| 35  | BB    | 1967 | C    | N1-C6   | -5.63 | 1.33        | 1.37     |
| 35  | BB    | 1997 | C    | C4-N4   | 5.63  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2028 | U    | C5-C6   | -5.63 | 1.29        | 1.34     |
| 35  | BB    | 2881 | U    | C4'-O4' | -5.63 | 1.38        | 1.45     |
| 40  | BG    | 60   | GLY  | CA-C    | -5.63 | 1.42        | 1.51     |
| 1   | AA    | 1166 | G    | C8-N7   | 5.62  | 1.34        | 1.30     |
| 35  | BB    | 19   | A    | N9-C4   | 5.62  | 1.41        | 1.37     |
| 35  | BB    | 651  | G    | C5-C4   | 5.62  | 1.42        | 1.38     |
| 35  | BB    | 1299 | G    | P-O5'   | -5.62 | 1.54        | 1.59     |
| 1   | AA    | 674  | G    | C6-N1   | 5.62  | 1.43        | 1.39     |
| 1   | AA    | 1159 | U    | C4-C5   | 5.62  | 1.48        | 1.43     |
| 1   | AA    | 1333 | A    | C5-C4   | 5.62  | 1.42        | 1.38     |
| 35  | BB    | 320  | A    | N9-C8   | 5.62  | 1.42        | 1.37     |
| 35  | BB    | 679  | C    | C4'-C3' | 5.62  | 1.59        | 1.53     |
| 35  | BB    | 2121 | G    | C2-N3   | 5.62  | 1.37        | 1.32     |
| 1   | AA    | 1167 | A    | C4'-O4' | 5.62  | 1.52        | 1.45     |
| 1   | AA    | 1279 | G    | O3'-P   | -5.62 | 1.54        | 1.61     |
| 1   | AA    | 1418 | A    | C6-N6   | 5.62  | 1.38        | 1.33     |
| 35  | BB    | 769  | U    | C4-O4   | -5.62 | 1.19        | 1.23     |
| 35  | BB    | 1091 | G    | P-O5'   | 5.62  | 1.65        | 1.59     |
| 35  | BB    | 1142 | A    | C3'-C2' | -5.62 | 1.46        | 1.52     |
| 35  | BB    | 1348 | C    | N1-C6   | 5.62  | 1.40        | 1.37     |
| 35  | BB    | 1494 | A    | N7-C5   | -5.62 | 1.35        | 1.39     |
| 35  | BB    | 1534 | U    | C3'-O3' | 5.62  | 1.50        | 1.42     |
| 35  | BB    | 2361 | G    | C5-C4   | -5.62 | 1.34        | 1.38     |
| 35  | BB    | 104  | A    | N9-C4   | -5.62 | 1.34        | 1.37     |
| 35  | BB    | 514  | A    | C4'-O4' | 5.62  | 1.52        | 1.45     |
| 35  | BB    | 357  | C    | C2'-C1' | -5.62 | 1.47        | 1.53     |
| 35  | BB    | 698  | C    | N3-C4   | 5.62  | 1.37        | 1.33     |
| 35  | BB    | 1244 | A    | C5-C4   | 5.62  | 1.42        | 1.38     |
| 35  | BB    | 1318 | U    | C2-N3   | 5.62  | 1.41        | 1.37     |
| 35  | BB    | 1407 | G    | P-O5'   | -5.62 | 1.54        | 1.59     |
| 35  | BB    | 1549 | A    | P-O5'   | -5.62 | 1.54        | 1.59     |
| 35  | BB    | 1595 | C    | C2-O2   | 5.62  | 1.29        | 1.24     |
| 35  | BB    | 2115 | G    | C5-C6   | -5.62 | 1.36        | 1.42     |
| 1   | AA    | 129  | A    | N9-C8   | 5.62  | 1.42        | 1.37     |
| 35  | BB    | 1266 | G    | C4'-O4' | 5.62  | 1.52        | 1.45     |
| 35  | BB    | 2704 | C    | N3-C4   | 5.62  | 1.37        | 1.33     |
| 1   | AA    | 1160 | G    | C6-N1   | 5.62  | 1.43        | 1.39     |
| 4   | AD    | 153  | ARG  | NE-CZ   | 5.62  | 1.40        | 1.33     |
| 35  | BB    | 451  | U    | N3-C4   | 5.62  | 1.43        | 1.38     |
| 35  | BB    | 841  | G    | N9-C4   | 5.62  | 1.42        | 1.38     |
| 35  | BB    | 1263 | U    | O3'-P   | -5.62 | 1.54        | 1.61     |
| 35  | BB    | 1578 | U    | O3'-P   | -5.62 | 1.54        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2827 | C    | C2-N3   | 5.62  | 1.40        | 1.35     |
| 52  | BS    | 8    | ARG  | CZ-NH2  | 5.62  | 1.40        | 1.33     |
| 1   | AA    | 577  | G    | C6-N1   | 5.61  | 1.43        | 1.39     |
| 1   | AA    | 759  | A    | C8-N7   | 5.61  | 1.35        | 1.31     |
| 1   | AA    | 1171 | A    | C8-N7   | 5.61  | 1.35        | 1.31     |
| 35  | BB    | 159  | G    | N9-C4   | 5.61  | 1.42        | 1.38     |
| 35  | BB    | 559  | G    | C5'-C4' | 5.61  | 1.58        | 1.51     |
| 35  | BB    | 1149 | G    | N9-C8   | -5.61 | 1.33        | 1.37     |
| 48  | BO    | 25   | ARG  | CZ-NH1  | 5.61  | 1.40        | 1.33     |
| 9   | AI    | 84   | ARG  | CD-NE   | 5.61  | 1.55        | 1.46     |
| 35  | BB    | 980  | A    | N9-C4   | -5.61 | 1.34        | 1.37     |
| 35  | BB    | 2428 | G    | N9-C8   | 5.61  | 1.41        | 1.37     |
| 1   | AA    | 104  | G    | N7-C5   | -5.61 | 1.35        | 1.39     |
| 1   | AA    | 245  | U    | P-O5'   | 5.61  | 1.65        | 1.59     |
| 1   | AA    | 1478 | U    | C3'-C2' | -5.61 | 1.46        | 1.52     |
| 10  | AJ    | 13   | PHE  | CB-CG   | 5.61  | 1.60        | 1.51     |
| 34  | BA    | 86   | G    | C2-N2   | 5.61  | 1.40        | 1.34     |
| 35  | BB    | 197  | A    | C6-N6   | 5.61  | 1.38        | 1.33     |
| 35  | BB    | 936  | A    | N1-C2   | -5.61 | 1.29        | 1.34     |
| 35  | BB    | 1463 | C    | N1-C6   | 5.61  | 1.40        | 1.37     |
| 35  | BB    | 1474 | U    | P-O5'   | -5.61 | 1.54        | 1.59     |
| 35  | BB    | 1723 | G    | C2-N2   | 5.61  | 1.40        | 1.34     |
| 35  | BB    | 1743 | G    | C8-N7   | 5.61  | 1.34        | 1.30     |
| 35  | BB    | 1973 | G    | N1-C2   | 5.61  | 1.42        | 1.37     |
| 35  | BB    | 2061 | G    | N1-C2   | 5.61  | 1.42        | 1.37     |
| 37  | BD    | 169  | ARG  | CZ-NH2  | 5.61  | 1.40        | 1.33     |
| 1   | AA    | 268  | U    | N3-C4   | 5.61  | 1.43        | 1.38     |
| 1   | AA    | 1279 | G    | N9-C8   | 5.61  | 1.41        | 1.37     |
| 35  | BB    | 342  | A    | O4'-C1' | 5.61  | 1.49        | 1.41     |
| 35  | BB    | 706  | A    | N9-C4   | -5.61 | 1.34        | 1.37     |
| 35  | BB    | 2333 | A    | N7-C5   | 5.61  | 1.42        | 1.39     |
| 38  | BE    | 40   | ARG  | NE-CZ   | 5.61  | 1.40        | 1.33     |
| 1   | AA    | 105  | G    | C2-N3   | 5.61  | 1.37        | 1.32     |
| 1   | AA    | 833  | G    | C6-N1   | 5.61  | 1.43        | 1.39     |
| 1   | AA    | 1160 | G    | C2-N2   | 5.61  | 1.40        | 1.34     |
| 22  | AV    | 6    | C    | C3'-C2' | 5.61  | 1.59        | 1.52     |
| 35  | BB    | 7    | G    | N1-C2   | 5.61  | 1.42        | 1.37     |
| 35  | BB    | 235  | U    | C4'-C3' | -5.61 | 1.47        | 1.52     |
| 35  | BB    | 590  | A    | C4'-O4' | 5.61  | 1.52        | 1.45     |
| 35  | BB    | 1011 | G    | C3'-C2' | -5.61 | 1.46        | 1.52     |
| 35  | BB    | 1242 | U    | C2-N3   | -5.61 | 1.33        | 1.37     |
| 35  | BB    | 1323 | C    | O3'-P   | -5.61 | 1.54        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1356 | G    | C3'-O3' | 5.61  | 1.50        | 1.42     |
| 35  | BB    | 1466 | U    | C1'-N1  | -5.61 | 1.39        | 1.46     |
| 35  | BB    | 1931 | U    | C2'-C1' | -5.61 | 1.47        | 1.53     |
| 35  | BB    | 1935 | G    | N9-C8   | 5.61  | 1.41        | 1.37     |
| 35  | BB    | 2854 | G    | C5'-C4' | 5.61  | 1.58        | 1.51     |
| 1   | AA    | 438  | U    | C2-N3   | 5.61  | 1.41        | 1.37     |
| 1   | AA    | 632  | U    | C2-O2   | 5.61  | 1.27        | 1.22     |
| 1   | AA    | 1086 | U    | C4'-C3' | -5.61 | 1.47        | 1.52     |
| 6   | AF    | 12   | PRO  | N-CD    | -5.61 | 1.40        | 1.47     |
| 35  | BB    | 56   | A    | O4'-C1' | -5.61 | 1.34        | 1.41     |
| 35  | BB    | 921  | C    | C5-C6   | -5.61 | 1.29        | 1.34     |
| 35  | BB    | 1095 | A    | C5'-C4' | 5.61  | 1.58        | 1.51     |
| 35  | BB    | 2226 | C    | C5-C6   | -5.61 | 1.29        | 1.34     |
| 1   | AA    | 680  | C    | O3'-P   | -5.60 | 1.54        | 1.61     |
| 35  | BB    | 291  | G    | C3'-O3' | 5.60  | 1.50        | 1.42     |
| 1   | AA    | 313  | A    | N9-C8   | 5.60  | 1.42        | 1.37     |
| 1   | AA    | 907  | A    | C1'-N9  | 5.60  | 1.57        | 1.48     |
| 1   | AA    | 1178 | G    | C5-C4   | 5.60  | 1.42        | 1.38     |
| 22  | AV    | 69   | G    | C8-N7   | -5.60 | 1.27        | 1.30     |
| 35  | BB    | 354  | A    | N3-C4   | -5.60 | 1.31        | 1.34     |
| 35  | BB    | 903  | C    | C5'-C4' | -5.60 | 1.44        | 1.51     |
| 35  | BB    | 1595 | C    | N1-C2   | 5.60  | 1.45        | 1.40     |
| 35  | BB    | 2222 | C    | C4-N4   | 5.60  | 1.39        | 1.33     |
| 35  | BB    | 2366 | A    | N9-C4   | 5.60  | 1.41        | 1.37     |
| 35  | BB    | 2471 | A    | C6-N6   | 5.60  | 1.38        | 1.33     |
| 1   | AA    | 128  | G    | O4'-C1' | -5.60 | 1.34        | 1.41     |
| 1   | AA    | 161  | A    | N9-C4   | -5.60 | 1.34        | 1.37     |
| 1   | AA    | 341  | C    | N1-C6   | -5.60 | 1.33        | 1.37     |
| 34  | BA    | 73   | A    | C5'-C4' | 5.60  | 1.58        | 1.51     |
| 35  | BB    | 2001 | C    | N3-C4   | 5.60  | 1.37        | 1.33     |
| 35  | BB    | 2255 | G    | C4'-O4' | 5.60  | 1.52        | 1.45     |
| 35  | BB    | 2829 | A    | N7-C5   | -5.60 | 1.35        | 1.39     |
| 35  | BB    | 2853 | C    | C2-O2   | 5.60  | 1.29        | 1.24     |
| 1   | AA    | 541  | G    | C8-N7   | -5.60 | 1.27        | 1.30     |
| 1   | AA    | 889  | A    | C6-N1   | 5.60  | 1.39        | 1.35     |
| 1   | AA    | 1102 | A    | C5-C6   | 5.60  | 1.46        | 1.41     |
| 7   | AG    | 3    | ARG  | CD-NE   | 5.60  | 1.55        | 1.46     |
| 21  | AU    | 17   | ARG  | NE-CZ   | 5.60  | 1.40        | 1.33     |
| 35  | BB    | 189  | G    | C6-N1   | 5.60  | 1.43        | 1.39     |
| 35  | BB    | 420  | C    | C4-N4   | 5.60  | 1.39        | 1.33     |
| 35  | BB    | 1008 | A    | C2-N3   | 5.60  | 1.38        | 1.33     |
| 35  | BB    | 1142 | A    | N1-C2   | 5.60  | 1.39        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1560 | G    | C6-O6   | -5.60 | 1.19        | 1.24     |
| 35  | BB    | 1613 | G    | P-O5'   | -5.60 | 1.54        | 1.59     |
| 35  | BB    | 1773 | A    | C3'-C2' | -5.60 | 1.46        | 1.52     |
| 35  | BB    | 2207 | C    | N1-C6   | 5.60  | 1.40        | 1.37     |
| 35  | BB    | 2526 | G    | C2'-C1' | -5.60 | 1.47        | 1.53     |
| 35  | BB    | 2552 | U    | C2'-C1' | -5.60 | 1.47        | 1.53     |
| 35  | BB    | 2604 | U    | C2-N3   | 5.60  | 1.41        | 1.37     |
| 1   | AA    | 331  | G    | N9-C8   | 5.60  | 1.41        | 1.37     |
| 1   | AA    | 484  | G    | C4'-C3' | 5.60  | 1.59        | 1.53     |
| 1   | AA    | 640  | A    | N7-C5   | -5.60 | 1.35        | 1.39     |
| 1   | AA    | 843  | U    | C2-O2   | 5.60  | 1.27        | 1.22     |
| 1   | AA    | 906  | A    | N1-C2   | 5.60  | 1.39        | 1.34     |
| 1   | AA    | 1081 | A    | C6-N6   | 5.60  | 1.38        | 1.33     |
| 35  | BB    | 326  | G    | O3'-P   | -5.60 | 1.54        | 1.61     |
| 35  | BB    | 494  | G    | C4'-O4' | -5.60 | 1.38        | 1.45     |
| 35  | BB    | 581  | C    | C2'-C1' | 5.60  | 1.59        | 1.53     |
| 35  | BB    | 830  | G    | C4'-O4' | -5.60 | 1.38        | 1.45     |
| 35  | BB    | 843  | G    | C3'-C2' | -5.60 | 1.46        | 1.52     |
| 35  | BB    | 2422 | C    | C4-N4   | 5.60  | 1.39        | 1.33     |
| 35  | BB    | 2567 | G    | C5'-C4' | 5.60  | 1.58        | 1.51     |
| 35  | BB    | 2887 | A    | C5-C4   | 5.60  | 1.42        | 1.38     |
| 1   | AA    | 617  | G    | N1-C2   | 5.60  | 1.42        | 1.37     |
| 1   | AA    | 983  | A    | C6-N6   | 5.60  | 1.38        | 1.33     |
| 35  | BB    | 370  | G    | C5'-C4' | 5.60  | 1.58        | 1.51     |
| 35  | BB    | 2146 | C    | O3'-P   | -5.60 | 1.54        | 1.61     |
| 1   | AA    | 1317 | C    | C4-C5   | 5.59  | 1.47        | 1.43     |
| 1   | AA    | 1425 | U    | C4'-C3' | -5.59 | 1.47        | 1.52     |
| 35  | BB    | 10   | A    | N9-C8   | 5.59  | 1.42        | 1.37     |
| 35  | BB    | 377  | G    | C2'-C1' | -5.59 | 1.47        | 1.53     |
| 35  | BB    | 519  | U    | C2'-C1' | -5.59 | 1.47        | 1.53     |
| 35  | BB    | 1007 | C    | N3-C4   | 5.59  | 1.37        | 1.33     |
| 35  | BB    | 1122 | G    | N9-C8   | 5.59  | 1.41        | 1.37     |
| 35  | BB    | 2120 | G    | N3-C4   | -5.59 | 1.31        | 1.35     |
| 35  | BB    | 2182 | U    | N3-C4   | 5.59  | 1.43        | 1.38     |
| 35  | BB    | 2280 | G    | C5'-C4' | 5.59  | 1.58        | 1.51     |
| 35  | BB    | 2577 | A    | N1-C2   | 5.59  | 1.39        | 1.34     |
| 1   | AA    | 1491 | G    | N3-C4   | 5.59  | 1.39        | 1.35     |
| 18  | AR    | 63   | TYR  | CE2-CZ  | 5.59  | 1.45        | 1.38     |
| 22  | AV    | 76   | A    | N1-C2   | -5.59 | 1.29        | 1.34     |
| 35  | BB    | 16   | C    | N1-C6   | 5.59  | 1.40        | 1.37     |
| 35  | BB    | 547  | A    | C8-N7   | -5.59 | 1.27        | 1.31     |
| 35  | BB    | 1746 | A    | C6-N6   | 5.59  | 1.38        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2246 | G    | N9-C4   | -5.59 | 1.33        | 1.38     |
| 46  | BM    | 6    | ARG  | CZ-NH1  | 5.59  | 1.40        | 1.33     |
| 46  | BM    | 81   | ARG  | CD-NE   | 5.59  | 1.55        | 1.46     |
| 1   | AA    | 165  | G    | C8-N7   | -5.59 | 1.27        | 1.30     |
| 1   | AA    | 434  | U    | C2-N3   | 5.59  | 1.41        | 1.37     |
| 1   | AA    | 537  | G    | C5-C4   | 5.59  | 1.42        | 1.38     |
| 35  | BB    | 234  | U    | C2'-C1' | -5.59 | 1.47        | 1.53     |
| 35  | BB    | 1555 | G    | C5-C6   | 5.59  | 1.48        | 1.42     |
| 35  | BB    | 1763 | G    | N1-C2   | 5.59  | 1.42        | 1.37     |
| 35  | BB    | 1978 | A    | O3'-P   | 5.59  | 1.67        | 1.61     |
| 35  | BB    | 2080 | A    | N1-C2   | 5.59  | 1.39        | 1.34     |
| 35  | BB    | 2306 | C    | O5'-C5' | 5.59  | 1.53        | 1.44     |
| 1   | AA    | 148  | G    | N9-C8   | 5.59  | 1.41        | 1.37     |
| 1   | AA    | 344  | A    | C2-N3   | -5.59 | 1.28        | 1.33     |
| 1   | AA    | 423  | G    | O3'-P   | -5.59 | 1.54        | 1.61     |
| 1   | AA    | 608  | A    | N3-C4   | -5.59 | 1.31        | 1.34     |
| 1   | AA    | 1087 | G    | C6-N1   | 5.59  | 1.43        | 1.39     |
| 1   | AA    | 1395 | C    | N1-C6   | -5.59 | 1.33        | 1.37     |
| 1   | AA    | 1449 | C    | C4-N4   | 5.59  | 1.39        | 1.33     |
| 35  | BB    | 223  | A    | N7-C5   | -5.59 | 1.35        | 1.39     |
| 35  | BB    | 304  | U    | N3-C4   | 5.59  | 1.43        | 1.38     |
| 35  | BB    | 857  | G    | C8-N7   | -5.59 | 1.27        | 1.30     |
| 35  | BB    | 1505 | A    | C5-C4   | 5.59  | 1.42        | 1.38     |
| 1   | AA    | 269  | C    | N3-C4   | 5.59  | 1.37        | 1.33     |
| 22  | AV    | 1    | C    | C3'-C2' | -5.59 | 1.46        | 1.52     |
| 34  | BA    | 32   | U    | C2-N3   | 5.59  | 1.41        | 1.37     |
| 35  | BB    | 2873 | A    | N7-C5   | -5.59 | 1.35        | 1.39     |
| 1   | AA    | 118  | U    | P-O5'   | -5.59 | 1.54        | 1.59     |
| 1   | AA    | 169  | C    | N1-C2   | 5.59  | 1.45        | 1.40     |
| 1   | AA    | 626  | G    | C5-C4   | 5.59  | 1.42        | 1.38     |
| 1   | AA    | 674  | G    | N9-C8   | -5.59 | 1.33        | 1.37     |
| 1   | AA    | 1157 | A    | C3'-O3' | 5.59  | 1.50        | 1.42     |
| 1   | AA    | 1166 | G    | C5'-C4' | 5.59  | 1.58        | 1.51     |
| 34  | BA    | 75   | G    | P-O5'   | -5.59 | 1.54        | 1.59     |
| 35  | BB    | 16   | C    | P-O5'   | -5.59 | 1.54        | 1.59     |
| 35  | BB    | 369  | U    | C4'-O4' | -5.59 | 1.38        | 1.45     |
| 35  | BB    | 438  | G    | N7-C5   | 5.59  | 1.42        | 1.39     |
| 35  | BB    | 481  | G    | C4'-C3' | 5.59  | 1.59        | 1.53     |
| 35  | BB    | 1403 | A    | C8-N7   | -5.59 | 1.27        | 1.31     |
| 35  | BB    | 2373 | G    | C2-N2   | -5.59 | 1.28        | 1.34     |
| 35  | BB    | 2670 | A    | N7-C5   | -5.59 | 1.35        | 1.39     |
| 35  | BB    | 2748 | A    | N7-C5   | -5.59 | 1.35        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2799 | A    | C2-N3   | 5.59  | 1.38        | 1.33     |
| 1   | AA    | 690  | G    | C5-C4   | 5.58  | 1.42        | 1.38     |
| 1   | AA    | 1296 | C    | N3-C4   | 5.58  | 1.37        | 1.33     |
| 35  | BB    | 459  | U    | C5'-C4' | 5.58  | 1.58        | 1.51     |
| 35  | BB    | 1699 | G    | N3-C4   | -5.58 | 1.31        | 1.35     |
| 35  | BB    | 2159 | G    | C4'-C3' | 5.58  | 1.59        | 1.53     |
| 35  | BB    | 2609 | U    | C4'-O4' | 5.58  | 1.52        | 1.45     |
| 35  | BB    | 2745 | C    | P-O5'   | -5.58 | 1.54        | 1.59     |
| 35  | BB    | 2843 | G    | N9-C8   | 5.58  | 1.41        | 1.37     |
| 1   | AA    | 760  | G    | N1-C2   | 5.58  | 1.42        | 1.37     |
| 1   | AA    | 1351 | U    | C5-C6   | 5.58  | 1.39        | 1.34     |
| 1   | AA    | 1387 | G    | N3-C4   | -5.58 | 1.31        | 1.35     |
| 35  | BB    | 1    | G    | N7-C5   | -5.58 | 1.35        | 1.39     |
| 35  | BB    | 103  | A    | O3'-P   | -5.58 | 1.54        | 1.61     |
| 35  | BB    | 668  | A    | C2'-O2' | -5.58 | 1.34        | 1.41     |
| 35  | BB    | 879  | G    | C2'-C1' | -5.58 | 1.47        | 1.53     |
| 35  | BB    | 1645 | G    | C5'-C4' | 5.58  | 1.58        | 1.51     |
| 35  | BB    | 1734 | G    | C2'-C1' | -5.58 | 1.47        | 1.53     |
| 35  | BB    | 2155 | U    | O3'-P   | -5.58 | 1.54        | 1.61     |
| 35  | BB    | 2336 | A    | O3'-P   | -5.58 | 1.54        | 1.61     |
| 35  | BB    | 2355 | G    | P-O5'   | -5.58 | 1.54        | 1.59     |
| 1   | AA    | 202  | G    | N3-C4   | -5.58 | 1.31        | 1.35     |
| 1   | AA    | 358  | U    | N1-C2   | -5.58 | 1.33        | 1.38     |
| 1   | AA    | 1048 | G    | C4'-C3' | -5.58 | 1.47        | 1.52     |
| 1   | AA    | 1371 | G    | N3-C4   | -5.58 | 1.31        | 1.35     |
| 35  | BB    | 432  | A    | N7-C5   | -5.58 | 1.35        | 1.39     |
| 35  | BB    | 673  | C    | C4-C5   | 5.58  | 1.47        | 1.43     |
| 35  | BB    | 777  | G    | C6-O6   | 5.58  | 1.29        | 1.24     |
| 35  | BB    | 918  | A    | C3'-C2' | 5.58  | 1.59        | 1.52     |
| 35  | BB    | 1816 | C    | N1-C6   | -5.58 | 1.33        | 1.37     |
| 35  | BB    | 1921 | G    | P-O5'   | -5.58 | 1.54        | 1.59     |
| 35  | BB    | 2187 | U    | C4'-O4' | 5.58  | 1.52        | 1.45     |
| 35  | BB    | 2607 | G    | C4'-C3' | 5.58  | 1.59        | 1.53     |
| 35  | BB    | 2702 | G    | C8-N7   | -5.58 | 1.27        | 1.30     |
| 35  | BB    | 2750 | A    | C2-N3   | 5.58  | 1.38        | 1.33     |
| 35  | BB    | 2839 | G    | N9-C8   | -5.58 | 1.33        | 1.37     |
| 37  | BD    | 3    | GLY  | N-CA    | -5.58 | 1.37        | 1.46     |
| 1   | AA    | 865  | A    | N7-C5   | -5.58 | 1.35        | 1.39     |
| 16  | AP    | 70   | ARG  | CZ-NH2  | 5.58  | 1.40        | 1.33     |
| 35  | BB    | 328  | U    | P-O5'   | -5.58 | 1.54        | 1.59     |
| 35  | BB    | 2285 | C    | C2'-C1' | -5.58 | 1.47        | 1.53     |
| 35  | BB    | 2828 | G    | O4'-C1' | 5.58  | 1.49        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 39   | G    | C2-N2   | 5.58  | 1.40        | 1.34     |
| 1   | AA    | 232  | G    | C2-N2   | 5.58  | 1.40        | 1.34     |
| 1   | AA    | 297  | G    | N9-C4   | 5.58  | 1.42        | 1.38     |
| 1   | AA    | 576  | C    | C4-N4   | 5.58  | 1.39        | 1.33     |
| 1   | AA    | 615  | G    | N9-C4   | 5.58  | 1.42        | 1.38     |
| 1   | AA    | 1517 | G    | N1-C2   | 5.58  | 1.42        | 1.37     |
| 35  | BB    | 85   | G    | N3-C4   | -5.58 | 1.31        | 1.35     |
| 35  | BB    | 1750 | G    | N7-C5   | -5.58 | 1.35        | 1.39     |
| 35  | BB    | 2406 | A    | N1-C2   | -5.58 | 1.29        | 1.34     |
| 1   | AA    | 128  | G    | C2-N2   | 5.58  | 1.40        | 1.34     |
| 1   | AA    | 171  | A    | N3-C4   | 5.58  | 1.38        | 1.34     |
| 1   | AA    | 360  | G    | C5-C6   | -5.58 | 1.36        | 1.42     |
| 1   | AA    | 1038 | C    | C2-N3   | 5.58  | 1.40        | 1.35     |
| 35  | BB    | 659  | G    | C5-C4   | 5.58  | 1.42        | 1.38     |
| 35  | BB    | 727  | A    | O3'-P   | -5.58 | 1.54        | 1.61     |
| 35  | BB    | 1063 | G    | C1'-N9  | 5.58  | 1.57        | 1.48     |
| 35  | BB    | 1835 | G    | C3'-C2' | -5.58 | 1.46        | 1.52     |
| 35  | BB    | 2216 | G    | N9-C8   | -5.58 | 1.33        | 1.37     |
| 1   | AA    | 678  | U    | C2'-C1' | -5.58 | 1.47        | 1.53     |
| 1   | AA    | 920  | U    | N3-C4   | 5.58  | 1.43        | 1.38     |
| 35  | BB    | 575  | A    | N1-C2   | 5.58  | 1.39        | 1.34     |
| 35  | BB    | 820  | A    | C6-N6   | -5.58 | 1.29        | 1.33     |
| 35  | BB    | 1785 | A    | N7-C5   | -5.58 | 1.35        | 1.39     |
| 35  | BB    | 2426 | A    | N9-C4   | 5.58  | 1.41        | 1.37     |
| 35  | BB    | 2598 | A    | C6-N6   | 5.58  | 1.38        | 1.33     |
| 35  | BB    | 2728 | U    | C4'-C3' | 5.58  | 1.59        | 1.53     |
| 1   | AA    | 45   | G    | C2-N3   | 5.57  | 1.37        | 1.32     |
| 1   | AA    | 69   | G    | N7-C5   | -5.57 | 1.35        | 1.39     |
| 1   | AA    | 84   | U    | P-O5'   | -5.57 | 1.54        | 1.59     |
| 1   | AA    | 1215 | G    | N1-C2   | 5.57  | 1.42        | 1.37     |
| 1   | AA    | 1503 | A    | C4'-C3' | 5.57  | 1.59        | 1.53     |
| 34  | BA    | 33   | G    | N3-C4   | 5.57  | 1.39        | 1.35     |
| 35  | BB    | 554  | U    | O3'-P   | -5.57 | 1.54        | 1.61     |
| 35  | BB    | 957  | C    | C3'-C2' | -5.57 | 1.46        | 1.52     |
| 35  | BB    | 1041 | G    | C2'-C1' | 5.57  | 1.59        | 1.53     |
| 35  | BB    | 1226 | A    | C3'-O3' | 5.57  | 1.50        | 1.42     |
| 35  | BB    | 2293 | G    | C5-C6   | -5.57 | 1.36        | 1.42     |
| 35  | BB    | 2320 | U    | C4'-C3' | 5.57  | 1.59        | 1.53     |
| 35  | BB    | 2509 | G    | C2-N3   | 5.57  | 1.37        | 1.32     |
| 1   | AA    | 1374 | A    | N7-C5   | -5.57 | 1.35        | 1.39     |
| 9   | AI    | 96   | GLU  | CD-OE1  | 5.57  | 1.31        | 1.25     |
| 35  | BB    | 1029 | A    | C2-N3   | 5.57  | 1.38        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1339 | G    | C5-C6   | -5.57 | 1.36        | 1.42     |
| 55  | BW    | 58   | SER  | CA-CB   | 5.57  | 1.61        | 1.52     |
| 1   | AA    | 494  | G    | C6-N1   | 5.57  | 1.43        | 1.39     |
| 1   | AA    | 714  | G    | C5'-C4' | 5.57  | 1.58        | 1.51     |
| 1   | AA    | 801  | U    | C2'-C1' | -5.57 | 1.47        | 1.53     |
| 1   | AA    | 1023 | U    | C4'-C3' | 5.57  | 1.59        | 1.53     |
| 1   | AA    | 1305 | G    | C6-N1   | 5.57  | 1.43        | 1.39     |
| 35  | BB    | 140  | C    | N3-C4   | 5.57  | 1.37        | 1.33     |
| 35  | BB    | 412  | A    | C6-N1   | 5.57  | 1.39        | 1.35     |
| 35  | BB    | 662  | G    | N9-C4   | -5.57 | 1.33        | 1.38     |
| 35  | BB    | 1234 | U    | N3-C4   | 5.57  | 1.43        | 1.38     |
| 35  | BB    | 1492 | G    | C5'-C4' | 5.57  | 1.58        | 1.51     |
| 32  | B7    | 7    | ARG  | CZ-NH2  | 5.57  | 1.40        | 1.33     |
| 35  | BB    | 1285 | A    | C5'-C4' | 5.57  | 1.58        | 1.51     |
| 35  | BB    | 2085 | U    | O3'-P   | -5.57 | 1.54        | 1.61     |
| 35  | BB    | 2381 | A    | N3-C4   | -5.57 | 1.31        | 1.34     |
| 1   | AA    | 532  | A    | C5-C4   | -5.57 | 1.34        | 1.38     |
| 1   | AA    | 692  | U    | N1-C6   | 5.57  | 1.43        | 1.38     |
| 1   | AA    | 1387 | G    | C6-N1   | 5.57  | 1.43        | 1.39     |
| 35  | BB    | 24   | G    | N1-C2   | 5.57  | 1.42        | 1.37     |
| 35  | BB    | 407  | G    | C4'-O4' | 5.57  | 1.52        | 1.45     |
| 22  | AV    | 32   | A    | C3'-C2' | 5.57  | 1.59        | 1.52     |
| 35  | BB    | 88   | G    | C5-C4   | -5.57 | 1.34        | 1.38     |
| 35  | BB    | 666  | A    | P-O5'   | -5.57 | 1.54        | 1.59     |
| 35  | BB    | 694  | U    | C3'-C2' | 5.57  | 1.59        | 1.52     |
| 35  | BB    | 1714 | U    | C2-N3   | 5.57  | 1.41        | 1.37     |
| 35  | BB    | 2276 | G    | C4'-C3' | -5.57 | 1.47        | 1.52     |
| 35  | BB    | 2858 | C    | C3'-O3' | 5.57  | 1.50        | 1.42     |
| 35  | BB    | 2862 | G    | C2-N3   | 5.57  | 1.37        | 1.32     |
| 44  | BK    | 17   | ARG  | NE-CZ   | 5.57  | 1.40        | 1.33     |
| 1   | AA    | 468  | A    | N9-C4   | -5.56 | 1.34        | 1.37     |
| 1   | AA    | 872  | A    | N9-C8   | -5.56 | 1.33        | 1.37     |
| 1   | AA    | 876  | C    | O3'-P   | -5.56 | 1.54        | 1.61     |
| 1   | AA    | 1423 | G    | C5'-C4' | -5.56 | 1.44        | 1.51     |
| 35  | BB    | 79   | C    | N1-C6   | 5.56  | 1.40        | 1.37     |
| 35  | BB    | 1406 | U    | C2'-C1' | -5.56 | 1.47        | 1.53     |
| 35  | BB    | 2626 | C    | C4'-C3' | -5.56 | 1.47        | 1.52     |
| 35  | BB    | 2735 | G    | C2'-C1' | -5.56 | 1.47        | 1.53     |
| 35  | BB    | 2770 | G    | N7-C5   | 5.56  | 1.42        | 1.39     |
| 1   | AA    | 33   | A    | N9-C8   | -5.56 | 1.33        | 1.37     |
| 1   | AA    | 555  | U    | O4'-C1' | 5.56  | 1.48        | 1.41     |
| 1   | AA    | 619  | U    | C2-N3   | 5.56  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 779  | C    | P-O5'   | -5.56 | 1.54        | 1.59     |
| 1   | AA    | 1107 | C    | C3'-C2' | -5.56 | 1.46        | 1.52     |
| 18  | AR    | 34   | GLU  | CB-CG   | 5.56  | 1.62        | 1.52     |
| 35  | BB    | 2129 | C    | C4-N4   | 5.56  | 1.39        | 1.33     |
| 35  | BB    | 2300 | C    | C1'-N1  | -5.56 | 1.39        | 1.46     |
| 35  | BB    | 2544 | G    | C8-N7   | -5.56 | 1.27        | 1.30     |
| 35  | BB    | 2767 | C    | C1'-N1  | 5.56  | 1.57        | 1.48     |
| 1   | AA    | 16   | A    | N3-C4   | 5.56  | 1.38        | 1.34     |
| 1   | AA    | 50   | A    | C6-N1   | 5.56  | 1.39        | 1.35     |
| 35  | BB    | 752  | A    | P-O5'   | -5.56 | 1.54        | 1.59     |
| 35  | BB    | 920  | A    | C2'-C1' | -5.56 | 1.47        | 1.53     |
| 35  | BB    | 2052 | A    | N3-C4   | 5.56  | 1.38        | 1.34     |
| 1   | AA    | 336  | A    | C5-C6   | 5.56  | 1.46        | 1.41     |
| 1   | AA    | 682  | G    | C5'-C4' | 5.56  | 1.58        | 1.51     |
| 1   | AA    | 713  | G    | C6-O6   | -5.56 | 1.19        | 1.24     |
| 1   | AA    | 792  | A    | C6-N6   | 5.56  | 1.38        | 1.33     |
| 1   | AA    | 1076 | U    | C4'-O4' | 5.56  | 1.52        | 1.45     |
| 21  | AU    | 34   | ARG  | CD-NE   | 5.56  | 1.55        | 1.46     |
| 34  | BA    | 12   | C    | C2'-C1' | -5.56 | 1.47        | 1.53     |
| 35  | BB    | 518  | G    | C6-N1   | 5.56  | 1.43        | 1.39     |
| 35  | BB    | 862  | G    | N3-C4   | -5.56 | 1.31        | 1.35     |
| 35  | BB    | 1114 | C    | C4-C5   | 5.56  | 1.47        | 1.43     |
| 35  | BB    | 1494 | A    | C5'-C4' | 5.56  | 1.58        | 1.51     |
| 35  | BB    | 1684 | G    | C5-C4   | 5.56  | 1.42        | 1.38     |
| 35  | BB    | 2157 | G    | C2-N3   | 5.56  | 1.37        | 1.32     |
| 35  | BB    | 2652 | C    | N1-C6   | 5.56  | 1.40        | 1.37     |
| 1   | AA    | 209  | U    | C5'-C4' | 5.56  | 1.58        | 1.51     |
| 1   | AA    | 603  | U    | C2-N3   | -5.56 | 1.33        | 1.37     |
| 1   | AA    | 762  | U    | C2-N3   | 5.56  | 1.41        | 1.37     |
| 1   | AA    | 855  | U    | C4'-C3' | -5.56 | 1.47        | 1.52     |
| 1   | AA    | 922  | G    | C2'-C1' | -5.56 | 1.47        | 1.53     |
| 22  | AV    | 68   | U    | C2'-C1' | -5.56 | 1.47        | 1.53     |
| 35  | BB    | 407  | G    | C5-C4   | 5.56  | 1.42        | 1.38     |
| 35  | BB    | 996  | A    | C3'-O3' | 5.56  | 1.50        | 1.42     |
| 35  | BB    | 1077 | A    | C5'-C4' | 5.56  | 1.58        | 1.51     |
| 35  | BB    | 1262 | A    | C2-N3   | 5.56  | 1.38        | 1.33     |
| 35  | BB    | 2549 | G    | O5'-C5' | -5.56 | 1.33        | 1.42     |
| 1   | AA    | 250  | A    | C2'-C1' | -5.56 | 1.47        | 1.53     |
| 1   | AA    | 1046 | A    | C2'-C1' | -5.56 | 1.47        | 1.53     |
| 35  | BB    | 639  | U    | C2'-C1' | -5.56 | 1.47        | 1.53     |
| 35  | BB    | 2053 | G    | C6-N1   | 5.56  | 1.43        | 1.39     |
| 1   | AA    | 176  | C    | O4'-C1' | -5.55 | 1.34        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 378  | G    | C6-N1   | 5.55  | 1.43        | 1.39     |
| 1   | AA    | 1130 | A    | C2'-C1' | -5.55 | 1.47        | 1.53     |
| 1   | AA    | 1323 | G    | N9-C4   | 5.55  | 1.42        | 1.38     |
| 1   | AA    | 1350 | A    | C5'-C4' | 5.55  | 1.58        | 1.51     |
| 35  | BB    | 303  | G    | N1-C2   | 5.55  | 1.42        | 1.37     |
| 35  | BB    | 970  | U    | C4-O4   | 5.55  | 1.28        | 1.23     |
| 35  | BB    | 1486 | U    | N3-C4   | 5.55  | 1.43        | 1.38     |
| 35  | BB    | 1738 | G    | C3'-O3' | 5.55  | 1.50        | 1.42     |
| 35  | BB    | 1938 | A    | C2-N3   | 5.55  | 1.38        | 1.33     |
| 35  | BB    | 2048 | G    | C1'-N9  | -5.55 | 1.39        | 1.46     |
| 35  | BB    | 2521 | C    | C2-N3   | 5.55  | 1.40        | 1.35     |
| 35  | BB    | 2554 | U    | C2'-C1' | -5.55 | 1.47        | 1.53     |
| 36  | BC    | 82   | TYR  | CD1-CE1 | 5.55  | 1.47        | 1.39     |
| 1   | AA    | 740  | U    | C2-N3   | 5.55  | 1.41        | 1.37     |
| 1   | AA    | 1280 | A    | N9-C8   | -5.55 | 1.33        | 1.37     |
| 1   | AA    | 1524 | C    | C4-N4   | 5.55  | 1.39        | 1.33     |
| 35  | BB    | 975  | A    | N7-C5   | -5.55 | 1.35        | 1.39     |
| 35  | BB    | 984  | A    | C6-N6   | 5.55  | 1.38        | 1.33     |
| 55  | BW    | 26   | PHE  | CG-CD1  | 5.55  | 1.47        | 1.38     |
| 1   | AA    | 169  | C    | C4-N4   | 5.55  | 1.39        | 1.33     |
| 1   | AA    | 626  | G    | C6-N1   | 5.55  | 1.43        | 1.39     |
| 1   | AA    | 1154 | G    | P-O5'   | -5.55 | 1.54        | 1.59     |
| 34  | BA    | 63   | C    | C2-N3   | 5.55  | 1.40        | 1.35     |
| 35  | BB    | 290  | U    | C2'-C1' | -5.55 | 1.47        | 1.53     |
| 35  | BB    | 536  | G    | C8-N7   | 5.55  | 1.34        | 1.30     |
| 35  | BB    | 566  | U    | C2'-O2' | -5.55 | 1.34        | 1.41     |
| 35  | BB    | 924  | G    | N7-C5   | -5.55 | 1.35        | 1.39     |
| 35  | BB    | 2190 | G    | C6-N1   | 5.55  | 1.43        | 1.39     |
| 35  | BB    | 2397 | G    | C4'-C3' | 5.55  | 1.59        | 1.53     |
| 1   | AA    | 127  | G    | N9-C4   | -5.55 | 1.33        | 1.38     |
| 1   | AA    | 369  | G    | O3'-P   | -5.55 | 1.54        | 1.61     |
| 1   | AA    | 482  | A    | N1-C2   | -5.55 | 1.29        | 1.34     |
| 1   | AA    | 1002 | G    | C2-N3   | 5.55  | 1.37        | 1.32     |
| 1   | AA    | 1181 | G    | N3-C4   | 5.55  | 1.39        | 1.35     |
| 1   | AA    | 1355 | G    | N7-C5   | -5.55 | 1.35        | 1.39     |
| 35  | BB    | 274  | C    | C3'-C2' | -5.55 | 1.46        | 1.52     |
| 35  | BB    | 361  | G    | C5'-C4' | 5.55  | 1.58        | 1.51     |
| 35  | BB    | 570  | G    | N9-C4   | -5.55 | 1.33        | 1.38     |
| 35  | BB    | 721  | A    | C2'-C1' | -5.55 | 1.47        | 1.53     |
| 35  | BB    | 1062 | G    | C5-C4   | -5.55 | 1.34        | 1.38     |
| 35  | BB    | 1786 | A    | C6-N1   | 5.55  | 1.39        | 1.35     |
| 35  | BB    | 2176 | A    | C5'-C4' | 5.55  | 1.58        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2561 | U    | P-O5'   | 5.55  | 1.65        | 1.59     |
| 35  | BB    | 2895 | G    | C5'-C4' | 5.55  | 1.58        | 1.51     |
| 47  | BN    | 90   | ARG  | NE-CZ   | 5.55  | 1.40        | 1.33     |
| 1   | AA    | 919  | A    | C5-C4   | 5.55  | 1.42        | 1.38     |
| 35  | BB    | 131  | A    | C6-N6   | 5.55  | 1.38        | 1.33     |
| 35  | BB    | 448  | U    | C4'-C3' | 5.55  | 1.59        | 1.53     |
| 35  | BB    | 721  | A    | N3-C4   | 5.55  | 1.38        | 1.34     |
| 35  | BB    | 1149 | G    | N7-C5   | -5.55 | 1.35        | 1.39     |
| 35  | BB    | 1555 | G    | N1-C2   | 5.55  | 1.42        | 1.37     |
| 35  | BB    | 2507 | C    | C2-N3   | 5.55  | 1.40        | 1.35     |
| 35  | BB    | 2653 | U    | C4'-C3' | 5.55  | 1.59        | 1.53     |
| 1   | AA    | 656  | G    | N9-C4   | -5.55 | 1.33        | 1.38     |
| 1   | AA    | 870  | U    | C4-C5   | 5.55  | 1.48        | 1.43     |
| 1   | AA    | 947  | G    | C6-N1   | 5.55  | 1.43        | 1.39     |
| 35  | BB    | 180  | G    | C2'-O2' | -5.55 | 1.34        | 1.41     |
| 35  | BB    | 606  | U    | C4'-C3' | 5.55  | 1.59        | 1.53     |
| 35  | BB    | 793  | A    | C2'-C1' | -5.55 | 1.47        | 1.53     |
| 35  | BB    | 1236 | G    | C5-C4   | 5.55  | 1.42        | 1.38     |
| 35  | BB    | 1722 | A    | C2-N3   | 5.55  | 1.38        | 1.33     |
| 35  | BB    | 2649 | C    | O3'-P   | -5.55 | 1.54        | 1.61     |
| 37  | BD    | 118  | PHE  | CG-CD1  | 5.55  | 1.47        | 1.38     |
| 1   | AA    | 1158 | C    | C2-O2   | -5.54 | 1.19        | 1.24     |
| 1   | AA    | 1302 | C    | N1-C2   | 5.54  | 1.45        | 1.40     |
| 30  | B5    | 117  | SER  | CA-CB   | 5.54  | 1.61        | 1.52     |
| 35  | BB    | 2336 | A    | C2'-C1' | -5.54 | 1.47        | 1.53     |
| 35  | BB    | 2393 | U    | C4'-C3' | 5.54  | 1.59        | 1.53     |
| 1   | AA    | 190  | A    | N7-C5   | -5.54 | 1.35        | 1.39     |
| 1   | AA    | 672  | U    | P-O5'   | -5.54 | 1.54        | 1.59     |
| 1   | AA    | 1141 | C    | C4-C5   | 5.54  | 1.47        | 1.43     |
| 1   | AA    | 1493 | A    | C5-C4   | 5.54  | 1.42        | 1.38     |
| 4   | AD    | 23   | GLY  | N-CA    | -5.54 | 1.37        | 1.46     |
| 35  | BB    | 89   | A    | C6-N6   | 5.54  | 1.38        | 1.33     |
| 35  | BB    | 1074 | G    | C2-N2   | 5.54  | 1.40        | 1.34     |
| 35  | BB    | 1162 | G    | C5-C6   | -5.54 | 1.36        | 1.42     |
| 35  | BB    | 1174 | U    | N1-C6   | -5.54 | 1.32        | 1.38     |
| 35  | BB    | 2273 | A    | C3'-O3' | 5.54  | 1.50        | 1.42     |
| 35  | BB    | 2723 | C    | C2'-C1' | -5.54 | 1.47        | 1.53     |
| 35  | BB    | 2788 | C    | O3'-P   | -5.54 | 1.54        | 1.61     |
| 1   | AA    | 304  | U    | O4'-C1' | 5.54  | 1.48        | 1.41     |
| 1   | AA    | 349  | A    | C6-N1   | 5.54  | 1.39        | 1.35     |
| 1   | AA    | 639  | G    | N7-C5   | -5.54 | 1.35        | 1.39     |
| 1   | AA    | 695  | A    | N9-C8   | 5.54  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1200 | C    | C4-N4   | 5.54  | 1.39        | 1.33     |
| 1   | AA    | 1350 | A    | C4'-C3' | -5.54 | 1.47        | 1.52     |
| 35  | BB    | 59   | U    | C2-O2   | 5.54  | 1.27        | 1.22     |
| 35  | BB    | 401  | A    | C5-C6   | 5.54  | 1.46        | 1.41     |
| 35  | BB    | 440  | C    | C3'-C2' | 5.54  | 1.59        | 1.52     |
| 35  | BB    | 713  | G    | N7-C5   | -5.54 | 1.35        | 1.39     |
| 35  | BB    | 750  | A    | O3'-P   | -5.54 | 1.54        | 1.61     |
| 35  | BB    | 799  | G    | N3-C4   | 5.54  | 1.39        | 1.35     |
| 35  | BB    | 1130 | U    | C4-C5   | -5.54 | 1.38        | 1.43     |
| 35  | BB    | 1202 | G    | C2-N3   | 5.54  | 1.37        | 1.32     |
| 35  | BB    | 1268 | A    | N9-C4   | -5.54 | 1.34        | 1.37     |
| 35  | BB    | 1315 | C    | N1-C2   | 5.54  | 1.45        | 1.40     |
| 35  | BB    | 1467 | U    | O3'-P   | -5.54 | 1.54        | 1.61     |
| 35  | BB    | 1794 | A    | N3-C4   | -5.54 | 1.31        | 1.34     |
| 36  | BC    | 268  | ARG  | CZ-NH1  | 5.54  | 1.40        | 1.33     |
| 1   | AA    | 374  | A    | N9-C4   | 5.54  | 1.41        | 1.37     |
| 1   | AA    | 518  | C    | C3'-C2' | 5.54  | 1.59        | 1.52     |
| 1   | AA    | 753  | A    | N3-C4   | 5.54  | 1.38        | 1.34     |
| 1   | AA    | 1150 | A    | C2'-C1' | -5.54 | 1.47        | 1.53     |
| 35  | BB    | 1819 | A    | P-O5'   | -5.54 | 1.54        | 1.59     |
| 35  | BB    | 2681 | C    | C2-N3   | 5.54  | 1.40        | 1.35     |
| 1   | AA    | 192  | A    | C5'-C4' | 5.54  | 1.57        | 1.51     |
| 1   | AA    | 195  | A    | C2-N3   | 5.54  | 1.38        | 1.33     |
| 35  | BB    | 300  | A    | N3-C4   | -5.54 | 1.31        | 1.34     |
| 35  | BB    | 376  | G    | C5-C4   | 5.54  | 1.42        | 1.38     |
| 35  | BB    | 501  | A    | N1-C2   | 5.54  | 1.39        | 1.34     |
| 35  | BB    | 860  | U    | N3-C4   | -5.54 | 1.33        | 1.38     |
| 35  | BB    | 943  | A    | C5'-C4' | 5.54  | 1.57        | 1.51     |
| 35  | BB    | 1169 | A    | C6-N1   | -5.54 | 1.31        | 1.35     |
| 35  | BB    | 1319 | C    | C3'-C2' | -5.54 | 1.46        | 1.52     |
| 35  | BB    | 1351 | C    | N3-C4   | 5.54  | 1.37        | 1.33     |
| 35  | BB    | 1439 | A    | C6-N6   | 5.54  | 1.38        | 1.33     |
| 35  | BB    | 1576 | U    | C3'-C2' | 5.54  | 1.59        | 1.52     |
| 35  | BB    | 2304 | G    | C6-N1   | 5.54  | 1.43        | 1.39     |
| 1   | AA    | 112  | G    | N9-C8   | -5.54 | 1.33        | 1.37     |
| 1   | AA    | 1104 | G    | C5-C6   | -5.54 | 1.36        | 1.42     |
| 8   | AH    | 14   | ARG  | CZ-NH2  | 5.54  | 1.40        | 1.33     |
| 27  | B2    | 10   | ARG  | NE-CZ   | 5.54  | 1.40        | 1.33     |
| 34  | BA    | 92   | C    | C2-N3   | 5.54  | 1.40        | 1.35     |
| 35  | BB    | 245  | G    | O3'-P   | -5.54 | 1.54        | 1.61     |
| 35  | BB    | 1526 | C    | C5-C6   | -5.54 | 1.29        | 1.34     |
| 1   | AA    | 372  | C    | N1-C2   | -5.54 | 1.34        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 395  | C    | C4-C5   | 5.54  | 1.47        | 1.43     |
| 1   | AA    | 589  | U    | N1-C6   | 5.54  | 1.43        | 1.38     |
| 1   | AA    | 660  | C    | C2-N3   | 5.54  | 1.40        | 1.35     |
| 1   | AA    | 1015 | G    | C5'-C4' | -5.54 | 1.44        | 1.51     |
| 35  | BB    | 1391 | U    | O3'-P   | -5.54 | 1.54        | 1.61     |
| 35  | BB    | 2024 | G    | C3'-C2' | -5.54 | 1.46        | 1.52     |
| 35  | BB    | 2053 | G    | C5-C4   | -5.54 | 1.34        | 1.38     |
| 1   | AA    | 112  | G    | C2'-C1' | -5.53 | 1.47        | 1.53     |
| 1   | AA    | 174  | A    | C4'-C3' | 5.53  | 1.59        | 1.53     |
| 1   | AA    | 1054 | C    | O4'-C1' | 5.53  | 1.48        | 1.41     |
| 1   | AA    | 1256 | A    | C4'-C3' | -5.53 | 1.47        | 1.52     |
| 12  | AL    | 67   | GLY  | N-CA    | -5.53 | 1.37        | 1.46     |
| 34  | BA    | 89   | U    | C3'-C2' | -5.53 | 1.46        | 1.52     |
| 35  | BB    | 432  | A    | C2'-C1' | -5.53 | 1.47        | 1.53     |
| 35  | BB    | 521  | U    | C4'-C3' | -5.53 | 1.47        | 1.52     |
| 35  | BB    | 1430 | G    | C8-N7   | -5.53 | 1.27        | 1.30     |
| 35  | BB    | 1618 | A    | N7-C5   | -5.53 | 1.35        | 1.39     |
| 35  | BB    | 1706 | C    | C4-N4   | 5.53  | 1.39        | 1.33     |
| 35  | BB    | 1724 | G    | N9-C8   | 5.53  | 1.41        | 1.37     |
| 35  | BB    | 2448 | A    | N9-C4   | 5.53  | 1.41        | 1.37     |
| 35  | BB    | 2616 | C    | N1-C2   | -5.53 | 1.34        | 1.40     |
| 1   | AA    | 188  | C    | C4-C5   | 5.53  | 1.47        | 1.43     |
| 1   | AA    | 655  | A    | P-O5'   | -5.53 | 1.54        | 1.59     |
| 35  | BB    | 497  | A    | C6-N6   | 5.53  | 1.38        | 1.33     |
| 35  | BB    | 748  | G    | C8-N7   | 5.53  | 1.34        | 1.30     |
| 35  | BB    | 1105 | U    | C4-C5   | 5.53  | 1.48        | 1.43     |
| 35  | BB    | 1401 | G    | N9-C8   | -5.53 | 1.33        | 1.37     |
| 35  | BB    | 2695 | U    | C5'-C4' | 5.53  | 1.57        | 1.51     |
| 1   | AA    | 142  | G    | C3'-C2' | 5.53  | 1.59        | 1.52     |
| 1   | AA    | 726  | C    | N1-C2   | 5.53  | 1.45        | 1.40     |
| 35  | BB    | 1395 | A    | N3-C4   | 5.53  | 1.38        | 1.34     |
| 35  | BB    | 2331 | G    | C4'-C3' | 5.53  | 1.59        | 1.53     |
| 1   | AA    | 120  | A    | N9-C8   | 5.53  | 1.42        | 1.37     |
| 35  | BB    | 1061 | U    | C2'-C1' | -5.53 | 1.47        | 1.53     |
| 35  | BB    | 1249 | U    | P-O5'   | -5.53 | 1.54        | 1.59     |
| 35  | BB    | 1251 | C    | C4-C5   | -5.53 | 1.38        | 1.43     |
| 35  | BB    | 1498 | C    | C2'-O2' | -5.53 | 1.34        | 1.41     |
| 35  | BB    | 1526 | C    | C4'-O4' | -5.53 | 1.38        | 1.45     |
| 35  | BB    | 2549 | G    | C6-N1   | 5.53  | 1.43        | 1.39     |
| 1   | AA    | 75   | G    | C2-N3   | 5.53  | 1.37        | 1.32     |
| 1   | AA    | 231  | U    | N1-C6   | 5.53  | 1.43        | 1.38     |
| 1   | AA    | 356  | A    | C5'-C4' | 5.53  | 1.57        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 540  | G    | C8-N7   | -5.53 | 1.27        | 1.30     |
| 1   | AA    | 720  | C    | C4'-C3' | -5.53 | 1.47        | 1.52     |
| 1   | AA    | 760  | G    | C4'-O4' | 5.53  | 1.52        | 1.45     |
| 1   | AA    | 910  | C    | C1'-N1  | 5.53  | 1.57        | 1.48     |
| 22  | AV    | 76   | A    | N9-C4   | 5.53  | 1.41        | 1.37     |
| 34  | BA    | 75   | G    | C5-C4   | -5.53 | 1.34        | 1.38     |
| 35  | BB    | 550  | C    | C2-N3   | 5.53  | 1.40        | 1.35     |
| 35  | BB    | 839  | U    | C2-O2   | 5.53  | 1.27        | 1.22     |
| 35  | BB    | 1045 | C    | P-O5'   | 5.53  | 1.65        | 1.59     |
| 35  | BB    | 2182 | U    | C4-C5   | 5.53  | 1.48        | 1.43     |
| 1   | AA    | 229  | U    | C2-N3   | 5.53  | 1.41        | 1.37     |
| 1   | AA    | 699  | C    | N1-C2   | -5.53 | 1.34        | 1.40     |
| 1   | AA    | 998  | C    | C4-N4   | 5.53  | 1.39        | 1.33     |
| 34  | BA    | 113  | C    | C5-C6   | 5.53  | 1.38        | 1.34     |
| 35  | BB    | 194  | G    | C5-C6   | -5.53 | 1.36        | 1.42     |
| 35  | BB    | 966  | G    | C8-N7   | 5.53  | 1.34        | 1.30     |
| 35  | BB    | 1483 | G    | C3'-C2' | 5.53  | 1.59        | 1.52     |
| 35  | BB    | 1622 | G    | O4'-C1' | 5.53  | 1.48        | 1.41     |
| 35  | BB    | 1903 | G    | N3-C4   | -5.53 | 1.31        | 1.35     |
| 35  | BB    | 2450 | A    | C2-N3   | 5.53  | 1.38        | 1.33     |
| 35  | BB    | 2458 | G    | N3-C4   | -5.53 | 1.31        | 1.35     |
| 1   | AA    | 741  | G    | O4'-C1' | 5.52  | 1.48        | 1.41     |
| 35  | BB    | 104  | A    | C5'-C4' | 5.52  | 1.57        | 1.51     |
| 35  | BB    | 715  | A    | N9-C4   | 5.52  | 1.41        | 1.37     |
| 35  | BB    | 2537 | U    | C2-N3   | -5.52 | 1.33        | 1.37     |
| 35  | BB    | 2890 | G    | C2-N2   | 5.52  | 1.40        | 1.34     |
| 1   | AA    | 970  | C    | C4'-O4' | 5.52  | 1.52        | 1.45     |
| 1   | AA    | 996  | A    | C2'-O2' | 5.52  | 1.48        | 1.41     |
| 34  | BA    | 9    | G    | N7-C5   | -5.52 | 1.35        | 1.39     |
| 34  | BA    | 33   | G    | P-O5'   | -5.52 | 1.54        | 1.59     |
| 34  | BA    | 53   | A    | N1-C2   | 5.52  | 1.39        | 1.34     |
| 35  | BB    | 111  | A    | P-O5'   | -5.52 | 1.54        | 1.59     |
| 35  | BB    | 361  | G    | N7-C5   | -5.52 | 1.35        | 1.39     |
| 35  | BB    | 1474 | U    | C5-C6   | 5.52  | 1.39        | 1.34     |
| 35  | BB    | 1587 | G    | N9-C8   | 5.52  | 1.41        | 1.37     |
| 35  | BB    | 2463 | C    | N1-C2   | 5.52  | 1.45        | 1.40     |
| 35  | BB    | 2816 | G    | N3-C4   | -5.52 | 1.31        | 1.35     |
| 37  | BD    | 128  | ARG  | CZ-NH2  | 5.52  | 1.40        | 1.33     |
| 41  | BH    | 34   | GLY  | CA-C    | -5.52 | 1.43        | 1.51     |
| 34  | BA    | 50   | A    | N9-C4   | -5.52 | 1.34        | 1.37     |
| 35  | BB    | 779  | U    | O3'-P   | -5.52 | 1.54        | 1.61     |
| 35  | BB    | 2093 | G    | N9-C8   | 5.52  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2380 | C    | N3-C4   | 5.52  | 1.37        | 1.33     |
| 1   | AA    | 325  | A    | C5'-C4' | 5.52  | 1.57        | 1.51     |
| 1   | AA    | 409  | U    | O3'-P   | -5.52 | 1.54        | 1.61     |
| 1   | AA    | 642  | A    | C8-N7   | -5.52 | 1.27        | 1.31     |
| 1   | AA    | 1401 | G    | C4'-C3' | -5.52 | 1.47        | 1.52     |
| 1   | AA    | 1502 | A    | C6-N1   | 5.52  | 1.39        | 1.35     |
| 35  | BB    | 466  | A    | C2'-C1' | -5.52 | 1.47        | 1.53     |
| 35  | BB    | 580  | U    | C2-O2   | 5.52  | 1.27        | 1.22     |
| 35  | BB    | 1112 | G    | N1-C2   | 5.52  | 1.42        | 1.37     |
| 35  | BB    | 1698 | A    | C3'-C2' | 5.52  | 1.59        | 1.52     |
| 35  | BB    | 2330 | G    | C5-C4   | 5.52  | 1.42        | 1.38     |
| 35  | BB    | 2683 | C    | C5-C6   | 5.52  | 1.38        | 1.34     |
| 35  | BB    | 2704 | C    | N1-C6   | 5.52  | 1.40        | 1.37     |
| 1   | AA    | 13   | U    | C4-O4   | -5.52 | 1.19        | 1.23     |
| 1   | AA    | 1271 | A    | C4'-O4' | -5.52 | 1.38        | 1.45     |
| 35  | BB    | 699  | A    | C5'-C4' | 5.52  | 1.57        | 1.51     |
| 35  | BB    | 887  | U    | O3'-P   | -5.52 | 1.54        | 1.61     |
| 35  | BB    | 915  | C    | C4'-O4' | 5.52  | 1.52        | 1.45     |
| 35  | BB    | 1442 | U    | C2-N3   | -5.52 | 1.33        | 1.37     |
| 35  | BB    | 1735 | A    | N9-C4   | -5.52 | 1.34        | 1.37     |
| 35  | BB    | 2270 | A    | C2-N3   | 5.52  | 1.38        | 1.33     |
| 35  | BB    | 2620 | C    | C4'-O4' | 5.52  | 1.52        | 1.45     |
| 1   | AA    | 554  | A    | C4'-C3' | 5.52  | 1.59        | 1.53     |
| 1   | AA    | 575  | G    | N1-C2   | 5.52  | 1.42        | 1.37     |
| 1   | AA    | 706  | A    | O3'-P   | -5.52 | 1.54        | 1.61     |
| 2   | AB    | 103  | TRP  | CD2-CE2 | -5.52 | 1.34        | 1.41     |
| 35  | BB    | 127  | A    | C4'-C3' | -5.52 | 1.47        | 1.52     |
| 35  | BB    | 172  | A    | C1'-N9  | -5.52 | 1.39        | 1.46     |
| 35  | BB    | 756  | A    | C5-C6   | -5.52 | 1.36        | 1.41     |
| 35  | BB    | 1134 | A    | P-O5'   | -5.52 | 1.54        | 1.59     |
| 35  | BB    | 1428 | C    | O3'-P   | -5.52 | 1.54        | 1.61     |
| 35  | BB    | 1523 | U    | C2'-C1' | -5.52 | 1.47        | 1.53     |
| 35  | BB    | 2176 | A    | C5-C4   | 5.52  | 1.42        | 1.38     |
| 35  | BB    | 2472 | G    | C2-N3   | 5.52  | 1.37        | 1.32     |
| 1   | AA    | 690  | G    | N9-C4   | -5.51 | 1.33        | 1.38     |
| 1   | AA    | 833  | G    | N9-C4   | -5.51 | 1.33        | 1.38     |
| 1   | AA    | 936  | C    | C3'-C2' | -5.51 | 1.46        | 1.52     |
| 1   | AA    | 1031 | C    | C4-C5   | 5.51  | 1.47        | 1.43     |
| 1   | AA    | 1067 | A    | C6-N6   | 5.51  | 1.38        | 1.33     |
| 1   | AA    | 1145 | A    | N3-C4   | 5.51  | 1.38        | 1.34     |
| 35  | BB    | 1946 | U    | P-O5'   | -5.51 | 1.54        | 1.59     |
| 35  | BB    | 2020 | A    | N3-C4   | -5.51 | 1.31        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2315 | G    | O3'-P   | -5.51 | 1.54        | 1.61     |
| 35  | BB    | 2610 | C    | C4-C5   | 5.51  | 1.47        | 1.43     |
| 1   | AA    | 120  | A    | C2'-O2' | 5.51  | 1.48        | 1.41     |
| 1   | AA    | 189  | A    | N1-C2   | -5.51 | 1.29        | 1.34     |
| 1   | AA    | 389  | A    | O3'-P   | -5.51 | 1.54        | 1.61     |
| 1   | AA    | 807  | A    | P-O5'   | -5.51 | 1.54        | 1.59     |
| 35  | BB    | 997  | G    | C2-N3   | 5.51  | 1.37        | 1.32     |
| 35  | BB    | 1457 | U    | C4'-O4' | 5.51  | 1.52        | 1.45     |
| 35  | BB    | 1972 | G    | C2-N2   | 5.51  | 1.40        | 1.34     |
| 1   | AA    | 228  | A    | N9-C4   | -5.51 | 1.34        | 1.37     |
| 1   | AA    | 529  | G    | O4'-C1' | 5.51  | 1.48        | 1.41     |
| 1   | AA    | 972  | C    | C3'-C2' | 5.51  | 1.59        | 1.52     |
| 35  | BB    | 132  | G    | C2-N2   | 5.51  | 1.40        | 1.34     |
| 35  | BB    | 936  | A    | N7-C5   | -5.51 | 1.35        | 1.39     |
| 35  | BB    | 1642 | G    | N9-C4   | -5.51 | 1.33        | 1.38     |
| 35  | BB    | 1897 | G    | C3'-C2' | 5.51  | 1.59        | 1.52     |
| 35  | BB    | 1997 | C    | C1'-N1  | -5.51 | 1.39        | 1.46     |
| 35  | BB    | 2526 | G    | C5-C4   | 5.51  | 1.42        | 1.38     |
| 35  | BB    | 2668 | G    | C3'-C2' | 5.51  | 1.59        | 1.52     |
| 1   | AA    | 232  | G    | N3-C4   | 5.51  | 1.39        | 1.35     |
| 1   | AA    | 310  | G    | C2-N3   | 5.51  | 1.37        | 1.32     |
| 1   | AA    | 651  | C    | C4-C5   | 5.51  | 1.47        | 1.43     |
| 35  | BB    | 340  | A    | N9-C8   | -5.51 | 1.33        | 1.37     |
| 35  | BB    | 624  | C    | C4-N4   | 5.51  | 1.39        | 1.33     |
| 35  | BB    | 903  | C    | P-O5'   | -5.51 | 1.54        | 1.59     |
| 35  | BB    | 909  | A    | C5'-C4' | 5.51  | 1.57        | 1.51     |
| 35  | BB    | 1000 | A    | C5'-C4' | 5.51  | 1.57        | 1.51     |
| 35  | BB    | 1384 | A    | N9-C4   | -5.51 | 1.34        | 1.37     |
| 35  | BB    | 1496 | A    | C2'-C1' | -5.51 | 1.47        | 1.53     |
| 35  | BB    | 2200 | C    | C3'-C2' | -5.51 | 1.46        | 1.52     |
| 35  | BB    | 2337 | G    | N9-C4   | 5.51  | 1.42        | 1.38     |
| 1   | AA    | 105  | G    | C4'-C3' | -5.51 | 1.47        | 1.52     |
| 1   | AA    | 338  | A    | C6-N1   | 5.51  | 1.39        | 1.35     |
| 1   | AA    | 1087 | G    | C2-N2   | 5.51  | 1.40        | 1.34     |
| 19  | AS    | 28   | LYS  | CD-CE   | 5.51  | 1.65        | 1.51     |
| 35  | BB    | 20   | C    | C5'-C4' | 5.51  | 1.57        | 1.51     |
| 35  | BB    | 869  | G    | C3'-C2' | -5.51 | 1.46        | 1.52     |
| 35  | BB    | 1374 | G    | N3-C4   | -5.51 | 1.31        | 1.35     |
| 35  | BB    | 1861 | G    | N9-C8   | 5.51  | 1.41        | 1.37     |
| 35  | BB    | 1998 | A    | C6-N1   | -5.51 | 1.31        | 1.35     |
| 35  | BB    | 2581 | G    | N3-C4   | 5.51  | 1.39        | 1.35     |
| 35  | BB    | 2620 | C    | O5'-C5' | -5.51 | 1.34        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 41  | BH    | 25   | TYR  | CG-CD2  | 5.51  | 1.46        | 1.39     |
| 1   | AA    | 332  | G    | N9-C8   | -5.51 | 1.33        | 1.37     |
| 1   | AA    | 585  | G    | C2'-C1' | -5.51 | 1.47        | 1.53     |
| 1   | AA    | 602  | A    | C2'-C1' | -5.51 | 1.47        | 1.53     |
| 1   | AA    | 728  | A    | N9-C8   | 5.51  | 1.42        | 1.37     |
| 1   | AA    | 820  | U    | C2-N3   | 5.51  | 1.41        | 1.37     |
| 1   | AA    | 898  | G    | C4'-C3' | -5.51 | 1.47        | 1.52     |
| 34  | BA    | 53   | A    | C4'-C3' | -5.51 | 1.47        | 1.52     |
| 35  | BB    | 4    | U    | P-O5'   | -5.51 | 1.54        | 1.59     |
| 35  | BB    | 35   | G    | N9-C8   | 5.51  | 1.41        | 1.37     |
| 35  | BB    | 168  | G    | N3-C4   | 5.51  | 1.39        | 1.35     |
| 35  | BB    | 260  | G    | N7-C5   | -5.51 | 1.35        | 1.39     |
| 35  | BB    | 457  | A    | P-O5'   | -5.51 | 1.54        | 1.59     |
| 35  | BB    | 850  | U    | N1-C6   | -5.51 | 1.32        | 1.38     |
| 35  | BB    | 862  | G    | C6-N1   | -5.51 | 1.35        | 1.39     |
| 35  | BB    | 1265 | A    | C5-C6   | -5.51 | 1.36        | 1.41     |
| 35  | BB    | 1736 | U    | N1-C6   | 5.51  | 1.43        | 1.38     |
| 35  | BB    | 2789 | C    | N3-C4   | 5.51  | 1.37        | 1.33     |
| 1   | AA    | 292  | G    | N7-C5   | -5.50 | 1.35        | 1.39     |
| 1   | AA    | 455  | G    | N3-C4   | -5.50 | 1.31        | 1.35     |
| 1   | AA    | 712  | A    | C8-N7   | -5.50 | 1.27        | 1.31     |
| 1   | AA    | 1506 | U    | C4-C5   | 5.50  | 1.48        | 1.43     |
| 35  | BB    | 1622 | G    | C5-C6   | -5.50 | 1.36        | 1.42     |
| 35  | BB    | 1761 | C    | C4-N4   | 5.50  | 1.39        | 1.33     |
| 1   | AA    | 86   | G    | C5-C4   | -5.50 | 1.34        | 1.38     |
| 1   | AA    | 491  | G    | C5-C4   | 5.50  | 1.42        | 1.38     |
| 1   | AA    | 573  | A    | C6-N6   | 5.50  | 1.38        | 1.33     |
| 1   | AA    | 861  | G    | N3-C4   | -5.50 | 1.31        | 1.35     |
| 35  | BB    | 869  | G    | P-O5'   | -5.50 | 1.54        | 1.59     |
| 35  | BB    | 1256 | G    | C4'-O4' | -5.50 | 1.38        | 1.45     |
| 35  | BB    | 1498 | C    | N1-C2   | 5.50  | 1.45        | 1.40     |
| 35  | BB    | 2143 | C    | C3'-O3' | 5.50  | 1.49        | 1.42     |
| 35  | BB    | 2461 | A    | C3'-C2' | -5.50 | 1.46        | 1.52     |
| 35  | BB    | 2735 | G    | C5-C4   | -5.50 | 1.34        | 1.38     |
| 35  | BB    | 2739 | U    | C2-N3   | 5.50  | 1.41        | 1.37     |
| 1   | AA    | 574  | A    | O4'-C1' | 5.50  | 1.48        | 1.41     |
| 1   | AA    | 1407 | C    | N3-C4   | 5.50  | 1.37        | 1.33     |
| 35  | BB    | 745  | G    | C3'-C2' | -5.50 | 1.46        | 1.52     |
| 35  | BB    | 1031 | G    | N9-C4   | 5.50  | 1.42        | 1.38     |
| 35  | BB    | 1635 | A    | N3-C4   | -5.50 | 1.31        | 1.34     |
| 35  | BB    | 1694 | C    | C5-C6   | 5.50  | 1.38        | 1.34     |
| 1   | AA    | 960  | U    | N3-C4   | -5.50 | 1.33        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1163 | G    | P-O5'   | -5.50 | 1.54        | 1.59     |
| 35  | BB    | 1863 | G    | C1'-N9  | -5.50 | 1.39        | 1.46     |
| 35  | BB    | 2310 | C    | O3'-P   | -5.50 | 1.54        | 1.61     |
| 1   | AA    | 425  | G    | N9-C8   | 5.50  | 1.41        | 1.37     |
| 1   | AA    | 716  | A    | N9-C4   | -5.50 | 1.34        | 1.37     |
| 1   | AA    | 733  | G    | C2'-O2' | -5.50 | 1.34        | 1.41     |
| 1   | AA    | 746  | A    | C2'-C1' | -5.50 | 1.47        | 1.53     |
| 1   | AA    | 1139 | G    | O3'-P   | -5.50 | 1.54        | 1.61     |
| 1   | AA    | 1299 | A    | C5'-C4' | 5.50  | 1.57        | 1.51     |
| 35  | BB    | 278  | A    | C6-N6   | 5.50  | 1.38        | 1.33     |
| 35  | BB    | 284  | U    | C2'-C1' | -5.50 | 1.47        | 1.53     |
| 35  | BB    | 500  | G    | C5-C4   | 5.50  | 1.42        | 1.38     |
| 35  | BB    | 715  | A    | C2'-C1' | -5.50 | 1.47        | 1.53     |
| 35  | BB    | 865  | C    | O4'-C1' | -5.50 | 1.34        | 1.41     |
| 35  | BB    | 1961 | C    | C3'-C2' | 5.50  | 1.58        | 1.52     |
| 35  | BB    | 1977 | A    | N3-C4   | -5.50 | 1.31        | 1.34     |
| 35  | BB    | 2114 | A    | N9-C8   | 5.50  | 1.42        | 1.37     |
| 35  | BB    | 2155 | U    | C3'-C2' | -5.50 | 1.46        | 1.52     |
| 35  | BB    | 2399 | G    | C2'-C1' | -5.50 | 1.47        | 1.53     |
| 35  | BB    | 2868 | A    | N3-C4   | -5.50 | 1.31        | 1.34     |
| 1   | AA    | 178  | C    | N3-C4   | 5.50  | 1.37        | 1.33     |
| 34  | BA    | 76   | G    | N1-C2   | 5.50  | 1.42        | 1.37     |
| 35  | BB    | 651  | G    | P-O5'   | -5.50 | 1.54        | 1.59     |
| 35  | BB    | 1025 | G    | P-O5'   | -5.50 | 1.54        | 1.59     |
| 35  | BB    | 1039 | A    | C3'-O3' | 5.50  | 1.49        | 1.42     |
| 35  | BB    | 2020 | A    | O3'-P   | -5.50 | 1.54        | 1.61     |
| 1   | AA    | 116  | A    | C6-N1   | 5.50  | 1.39        | 1.35     |
| 1   | AA    | 487  | A    | O3'-P   | -5.50 | 1.54        | 1.61     |
| 1   | AA    | 1493 | A    | C5'-C4' | 5.50  | 1.57        | 1.51     |
| 35  | BB    | 48   | G    | N1-C2   | 5.50  | 1.42        | 1.37     |
| 35  | BB    | 616  | A    | P-O5'   | -5.50 | 1.54        | 1.59     |
| 35  | BB    | 1446 | C    | C4'-C3' | 5.50  | 1.59        | 1.53     |
| 35  | BB    | 1516 | G    | C5-C6   | -5.50 | 1.36        | 1.42     |
| 35  | BB    | 2241 | A    | C5-C4   | -5.50 | 1.34        | 1.38     |
| 35  | BB    | 2679 | A    | C6-N1   | 5.50  | 1.39        | 1.35     |
| 1   | AA    | 391  | G    | N1-C2   | 5.49  | 1.42        | 1.37     |
| 1   | AA    | 528  | C    | P-O5'   | -5.49 | 1.54        | 1.59     |
| 1   | AA    | 780  | A    | C6-N6   | 5.49  | 1.38        | 1.33     |
| 1   | AA    | 846  | G    | C8-N7   | -5.49 | 1.27        | 1.30     |
| 1   | AA    | 1289 | A    | N3-C4   | -5.49 | 1.31        | 1.34     |
| 4   | AD    | 43   | ARG  | NE-CZ   | 5.49  | 1.40        | 1.33     |
| 35  | BB    | 458  | G    | C6-N1   | 5.49  | 1.43        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 502  | A    | N3-C4   | -5.49 | 1.31        | 1.34     |
| 35  | BB    | 514  | A    | C2'-C1' | -5.49 | 1.47        | 1.53     |
| 35  | BB    | 547  | A    | C6-N6   | 5.49  | 1.38        | 1.33     |
| 35  | BB    | 1669 | A    | N9-C4   | -5.49 | 1.34        | 1.37     |
| 35  | BB    | 1678 | A    | C3'-C2' | -5.49 | 1.46        | 1.52     |
| 35  | BB    | 2636 | C    | N3-C4   | 5.49  | 1.37        | 1.33     |
| 35  | BB    | 2796 | U    | O3'-P   | -5.49 | 1.54        | 1.61     |
| 1   | AA    | 1367 | C    | C4-C5   | -5.49 | 1.38        | 1.43     |
| 35  | BB    | 970  | U    | N3-C4   | 5.49  | 1.43        | 1.38     |
| 35  | BB    | 1291 | C    | C2-O2   | 5.49  | 1.29        | 1.24     |
| 35  | BB    | 2479 | U    | C2-O2   | 5.49  | 1.27        | 1.22     |
| 1   | AA    | 716  | A    | O3'-P   | -5.49 | 1.54        | 1.61     |
| 1   | AA    | 840  | C    | C5'-C4' | 5.49  | 1.57        | 1.51     |
| 1   | AA    | 1101 | A    | N9-C4   | -5.49 | 1.34        | 1.37     |
| 35  | BB    | 888  | C    | C5-C6   | 5.49  | 1.38        | 1.34     |
| 35  | BB    | 1476 | U    | N3-C4   | 5.49  | 1.43        | 1.38     |
| 35  | BB    | 1682 | G    | N9-C4   | -5.49 | 1.33        | 1.38     |
| 35  | BB    | 1830 | C    | C4-N4   | 5.49  | 1.38        | 1.33     |
| 35  | BB    | 1918 | A    | N1-C2   | -5.49 | 1.29        | 1.34     |
| 35  | BB    | 2061 | G    | O4'-C1' | 5.49  | 1.48        | 1.41     |
| 35  | BB    | 2065 | C    | N3-C4   | 5.49  | 1.37        | 1.33     |
| 35  | BB    | 2100 | G    | C4'-C3' | 5.49  | 1.59        | 1.53     |
| 35  | BB    | 2164 | C    | C5'-C4' | 5.49  | 1.57        | 1.51     |
| 35  | BB    | 2419 | U    | C4-C5   | 5.49  | 1.48        | 1.43     |
| 35  | BB    | 274  | C    | C5-C6   | -5.49 | 1.29        | 1.34     |
| 35  | BB    | 957  | C    | C2-O2   | 5.49  | 1.29        | 1.24     |
| 35  | BB    | 1341 | G    | N1-C2   | 5.49  | 1.42        | 1.37     |
| 35  | BB    | 1700 | A    | O3'-P   | -5.49 | 1.54        | 1.61     |
| 35  | BB    | 1919 | A    | O3'-P   | 5.49  | 1.67        | 1.61     |
| 35  | BB    | 2148 | G    | C2-N3   | 5.49  | 1.37        | 1.32     |
| 35  | BB    | 2    | G    | C5-C4   | 5.49  | 1.42        | 1.38     |
| 35  | BB    | 1005 | C    | C3'-C2' | -5.49 | 1.46        | 1.52     |
| 35  | BB    | 1577 | C    | C4-C5   | 5.49  | 1.47        | 1.43     |
| 1   | AA    | 439  | U    | P-O5'   | -5.49 | 1.54        | 1.59     |
| 1   | AA    | 569  | C    | C5-C6   | 5.49  | 1.38        | 1.34     |
| 1   | AA    | 1515 | G    | C2-N3   | 5.49  | 1.37        | 1.32     |
| 29  | B4    | 15   | GLY  | CA-C    | -5.49 | 1.43        | 1.51     |
| 35  | BB    | 1032 | A    | N1-C2   | -5.49 | 1.29        | 1.34     |
| 35  | BB    | 1171 | G    | N7-C5   | -5.49 | 1.35        | 1.39     |
| 35  | BB    | 1219 | U    | N1-C2   | -5.49 | 1.33        | 1.38     |
| 35  | BB    | 1324 | G    | N1-C2   | 5.49  | 1.42        | 1.37     |
| 35  | BB    | 1776 | G    | C5-C6   | -5.49 | 1.36        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1804 | C    | O3'-P   | -5.49 | 1.54        | 1.61     |
| 35  | BB    | 1808 | A    | C5-C4   | 5.49  | 1.42        | 1.38     |
| 35  | BB    | 2398 | U    | O3'-P   | -5.49 | 1.54        | 1.61     |
| 35  | BB    | 2849 | U    | N1-C6   | 5.49  | 1.42        | 1.38     |
| 1   | AA    | 809  | G    | C2'-C1' | -5.48 | 1.47        | 1.53     |
| 35  | BB    | 440  | C    | N1-C6   | -5.48 | 1.33        | 1.37     |
| 35  | BB    | 672  | C    | N1-C6   | -5.48 | 1.33        | 1.37     |
| 35  | BB    | 1213 | A    | N9-C8   | -5.48 | 1.33        | 1.37     |
| 35  | BB    | 2235 | G    | P-O5'   | -5.48 | 1.54        | 1.59     |
| 35  | BB    | 2503 | A    | O3'-P   | -5.48 | 1.54        | 1.61     |
| 1   | AA    | 262  | A    | C5'-C4' | 5.48  | 1.57        | 1.51     |
| 1   | AA    | 442  | G    | N9-C4   | 5.48  | 1.42        | 1.38     |
| 1   | AA    | 566  | G    | N7-C5   | -5.48 | 1.35        | 1.39     |
| 1   | AA    | 1281 | C    | N1-C2   | -5.48 | 1.34        | 1.40     |
| 35  | BB    | 114  | U    | C4-O4   | -5.48 | 1.19        | 1.23     |
| 35  | BB    | 697  | G    | C2'-C1' | -5.48 | 1.47        | 1.53     |
| 35  | BB    | 937  | C    | N3-C4   | 5.48  | 1.37        | 1.33     |
| 35  | BB    | 1964 | G    | C5'-C4' | 5.48  | 1.57        | 1.51     |
| 1   | AA    | 291  | U    | C2'-C1' | -5.48 | 1.47        | 1.53     |
| 1   | AA    | 473  | U    | N1-C2   | -5.48 | 1.33        | 1.38     |
| 34  | BA    | 32   | U    | C4-O4   | -5.48 | 1.19        | 1.23     |
| 35  | BB    | 142  | A    | N1-C2   | -5.48 | 1.29        | 1.34     |
| 35  | BB    | 363  | G    | C5'-C4' | 5.48  | 1.57        | 1.51     |
| 35  | BB    | 553  | G    | N7-C5   | 5.48  | 1.42        | 1.39     |
| 35  | BB    | 896  | A    | N9-C8   | 5.48  | 1.42        | 1.37     |
| 35  | BB    | 2774 | C    | O4'-C1' | 5.48  | 1.48        | 1.41     |
| 35  | BB    | 2864 | G    | O3'-P   | -5.48 | 1.54        | 1.61     |
| 35  | BB    | 319  | G    | C2'-C1' | -5.48 | 1.47        | 1.53     |
| 35  | BB    | 2176 | A    | C2'-O2' | 5.48  | 1.48        | 1.41     |
| 35  | BB    | 2846 | G    | N3-C4   | -5.48 | 1.31        | 1.35     |
| 1   | AA    | 792  | A    | N7-C5   | -5.48 | 1.35        | 1.39     |
| 1   | AA    | 975  | A    | C6-N6   | 5.48  | 1.38        | 1.33     |
| 1   | AA    | 1356 | G    | O3'-P   | -5.48 | 1.54        | 1.61     |
| 16  | AP    | 8    | ARG  | CD-NE   | 5.48  | 1.55        | 1.46     |
| 22  | AV    | 69   | G    | C5-C6   | -5.48 | 1.36        | 1.42     |
| 34  | BA    | 80   | U    | C5'-C4' | 5.48  | 1.57        | 1.51     |
| 35  | BB    | 700  | G    | N3-C4   | -5.48 | 1.31        | 1.35     |
| 35  | BB    | 2009 | A    | C5'-C4' | 5.48  | 1.57        | 1.51     |
| 35  | BB    | 2529 | G    | C2-N2   | 5.48  | 1.40        | 1.34     |
| 35  | BB    | 2721 | A    | O3'-P   | -5.48 | 1.54        | 1.61     |
| 1   | AA    | 235  | C    | C2'-C1' | -5.48 | 1.47        | 1.53     |
| 34  | BA    | 77   | U    | O3'-P   | -5.48 | 1.54        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1497 | U    | N1-C2   | 5.48  | 1.43        | 1.38     |
| 35  | BB    | 2442 | C    | C4-N4   | 5.48  | 1.38        | 1.33     |
| 1   | AA    | 914  | A    | C2'-C1' | -5.47 | 1.47        | 1.53     |
| 1   | AA    | 1027 | C    | C5-C6   | -5.47 | 1.29        | 1.34     |
| 19  | AS    | 79   | TYR  | CD2-CE2 | 5.47  | 1.47        | 1.39     |
| 35  | BB    | 281  | C    | C4'-O4' | -5.47 | 1.38        | 1.45     |
| 35  | BB    | 691  | C    | C3'-C2' | -5.47 | 1.46        | 1.52     |
| 35  | BB    | 838  | C    | C4-C5   | 5.47  | 1.47        | 1.43     |
| 35  | BB    | 960  | A    | P-O5'   | -5.47 | 1.54        | 1.59     |
| 35  | BB    | 1071 | G    | C2'-C1' | -5.47 | 1.47        | 1.53     |
| 35  | BB    | 1170 | C    | C2-N3   | 5.47  | 1.40        | 1.35     |
| 35  | BB    | 1547 | C    | C5'-C4' | 5.47  | 1.57        | 1.51     |
| 35  | BB    | 1852 | U    | C4'-O4' | -5.47 | 1.38        | 1.45     |
| 35  | BB    | 2502 | G    | C8-N7   | 5.47  | 1.34        | 1.30     |
| 35  | BB    | 2615 | U    | C4-C5   | 5.47  | 1.48        | 1.43     |
| 56  | BY    | 76   | ARG  | CZ-NH2  | 5.47  | 1.40        | 1.33     |
| 1   | AA    | 1413 | A    | N9-C4   | 5.47  | 1.41        | 1.37     |
| 1   | AA    | 1461 | G    | C2-N3   | 5.47  | 1.37        | 1.32     |
| 11  | AK    | 105  | ARG  | CZ-NH2  | 5.47  | 1.40        | 1.33     |
| 35  | BB    | 730  | A    | O4'-C1' | -5.47 | 1.34        | 1.41     |
| 35  | BB    | 1154 | G    | C2-N3   | 5.47  | 1.37        | 1.32     |
| 35  | BB    | 1270 | C    | C3'-O3' | 5.47  | 1.49        | 1.42     |
| 35  | BB    | 1610 | A    | C5-C4   | -5.47 | 1.34        | 1.38     |
| 35  | BB    | 1740 | G    | P-O5'   | -5.47 | 1.54        | 1.59     |
| 35  | BB    | 1787 | A    | P-O5'   | -5.47 | 1.54        | 1.59     |
| 35  | BB    | 2836 | U    | N1-C6   | 5.47  | 1.42        | 1.38     |
| 1   | AA    | 177  | G    | C2-N2   | 5.47  | 1.40        | 1.34     |
| 1   | AA    | 1193 | G    | N3-C4   | -5.47 | 1.31        | 1.35     |
| 1   | AA    | 1422 | G    | O4'-C1' | -5.47 | 1.34        | 1.41     |
| 34  | BA    | 108  | A    | C6-N6   | 5.47  | 1.38        | 1.33     |
| 35  | BB    | 63   | A    | C4'-C3' | 5.47  | 1.59        | 1.53     |
| 35  | BB    | 937  | C    | P-O5'   | -5.47 | 1.54        | 1.59     |
| 35  | BB    | 1520 | U    | C4-C5   | 5.47  | 1.48        | 1.43     |
| 35  | BB    | 1760 | C    | N1-C6   | 5.47  | 1.40        | 1.37     |
| 35  | BB    | 668  | A    | C4'-C3' | 5.47  | 1.59        | 1.53     |
| 35  | BB    | 1418 | G    | C5'-C4' | 5.47  | 1.57        | 1.51     |
| 1   | AA    | 1183 | U    | C4-C5   | 5.47  | 1.48        | 1.43     |
| 35  | BB    | 1074 | G    | C6-N1   | 5.47  | 1.43        | 1.39     |
| 35  | BB    | 1386 | C    | C4-C5   | 5.47  | 1.47        | 1.43     |
| 35  | BB    | 1578 | U    | C2'-O2' | 5.47  | 1.48        | 1.41     |
| 51  | BR    | 13   | ARG  | CD-NE   | 5.47  | 1.55        | 1.46     |
| 1   | AA    | 447  | G    | C5-C4   | -5.47 | 1.34        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1132 | C    | C4-C5   | 5.47  | 1.47        | 1.43     |
| 1   | AA    | 1482 | G    | C4'-O4' | 5.47  | 1.52        | 1.45     |
| 22  | AV    | 38   | U    | N1-C6   | 5.47  | 1.42        | 1.38     |
| 22  | AV    | 67   | G    | P-O5'   | -5.47 | 1.54        | 1.59     |
| 35  | BB    | 81   | G    | N1-C2   | 5.47  | 1.42        | 1.37     |
| 35  | BB    | 303  | G    | C2-N3   | 5.47  | 1.37        | 1.32     |
| 35  | BB    | 1918 | A    | C5-C6   | -5.47 | 1.36        | 1.41     |
| 35  | BB    | 2135 | A    | C5'-C4' | 5.47  | 1.57        | 1.51     |
| 38  | BE    | 102  | ARG  | CD-NE   | 5.47  | 1.55        | 1.46     |
| 1   | AA    | 368  | U    | N1-C2   | 5.46  | 1.43        | 1.38     |
| 1   | AA    | 838  | G    | C6-N1   | 5.46  | 1.43        | 1.39     |
| 1   | AA    | 1093 | A    | C3'-C2' | -5.46 | 1.46        | 1.52     |
| 1   | AA    | 1409 | C    | C2'-C1' | -5.46 | 1.47        | 1.53     |
| 7   | AG    | 4    | ARG  | CD-NE   | 5.46  | 1.55        | 1.46     |
| 30  | B5    | 208  | TYR  | CG-CD1  | 5.46  | 1.46        | 1.39     |
| 35  | BB    | 200  | U    | C2-N3   | 5.46  | 1.41        | 1.37     |
| 35  | BB    | 432  | A    | N9-C4   | 5.46  | 1.41        | 1.37     |
| 35  | BB    | 725  | G    | C4'-C3' | 5.46  | 1.59        | 1.53     |
| 35  | BB    | 797  | G    | N7-C5   | -5.46 | 1.35        | 1.39     |
| 35  | BB    | 1221 | C    | N1-C2   | -5.46 | 1.34        | 1.40     |
| 35  | BB    | 2329 | U    | N1-C2   | -5.46 | 1.33        | 1.38     |
| 35  | BB    | 2733 | A    | C2-N3   | 5.46  | 1.38        | 1.33     |
| 35  | BB    | 2866 | U    | C2-N3   | 5.46  | 1.41        | 1.37     |
| 41  | BH    | 16   | GLY  | N-CA    | -5.46 | 1.37        | 1.46     |
| 1   | AA    | 212  | G    | C2-N3   | 5.46  | 1.37        | 1.32     |
| 1   | AA    | 265  | G    | N1-C2   | 5.46  | 1.42        | 1.37     |
| 1   | AA    | 1327 | C    | C2-N3   | 5.46  | 1.40        | 1.35     |
| 35  | BB    | 1539 | U    | C4-C5   | 5.46  | 1.48        | 1.43     |
| 35  | BB    | 2148 | G    | N7-C5   | -5.46 | 1.35        | 1.39     |
| 35  | BB    | 2294 | G    | C5-C6   | -5.46 | 1.36        | 1.42     |
| 35  | BB    | 2409 | G    | N1-C2   | 5.46  | 1.42        | 1.37     |
| 35  | BB    | 2434 | A    | N9-C4   | -5.46 | 1.34        | 1.37     |
| 1   | AA    | 187  | G    | C6-N1   | -5.46 | 1.35        | 1.39     |
| 1   | AA    | 203  | G    | C2-N3   | 5.46  | 1.37        | 1.32     |
| 1   | AA    | 463  | U    | N3-C4   | 5.46  | 1.43        | 1.38     |
| 1   | AA    | 595  | A    | C5-C4   | -5.46 | 1.34        | 1.38     |
| 1   | AA    | 606  | G    | P-O5'   | -5.46 | 1.54        | 1.59     |
| 34  | BA    | 64   | G    | C3'-O3' | 5.46  | 1.49        | 1.42     |
| 35  | BB    | 429  | A    | C8-N7   | 5.46  | 1.35        | 1.31     |
| 35  | BB    | 1789 | A    | N9-C8   | -5.46 | 1.33        | 1.37     |
| 35  | BB    | 2060 | A    | N9-C8   | 5.46  | 1.42        | 1.37     |
| 50  | BQ    | 91   | ARG  | NE-CZ   | 5.46  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 697  | U    | C4'-C3' | 5.46  | 1.59        | 1.53     |
| 1   | AA    | 1036 | A    | O3'-P   | -5.46 | 1.54        | 1.61     |
| 35  | BB    | 356  | G    | C2'-C1' | -5.46 | 1.47        | 1.53     |
| 35  | BB    | 559  | G    | C8-N7   | -5.46 | 1.27        | 1.30     |
| 35  | BB    | 806  | C    | C4-N4   | 5.46  | 1.38        | 1.33     |
| 35  | BB    | 1673 | G    | C4'-C3' | 5.46  | 1.59        | 1.53     |
| 35  | BB    | 2627 | G    | N1-C2   | 5.46  | 1.42        | 1.37     |
| 35  | BB    | 2807 | U    | C2-O2   | 5.46  | 1.27        | 1.22     |
| 35  | BB    | 2835 | A    | N1-C2   | -5.46 | 1.29        | 1.34     |
| 39  | BF    | 79   | ARG  | CZ-NH1  | 5.46  | 1.40        | 1.33     |
| 1   | AA    | 227  | G    | N9-C8   | 5.46  | 1.41        | 1.37     |
| 1   | AA    | 697  | U    | N1-C6   | 5.46  | 1.42        | 1.38     |
| 1   | AA    | 1272 | G    | C2-N3   | 5.46  | 1.37        | 1.32     |
| 34  | BA    | 49   | C    | C4-N4   | 5.46  | 1.38        | 1.33     |
| 35  | BB    | 219  | A    | C3'-C2' | 5.46  | 1.58        | 1.52     |
| 35  | BB    | 903  | C    | C5-C6   | -5.46 | 1.29        | 1.34     |
| 35  | BB    | 1514 | G    | C5-C4   | 5.46  | 1.42        | 1.38     |
| 35  | BB    | 2212 | A    | C6-N6   | 5.46  | 1.38        | 1.33     |
| 35  | BB    | 2861 | U    | C5'-C4' | 5.46  | 1.57        | 1.51     |
| 36  | BC    | 204  | LEU  | CA-CB   | 5.46  | 1.66        | 1.53     |
| 1   | AA    | 101  | A    | N9-C4   | 5.46  | 1.41        | 1.37     |
| 1   | AA    | 164  | G    | C4'-O4' | 5.46  | 1.52        | 1.45     |
| 1   | AA    | 419  | C    | C4-C5   | 5.46  | 1.47        | 1.43     |
| 1   | AA    | 677  | U    | C3'-C2' | 5.46  | 1.58        | 1.52     |
| 1   | AA    | 686  | U    | C4-O4   | 5.46  | 1.28        | 1.23     |
| 1   | AA    | 750  | C    | C4'-C3' | 5.46  | 1.59        | 1.53     |
| 1   | AA    | 1350 | A    | C6-N6   | 5.46  | 1.38        | 1.33     |
| 1   | AA    | 1443 | C    | C2-N3   | 5.46  | 1.40        | 1.35     |
| 34  | BA    | 115  | A    | C6-N1   | -5.46 | 1.31        | 1.35     |
| 35  | BB    | 109  | C    | C2-N3   | 5.46  | 1.40        | 1.35     |
| 35  | BB    | 374  | A    | C6-N6   | 5.46  | 1.38        | 1.33     |
| 35  | BB    | 999  | U    | C2'-C1' | -5.46 | 1.47        | 1.53     |
| 35  | BB    | 1200 | C    | C3'-C2' | 5.46  | 1.58        | 1.52     |
| 35  | BB    | 1468 | U    | N1-C2   | -5.46 | 1.33        | 1.38     |
| 35  | BB    | 2339 | C    | C2-N3   | 5.46  | 1.40        | 1.35     |
| 35  | BB    | 2802 | G    | C5-C4   | -5.46 | 1.34        | 1.38     |
| 35  | BB    | 2895 | G    | C6-N1   | 5.46  | 1.43        | 1.39     |
| 1   | AA    | 508  | U    | C4'-O4' | -5.46 | 1.38        | 1.45     |
| 34  | BA    | 107  | G    | N9-C4   | -5.46 | 1.33        | 1.38     |
| 35  | BB    | 1519 | G    | C8-N7   | 5.46  | 1.34        | 1.30     |
| 35  | BB    | 1620 | G    | N7-C5   | -5.46 | 1.35        | 1.39     |
| 46  | BM    | 18   | ARG  | NE-CZ   | 5.46  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 85   | U    | C4-C5   | 5.45  | 1.48        | 1.43     |
| 1   | AA    | 500  | G    | C8-N7   | -5.45 | 1.27        | 1.30     |
| 1   | AA    | 651  | C    | P-O5'   | -5.45 | 1.54        | 1.59     |
| 1   | AA    | 1395 | C    | C4'-C3' | 5.45  | 1.59        | 1.53     |
| 35  | BB    | 1195 | G    | C8-N7   | -5.45 | 1.27        | 1.30     |
| 35  | BB    | 1216 | G    | C6-N1   | 5.45  | 1.43        | 1.39     |
| 35  | BB    | 1873 | G    | C2-N3   | 5.45  | 1.37        | 1.32     |
| 35  | BB    | 2582 | G    | C5-C4   | 5.45  | 1.42        | 1.38     |
| 35  | BB    | 2828 | G    | N3-C4   | -5.45 | 1.31        | 1.35     |
| 38  | BE    | 170  | ARG  | CZ-NH2  | 5.45  | 1.40        | 1.33     |
| 1   | AA    | 954  | G    | N9-C4   | -5.45 | 1.33        | 1.38     |
| 1   | AA    | 1335 | U    | N1-C6   | 5.45  | 1.42        | 1.38     |
| 35  | BB    | 496  | G    | C5-C6   | -5.45 | 1.36        | 1.42     |
| 35  | BB    | 730  | A    | O3'-P   | -5.45 | 1.54        | 1.61     |
| 35  | BB    | 1689 | A    | C2'-C1' | -5.45 | 1.47        | 1.53     |
| 1   | AA    | 109  | A    | C2'-C1' | -5.45 | 1.47        | 1.53     |
| 1   | AA    | 312  | C    | O4'-C1' | 5.45  | 1.48        | 1.41     |
| 1   | AA    | 515  | G    | C8-N7   | -5.45 | 1.27        | 1.30     |
| 16  | AP    | 51   | ARG  | CZ-NH1  | 5.45  | 1.40        | 1.33     |
| 35  | BB    | 373  | U    | N1-C6   | 5.45  | 1.42        | 1.38     |
| 35  | BB    | 583  | G    | C6-N1   | 5.45  | 1.43        | 1.39     |
| 35  | BB    | 744  | U    | C4-O4   | 5.45  | 1.28        | 1.23     |
| 35  | BB    | 810  | U    | C2'-C1' | -5.45 | 1.47        | 1.53     |
| 35  | BB    | 870  | U    | C3'-O3' | 5.45  | 1.49        | 1.42     |
| 35  | BB    | 1140 | C    | C4-N4   | 5.45  | 1.38        | 1.33     |
| 35  | BB    | 1691 | C    | N3-C4   | 5.45  | 1.37        | 1.33     |
| 1   | AA    | 71   | A    | C8-N7   | 5.45  | 1.35        | 1.31     |
| 1   | AA    | 350  | G    | C2-N2   | 5.45  | 1.40        | 1.34     |
| 1   | AA    | 607  | A    | C8-N7   | -5.45 | 1.27        | 1.31     |
| 1   | AA    | 818  | G    | N1-C2   | 5.45  | 1.42        | 1.37     |
| 1   | AA    | 1030 | U    | O3'-P   | -5.45 | 1.54        | 1.61     |
| 1   | AA    | 1313 | U    | C4'-C3' | -5.45 | 1.47        | 1.52     |
| 35  | BB    | 313  | G    | N3-C4   | -5.45 | 1.31        | 1.35     |
| 35  | BB    | 552  | U    | C4-C5   | 5.45  | 1.48        | 1.43     |
| 35  | BB    | 588  | U    | C2'-C1' | -5.45 | 1.47        | 1.53     |
| 35  | BB    | 919  | U    | C5'-C4' | 5.45  | 1.57        | 1.51     |
| 35  | BB    | 1411 | U    | C3'-C2' | 5.45  | 1.58        | 1.52     |
| 35  | BB    | 2793 | C    | C5'-C4' | 5.45  | 1.57        | 1.51     |
| 1   | AA    | 1366 | C    | O3'-P   | 5.45  | 1.67        | 1.61     |
| 35  | BB    | 637  | A    | C2'-C1' | -5.45 | 1.47        | 1.53     |
| 35  | BB    | 726  | G    | C2'-C1' | -5.45 | 1.47        | 1.53     |
| 1   | AA    | 402  | G    | C8-N7   | 5.45  | 1.34        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21  | AU    | 20   | ARG  | CZ-NH1  | 5.45  | 1.40        | 1.33     |
| 35  | BB    | 29   | U    | C2-O2   | 5.45  | 1.27        | 1.22     |
| 35  | BB    | 294  | A    | C5'-C4' | 5.45  | 1.57        | 1.51     |
| 35  | BB    | 554  | U    | C4-C5   | 5.45  | 1.48        | 1.43     |
| 35  | BB    | 756  | A    | N1-C2   | -5.45 | 1.29        | 1.34     |
| 35  | BB    | 797  | G    | C3'-O3' | 5.45  | 1.49        | 1.42     |
| 35  | BB    | 958  | U    | C3'-C2' | -5.45 | 1.46        | 1.52     |
| 35  | BB    | 1077 | A    | C2-N3   | 5.45  | 1.38        | 1.33     |
| 35  | BB    | 1294 | U    | O3'-P   | -5.45 | 1.54        | 1.61     |
| 35  | BB    | 1295 | C    | C2-N3   | -5.45 | 1.31        | 1.35     |
| 35  | BB    | 1309 | G    | C2-N3   | 5.45  | 1.37        | 1.32     |
| 35  | BB    | 1426 | G    | C2-N2   | 5.45  | 1.40        | 1.34     |
| 35  | BB    | 1477 | A    | C5-C4   | -5.45 | 1.34        | 1.38     |
| 35  | BB    | 1501 | G    | N3-C4   | -5.45 | 1.31        | 1.35     |
| 35  | BB    | 1555 | G    | C5'-C4' | 5.45  | 1.57        | 1.51     |
| 35  | BB    | 1719 | G    | C6-N1   | 5.45  | 1.43        | 1.39     |
| 35  | BB    | 2353 | G    | N1-C2   | 5.45  | 1.42        | 1.37     |
| 35  | BB    | 2558 | C    | N1-C6   | -5.45 | 1.33        | 1.37     |
| 35  | BB    | 2830 | C    | N3-C4   | 5.45  | 1.37        | 1.33     |
| 1   | AA    | 634  | C    | C4'-C3' | -5.44 | 1.47        | 1.52     |
| 1   | AA    | 1317 | C    | P-O5'   | -5.44 | 1.54        | 1.59     |
| 3   | AC    | 57   | GLU  | CA-CB   | -5.44 | 1.42        | 1.53     |
| 35  | BB    | 685  | A    | N7-C5   | -5.44 | 1.35        | 1.39     |
| 35  | BB    | 703  | U    | N3-C4   | 5.44  | 1.43        | 1.38     |
| 1   | AA    | 870  | U    | O3'-P   | -5.44 | 1.54        | 1.61     |
| 1   | AA    | 1434 | A    | C5-C4   | 5.44  | 1.42        | 1.38     |
| 28  | B3    | 16   | ARG  | CZ-NH2  | 5.44  | 1.40        | 1.33     |
| 35  | BB    | 248  | G    | N9-C4   | 5.44  | 1.42        | 1.38     |
| 35  | BB    | 2066 | C    | N1-C6   | 5.44  | 1.40        | 1.37     |
| 35  | BB    | 2112 | G    | O4'-C1' | 5.44  | 1.48        | 1.41     |
| 1   | AA    | 102  | G    | N1-C2   | 5.44  | 1.42        | 1.37     |
| 1   | AA    | 291  | U    | C2-N3   | 5.44  | 1.41        | 1.37     |
| 1   | AA    | 761  | G    | P-O5'   | -5.44 | 1.54        | 1.59     |
| 1   | AA    | 893  | C    | C3'-O3' | 5.44  | 1.49        | 1.42     |
| 1   | AA    | 1047 | G    | N9-C4   | 5.44  | 1.42        | 1.38     |
| 35  | BB    | 28   | A    | N9-C4   | -5.44 | 1.34        | 1.37     |
| 35  | BB    | 228  | C    | C2-N3   | 5.44  | 1.40        | 1.35     |
| 35  | BB    | 914  | G    | C5-C6   | -5.44 | 1.36        | 1.42     |
| 35  | BB    | 966  | G    | P-O5'   | -5.44 | 1.54        | 1.59     |
| 35  | BB    | 1090 | A    | C6-N1   | 5.44  | 1.39        | 1.35     |
| 35  | BB    | 1138 | G    | N9-C4   | -5.44 | 1.33        | 1.38     |
| 35  | BB    | 1156 | A    | C6-N1   | 5.44  | 1.39        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1469 | A    | C6-N1   | -5.44 | 1.31        | 1.35     |
| 35  | BB    | 1674 | G    | C2-N3   | 5.44  | 1.37        | 1.32     |
| 35  | BB    | 2526 | G    | N9-C4   | -5.44 | 1.33        | 1.38     |
| 1   | AA    | 342  | C    | N1-C6   | 5.44  | 1.40        | 1.37     |
| 1   | AA    | 1203 | C    | C4'-C3' | -5.44 | 1.47        | 1.52     |
| 35  | BB    | 217  | A    | N9-C8   | -5.44 | 1.33        | 1.37     |
| 35  | BB    | 900  | A    | O4'-C1' | 5.44  | 1.48        | 1.41     |
| 35  | BB    | 1040 | A    | C6-N6   | 5.44  | 1.38        | 1.33     |
| 35  | BB    | 1394 | U    | C4-O4   | -5.44 | 1.19        | 1.23     |
| 1   | AA    | 129  | A    | O3'-P   | -5.44 | 1.54        | 1.61     |
| 1   | AA    | 473  | U    | N1-C6   | 5.44  | 1.42        | 1.38     |
| 1   | AA    | 628  | G    | C2-N2   | 5.44  | 1.40        | 1.34     |
| 1   | AA    | 770  | C    | P-O5'   | -5.44 | 1.54        | 1.59     |
| 1   | AA    | 1083 | U    | C4'-O4' | 5.44  | 1.52        | 1.45     |
| 1   | AA    | 1217 | C    | C5-C6   | 5.44  | 1.38        | 1.34     |
| 35  | BB    | 20   | C    | C4-C5   | 5.44  | 1.47        | 1.43     |
| 35  | BB    | 192  | C    | C4-C5   | -5.44 | 1.38        | 1.43     |
| 35  | BB    | 288  | U    | C2-N3   | 5.44  | 1.41        | 1.37     |
| 35  | BB    | 439  | A    | O3'-P   | -5.44 | 1.54        | 1.61     |
| 35  | BB    | 501  | A    | O5'-C5' | -5.44 | 1.34        | 1.42     |
| 35  | BB    | 1228 | G    | C3'-O3' | 5.44  | 1.49        | 1.42     |
| 35  | BB    | 1236 | G    | C3'-O3' | 5.44  | 1.49        | 1.42     |
| 35  | BB    | 1542 | U    | C4-C5   | 5.44  | 1.48        | 1.43     |
| 1   | AA    | 176  | C    | C2'-C1' | -5.44 | 1.47        | 1.53     |
| 35  | BB    | 1250 | G    | C3'-O3' | 5.44  | 1.49        | 1.42     |
| 35  | BB    | 1423 | G    | C2-N3   | 5.44  | 1.37        | 1.32     |
| 35  | BB    | 2388 | A    | O3'-P   | -5.44 | 1.54        | 1.61     |
| 35  | BB    | 2876 | G    | C5'-C4' | 5.44  | 1.57        | 1.51     |
| 1   | AA    | 693  | G    | N9-C8   | -5.43 | 1.34        | 1.37     |
| 1   | AA    | 880  | C    | C5-C6   | 5.43  | 1.38        | 1.34     |
| 1   | AA    | 1065 | U    | C4'-C3' | -5.43 | 1.47        | 1.52     |
| 22  | AV    | 67   | G    | C5-C4   | -5.43 | 1.34        | 1.38     |
| 34  | BA    | 94   | A    | N9-C4   | -5.43 | 1.34        | 1.37     |
| 35  | BB    | 370  | G    | N9-C4   | 5.43  | 1.42        | 1.38     |
| 35  | BB    | 415  | A    | N7-C5   | -5.43 | 1.35        | 1.39     |
| 35  | BB    | 430  | A    | C5-C6   | -5.43 | 1.36        | 1.41     |
| 35  | BB    | 488  | G    | C5-C4   | 5.43  | 1.42        | 1.38     |
| 35  | BB    | 540  | C    | C4-N4   | -5.43 | 1.29        | 1.33     |
| 35  | BB    | 704  | G    | C5-C4   | -5.43 | 1.34        | 1.38     |
| 35  | BB    | 1759 | A    | N3-C4   | -5.43 | 1.31        | 1.34     |
| 35  | BB    | 2315 | G    | C5-C6   | -5.43 | 1.36        | 1.42     |
| 1   | AA    | 18   | C    | N1-C6   | 5.43  | 1.40        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 593  | U    | C1'-N1  | 5.43  | 1.56        | 1.48     |
| 1   | AA    | 732  | C    | C1'-N1  | 5.43  | 1.56        | 1.48     |
| 1   | AA    | 784  | A    | N9-C4   | 5.43  | 1.41        | 1.37     |
| 1   | AA    | 1033 | G    | O4'-C1' | 5.43  | 1.48        | 1.41     |
| 1   | AA    | 1185 | G    | N9-C4   | -5.43 | 1.33        | 1.38     |
| 1   | AA    | 1366 | C    | C2-O2   | 5.43  | 1.29        | 1.24     |
| 4   | AD    | 171  | GLU  | CD-OE1  | 5.43  | 1.31        | 1.25     |
| 15  | AO    | 79   | ARG  | CZ-NH2  | 5.43  | 1.40        | 1.33     |
| 35  | BB    | 989  | G    | C3'-O3' | 5.43  | 1.49        | 1.42     |
| 35  | BB    | 2145 | C    | C5-C6   | 5.43  | 1.38        | 1.34     |
| 35  | BB    | 2294 | G    | N1-C2   | 5.43  | 1.42        | 1.37     |
| 35  | BB    | 2742 | G    | N3-C4   | -5.43 | 1.31        | 1.35     |
| 1   | AA    | 514  | C    | O3'-P   | -5.43 | 1.54        | 1.61     |
| 1   | AA    | 763  | G    | C5-C4   | -5.43 | 1.34        | 1.38     |
| 1   | AA    | 890  | G    | C2-N3   | 5.43  | 1.37        | 1.32     |
| 1   | AA    | 1457 | G    | C2'-C1' | -5.43 | 1.47        | 1.53     |
| 35  | BB    | 158  | U    | C4-C5   | -5.43 | 1.38        | 1.43     |
| 35  | BB    | 181  | A    | P-O5'   | 5.43  | 1.65        | 1.59     |
| 35  | BB    | 1088 | A    | C2-N3   | 5.43  | 1.38        | 1.33     |
| 35  | BB    | 1846 | G    | C3'-C2' | 5.43  | 1.58        | 1.52     |
| 35  | BB    | 2512 | C    | C2-N3   | 5.43  | 1.40        | 1.35     |
| 44  | BK    | 64   | ARG  | CZ-NH1  | 5.43  | 1.40        | 1.33     |
| 1   | AA    | 35   | G    | C2-N3   | 5.43  | 1.37        | 1.32     |
| 1   | AA    | 469  | C    | N1-C6   | 5.43  | 1.40        | 1.37     |
| 1   | AA    | 625  | U    | C5-C6   | -5.43 | 1.29        | 1.34     |
| 1   | AA    | 769  | G    | C8-N7   | -5.43 | 1.27        | 1.30     |
| 35  | BB    | 23   | G    | C6-N1   | 5.43  | 1.43        | 1.39     |
| 35  | BB    | 1144 | A    | C8-N7   | -5.43 | 1.27        | 1.31     |
| 35  | BB    | 1867 | G    | P-O5'   | -5.43 | 1.54        | 1.59     |
| 35  | BB    | 2247 | A    | P-O5'   | -5.43 | 1.54        | 1.59     |
| 35  | BB    | 2326 | C    | C3'-C2' | 5.43  | 1.58        | 1.52     |
| 35  | BB    | 2822 | G    | C5-C4   | 5.43  | 1.42        | 1.38     |
| 1   | AA    | 11   | G    | C6-N1   | 5.43  | 1.43        | 1.39     |
| 1   | AA    | 141  | G    | C5-C6   | -5.43 | 1.36        | 1.42     |
| 1   | AA    | 1166 | G    | N9-C8   | 5.43  | 1.41        | 1.37     |
| 35  | BB    | 1067 | A    | N7-C5   | -5.43 | 1.35        | 1.39     |
| 35  | BB    | 1677 | A    | N1-C2   | -5.43 | 1.29        | 1.34     |
| 35  | BB    | 1833 | C    | C4-N4   | 5.43  | 1.38        | 1.33     |
| 35  | BB    | 1901 | A    | C5-C6   | -5.43 | 1.36        | 1.41     |
| 35  | BB    | 2080 | A    | C6-N6   | 5.43  | 1.38        | 1.33     |
| 35  | BB    | 2122 | U    | N1-C2   | 5.43  | 1.43        | 1.38     |
| 35  | BB    | 2791 | G    | N9-C8   | 5.43  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 566  | G    | C2'-C1' | -5.43 | 1.47        | 1.53     |
| 1   | AA    | 1105 | A    | N9-C4   | -5.43 | 1.34        | 1.37     |
| 35  | BB    | 551  | G    | C8-N7   | -5.43 | 1.27        | 1.30     |
| 35  | BB    | 1225 | G    | O3'-P   | -5.43 | 1.54        | 1.61     |
| 35  | BB    | 1832 | C    | C2-N3   | 5.43  | 1.40        | 1.35     |
| 35  | BB    | 2040 | G    | C5-C4   | -5.43 | 1.34        | 1.38     |
| 35  | BB    | 2527 | C    | C2'-C1' | -5.43 | 1.47        | 1.53     |
| 35  | BB    | 2775 | G    | C2-N3   | 5.43  | 1.37        | 1.32     |
| 1   | AA    | 253  | A    | C5-C4   | 5.42  | 1.42        | 1.38     |
| 1   | AA    | 728  | A    | O4'-C1' | -5.42 | 1.34        | 1.41     |
| 1   | AA    | 1216 | A    | P-O5'   | -5.42 | 1.54        | 1.59     |
| 1   | AA    | 1416 | G    | O3'-P   | -5.42 | 1.54        | 1.61     |
| 35  | BB    | 268  | C    | C1'-N1  | 5.42  | 1.56        | 1.48     |
| 35  | BB    | 347  | A    | C8-N7   | -5.42 | 1.27        | 1.31     |
| 35  | BB    | 485  | C    | N1-C2   | 5.42  | 1.45        | 1.40     |
| 35  | BB    | 656  | G    | C1'-N9  | -5.42 | 1.39        | 1.46     |
| 35  | BB    | 889  | C    | N1-C2   | 5.42  | 1.45        | 1.40     |
| 35  | BB    | 1169 | A    | N7-C5   | -5.42 | 1.35        | 1.39     |
| 35  | BB    | 1434 | A    | N1-C2   | 5.42  | 1.39        | 1.34     |
| 35  | BB    | 2243 | U    | C4-O4   | 5.42  | 1.27        | 1.23     |
| 35  | BB    | 2428 | G    | N3-C4   | 5.42  | 1.39        | 1.35     |
| 48  | BO    | 33   | ARG  | CD-NE   | 5.42  | 1.55        | 1.46     |
| 1   | AA    | 447  | G    | C2-N3   | 5.42  | 1.37        | 1.32     |
| 35  | BB    | 645  | C    | C4-N4   | 5.42  | 1.38        | 1.33     |
| 35  | BB    | 2817 | U    | P-O5'   | -5.42 | 1.54        | 1.59     |
| 1   | AA    | 319  | G    | P-O5'   | -5.42 | 1.54        | 1.59     |
| 1   | AA    | 450  | G    | C5-C6   | -5.42 | 1.36        | 1.42     |
| 1   | AA    | 501  | C    | P-O5'   | -5.42 | 1.54        | 1.59     |
| 1   | AA    | 1146 | A    | C2-N3   | -5.42 | 1.28        | 1.33     |
| 1   | AA    | 1379 | G    | C4'-C3' | -5.42 | 1.47        | 1.52     |
| 1   | AA    | 1415 | G    | C6-O6   | -5.42 | 1.19        | 1.24     |
| 35  | BB    | 14   | A    | P-O5'   | -5.42 | 1.54        | 1.59     |
| 35  | BB    | 191  | A    | N9-C8   | -5.42 | 1.33        | 1.37     |
| 35  | BB    | 454  | A    | P-O5'   | -5.42 | 1.54        | 1.59     |
| 35  | BB    | 494  | G    | C6-N1   | -5.42 | 1.35        | 1.39     |
| 35  | BB    | 541  | A    | C5-C6   | -5.42 | 1.36        | 1.41     |
| 35  | BB    | 639  | U    | C4'-C3' | -5.42 | 1.47        | 1.52     |
| 35  | BB    | 675  | A    | N3-C4   | -5.42 | 1.31        | 1.34     |
| 35  | BB    | 1460 | U    | N3-C4   | 5.42  | 1.43        | 1.38     |
| 35  | BB    | 2412 | A    | O3'-P   | -5.42 | 1.54        | 1.61     |
| 35  | BB    | 2484 | G    | C2-N3   | 5.42  | 1.37        | 1.32     |
| 35  | BB    | 2745 | C    | C3'-C2' | -5.42 | 1.46        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 50  | BQ    | 12   | ARG  | CZ-NH2  | 5.42  | 1.40        | 1.33     |
| 1   | AA    | 78   | A    | O3'-P   | -5.42 | 1.54        | 1.61     |
| 35  | BB    | 615  | U    | N1-C2   | -5.42 | 1.33        | 1.38     |
| 35  | BB    | 1538 | G    | N1-C2   | 5.42  | 1.42        | 1.37     |
| 1   | AA    | 59   | A    | N3-C4   | -5.42 | 1.31        | 1.34     |
| 1   | AA    | 378  | G    | C5-C4   | -5.42 | 1.34        | 1.38     |
| 1   | AA    | 529  | G    | C8-N7   | 5.42  | 1.34        | 1.30     |
| 1   | AA    | 786  | G    | C8-N7   | 5.42  | 1.34        | 1.30     |
| 1   | AA    | 1205 | U    | C1'-N1  | 5.42  | 1.56        | 1.48     |
| 1   | AA    | 1441 | A    | C5-C4   | -5.42 | 1.34        | 1.38     |
| 35  | BB    | 220  | G    | C6-O6   | -5.42 | 1.19        | 1.24     |
| 35  | BB    | 953  | G    | C8-N7   | -5.42 | 1.27        | 1.30     |
| 35  | BB    | 1111 | A    | C6-N6   | 5.42  | 1.38        | 1.33     |
| 35  | BB    | 1413 | A    | C6-N6   | 5.42  | 1.38        | 1.33     |
| 35  | BB    | 1833 | C    | N3-C4   | 5.42  | 1.37        | 1.33     |
| 35  | BB    | 1949 | G    | C6-N1   | 5.42  | 1.43        | 1.39     |
| 35  | BB    | 2171 | A    | N3-C4   | 5.42  | 1.38        | 1.34     |
| 35  | BB    | 2468 | A    | C6-N6   | 5.42  | 1.38        | 1.33     |
| 1   | AA    | 425  | G    | N9-C4   | -5.42 | 1.33        | 1.38     |
| 3   | AC    | 21   | TRP  | CD2-CE2 | 5.42  | 1.47        | 1.41     |
| 35  | BB    | 96   | C    | N3-C4   | 5.42  | 1.37        | 1.33     |
| 35  | BB    | 102  | U    | C2'-C1' | -5.42 | 1.47        | 1.53     |
| 35  | BB    | 787  | C    | N1-C2   | -5.42 | 1.34        | 1.40     |
| 35  | BB    | 967  | U    | C3'-O3' | 5.42  | 1.49        | 1.42     |
| 35  | BB    | 1380 | G    | N1-C2   | 5.42  | 1.42        | 1.37     |
| 35  | BB    | 1728 | C    | C4-N4   | 5.42  | 1.38        | 1.33     |
| 35  | BB    | 2144 | G    | C4'-C3' | 5.42  | 1.59        | 1.53     |
| 35  | BB    | 2348 | U    | N1-C2   | 5.42  | 1.43        | 1.38     |
| 35  | BB    | 2696 | U    | P-O5'   | -5.42 | 1.54        | 1.59     |
| 1   | AA    | 378  | G    | C6-O6   | -5.42 | 1.19        | 1.24     |
| 1   | AA    | 429  | U    | P-O5'   | -5.42 | 1.54        | 1.59     |
| 1   | AA    | 439  | U    | C2'-C1' | -5.42 | 1.47        | 1.53     |
| 34  | BA    | 27   | C    | C4-C5   | -5.42 | 1.38        | 1.43     |
| 35  | BB    | 513  | A    | C5'-C4' | 5.42  | 1.57        | 1.51     |
| 35  | BB    | 742  | A    | C8-N7   | -5.42 | 1.27        | 1.31     |
| 35  | BB    | 1157 | G    | N7-C5   | -5.42 | 1.36        | 1.39     |
| 35  | BB    | 2430 | A    | C2-N3   | 5.42  | 1.38        | 1.33     |
| 35  | BB    | 2564 | A    | N7-C5   | -5.42 | 1.36        | 1.39     |
| 1   | AA    | 203  | G    | N9-C4   | -5.41 | 1.33        | 1.38     |
| 1   | AA    | 376  | G    | C6-N1   | 5.41  | 1.43        | 1.39     |
| 1   | AA    | 393  | A    | C2-N3   | -5.41 | 1.28        | 1.33     |
| 1   | AA    | 1410 | A    | P-O5'   | -5.41 | 1.54        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 105  | C    | C4'-O4' | 5.41  | 1.52        | 1.45     |
| 35  | BB    | 196  | A    | C2'-C1' | -5.41 | 1.47        | 1.53     |
| 35  | BB    | 1418 | G    | C2'-C1' | -5.41 | 1.47        | 1.53     |
| 35  | BB    | 1746 | A    | O3'-P   | -5.41 | 1.54        | 1.61     |
| 35  | BB    | 2252 | G    | C6-O6   | -5.41 | 1.19        | 1.24     |
| 35  | BB    | 2403 | C    | P-O5'   | 5.41  | 1.65        | 1.59     |
| 35  | BB    | 2835 | A    | C4'-C3' | -5.41 | 1.47        | 1.52     |
| 1   | AA    | 338  | A    | N7-C5   | -5.41 | 1.36        | 1.39     |
| 1   | AA    | 1197 | A    | C2'-C1' | -5.41 | 1.47        | 1.53     |
| 22  | AV    | 4    | C    | O4'-C1' | -5.41 | 1.34        | 1.41     |
| 34  | BA    | 108  | A    | N9-C4   | -5.41 | 1.34        | 1.37     |
| 35  | BB    | 364  | C    | C4-C5   | -5.41 | 1.38        | 1.43     |
| 35  | BB    | 1539 | U    | O3'-P   | -5.41 | 1.54        | 1.61     |
| 35  | BB    | 2700 | A    | C2'-C1' | -5.41 | 1.47        | 1.53     |
| 1   | AA    | 877  | G    | N9-C4   | -5.41 | 1.33        | 1.38     |
| 1   | AA    | 1029 | U    | C4-O4   | 5.41  | 1.27        | 1.23     |
| 35  | BB    | 142  | A    | C5'-C4' | 5.41  | 1.57        | 1.51     |
| 35  | BB    | 224  | U    | C2-N3   | 5.41  | 1.41        | 1.37     |
| 35  | BB    | 711  | G    | C2'-C1' | -5.41 | 1.47        | 1.53     |
| 35  | BB    | 724  | U    | O3'-P   | -5.41 | 1.54        | 1.61     |
| 35  | BB    | 1572 | A    | N9-C8   | -5.41 | 1.33        | 1.37     |
| 35  | BB    | 1712 | U    | C4-C5   | -5.41 | 1.38        | 1.43     |
| 35  | BB    | 2200 | C    | C2-N3   | -5.41 | 1.31        | 1.35     |
| 35  | BB    | 2238 | G    | C5'-C4' | 5.41  | 1.57        | 1.51     |
| 35  | BB    | 2890 | G    | C8-N7   | -5.41 | 1.27        | 1.30     |
| 1   | AA    | 379  | C    | N1-C6   | 5.41  | 1.40        | 1.37     |
| 1   | AA    | 574  | A    | N1-C2   | 5.41  | 1.39        | 1.34     |
| 1   | AA    | 978  | A    | C5-C6   | -5.41 | 1.36        | 1.41     |
| 26  | B1    | 21   | LEU  | CA-CB   | 5.41  | 1.66        | 1.53     |
| 35  | BB    | 53   | A    | N9-C8   | -5.41 | 1.33        | 1.37     |
| 35  | BB    | 1269 | A    | N1-C2   | 5.41  | 1.39        | 1.34     |
| 35  | BB    | 1319 | C    | N3-C4   | 5.41  | 1.37        | 1.33     |
| 35  | BB    | 2103 | C    | C2-N3   | 5.41  | 1.40        | 1.35     |
| 35  | BB    | 2573 | C    | C5'-C4' | 5.41  | 1.57        | 1.51     |
| 35  | BB    | 2625 | G    | N3-C4   | 5.41  | 1.39        | 1.35     |
| 1   | AA    | 1162 | C    | C2-N3   | 5.41  | 1.40        | 1.35     |
| 1   | AA    | 1264 | U    | C4'-C3' | 5.41  | 1.59        | 1.53     |
| 35  | BB    | 1129 | A    | C5-C6   | -5.41 | 1.36        | 1.41     |
| 35  | BB    | 1479 | G    | C6-N1   | -5.41 | 1.35        | 1.39     |
| 35  | BB    | 1564 | C    | C3'-O3' | 5.41  | 1.49        | 1.42     |
| 35  | BB    | 2018 | G    | C2-N3   | 5.41  | 1.37        | 1.32     |
| 47  | BN    | 119  | SER  | CA-CB   | 5.41  | 1.61        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 555  | U    | O3'-P   | -5.41 | 1.54        | 1.61     |
| 1   | AA    | 1176 | A    | C6-N1   | 5.41  | 1.39        | 1.35     |
| 1   | AA    | 1369 | C    | C4-N4   | 5.41  | 1.38        | 1.33     |
| 1   | AA    | 1445 | U    | C4-C5   | -5.41 | 1.38        | 1.43     |
| 17  | AQ    | 26   | ARG  | NE-CZ   | 5.41  | 1.40        | 1.33     |
| 34  | BA    | 35   | C    | P-O5'   | 5.41  | 1.65        | 1.59     |
| 35  | BB    | 1334 | G    | N9-C4   | -5.41 | 1.33        | 1.38     |
| 35  | BB    | 1997 | C    | N3-C4   | 5.41  | 1.37        | 1.33     |
| 35  | BB    | 2173 | A    | C5-C4   | 5.41  | 1.42        | 1.38     |
| 43  | BJ    | 44   | TYR  | N-CA    | -5.41 | 1.35        | 1.46     |
| 1   | AA    | 314  | C    | C2-N3   | 5.40  | 1.40        | 1.35     |
| 1   | AA    | 769  | G    | N9-C4   | -5.40 | 1.33        | 1.38     |
| 9   | AI    | 63   | TYR  | CZ-OH   | 5.40  | 1.47        | 1.37     |
| 27  | B2    | 55   | LYS  | N-CA    | -5.40 | 1.35        | 1.46     |
| 35  | BB    | 173  | A    | C2'-C1' | -5.40 | 1.47        | 1.53     |
| 35  | BB    | 341  | C    | C3'-C2' | -5.40 | 1.46        | 1.52     |
| 35  | BB    | 1290 | C    | N1-C2   | -5.40 | 1.34        | 1.40     |
| 35  | BB    | 1953 | A    | N3-C4   | -5.40 | 1.31        | 1.34     |
| 35  | BB    | 1972 | G    | C3'-O3' | 5.40  | 1.49        | 1.42     |
| 35  | BB    | 2528 | U    | C2'-C1' | -5.40 | 1.47        | 1.53     |
| 1   | AA    | 592  | G    | N9-C4   | -5.40 | 1.33        | 1.38     |
| 1   | AA    | 1063 | C    | C4'-C3' | -5.40 | 1.47        | 1.52     |
| 1   | AA    | 1355 | G    | C5'-C4' | -5.40 | 1.44        | 1.51     |
| 1   | AA    | 1416 | G    | C3'-C2' | -5.40 | 1.46        | 1.52     |
| 35  | BB    | 1147 | A    | C3'-O3' | 5.40  | 1.49        | 1.42     |
| 35  | BB    | 1160 | G    | C6-N1   | 5.40  | 1.43        | 1.39     |
| 35  | BB    | 1518 | C    | C3'-C2' | -5.40 | 1.46        | 1.52     |
| 35  | BB    | 1541 | C    | N3-C4   | 5.40  | 1.37        | 1.33     |
| 35  | BB    | 1592 | C    | O4'-C1' | 5.40  | 1.48        | 1.41     |
| 35  | BB    | 1666 | G    | N9-C4   | -5.40 | 1.33        | 1.38     |
| 35  | BB    | 1962 | C    | C5-C6   | -5.40 | 1.30        | 1.34     |
| 35  | BB    | 2568 | U    | C5-C6   | 5.40  | 1.39        | 1.34     |
| 35  | BB    | 2630 | G    | C4'-C3' | 5.40  | 1.59        | 1.53     |
| 35  | BB    | 2845 | U    | P-O5'   | -5.40 | 1.54        | 1.59     |
| 1   | AA    | 911  | U    | O4'-C1' | 5.40  | 1.48        | 1.41     |
| 1   | AA    | 1485 | U    | C2'-C1' | -5.40 | 1.47        | 1.53     |
| 35  | BB    | 1022 | G    | N9-C4   | -5.40 | 1.33        | 1.38     |
| 35  | BB    | 1039 | A    | C6-N6   | 5.40  | 1.38        | 1.33     |
| 35  | BB    | 1772 | A    | C3'-O3' | 5.40  | 1.49        | 1.42     |
| 35  | BB    | 1919 | A    | C2'-C1' | -5.40 | 1.47        | 1.53     |
| 35  | BB    | 2502 | G    | N7-C5   | -5.40 | 1.36        | 1.39     |
| 1   | AA    | 388  | G    | C5-C6   | -5.40 | 1.36        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1220 | G    | N9-C8   | 5.40  | 1.41        | 1.37     |
| 1   | AA    | 1366 | C    | C2'-C1' | -5.40 | 1.47        | 1.53     |
| 35  | BB    | 1277 | G    | C4'-C3' | 5.40  | 1.59        | 1.53     |
| 35  | BB    | 1645 | G    | C2'-C1' | -5.40 | 1.47        | 1.53     |
| 35  | BB    | 1928 | A    | C5'-C4' | 5.40  | 1.57        | 1.51     |
| 35  | BB    | 2193 | G    | P-O5'   | 5.40  | 1.65        | 1.59     |
| 35  | BB    | 2319 | G    | N1-C2   | 5.40  | 1.42        | 1.37     |
| 1   | AA    | 525  | C    | C4'-O4' | -5.40 | 1.38        | 1.45     |
| 35  | BB    | 240  | C    | N1-C2   | -5.40 | 1.34        | 1.40     |
| 35  | BB    | 808  | G    | C5-C4   | -5.40 | 1.34        | 1.38     |
| 35  | BB    | 1138 | G    | C6-N1   | 5.40  | 1.43        | 1.39     |
| 35  | BB    | 1286 | A    | C6-N6   | 5.40  | 1.38        | 1.33     |
| 35  | BB    | 1513 | U    | O4'-C1' | 5.40  | 1.48        | 1.41     |
| 35  | BB    | 1821 | A    | O4'-C1' | 5.40  | 1.48        | 1.41     |
| 35  | BB    | 2150 | C    | C4-N4   | 5.40  | 1.38        | 1.33     |
| 35  | BB    | 2307 | G    | N3-C4   | 5.40  | 1.39        | 1.35     |
| 35  | BB    | 2510 | C    | C5'-C4' | 5.40  | 1.57        | 1.51     |
| 35  | BB    | 2718 | G    | C5'-C4' | 5.40  | 1.57        | 1.51     |
| 35  | BB    | 2886 | A    | C6-N1   | 5.40  | 1.39        | 1.35     |
| 1   | AA    | 55   | A    | C3'-O3' | 5.40  | 1.49        | 1.42     |
| 1   | AA    | 71   | A    | C6-N6   | 5.40  | 1.38        | 1.33     |
| 1   | AA    | 402  | G    | C6-N1   | 5.40  | 1.43        | 1.39     |
| 35  | BB    | 1224 | U    | N3-C4   | 5.40  | 1.43        | 1.38     |
| 1   | AA    | 32   | A    | C6-N6   | 5.39  | 1.38        | 1.33     |
| 1   | AA    | 57   | G    | C6-N1   | 5.39  | 1.43        | 1.39     |
| 1   | AA    | 78   | A    | C4'-C3' | -5.39 | 1.47        | 1.52     |
| 1   | AA    | 245  | U    | N3-C4   | 5.39  | 1.43        | 1.38     |
| 1   | AA    | 736  | C    | C5'-C4' | 5.39  | 1.57        | 1.51     |
| 1   | AA    | 1225 | A    | C5-C6   | -5.39 | 1.36        | 1.41     |
| 15  | AO    | 5    | GLU  | CD-OE1  | 5.39  | 1.31        | 1.25     |
| 22  | AV    | 72   | G    | O3'-P   | -5.39 | 1.54        | 1.61     |
| 34  | BA    | 103  | U    | C4-O4   | -5.39 | 1.19        | 1.23     |
| 35  | BB    | 57   | C    | C2'-C1' | -5.39 | 1.47        | 1.53     |
| 35  | BB    | 559  | G    | N7-C5   | -5.39 | 1.36        | 1.39     |
| 35  | BB    | 1382 | G    | C8-N7   | -5.39 | 1.27        | 1.30     |
| 35  | BB    | 2129 | C    | C4-C5   | 5.39  | 1.47        | 1.43     |
| 35  | BB    | 2408 | U    | C5-C6   | 5.39  | 1.39        | 1.34     |
| 1   | AA    | 280  | C    | O3'-P   | -5.39 | 1.54        | 1.61     |
| 1   | AA    | 484  | G    | C2-N2   | 5.39  | 1.40        | 1.34     |
| 1   | AA    | 973  | G    | P-O5'   | -5.39 | 1.54        | 1.59     |
| 8   | AH    | 64   | TYR  | CG-CD2  | 5.39  | 1.46        | 1.39     |
| 10  | AJ    | 15   | HIS  | N-CA    | -5.39 | 1.35        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1285 | A    | P-O5'   | -5.39 | 1.54        | 1.59     |
| 35  | BB    | 1545 | A    | C8-N7   | -5.39 | 1.27        | 1.31     |
| 35  | BB    | 1913 | A    | C2'-C1' | -5.39 | 1.47        | 1.53     |
| 1   | AA    | 258  | G    | P-O5'   | 5.39  | 1.65        | 1.59     |
| 35  | BB    | 325  | G    | P-O5'   | -5.39 | 1.54        | 1.59     |
| 35  | BB    | 1078 | U    | C2-O2   | 5.39  | 1.27        | 1.22     |
| 35  | BB    | 1981 | A    | C5-C4   | 5.39  | 1.42        | 1.38     |
| 1   | AA    | 468  | A    | P-O5'   | 5.39  | 1.65        | 1.59     |
| 1   | AA    | 1079 | G    | C5'-C4' | 5.39  | 1.57        | 1.51     |
| 1   | AA    | 1143 | G    | N7-C5   | -5.39 | 1.36        | 1.39     |
| 5   | AE    | 64   | GLU  | CG-CD   | 5.39  | 1.60        | 1.51     |
| 20  | AT    | 73   | ARG  | NE-CZ   | 5.39  | 1.40        | 1.33     |
| 22  | AV    | 36   | G    | C4'-C3' | -5.39 | 1.47        | 1.52     |
| 35  | BB    | 875  | G    | C8-N7   | 5.39  | 1.34        | 1.30     |
| 35  | BB    | 1146 | C    | C3'-O3' | 5.39  | 1.49        | 1.42     |
| 35  | BB    | 1634 | A    | C4'-O4' | -5.39 | 1.38        | 1.45     |
| 35  | BB    | 2494 | G    | C1'-N9  | 5.39  | 1.56        | 1.48     |
| 35  | BB    | 2598 | A    | C5'-C4' | -5.39 | 1.44        | 1.51     |
| 1   | AA    | 82   | G    | P-O5'   | 5.39  | 1.65        | 1.59     |
| 1   | AA    | 309  | A    | C1'-N9  | -5.39 | 1.39        | 1.46     |
| 34  | BA    | 106  | G    | N9-C4   | -5.39 | 1.33        | 1.38     |
| 35  | BB    | 1081 | U    | C4'-O4' | -5.39 | 1.38        | 1.45     |
| 35  | BB    | 1842 | G    | C1'-N9  | -5.39 | 1.39        | 1.46     |
| 35  | BB    | 2365 | G    | N9-C4   | 5.39  | 1.42        | 1.38     |
| 35  | BB    | 2627 | G    | C2'-C1' | -5.39 | 1.47        | 1.53     |
| 35  | BB    | 2860 | A    | C6-N6   | 5.39  | 1.38        | 1.33     |
| 47  | BN    | 71   | ARG  | NE-CZ   | 5.39  | 1.40        | 1.33     |
| 1   | AA    | 166  | U    | C2-N3   | -5.39 | 1.33        | 1.37     |
| 1   | AA    | 182  | A    | C3'-C2' | 5.39  | 1.58        | 1.52     |
| 1   | AA    | 424  | G    | C5'-C4' | 5.39  | 1.57        | 1.51     |
| 1   | AA    | 446  | G    | N9-C4   | 5.39  | 1.42        | 1.38     |
| 1   | AA    | 782  | A    | C8-N7   | -5.39 | 1.27        | 1.31     |
| 1   | AA    | 1162 | C    | C5-C6   | -5.39 | 1.30        | 1.34     |
| 1   | AA    | 1428 | A    | N3-C4   | -5.39 | 1.31        | 1.34     |
| 1   | AA    | 1498 | U    | C2-N3   | 5.39  | 1.41        | 1.37     |
| 34  | BA    | 33   | G    | C5-C4   | 5.39  | 1.42        | 1.38     |
| 35  | BB    | 74   | A    | N9-C8   | -5.39 | 1.33        | 1.37     |
| 35  | BB    | 95   | A    | C6-N6   | 5.39  | 1.38        | 1.33     |
| 35  | BB    | 420  | C    | C5'-C4' | 5.39  | 1.57        | 1.51     |
| 35  | BB    | 572  | A    | N9-C4   | -5.39 | 1.34        | 1.37     |
| 35  | BB    | 588  | U    | C2-N3   | 5.39  | 1.41        | 1.37     |
| 35  | BB    | 1341 | G    | C2-N3   | 5.39  | 1.37        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1565 | C    | N1-C6   | 5.39  | 1.40        | 1.37     |
| 35  | BB    | 1910 | G    | N7-C5   | -5.39 | 1.36        | 1.39     |
| 35  | BB    | 2041 | U    | N3-C4   | -5.39 | 1.33        | 1.38     |
| 1   | AA    | 27   | G    | N1-C2   | 5.38  | 1.42        | 1.37     |
| 1   | AA    | 130  | A    | C5-C6   | 5.38  | 1.45        | 1.41     |
| 1   | AA    | 375  | U    | C4-C5   | -5.38 | 1.38        | 1.43     |
| 1   | AA    | 383  | A    | O4'-C1' | -5.38 | 1.34        | 1.41     |
| 1   | AA    | 791  | G    | C4'-C3' | -5.38 | 1.47        | 1.52     |
| 1   | AA    | 1276 | G    | C6-N1   | 5.38  | 1.43        | 1.39     |
| 30  | B5    | 53   | ARG  | CZ-NH1  | 5.38  | 1.40        | 1.33     |
| 35  | BB    | 470  | A    | C5-C4   | -5.38 | 1.34        | 1.38     |
| 35  | BB    | 885  | C    | C2-O2   | 5.38  | 1.29        | 1.24     |
| 48  | BO    | 16   | ARG  | NE-CZ   | 5.38  | 1.40        | 1.33     |
| 1   | AA    | 33   | A    | P-O5'   | -5.38 | 1.54        | 1.59     |
| 1   | AA    | 480  | U    | C2-N3   | 5.38  | 1.41        | 1.37     |
| 1   | AA    | 1386 | G    | N7-C5   | -5.38 | 1.36        | 1.39     |
| 35  | BB    | 2536 | G    | C2-N3   | 5.38  | 1.37        | 1.32     |
| 35  | BB    | 2779 | U    | C4-O4   | -5.38 | 1.19        | 1.23     |
| 1   | AA    | 228  | A    | N3-C4   | -5.38 | 1.31        | 1.34     |
| 1   | AA    | 447  | G    | C4'-C3' | -5.38 | 1.47        | 1.52     |
| 1   | AA    | 527  | G    | C2-N3   | -5.38 | 1.28        | 1.32     |
| 1   | AA    | 1063 | C    | C3'-C2' | 5.38  | 1.58        | 1.52     |
| 35  | BB    | 371  | A    | N7-C5   | -5.38 | 1.36        | 1.39     |
| 35  | BB    | 935  | C    | C2'-C1' | -5.38 | 1.47        | 1.53     |
| 35  | BB    | 1192 | G    | N3-C4   | 5.38  | 1.39        | 1.35     |
| 35  | BB    | 1422 | G    | C8-N7   | 5.38  | 1.34        | 1.30     |
| 35  | BB    | 2197 | U    | O3'-P   | -5.38 | 1.54        | 1.61     |
| 35  | BB    | 2483 | C    | C4'-O4' | 5.38  | 1.52        | 1.45     |
| 35  | BB    | 2547 | A    | O4'-C1' | -5.38 | 1.34        | 1.41     |
| 35  | BB    | 2597 | G    | N1-C2   | 5.38  | 1.42        | 1.37     |
| 53  | BT    | 77   | ARG  | NE-CZ   | 5.38  | 1.40        | 1.33     |
| 1   | AA    | 1300 | G    | C4'-C3' | 5.38  | 1.59        | 1.53     |
| 3   | AC    | 127  | VAL  | CB-CG1  | 5.38  | 1.64        | 1.52     |
| 35  | BB    | 644  | A    | N9-C8   | -5.38 | 1.33        | 1.37     |
| 1   | AA    | 358  | U    | C5'-C4' | 5.38  | 1.57        | 1.51     |
| 1   | AA    | 588  | G    | C4'-O4' | -5.38 | 1.38        | 1.45     |
| 1   | AA    | 660  | C    | C2'-C1' | -5.38 | 1.47        | 1.53     |
| 1   | AA    | 1033 | G    | N9-C8   | 5.38  | 1.41        | 1.37     |
| 1   | AA    | 1359 | C    | C2'-C1' | -5.38 | 1.47        | 1.53     |
| 35  | BB    | 169  | G    | C2-N3   | 5.38  | 1.37        | 1.32     |
| 35  | BB    | 204  | A    | C5-C4   | -5.38 | 1.34        | 1.38     |
| 35  | BB    | 477  | A    | O3'-P   | -5.38 | 1.54        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 622  | G    | C6-N1   | 5.38  | 1.43        | 1.39     |
| 35  | BB    | 649  | G    | C5-C6   | -5.38 | 1.36        | 1.42     |
| 35  | BB    | 1788 | C    | C4'-O4' | 5.38  | 1.52        | 1.45     |
| 35  | BB    | 2418 | A    | N1-C2   | -5.38 | 1.29        | 1.34     |
| 35  | BB    | 2792 | A    | N7-C5   | -5.38 | 1.36        | 1.39     |
| 55  | BW    | 19   | ARG  | CZ-NH1  | 5.38  | 1.40        | 1.33     |
| 1   | AA    | 36   | C    | C3'-O3' | 5.38  | 1.49        | 1.42     |
| 1   | AA    | 268  | U    | C2-N3   | 5.38  | 1.41        | 1.37     |
| 1   | AA    | 362  | G    | N9-C8   | 5.38  | 1.41        | 1.37     |
| 1   | AA    | 951  | G    | N1-C2   | 5.38  | 1.42        | 1.37     |
| 1   | AA    | 1223 | C    | N3-C4   | 5.38  | 1.37        | 1.33     |
| 35  | BB    | 104  | A    | N7-C5   | -5.38 | 1.36        | 1.39     |
| 35  | BB    | 145  | C    | C5-C6   | -5.38 | 1.30        | 1.34     |
| 35  | BB    | 699  | A    | C8-N7   | -5.38 | 1.27        | 1.31     |
| 35  | BB    | 822  | G    | N9-C4   | -5.38 | 1.33        | 1.38     |
| 35  | BB    | 838  | C    | C2-N3   | -5.38 | 1.31        | 1.35     |
| 35  | BB    | 1181 | U    | C1'-N1  | 5.38  | 1.56        | 1.48     |
| 35  | BB    | 1398 | C    | C2'-O2' | -5.38 | 1.34        | 1.41     |
| 35  | BB    | 2090 | A    | C6-N6   | 5.38  | 1.38        | 1.33     |
| 35  | BB    | 2509 | G    | N3-C4   | 5.38  | 1.39        | 1.35     |
| 1   | AA    | 178  | C    | N1-C2   | -5.38 | 1.34        | 1.40     |
| 1   | AA    | 803  | G    | C2-N3   | 5.38  | 1.37        | 1.32     |
| 1   | AA    | 830  | G    | N7-C5   | -5.38 | 1.36        | 1.39     |
| 35  | BB    | 27   | G    | C6-N1   | -5.38 | 1.35        | 1.39     |
| 35  | BB    | 539  | G    | C1'-N9  | 5.38  | 1.56        | 1.48     |
| 35  | BB    | 580  | U    | C2'-O2' | -5.38 | 1.34        | 1.41     |
| 35  | BB    | 1279 | G    | N1-C2   | 5.38  | 1.42        | 1.37     |
| 35  | BB    | 1313 | U    | N1-C2   | 5.38  | 1.43        | 1.38     |
| 35  | BB    | 1756 | G    | N9-C8   | 5.38  | 1.41        | 1.37     |
| 35  | BB    | 2421 | G    | C8-N7   | -5.38 | 1.27        | 1.30     |
| 35  | BB    | 2478 | A    | C8-N7   | -5.38 | 1.27        | 1.31     |
| 1   | AA    | 44   | A    | C5-C6   | 5.37  | 1.45        | 1.41     |
| 1   | AA    | 799  | G    | N9-C4   | 5.37  | 1.42        | 1.38     |
| 35  | BB    | 32   | C    | C4-N4   | -5.37 | 1.29        | 1.33     |
| 35  | BB    | 315  | G    | C2-N2   | 5.37  | 1.40        | 1.34     |
| 35  | BB    | 387  | U    | O3'-P   | -5.37 | 1.54        | 1.61     |
| 35  | BB    | 466  | A    | N9-C8   | 5.37  | 1.42        | 1.37     |
| 35  | BB    | 922  | C    | C2'-C1' | -5.37 | 1.47        | 1.53     |
| 35  | BB    | 1659 | G    | O4'-C1' | -5.37 | 1.34        | 1.41     |
| 35  | BB    | 2401 | U    | C2'-C1' | -5.37 | 1.47        | 1.53     |
| 1   | AA    | 452  | A    | N3-C4   | -5.37 | 1.31        | 1.34     |
| 1   | AA    | 454  | G    | C4'-C3' | 5.37  | 1.59        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 671  | G    | C4'-O4' | 5.37  | 1.52        | 1.45     |
| 35  | BB    | 1250 | G    | C6-O6   | 5.37  | 1.28        | 1.24     |
| 35  | BB    | 1359 | A    | O4'-C1' | -5.37 | 1.34        | 1.41     |
| 35  | BB    | 1514 | G    | C2-N2   | -5.37 | 1.29        | 1.34     |
| 35  | BB    | 1525 | A    | C8-N7   | -5.37 | 1.27        | 1.31     |
| 35  | BB    | 2112 | G    | C5-C4   | 5.37  | 1.42        | 1.38     |
| 35  | BB    | 2809 | A    | N9-C8   | -5.37 | 1.33        | 1.37     |
| 35  | BB    | 2827 | C    | O3'-P   | -5.37 | 1.54        | 1.61     |
| 43  | BJ    | 13   | ARG  | NE-CZ   | 5.37  | 1.40        | 1.33     |
| 43  | BJ    | 77   | HIS  | N-CA    | -5.37 | 1.35        | 1.46     |
| 50  | BQ    | 44   | TYR  | CG-CD1  | 5.37  | 1.46        | 1.39     |
| 1   | AA    | 21   | G    | N9-C4   | -5.37 | 1.33        | 1.38     |
| 1   | AA    | 861  | G    | C5-C6   | -5.37 | 1.36        | 1.42     |
| 35  | BB    | 1997 | C    | C2'-C1' | -5.37 | 1.47        | 1.53     |
| 35  | BB    | 2235 | G    | N9-C8   | 5.37  | 1.41        | 1.37     |
| 35  | BB    | 2528 | U    | N1-C6   | 5.37  | 1.42        | 1.38     |
| 1   | AA    | 1045 | C    | C4'-O4' | 5.37  | 1.52        | 1.45     |
| 2   | AB    | 207  | ARG  | CZ-NH1  | 5.37  | 1.40        | 1.33     |
| 26  | B1    | 5    | GLU  | CD-OE2  | 5.37  | 1.31        | 1.25     |
| 35  | BB    | 740  | C    | C2'-C1' | -5.37 | 1.47        | 1.53     |
| 35  | BB    | 1021 | A    | C5-C6   | 5.37  | 1.45        | 1.41     |
| 35  | BB    | 1246 | A    | O4'-C1' | -5.37 | 1.34        | 1.41     |
| 35  | BB    | 1676 | A    | N7-C5   | -5.37 | 1.36        | 1.39     |
| 35  | BB    | 2447 | G    | C2-N2   | 5.37  | 1.40        | 1.34     |
| 35  | BB    | 2460 | U    | N3-C4   | 5.37  | 1.43        | 1.38     |
| 35  | BB    | 2525 | G    | C2-N2   | 5.37  | 1.40        | 1.34     |
| 35  | BB    | 2639 | A    | C8-N7   | -5.37 | 1.27        | 1.31     |
| 1   | AA    | 1407 | C    | O4'-C1' | 5.37  | 1.48        | 1.41     |
| 35  | BB    | 108  | G    | N9-C4   | -5.37 | 1.33        | 1.38     |
| 35  | BB    | 121  | G    | N1-C2   | 5.37  | 1.42        | 1.37     |
| 35  | BB    | 1034 | G    | P-O5'   | -5.37 | 1.54        | 1.59     |
| 35  | BB    | 1817 | G    | C6-O6   | -5.37 | 1.19        | 1.24     |
| 35  | BB    | 2346 | A    | C4'-O4' | -5.37 | 1.38        | 1.45     |
| 35  | BB    | 2822 | G    | N7-C5   | -5.37 | 1.36        | 1.39     |
| 1   | AA    | 163  | C    | C1'-N1  | 5.37  | 1.56        | 1.48     |
| 1   | AA    | 224  | U    | O4'-C1' | -5.37 | 1.34        | 1.41     |
| 1   | AA    | 395  | C    | O4'-C1' | 5.37  | 1.48        | 1.41     |
| 1   | AA    | 776  | G    | C5-C6   | -5.37 | 1.36        | 1.42     |
| 1   | AA    | 1192 | C    | C5'-C4' | 5.37  | 1.57        | 1.51     |
| 35  | BB    | 164  | C    | C1'-N1  | 5.37  | 1.56        | 1.48     |
| 35  | BB    | 570  | G    | C2-N2   | 5.37  | 1.40        | 1.34     |
| 35  | BB    | 1980 | G    | P-O5'   | -5.37 | 1.54        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2734 | A    | C2-N3   | 5.37  | 1.38        | 1.33     |
| 35  | BB    | 2854 | G    | C2-N2   | -5.37 | 1.29        | 1.34     |
| 1   | AA    | 477  | C    | N1-C6   | -5.36 | 1.33        | 1.37     |
| 1   | AA    | 553  | A    | P-O5'   | -5.36 | 1.54        | 1.59     |
| 1   | AA    | 761  | G    | C3'-C2' | -5.36 | 1.46        | 1.52     |
| 1   | AA    | 1065 | U    | N3-C4   | 5.36  | 1.43        | 1.38     |
| 1   | AA    | 1266 | G    | C8-N7   | -5.36 | 1.27        | 1.30     |
| 5   | AE    | 68   | ARG  | CZ-NH2  | 5.36  | 1.40        | 1.33     |
| 35  | BB    | 2    | G    | C5-C6   | -5.36 | 1.36        | 1.42     |
| 35  | BB    | 441  | U    | C4-C5   | 5.36  | 1.48        | 1.43     |
| 35  | BB    | 2031 | A    | C2'-C1' | -5.36 | 1.47        | 1.53     |
| 35  | BB    | 2201 | G    | C2'-O2' | -5.36 | 1.34        | 1.41     |
| 35  | BB    | 2309 | A    | C6-N6   | 5.36  | 1.38        | 1.33     |
| 35  | BB    | 2373 | G    | C6-O6   | 5.36  | 1.28        | 1.24     |
| 50  | BQ    | 63   | ARG  | CZ-NH2  | 5.36  | 1.40        | 1.33     |
| 9   | AI    | 48   | ARG  | CZ-NH1  | 5.36  | 1.40        | 1.33     |
| 35  | BB    | 358  | U    | C3'-C2' | -5.36 | 1.46        | 1.52     |
| 35  | BB    | 385  | C    | C5'-C4' | 5.36  | 1.57        | 1.51     |
| 35  | BB    | 2303 | G    | C5'-C4' | 5.36  | 1.57        | 1.51     |
| 35  | BB    | 2755 | C    | C5'-C4' | 5.36  | 1.57        | 1.51     |
| 1   | AA    | 128  | G    | C8-N7   | -5.36 | 1.27        | 1.30     |
| 1   | AA    | 175  | C    | N1-C2   | -5.36 | 1.34        | 1.40     |
| 1   | AA    | 198  | G    | N3-C4   | -5.36 | 1.31        | 1.35     |
| 1   | AA    | 864  | A    | N9-C8   | -5.36 | 1.33        | 1.37     |
| 1   | AA    | 1082 | A    | C5-C6   | 5.36  | 1.45        | 1.41     |
| 35  | BB    | 785  | G    | C2-N3   | 5.36  | 1.37        | 1.32     |
| 35  | BB    | 1507 | C    | N3-C4   | 5.36  | 1.37        | 1.33     |
| 35  | BB    | 2794 | C    | C4'-O4' | 5.36  | 1.52        | 1.45     |
| 1   | AA    | 82   | G    | C8-N7   | -5.36 | 1.27        | 1.30     |
| 35  | BB    | 932  | U    | N3-C4   | 5.36  | 1.43        | 1.38     |
| 35  | BB    | 2456 | C    | C4-C5   | -5.36 | 1.38        | 1.43     |
| 35  | BB    | 2763 | G    | C6-N1   | 5.36  | 1.43        | 1.39     |
| 39  | BF    | 29   | ARG  | CD-NE   | 5.36  | 1.55        | 1.46     |
| 1   | AA    | 139  | A    | C5-C6   | -5.36 | 1.36        | 1.41     |
| 1   | AA    | 366  | A    | N7-C5   | -5.36 | 1.36        | 1.39     |
| 1   | AA    | 821  | G    | P-O5'   | -5.36 | 1.54        | 1.59     |
| 1   | AA    | 1004 | A    | C3'-C2' | -5.36 | 1.46        | 1.52     |
| 1   | AA    | 1259 | C    | C3'-O3' | 5.36  | 1.49        | 1.42     |
| 1   | AA    | 1387 | G    | N1-C2   | 5.36  | 1.42        | 1.37     |
| 35  | BB    | 16   | C    | C2-N3   | 5.36  | 1.40        | 1.35     |
| 35  | BB    | 590  | A    | P-O5'   | -5.36 | 1.54        | 1.59     |
| 35  | BB    | 944  | C    | N1-C2   | -5.36 | 1.34        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1231 | U    | C4'-O4' | 5.36  | 1.52        | 1.45     |
| 35  | BB    | 1763 | G    | N9-C8   | -5.36 | 1.34        | 1.37     |
| 35  | BB    | 2711 | A    | C4'-O4' | -5.36 | 1.38        | 1.45     |
| 35  | BB    | 2847 | U    | C5-C6   | 5.36  | 1.39        | 1.34     |
| 35  | BB    | 2899 | A    | N3-C4   | -5.36 | 1.31        | 1.34     |
| 1   | AA    | 31   | G    | N9-C8   | 5.36  | 1.41        | 1.37     |
| 1   | AA    | 812  | G    | P-O5'   | -5.36 | 1.54        | 1.59     |
| 1   | AA    | 1510 | C    | C5-C6   | -5.36 | 1.30        | 1.34     |
| 35  | BB    | 1250 | G    | C5'-C4' | 5.36  | 1.57        | 1.51     |
| 35  | BB    | 1636 | U    | O3'-P   | -5.36 | 1.54        | 1.61     |
| 35  | BB    | 1645 | G    | C3'-C2' | -5.36 | 1.46        | 1.52     |
| 35  | BB    | 2216 | G    | P-O5'   | 5.36  | 1.65        | 1.59     |
| 35  | BB    | 2375 | G    | N9-C8   | 5.36  | 1.41        | 1.37     |
| 35  | BB    | 2816 | G    | C5-C6   | -5.36 | 1.36        | 1.42     |
| 1   | AA    | 1020 | G    | C5'-C4' | 5.35  | 1.57        | 1.51     |
| 1   | AA    | 1534 | A    | C2-N3   | 5.35  | 1.38        | 1.33     |
| 1   | AA    | 273  | U    | C5'-C4' | 5.35  | 1.57        | 1.51     |
| 1   | AA    | 695  | A    | C6-N6   | 5.35  | 1.38        | 1.33     |
| 1   | AA    | 1153 | G    | C6-N1   | 5.35  | 1.43        | 1.39     |
| 5   | AE    | 115  | GLU  | CG-CD   | 5.35  | 1.59        | 1.51     |
| 35  | BB    | 115  | C    | O4'-C1' | 5.35  | 1.48        | 1.41     |
| 35  | BB    | 203  | A    | O3'-P   | -5.35 | 1.54        | 1.61     |
| 35  | BB    | 257  | C    | C2'-C1' | -5.35 | 1.47        | 1.53     |
| 35  | BB    | 388  | G    | C5-C4   | -5.35 | 1.34        | 1.38     |
| 35  | BB    | 1020 | A    | N9-C4   | -5.35 | 1.34        | 1.37     |
| 35  | BB    | 1882 | U    | P-O5'   | -5.35 | 1.54        | 1.59     |
| 35  | BB    | 2841 | C    | P-O5'   | -5.35 | 1.54        | 1.59     |
| 1   | AA    | 919  | A    | C2'-C1' | -5.35 | 1.47        | 1.53     |
| 35  | BB    | 1094 | U    | C3'-C2' | -5.35 | 1.46        | 1.52     |
| 35  | BB    | 2318 | G    | C8-N7   | -5.35 | 1.27        | 1.30     |
| 1   | AA    | 564  | C    | N3-C4   | 5.35  | 1.37        | 1.33     |
| 1   | AA    | 899  | C    | C4-N4   | 5.35  | 1.38        | 1.33     |
| 1   | AA    | 980  | C    | C5'-C4' | 5.35  | 1.57        | 1.51     |
| 1   | AA    | 996  | A    | C6-N6   | 5.35  | 1.38        | 1.33     |
| 1   | AA    | 1438 | G    | C5-C6   | -5.35 | 1.37        | 1.42     |
| 7   | AG    | 81   | GLY  | CA-C    | -5.35 | 1.43        | 1.51     |
| 34  | BA    | 68   | C    | P-O5'   | -5.35 | 1.54        | 1.59     |
| 35  | BB    | 31   | C    | C4'-O4' | 5.35  | 1.52        | 1.45     |
| 35  | BB    | 214  | G    | N9-C4   | -5.35 | 1.33        | 1.38     |
| 35  | BB    | 550  | C    | C4-N4   | -5.35 | 1.29        | 1.33     |
| 35  | BB    | 792  | A    | C3'-C2' | -5.35 | 1.46        | 1.52     |
| 35  | BB    | 823  | C    | P-O5'   | -5.35 | 1.54        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 844  | A    | C6-N6   | 5.35  | 1.38        | 1.33     |
| 35  | BB    | 897  | C    | C2'-C1' | -5.35 | 1.47        | 1.53     |
| 35  | BB    | 1227 | G    | N9-C8   | -5.35 | 1.34        | 1.37     |
| 35  | BB    | 1849 | G    | C2-N3   | 5.35  | 1.37        | 1.32     |
| 35  | BB    | 2645 | G    | C6-N1   | -5.35 | 1.35        | 1.39     |
| 1   | AA    | 505  | G    | C5-C4   | -5.35 | 1.34        | 1.38     |
| 1   | AA    | 637  | C    | C2-N3   | 5.35  | 1.40        | 1.35     |
| 35  | BB    | 83   | A    | C5'-C4' | 5.35  | 1.57        | 1.51     |
| 35  | BB    | 403  | U    | P-O5'   | 5.35  | 1.65        | 1.59     |
| 35  | BB    | 588  | U    | C5-C6   | 5.35  | 1.39        | 1.34     |
| 35  | BB    | 719  | C    | N1-C6   | -5.35 | 1.33        | 1.37     |
| 35  | BB    | 776  | G    | C2'-O2' | -5.35 | 1.34        | 1.41     |
| 35  | BB    | 1789 | A    | O3'-P   | -5.35 | 1.54        | 1.61     |
| 35  | BB    | 1975 | G    | C4'-O4' | -5.35 | 1.38        | 1.45     |
| 35  | BB    | 2437 | G    | C3'-C2' | -5.35 | 1.46        | 1.52     |
| 1   | AA    | 172  | A    | C5-C6   | 5.35  | 1.45        | 1.41     |
| 1   | AA    | 1324 | A    | P-O5'   | -5.35 | 1.54        | 1.59     |
| 1   | AA    | 1429 | A    | C2'-C1' | -5.35 | 1.47        | 1.53     |
| 35  | BB    | 1280 | G    | N1-C2   | 5.35  | 1.42        | 1.37     |
| 35  | BB    | 1501 | G    | C2-N2   | 5.35  | 1.39        | 1.34     |
| 35  | BB    | 1524 | G    | N9-C8   | -5.35 | 1.34        | 1.37     |
| 35  | BB    | 1665 | A    | C2'-C1' | -5.35 | 1.47        | 1.53     |
| 1   | AA    | 913  | A    | C6-N1   | 5.34  | 1.39        | 1.35     |
| 34  | BA    | 90   | C    | C1'-N1  | 5.34  | 1.56        | 1.48     |
| 35  | BB    | 282  | A    | C5-C4   | -5.34 | 1.35        | 1.38     |
| 35  | BB    | 304  | U    | P-O5'   | -5.34 | 1.54        | 1.59     |
| 35  | BB    | 359  | G    | N9-C4   | -5.34 | 1.33        | 1.38     |
| 35  | BB    | 599  | A    | N1-C2   | -5.34 | 1.29        | 1.34     |
| 35  | BB    | 1278 | C    | N1-C6   | 5.34  | 1.40        | 1.37     |
| 35  | BB    | 1279 | G    | C4'-C3' | -5.34 | 1.47        | 1.52     |
| 35  | BB    | 1805 | A    | C6-N1   | -5.34 | 1.31        | 1.35     |
| 35  | BB    | 1886 | U    | C2-N3   | 5.34  | 1.41        | 1.37     |
| 35  | BB    | 2214 | C    | C4'-C3' | 5.34  | 1.59        | 1.53     |
| 35  | BB    | 2731 | G    | N9-C4   | -5.34 | 1.33        | 1.38     |
| 1   | AA    | 958  | A    | C6-N1   | 5.34  | 1.39        | 1.35     |
| 35  | BB    | 245  | G    | N1-C2   | 5.34  | 1.42        | 1.37     |
| 35  | BB    | 770  | G    | P-O5'   | 5.34  | 1.65        | 1.59     |
| 35  | BB    | 1285 | A    | C8-N7   | -5.34 | 1.27        | 1.31     |
| 35  | BB    | 1608 | A    | P-O5'   | -5.34 | 1.54        | 1.59     |
| 35  | BB    | 1875 | G    | C6-N1   | -5.34 | 1.35        | 1.39     |
| 1   | AA    | 559  | A    | C4'-C3' | 5.34  | 1.59        | 1.53     |
| 1   | AA    | 1132 | C    | C4'-C3' | 5.34  | 1.59        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | AH    | 56   | PRO  | N-CD    | -5.34 | 1.40        | 1.47     |
| 35  | BB    | 1224 | U    | N1-C6   | 5.34  | 1.42        | 1.38     |
| 35  | BB    | 1239 | G    | O3'-P   | -5.34 | 1.54        | 1.61     |
| 35  | BB    | 1684 | G    | C4'-C3' | 5.34  | 1.59        | 1.53     |
| 35  | BB    | 1811 | G    | C2-N3   | 5.34  | 1.37        | 1.32     |
| 35  | BB    | 2250 | G    | C6-N1   | 5.34  | 1.43        | 1.39     |
| 35  | BB    | 2787 | C    | C2-N3   | 5.34  | 1.40        | 1.35     |
| 1   | AA    | 152  | A    | C6-N1   | 5.34  | 1.39        | 1.35     |
| 1   | AA    | 318  | G    | C5'-C4' | -5.34 | 1.45        | 1.51     |
| 1   | AA    | 637  | C    | C4-C5   | -5.34 | 1.38        | 1.43     |
| 1   | AA    | 1271 | A    | C6-N1   | 5.34  | 1.39        | 1.35     |
| 34  | BA    | 114  | C    | P-O5'   | -5.34 | 1.54        | 1.59     |
| 35  | BB    | 184  | C    | C3'-C2' | -5.34 | 1.46        | 1.52     |
| 35  | BB    | 434  | U    | N3-C4   | 5.34  | 1.43        | 1.38     |
| 35  | BB    | 1409 | U    | P-O5'   | -5.34 | 1.54        | 1.59     |
| 35  | BB    | 1421 | G    | N9-C8   | 5.34  | 1.41        | 1.37     |
| 35  | BB    | 1426 | G    | C2-N3   | 5.34  | 1.37        | 1.32     |
| 35  | BB    | 2197 | U    | N1-C2   | 5.34  | 1.43        | 1.38     |
| 1   | AA    | 231  | U    | C3'-C2' | 5.34  | 1.58        | 1.52     |
| 35  | BB    | 2491 | U    | C2'-C1' | -5.34 | 1.47        | 1.53     |
| 35  | BB    | 2568 | U    | C2'-C1' | -5.34 | 1.47        | 1.53     |
| 1   | AA    | 287  | U    | C3'-O3' | 5.34  | 1.49        | 1.42     |
| 1   | AA    | 552  | U    | C2-N3   | 5.34  | 1.41        | 1.37     |
| 1   | AA    | 839  | C    | O3'-P   | -5.34 | 1.54        | 1.61     |
| 1   | AA    | 888  | G    | C2'-C1' | -5.34 | 1.47        | 1.53     |
| 1   | AA    | 1167 | A    | N9-C4   | 5.34  | 1.41        | 1.37     |
| 1   | AA    | 1242 | G    | N9-C8   | 5.34  | 1.41        | 1.37     |
| 1   | AA    | 1298 | U    | C4-C5   | 5.34  | 1.48        | 1.43     |
| 27  | B2    | 37   | ARG  | CZ-NH1  | 5.34  | 1.40        | 1.33     |
| 35  | BB    | 900  | A    | N9-C4   | 5.34  | 1.41        | 1.37     |
| 35  | BB    | 956  | G    | C4'-O4' | -5.34 | 1.38        | 1.45     |
| 35  | BB    | 1940 | U    | C2'-C1' | -5.34 | 1.47        | 1.53     |
| 35  | BB    | 2845 | U    | N1-C2   | 5.34  | 1.43        | 1.38     |
| 1   | AA    | 874  | G    | C2'-C1' | -5.33 | 1.47        | 1.53     |
| 35  | BB    | 1480 | C    | C4-N4   | 5.33  | 1.38        | 1.33     |
| 35  | BB    | 1713 | A    | C5'-C4' | 5.33  | 1.57        | 1.51     |
| 1   | AA    | 410  | G    | N9-C8   | -5.33 | 1.34        | 1.37     |
| 1   | AA    | 414  | A    | C5-C6   | 5.33  | 1.45        | 1.41     |
| 1   | AA    | 914  | A    | N9-C8   | 5.33  | 1.42        | 1.37     |
| 35  | BB    | 1730 | C    | C3'-C2' | 5.33  | 1.58        | 1.52     |
| 35  | BB    | 1934 | C    | C1'-N1  | 5.33  | 1.56        | 1.48     |
| 35  | BB    | 2269 | G    | O3'-P   | -5.33 | 1.54        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2480 | C    | C3'-C2' | -5.33 | 1.46        | 1.52     |
| 1   | AA    | 116  | A    | N9-C4   | 5.33  | 1.41        | 1.37     |
| 1   | AA    | 1333 | A    | C3'-C2' | -5.33 | 1.46        | 1.52     |
| 8   | AH    | 58   | LEU  | N-CA    | -5.33 | 1.35        | 1.46     |
| 35  | BB    | 30   | G    | C2-N2   | 5.33  | 1.39        | 1.34     |
| 35  | BB    | 129  | C    | P-O5'   | -5.33 | 1.54        | 1.59     |
| 35  | BB    | 163  | C    | C4-N4   | 5.33  | 1.38        | 1.33     |
| 35  | BB    | 1380 | G    | C2-N3   | 5.33  | 1.37        | 1.32     |
| 35  | BB    | 1688 | U    | C2-N3   | 5.33  | 1.41        | 1.37     |
| 35  | BB    | 2685 | G    | N3-C4   | 5.33  | 1.39        | 1.35     |
| 1   | AA    | 76   | G    | N9-C4   | 5.33  | 1.42        | 1.38     |
| 1   | AA    | 189  | A    | N7-C5   | -5.33 | 1.36        | 1.39     |
| 1   | AA    | 1505 | G    | C8-N7   | -5.33 | 1.27        | 1.30     |
| 1   | AA    | 363  | A    | O3'-P   | -5.33 | 1.54        | 1.61     |
| 1   | AA    | 851  | G    | N1-C2   | 5.33  | 1.42        | 1.37     |
| 1   | AA    | 1168 | U    | C3'-O3' | 5.33  | 1.49        | 1.42     |
| 1   | AA    | 1473 | G    | N9-C8   | -5.33 | 1.34        | 1.37     |
| 3   | AC    | 192  | TYR  | CE2-CZ  | 5.33  | 1.45        | 1.38     |
| 35  | BB    | 421  | C    | C5'-C4' | -5.33 | 1.45        | 1.51     |
| 35  | BB    | 746  | U    | N3-C4   | 5.33  | 1.43        | 1.38     |
| 35  | BB    | 966  | G    | N3-C4   | -5.33 | 1.31        | 1.35     |
| 35  | BB    | 1121 | C    | C4-C5   | -5.33 | 1.38        | 1.43     |
| 35  | BB    | 1289 | C    | C2-N3   | 5.33  | 1.40        | 1.35     |
| 35  | BB    | 1486 | U    | C2-N3   | 5.33  | 1.41        | 1.37     |
| 35  | BB    | 1635 | A    | C2'-O2' | -5.33 | 1.34        | 1.41     |
| 35  | BB    | 1705 | A    | N1-C2   | 5.33  | 1.39        | 1.34     |
| 35  | BB    | 1767 | G    | C8-N7   | -5.33 | 1.27        | 1.30     |
| 35  | BB    | 1957 | C    | C2'-C1' | -5.33 | 1.47        | 1.53     |
| 35  | BB    | 2208 | C    | C3'-O3' | 5.33  | 1.49        | 1.42     |
| 35  | BB    | 2383 | G    | C8-N7   | -5.33 | 1.27        | 1.30     |
| 35  | BB    | 2760 | C    | C5'-C4' | 5.33  | 1.57        | 1.51     |
| 1   | AA    | 674  | G    | C4'-C3' | -5.33 | 1.47        | 1.52     |
| 1   | AA    | 831  | A    | C5-C6   | -5.33 | 1.36        | 1.41     |
| 34  | BA    | 62   | C    | N3-C4   | 5.33  | 1.37        | 1.33     |
| 35  | BB    | 773  | U    | C1'-N1  | 5.33  | 1.56        | 1.48     |
| 35  | BB    | 1342 | A    | C2-N3   | 5.33  | 1.38        | 1.33     |
| 35  | BB    | 2224 | G    | N1-C2   | 5.33  | 1.42        | 1.37     |
| 35  | BB    | 2264 | C    | N3-C4   | 5.33  | 1.37        | 1.33     |
| 35  | BB    | 2530 | A    | N3-C4   | -5.33 | 1.31        | 1.34     |
| 35  | BB    | 2875 | C    | C2-N3   | 5.33  | 1.40        | 1.35     |
| 1   | AA    | 601  | G    | C5'-C4' | 5.33  | 1.57        | 1.51     |
| 1   | AA    | 1148 | U    | C2'-C1' | -5.33 | 1.47        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1236 | A    | O3'-P   | -5.33 | 1.54        | 1.61     |
| 35  | BB    | 631  | A    | N7-C5   | -5.33 | 1.36        | 1.39     |
| 35  | BB    | 762  | U    | N3-C4   | 5.33  | 1.43        | 1.38     |
| 35  | BB    | 908  | C    | N3-C4   | 5.33  | 1.37        | 1.33     |
| 35  | BB    | 1311 | G    | C4'-O4' | 5.33  | 1.52        | 1.45     |
| 35  | BB    | 1538 | G    | P-O5'   | -5.33 | 1.54        | 1.59     |
| 35  | BB    | 2289 | G    | C2-N2   | 5.33  | 1.39        | 1.34     |
| 35  | BB    | 2316 | G    | C5-C6   | -5.33 | 1.37        | 1.42     |
| 35  | BB    | 2826 | A    | N9-C4   | 5.33  | 1.41        | 1.37     |
| 1   | AA    | 949  | A    | C4'-C3' | 5.32  | 1.59        | 1.53     |
| 1   | AA    | 978  | A    | C6-N6   | 5.32  | 1.38        | 1.33     |
| 1   | AA    | 1067 | A    | P-O5'   | -5.32 | 1.54        | 1.59     |
| 1   | AA    | 1246 | A    | C6-N6   | 5.32  | 1.38        | 1.33     |
| 1   | AA    | 1475 | G    | N9-C4   | 5.32  | 1.42        | 1.38     |
| 34  | BA    | 99   | A    | O3'-P   | -5.32 | 1.54        | 1.61     |
| 35  | BB    | 171  | U    | O4'-C1' | 5.32  | 1.48        | 1.41     |
| 35  | BB    | 446  | G    | N7-C5   | -5.32 | 1.36        | 1.39     |
| 35  | BB    | 726  | G    | C5-C4   | -5.32 | 1.34        | 1.38     |
| 35  | BB    | 979  | A    | N9-C4   | -5.32 | 1.34        | 1.37     |
| 35  | BB    | 1050 | A    | O4'-C1' | 5.32  | 1.48        | 1.41     |
| 35  | BB    | 1474 | U    | N3-C4   | 5.32  | 1.43        | 1.38     |
| 35  | BB    | 1611 | C    | N3-C4   | 5.32  | 1.37        | 1.33     |
| 35  | BB    | 1693 | U    | N3-C4   | 5.32  | 1.43        | 1.38     |
| 35  | BB    | 2682 | A    | N3-C4   | -5.32 | 1.31        | 1.34     |
| 1   | AA    | 657  | U    | P-O5'   | -5.32 | 1.54        | 1.59     |
| 1   | AA    | 1337 | G    | C6-N1   | 5.32  | 1.43        | 1.39     |
| 35  | BB    | 992  | C    | C5'-C4' | 5.32  | 1.57        | 1.51     |
| 35  | BB    | 1898 | U    | C4-C5   | 5.32  | 1.48        | 1.43     |
| 35  | BB    | 2228 | G    | C6-O6   | -5.32 | 1.19        | 1.24     |
| 35  | BB    | 2565 | A    | C3'-O3' | 5.32  | 1.49        | 1.42     |
| 1   | AA    | 191  | G    | N1-C2   | 5.32  | 1.42        | 1.37     |
| 1   | AA    | 347  | G    | C5'-C4' | 5.32  | 1.57        | 1.51     |
| 1   | AA    | 1162 | C    | C4-C5   | -5.32 | 1.38        | 1.43     |
| 35  | BB    | 121  | G    | C8-N7   | 5.32  | 1.34        | 1.30     |
| 35  | BB    | 693  | A    | N3-C4   | -5.32 | 1.31        | 1.34     |
| 35  | BB    | 1234 | U    | C5'-C4' | 5.32  | 1.57        | 1.51     |
| 35  | BB    | 1455 | G    | C2-N3   | 5.32  | 1.37        | 1.32     |
| 35  | BB    | 1844 | C    | N1-C6   | -5.32 | 1.33        | 1.37     |
| 35  | BB    | 2474 | U    | P-O5'   | -5.32 | 1.54        | 1.59     |
| 35  | BB    | 2778 | A    | C5'-C4' | 5.32  | 1.57        | 1.51     |
| 35  | BB    | 2887 | A    | C5-C6   | -5.32 | 1.36        | 1.41     |
| 1   | AA    | 1094 | G    | P-O5'   | -5.32 | 1.54        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 96   | C    | O4'-C1' | 5.32  | 1.48        | 1.41     |
| 35  | BB    | 1373 | A    | N9-C4   | -5.32 | 1.34        | 1.37     |
| 35  | BB    | 1531 | C    | C5-C6   | -5.32 | 1.30        | 1.34     |
| 49  | BP    | 8    | GLU  | CB-CG   | 5.32  | 1.62        | 1.52     |
| 1   | AA    | 52   | C    | C4'-C3' | 5.32  | 1.58        | 1.53     |
| 1   | AA    | 602  | A    | C5-C4   | 5.32  | 1.42        | 1.38     |
| 1   | AA    | 758  | C    | C4'-O4' | -5.32 | 1.38        | 1.45     |
| 1   | AA    | 838  | G    | C2'-C1' | -5.32 | 1.47        | 1.53     |
| 1   | AA    | 1312 | G    | N9-C8   | -5.32 | 1.34        | 1.37     |
| 35  | BB    | 1223 | G    | C8-N7   | 5.32  | 1.34        | 1.30     |
| 35  | BB    | 1500 | G    | C5-C6   | -5.32 | 1.37        | 1.42     |
| 35  | BB    | 1500 | G    | C4'-O4' | 5.32  | 1.52        | 1.45     |
| 35  | BB    | 1750 | G    | N1-C2   | 5.32  | 1.42        | 1.37     |
| 35  | BB    | 1862 | G    | N7-C5   | -5.32 | 1.36        | 1.39     |
| 35  | BB    | 2365 | G    | C2'-C1' | -5.32 | 1.47        | 1.53     |
| 35  | BB    | 2516 | A    | N7-C5   | -5.32 | 1.36        | 1.39     |
| 47  | BN    | 46   | ARG  | CZ-NH1  | 5.32  | 1.40        | 1.33     |
| 1   | AA    | 22   | G    | P-O5'   | 5.32  | 1.65        | 1.59     |
| 1   | AA    | 177  | G    | C5-C6   | -5.32 | 1.37        | 1.42     |
| 1   | AA    | 633  | G    | C2-N2   | 5.32  | 1.39        | 1.34     |
| 1   | AA    | 637  | C    | C3'-O3' | 5.32  | 1.49        | 1.42     |
| 1   | AA    | 1258 | G    | C5-C6   | -5.32 | 1.37        | 1.42     |
| 1   | AA    | 1298 | U    | N1-C2   | 5.32  | 1.43        | 1.38     |
| 35  | BB    | 306  | U    | C4'-C3' | -5.32 | 1.47        | 1.52     |
| 35  | BB    | 1345 | C    | C3'-C2' | -5.32 | 1.47        | 1.52     |
| 35  | BB    | 1976 | U    | O3'-P   | -5.32 | 1.54        | 1.61     |
| 35  | BB    | 2334 | U    | P-O5'   | -5.32 | 1.54        | 1.59     |
| 35  | BB    | 2452 | C    | C4'-C3' | 5.32  | 1.58        | 1.53     |
| 35  | BB    | 2673 | G    | C3'-C2' | 5.32  | 1.58        | 1.52     |
| 35  | BB    | 2692 | G    | O5'-C5' | 5.32  | 1.52        | 1.44     |
| 35  | BB    | 2767 | C    | N3-C4   | 5.32  | 1.37        | 1.33     |
| 1   | AA    | 338  | A    | C3'-C2' | -5.31 | 1.47        | 1.52     |
| 1   | AA    | 923  | A    | O3'-P   | -5.31 | 1.54        | 1.61     |
| 1   | AA    | 1305 | G    | C5'-C4' | 5.31  | 1.57        | 1.51     |
| 34  | BA    | 96   | G    | N1-C2   | 5.31  | 1.42        | 1.37     |
| 35  | BB    | 882  | G    | N3-C4   | -5.31 | 1.31        | 1.35     |
| 35  | BB    | 2020 | A    | N1-C2   | 5.31  | 1.39        | 1.34     |
| 35  | BB    | 2108 | A    | C2'-C1' | 5.31  | 1.59        | 1.53     |
| 35  | BB    | 2875 | C    | C2'-C1' | -5.31 | 1.47        | 1.53     |
| 1   | AA    | 513  | C    | C2-N3   | 5.31  | 1.40        | 1.35     |
| 1   | AA    | 645  | G    | C3'-O3' | 5.31  | 1.49        | 1.42     |
| 1   | AA    | 933  | G    | C5-C4   | 5.31  | 1.42        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 185  | G    | N9-C8   | 5.31  | 1.41        | 1.37     |
| 35  | BB    | 1228 | G    | C2-N3   | 5.31  | 1.37        | 1.32     |
| 35  | BB    | 1774 | C    | C4-N4   | 5.31  | 1.38        | 1.33     |
| 35  | BB    | 1889 | A    | C2-N3   | 5.31  | 1.38        | 1.33     |
| 35  | BB    | 1910 | G    | N1-C2   | 5.31  | 1.42        | 1.37     |
| 35  | BB    | 2048 | G    | N9-C4   | 5.31  | 1.42        | 1.38     |
| 35  | BB    | 2676 | C    | C4-N4   | 5.31  | 1.38        | 1.33     |
| 46  | BM    | 51   | ARG  | NE-CZ   | 5.31  | 1.40        | 1.33     |
| 1   | AA    | 920  | U    | P-O5'   | -5.31 | 1.54        | 1.59     |
| 35  | BB    | 644  | A    | P-O5'   | 5.31  | 1.65        | 1.59     |
| 35  | BB    | 742  | A    | O4'-C1' | 5.31  | 1.48        | 1.41     |
| 35  | BB    | 783  | A    | N3-C4   | -5.31 | 1.31        | 1.34     |
| 35  | BB    | 1226 | A    | P-O5'   | -5.31 | 1.54        | 1.59     |
| 35  | BB    | 2781 | A    | O3'-P   | -5.31 | 1.54        | 1.61     |
| 1   | AA    | 633  | G    | C2'-C1' | -5.31 | 1.47        | 1.53     |
| 1   | AA    | 852  | G    | C5-C6   | -5.31 | 1.37        | 1.42     |
| 1   | AA    | 1217 | C    | P-O5'   | -5.31 | 1.54        | 1.59     |
| 1   | AA    | 1288 | A    | N3-C4   | 5.31  | 1.38        | 1.34     |
| 1   | AA    | 1403 | C    | C2'-C1' | -5.31 | 1.47        | 1.53     |
| 3   | AC    | 129  | PHE  | CG-CD2  | 5.31  | 1.46        | 1.38     |
| 22  | AV    | 37   | G    | C2'-C1' | -5.31 | 1.47        | 1.53     |
| 25  | B0    | 26   | ARG  | NE-CZ   | 5.31  | 1.40        | 1.33     |
| 35  | BB    | 68   | G    | N9-C4   | 5.31  | 1.42        | 1.38     |
| 35  | BB    | 387  | U    | C4-C5   | 5.31  | 1.48        | 1.43     |
| 35  | BB    | 957  | C    | C2'-C1' | -5.31 | 1.47        | 1.53     |
| 35  | BB    | 1611 | C    | N1-C2   | 5.31  | 1.45        | 1.40     |
| 35  | BB    | 1621 | U    | C4-C5   | 5.31  | 1.48        | 1.43     |
| 35  | BB    | 1629 | U    | C5-C6   | 5.31  | 1.39        | 1.34     |
| 35  | BB    | 2401 | U    | N1-C6   | 5.31  | 1.42        | 1.38     |
| 35  | BB    | 2722 | G    | C6-O6   | -5.31 | 1.19        | 1.24     |
| 39  | BF    | 6    | TYR  | CE2-CZ  | 5.31  | 1.45        | 1.38     |
| 1   | AA    | 89   | U    | C5'-C4' | 5.31  | 1.57        | 1.51     |
| 1   | AA    | 1070 | U    | C2-N3   | -5.31 | 1.34        | 1.37     |
| 1   | AA    | 1087 | G    | C5-C4   | 5.31  | 1.42        | 1.38     |
| 1   | AA    | 1100 | C    | C4'-O4' | 5.31  | 1.52        | 1.45     |
| 1   | AA    | 1249 | C    | C5'-C4' | 5.31  | 1.57        | 1.51     |
| 35  | BB    | 94   | A    | O3'-P   | -5.31 | 1.54        | 1.61     |
| 35  | BB    | 511  | U    | O4'-C1' | 5.31  | 1.48        | 1.41     |
| 35  | BB    | 733  | G    | C3'-O3' | 5.31  | 1.49        | 1.42     |
| 35  | BB    | 1346 | G    | C2-N3   | 5.31  | 1.36        | 1.32     |
| 35  | BB    | 1487 | U    | C5'-C4' | 5.31  | 1.57        | 1.51     |
| 35  | BB    | 1718 | G    | N1-C2   | 5.31  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2417 | C    | C3'-O3' | 5.31  | 1.49        | 1.42     |
| 35  | BB    | 2486 | C    | N3-C4   | 5.31  | 1.37        | 1.33     |
| 35  | BB    | 2497 | A    | N3-C4   | -5.31 | 1.31        | 1.34     |
| 10  | AJ    | 45   | ARG  | CD-NE   | 5.31  | 1.55        | 1.46     |
| 35  | BB    | 1368 | G    | C6-N1   | 5.31  | 1.43        | 1.39     |
| 35  | BB    | 1972 | G    | C8-N7   | -5.31 | 1.27        | 1.30     |
| 35  | BB    | 2470 | G    | O3'-P   | -5.31 | 1.54        | 1.61     |
| 1   | AA    | 222  | C    | C5-C6   | 5.30  | 1.38        | 1.34     |
| 1   | AA    | 790  | A    | N9-C4   | -5.30 | 1.34        | 1.37     |
| 1   | AA    | 1072 | G    | C2-N2   | -5.30 | 1.29        | 1.34     |
| 30  | B5    | 180  | PHE  | CB-CG   | 5.30  | 1.60        | 1.51     |
| 34  | BA    | 18   | G    | N7-C5   | -5.30 | 1.36        | 1.39     |
| 34  | BA    | 107  | G    | C6-N1   | 5.30  | 1.43        | 1.39     |
| 34  | BA    | 110  | C    | C2-N3   | 5.30  | 1.40        | 1.35     |
| 34  | BA    | 117  | G    | N9-C8   | 5.30  | 1.41        | 1.37     |
| 35  | BB    | 1809 | A    | C2-N3   | 5.30  | 1.38        | 1.33     |
| 35  | BB    | 1872 | A    | C5-C4   | 5.30  | 1.42        | 1.38     |
| 35  | BB    | 1902 | C    | N1-C2   | -5.30 | 1.34        | 1.40     |
| 35  | BB    | 1983 | G    | N3-C4   | 5.30  | 1.39        | 1.35     |
| 35  | BB    | 2050 | C    | O4'-C1' | -5.30 | 1.34        | 1.41     |
| 35  | BB    | 2116 | G    | C6-N1   | 5.30  | 1.43        | 1.39     |
| 35  | BB    | 2703 | C    | C2'-C1' | 5.30  | 1.59        | 1.53     |
| 35  | BB    | 2716 | C    | N1-C6   | -5.30 | 1.33        | 1.37     |
| 51  | BR    | 80   | ARG  | CZ-NH1  | 5.30  | 1.40        | 1.33     |
| 1   | AA    | 77   | A    | C5-C4   | -5.30 | 1.35        | 1.38     |
| 1   | AA    | 358  | U    | C3'-C2' | 5.30  | 1.58        | 1.52     |
| 1   | AA    | 1200 | C    | C4'-C3' | 5.30  | 1.58        | 1.53     |
| 1   | AA    | 1334 | G    | N9-C4   | 5.30  | 1.42        | 1.38     |
| 35  | BB    | 255  | A    | C2'-C1' | -5.30 | 1.47        | 1.53     |
| 35  | BB    | 1038 | G    | C5-C4   | 5.30  | 1.42        | 1.38     |
| 35  | BB    | 1908 | C    | N1-C6   | 5.30  | 1.40        | 1.37     |
| 35  | BB    | 2524 | G    | O3'-P   | -5.30 | 1.54        | 1.61     |
| 35  | BB    | 2665 | A    | C6-N1   | 5.30  | 1.39        | 1.35     |
| 1   | AA    | 196  | A    | N9-C8   | -5.30 | 1.33        | 1.37     |
| 1   | AA    | 413  | G    | O4'-C1' | -5.30 | 1.34        | 1.41     |
| 1   | AA    | 742  | G    | C5'-C4' | 5.30  | 1.57        | 1.51     |
| 1   | AA    | 919  | A    | C5-C6   | -5.30 | 1.36        | 1.41     |
| 1   | AA    | 938  | A    | N9-C4   | -5.30 | 1.34        | 1.37     |
| 35  | BB    | 50   | U    | C2'-C1' | -5.30 | 1.47        | 1.53     |
| 35  | BB    | 342  | A    | C5-C4   | -5.30 | 1.35        | 1.38     |
| 35  | BB    | 500  | G    | P-O5'   | -5.30 | 1.54        | 1.59     |
| 35  | BB    | 870  | U    | C1'-N1  | 5.30  | 1.56        | 1.48     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1698 | A    | C8-N7   | -5.30 | 1.27        | 1.31     |
| 35  | BB    | 2016 | U    | O3'-P   | -5.30 | 1.54        | 1.61     |
| 35  | BB    | 2732 | G    | C6-O6   | -5.30 | 1.19        | 1.24     |
| 55  | BW    | 12   | GLN  | C-N     | 5.30  | 1.42        | 1.33     |
| 1   | AA    | 196  | A    | C6-N6   | 5.30  | 1.38        | 1.33     |
| 1   | AA    | 219  | U    | C4-O4   | 5.30  | 1.27        | 1.23     |
| 6   | AF    | 5    | GLU  | CB-CG   | 5.30  | 1.62        | 1.52     |
| 35  | BB    | 9    | G    | P-O5'   | -5.30 | 1.54        | 1.59     |
| 35  | BB    | 206  | U    | C2-N3   | 5.30  | 1.41        | 1.37     |
| 35  | BB    | 273  | G    | C8-N7   | -5.30 | 1.27        | 1.30     |
| 35  | BB    | 738  | G    | C3'-C2' | 5.30  | 1.58        | 1.52     |
| 35  | BB    | 823  | C    | N1-C2   | 5.30  | 1.45        | 1.40     |
| 35  | BB    | 1185 | G    | C8-N7   | -5.30 | 1.27        | 1.30     |
| 35  | BB    | 1215 | G    | C5-C4   | -5.30 | 1.34        | 1.38     |
| 35  | BB    | 2855 | C    | C4-N4   | 5.30  | 1.38        | 1.33     |
| 1   | AA    | 398  | U    | P-O5'   | -5.30 | 1.54        | 1.59     |
| 1   | AA    | 413  | G    | C2'-O2' | -5.30 | 1.34        | 1.41     |
| 1   | AA    | 689  | C    | N3-C4   | 5.30  | 1.37        | 1.33     |
| 1   | AA    | 1093 | A    | C4'-O4' | -5.30 | 1.38        | 1.45     |
| 35  | BB    | 734  | A    | N7-C5   | -5.30 | 1.36        | 1.39     |
| 35  | BB    | 793  | A    | N9-C8   | 5.30  | 1.42        | 1.37     |
| 35  | BB    | 1038 | G    | N9-C4   | 5.30  | 1.42        | 1.38     |
| 35  | BB    | 1482 | G    | C6-N1   | 5.30  | 1.43        | 1.39     |
| 35  | BB    | 1881 | C    | N1-C6   | -5.30 | 1.33        | 1.37     |
| 1   | AA    | 1328 | C    | N3-C4   | -5.30 | 1.30        | 1.33     |
| 5   | AE    | 81   | GLN  | CA-CB   | 5.30  | 1.65        | 1.53     |
| 13  | AM    | 100  | ARG  | CZ-NH2  | 5.30  | 1.40        | 1.33     |
| 35  | BB    | 1174 | U    | C4-O4   | 5.30  | 1.27        | 1.23     |
| 35  | BB    | 2081 | U    | C2-N3   | 5.30  | 1.41        | 1.37     |
| 35  | BB    | 2197 | U    | N3-C4   | 5.30  | 1.43        | 1.38     |
| 35  | BB    | 2263 | C    | O3'-P   | -5.30 | 1.54        | 1.61     |
| 35  | BB    | 2412 | A    | C3'-C2' | -5.30 | 1.47        | 1.52     |
| 1   | AA    | 64   | G    | C8-N7   | -5.29 | 1.27        | 1.30     |
| 1   | AA    | 152  | A    | C5'-C4' | 5.29  | 1.57        | 1.51     |
| 1   | AA    | 701  | U    | C3'-C2' | 5.29  | 1.58        | 1.52     |
| 1   | AA    | 933  | G    | N7-C5   | -5.29 | 1.36        | 1.39     |
| 35  | BB    | 886  | A    | C3'-C2' | -5.29 | 1.47        | 1.52     |
| 35  | BB    | 1393 | A    | O3'-P   | -5.29 | 1.54        | 1.61     |
| 35  | BB    | 1532 | A    | C2'-C1' | -5.29 | 1.47        | 1.53     |
| 35  | BB    | 2214 | C    | N1-C6   | 5.29  | 1.40        | 1.37     |
| 35  | BB    | 2564 | A    | C3'-O3' | 5.29  | 1.49        | 1.42     |
| 36  | BC    | 86   | ARG  | CD-NE   | 5.29  | 1.55        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 323  | U    | C2'-C1' | 5.29  | 1.59        | 1.53     |
| 1   | AA    | 557  | G    | C2'-C1' | -5.29 | 1.47        | 1.53     |
| 1   | AA    | 823  | C    | C2'-C1' | -5.29 | 1.47        | 1.53     |
| 35  | BB    | 659  | G    | N3-C4   | 5.29  | 1.39        | 1.35     |
| 35  | BB    | 1189 | A    | N1-C2   | 5.29  | 1.39        | 1.34     |
| 35  | BB    | 1525 | A    | N9-C4   | -5.29 | 1.34        | 1.37     |
| 35  | BB    | 1670 | C    | C5-C6   | -5.29 | 1.30        | 1.34     |
| 35  | BB    | 1692 | U    | C2-N3   | 5.29  | 1.41        | 1.37     |
| 35  | BB    | 1963 | U    | P-O5'   | -5.29 | 1.54        | 1.59     |
| 35  | BB    | 2238 | G    | C2'-C1' | -5.29 | 1.47        | 1.53     |
| 35  | BB    | 2308 | G    | C2-N2   | 5.29  | 1.39        | 1.34     |
| 35  | BB    | 2403 | C    | C4'-O4' | -5.29 | 1.38        | 1.45     |
| 1   | AA    | 377  | G    | N1-C2   | 5.29  | 1.42        | 1.37     |
| 1   | AA    | 1041 | G    | C3'-C2' | 5.29  | 1.58        | 1.52     |
| 1   | AA    | 1246 | A    | C2'-C1' | -5.29 | 1.47        | 1.53     |
| 1   | AA    | 1498 | U    | C4-O4   | -5.29 | 1.19        | 1.23     |
| 35  | BB    | 190  | A    | C2'-C1' | 5.29  | 1.59        | 1.53     |
| 35  | BB    | 532  | A    | N1-C2   | 5.29  | 1.39        | 1.34     |
| 35  | BB    | 905  | A    | C2'-C1' | -5.29 | 1.47        | 1.53     |
| 35  | BB    | 1137 | G    | N7-C5   | -5.29 | 1.36        | 1.39     |
| 35  | BB    | 1223 | G    | C4'-O4' | 5.29  | 1.52        | 1.45     |
| 35  | BB    | 1230 | A    | C3'-O3' | 5.29  | 1.49        | 1.42     |
| 35  | BB    | 1642 | G    | C2-N2   | 5.29  | 1.39        | 1.34     |
| 35  | BB    | 1963 | U    | C4'-O4' | -5.29 | 1.38        | 1.45     |
| 35  | BB    | 2773 | C    | C4'-O4' | 5.29  | 1.52        | 1.45     |
| 1   | AA    | 203  | G    | C5-C4   | 5.29  | 1.42        | 1.38     |
| 1   | AA    | 221  | C    | N3-C4   | 5.29  | 1.37        | 1.33     |
| 1   | AA    | 328  | C    | C5'-C4' | 5.29  | 1.57        | 1.51     |
| 1   | AA    | 543  | U    | C2-N3   | 5.29  | 1.41        | 1.37     |
| 1   | AA    | 625  | U    | C4-O4   | 5.29  | 1.27        | 1.23     |
| 1   | AA    | 641  | U    | O3'-P   | -5.29 | 1.54        | 1.61     |
| 35  | BB    | 1335 | C    | C4-N4   | 5.29  | 1.38        | 1.33     |
| 35  | BB    | 1818 | U    | O3'-P   | -5.29 | 1.54        | 1.61     |
| 35  | BB    | 1961 | C    | N1-C6   | -5.29 | 1.33        | 1.37     |
| 1   | AA    | 77   | A    | C6-N1   | 5.29  | 1.39        | 1.35     |
| 1   | AA    | 648  | A    | N7-C5   | -5.29 | 1.36        | 1.39     |
| 1   | AA    | 1281 | C    | C5'-C4' | 5.29  | 1.57        | 1.51     |
| 35  | BB    | 1069 | A    | C6-N6   | 5.29  | 1.38        | 1.33     |
| 35  | BB    | 1514 | G    | N9-C8   | 5.29  | 1.41        | 1.37     |
| 35  | BB    | 1726 | C    | C3'-C2' | -5.29 | 1.47        | 1.52     |
| 35  | BB    | 2090 | A    | C2-N3   | -5.29 | 1.28        | 1.33     |
| 35  | BB    | 2101 | A    | C2'-C1' | -5.29 | 1.47        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2865 | U    | P-O5'   | -5.29 | 1.54        | 1.59     |
| 48  | BO    | 25   | ARG  | CZ-NH2  | 5.29  | 1.40        | 1.33     |
| 55  | BW    | 5    | ASN  | CB-CG   | 5.29  | 1.63        | 1.51     |
| 1   | AA    | 304  | U    | O3'-P   | -5.29 | 1.54        | 1.61     |
| 1   | AA    | 1204 | A    | N7-C5   | -5.29 | 1.36        | 1.39     |
| 1   | AA    | 1246 | A    | C5'-C4' | 5.29  | 1.57        | 1.51     |
| 35  | BB    | 508  | A    | C6-N1   | 5.29  | 1.39        | 1.35     |
| 35  | BB    | 559  | G    | N1-C2   | 5.29  | 1.42        | 1.37     |
| 35  | BB    | 1442 | U    | C4'-C3' | -5.29 | 1.47        | 1.52     |
| 35  | BB    | 2643 | G    | C8-N7   | -5.29 | 1.27        | 1.30     |
| 1   | AA    | 260  | G    | C3'-O3' | 5.29  | 1.49        | 1.42     |
| 1   | AA    | 630  | A    | C2'-O2' | 5.29  | 1.48        | 1.41     |
| 1   | AA    | 635  | A    | C1'-N9  | -5.29 | 1.39        | 1.46     |
| 1   | AA    | 824  | G    | N9-C8   | 5.29  | 1.41        | 1.37     |
| 13  | AM    | 70   | ARG  | CD-NE   | 5.29  | 1.55        | 1.46     |
| 34  | BA    | 89   | U    | N1-C2   | 5.29  | 1.43        | 1.38     |
| 35  | BB    | 1147 | A    | C6-N6   | 5.29  | 1.38        | 1.33     |
| 35  | BB    | 1430 | G    | C4'-O4' | 5.29  | 1.52        | 1.45     |
| 35  | BB    | 1452 | G    | O4'-C1' | -5.29 | 1.34        | 1.41     |
| 35  | BB    | 2000 | C    | C4'-C3' | 5.29  | 1.58        | 1.53     |
| 35  | BB    | 2255 | G    | N1-C2   | 5.29  | 1.42        | 1.37     |
| 1   | AA    | 645  | G    | C5-C4   | -5.28 | 1.34        | 1.38     |
| 1   | AA    | 825  | A    | C6-N1   | 5.28  | 1.39        | 1.35     |
| 3   | AC    | 154  | GLY  | N-CA    | -5.28 | 1.38        | 1.46     |
| 35  | BB    | 60   | G    | C5'-C4' | 5.28  | 1.57        | 1.51     |
| 35  | BB    | 219  | A    | C2-N3   | 5.28  | 1.38        | 1.33     |
| 35  | BB    | 327  | G    | C4'-O4' | -5.28 | 1.38        | 1.45     |
| 35  | BB    | 506  | G    | N1-C2   | 5.28  | 1.42        | 1.37     |
| 35  | BB    | 630  | G    | C6-O6   | -5.28 | 1.19        | 1.24     |
| 35  | BB    | 1036 | G    | O3'-P   | -5.28 | 1.54        | 1.61     |
| 35  | BB    | 1164 | C    | C3'-C2' | -5.28 | 1.47        | 1.52     |
| 35  | BB    | 1270 | C    | C5'-C4' | 5.28  | 1.57        | 1.51     |
| 35  | BB    | 2852 | G    | N7-C5   | -5.28 | 1.36        | 1.39     |
| 41  | BH    | 137  | GLU  | CD-OE1  | 5.28  | 1.31        | 1.25     |
| 52  | BS    | 5    | ALA  | CA-C    | -5.28 | 1.39        | 1.52     |
| 1   | AA    | 226  | G    | C4'-C3' | -5.28 | 1.47        | 1.52     |
| 35  | BB    | 2307 | G    | N1-C2   | 5.28  | 1.42        | 1.37     |
| 1   | AA    | 226  | G    | N3-C4   | 5.28  | 1.39        | 1.35     |
| 1   | AA    | 1153 | G    | N9-C8   | 5.28  | 1.41        | 1.37     |
| 1   | AA    | 1209 | C    | C4-N4   | 5.28  | 1.38        | 1.33     |
| 35  | BB    | 86   | G    | C5-C6   | -5.28 | 1.37        | 1.42     |
| 35  | BB    | 314  | C    | N1-C6   | 5.28  | 1.40        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 455  | C    | P-O5'   | -5.28 | 1.54        | 1.59     |
| 35  | BB    | 1167 | C    | C2'-C1' | -5.28 | 1.47        | 1.53     |
| 35  | BB    | 1345 | C    | C4-N4   | 5.28  | 1.38        | 1.33     |
| 35  | BB    | 1521 | G    | C1'-N9  | 5.28  | 1.56        | 1.48     |
| 35  | BB    | 1543 | G    | C5-C4   | 5.28  | 1.42        | 1.38     |
| 35  | BB    | 1554 | U    | O3'-P   | -5.28 | 1.54        | 1.61     |
| 35  | BB    | 1659 | G    | C5'-C4' | 5.28  | 1.57        | 1.51     |
| 35  | BB    | 1881 | C    | N3-C4   | 5.28  | 1.37        | 1.33     |
| 35  | BB    | 1964 | G    | N1-C2   | 5.28  | 1.42        | 1.37     |
| 35  | BB    | 2048 | G    | N3-C4   | -5.28 | 1.31        | 1.35     |
| 1   | AA    | 1060 | U    | N1-C2   | -5.28 | 1.33        | 1.38     |
| 35  | BB    | 842  | U    | P-O5'   | -5.28 | 1.54        | 1.59     |
| 35  | BB    | 1125 | G    | N7-C5   | -5.28 | 1.36        | 1.39     |
| 35  | BB    | 1280 | G    | C6-O6   | 5.28  | 1.28        | 1.24     |
| 35  | BB    | 1835 | G    | P-O5'   | -5.28 | 1.54        | 1.59     |
| 40  | BG    | 163  | TYR  | CB-CG   | -5.28 | 1.43        | 1.51     |
| 1   | AA    | 455  | G    | C2-N3   | 5.28  | 1.36        | 1.32     |
| 1   | AA    | 1294 | G    | C2-N3   | 5.28  | 1.36        | 1.32     |
| 1   | AA    | 1331 | G    | N9-C8   | -5.28 | 1.34        | 1.37     |
| 1   | AA    | 1502 | A    | N9-C4   | -5.28 | 1.34        | 1.37     |
| 25  | B0    | 77   | TYR  | CG-CD2  | 5.28  | 1.46        | 1.39     |
| 35  | BB    | 139  | U    | C4'-C3' | 5.28  | 1.58        | 1.53     |
| 35  | BB    | 1255 | U    | C3'-C2' | 5.28  | 1.58        | 1.52     |
| 35  | BB    | 1360 | G    | O3'-P   | -5.28 | 1.54        | 1.61     |
| 35  | BB    | 1821 | A    | C6-N1   | -5.28 | 1.31        | 1.35     |
| 35  | BB    | 1844 | C    | C4'-O4' | -5.28 | 1.38        | 1.45     |
| 1   | AA    | 372  | C    | C3'-C2' | 5.28  | 1.58        | 1.52     |
| 1   | AA    | 915  | A    | C2'-C1' | 5.28  | 1.59        | 1.53     |
| 35  | BB    | 110  | G    | C2-N3   | 5.28  | 1.36        | 1.32     |
| 35  | BB    | 474  | G    | C2-N3   | 5.28  | 1.36        | 1.32     |
| 35  | BB    | 520  | G    | C3'-O3' | 5.28  | 1.49        | 1.42     |
| 35  | BB    | 1354 | A    | C5'-C4' | 5.28  | 1.57        | 1.51     |
| 35  | BB    | 2241 | A    | C6-N6   | 5.28  | 1.38        | 1.33     |
| 35  | BB    | 2638 | G    | C5-C4   | 5.28  | 1.42        | 1.38     |
| 35  | BB    | 2856 | A    | C6-N6   | 5.28  | 1.38        | 1.33     |
| 1   | AA    | 595  | A    | C4'-O4' | -5.27 | 1.38        | 1.45     |
| 1   | AA    | 673  | A    | C8-N7   | -5.27 | 1.27        | 1.31     |
| 35  | BB    | 117  | G    | C5-C6   | -5.27 | 1.37        | 1.42     |
| 35  | BB    | 1848 | A    | C6-N6   | 5.27  | 1.38        | 1.33     |
| 35  | BB    | 2810 | A    | C2'-C1' | -5.27 | 1.47        | 1.53     |
| 1   | AA    | 445  | G    | C2-N2   | 5.27  | 1.39        | 1.34     |
| 10  | AJ    | 31   | ARG  | CZ-NH1  | 5.27  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34  | BA    | 19   | C    | C4-C5   | -5.27 | 1.38        | 1.43     |
| 34  | BA    | 96   | G    | C2'-C1' | -5.27 | 1.47        | 1.53     |
| 35  | BB    | 251  | A    | C2-N3   | 5.27  | 1.38        | 1.33     |
| 35  | BB    | 459  | U    | C4'-C3' | -5.27 | 1.47        | 1.52     |
| 35  | BB    | 538  | A    | N9-C8   | -5.27 | 1.33        | 1.37     |
| 35  | BB    | 942  | G    | C2'-C1' | -5.27 | 1.47        | 1.53     |
| 35  | BB    | 1011 | G    | N7-C5   | -5.27 | 1.36        | 1.39     |
| 35  | BB    | 1014 | A    | N3-C4   | -5.27 | 1.31        | 1.34     |
| 35  | BB    | 1178 | C    | N3-C4   | 5.27  | 1.37        | 1.33     |
| 35  | BB    | 1741 | C    | C3'-O3' | 5.27  | 1.49        | 1.42     |
| 35  | BB    | 1902 | C    | C4'-C3' | 5.27  | 1.58        | 1.53     |
| 35  | BB    | 2146 | C    | C3'-C2' | 5.27  | 1.58        | 1.52     |
| 48  | BO    | 55   | GLU  | CD-OE2  | -5.27 | 1.19        | 1.25     |
| 1   | AA    | 1401 | G    | N3-C4   | 5.27  | 1.39        | 1.35     |
| 35  | BB    | 743  | A    | C6-N6   | 5.27  | 1.38        | 1.33     |
| 35  | BB    | 1082 | U    | C4'-C3' | -5.27 | 1.47        | 1.52     |
| 35  | BB    | 1303 | G    | C3'-C2' | -5.27 | 1.47        | 1.52     |
| 37  | BD    | 183  | GLU  | CD-OE2  | -5.27 | 1.19        | 1.25     |
| 1   | AA    | 488  | C    | N3-C4   | 5.27  | 1.37        | 1.33     |
| 1   | AA    | 498  | A    | C6-N1   | 5.27  | 1.39        | 1.35     |
| 1   | AA    | 836  | G    | C6-O6   | 5.27  | 1.28        | 1.24     |
| 35  | BB    | 51   | G    | N1-C2   | 5.27  | 1.42        | 1.37     |
| 35  | BB    | 364  | C    | N1-C6   | 5.27  | 1.40        | 1.37     |
| 35  | BB    | 981  | A    | N3-C4   | 5.27  | 1.38        | 1.34     |
| 35  | BB    | 1663 | G    | C5-C4   | 5.27  | 1.42        | 1.38     |
| 35  | BB    | 1918 | A    | C2'-C1' | -5.27 | 1.47        | 1.53     |
| 35  | BB    | 2532 | G    | C4'-C3' | 5.27  | 1.58        | 1.53     |
| 35  | BB    | 2566 | A    | N1-C2   | 5.27  | 1.39        | 1.34     |
| 1   | AA    | 161  | A    | C5-C4   | 5.27  | 1.42        | 1.38     |
| 1   | AA    | 557  | G    | C2'-O2' | 5.27  | 1.48        | 1.41     |
| 1   | AA    | 988  | G    | N1-C2   | 5.27  | 1.42        | 1.37     |
| 1   | AA    | 1342 | C    | N1-C6   | 5.27  | 1.40        | 1.37     |
| 1   | AA    | 1379 | G    | C4'-O4' | 5.27  | 1.52        | 1.45     |
| 1   | AA    | 1411 | C    | C2-N3   | 5.27  | 1.40        | 1.35     |
| 1   | AA    | 1436 | U    | C5'-C4' | 5.27  | 1.57        | 1.51     |
| 9   | AI    | 19   | PHE  | CB-CG   | -5.27 | 1.42        | 1.51     |
| 12  | AL    | 82   | ARG  | CD-NE   | 5.27  | 1.55        | 1.46     |
| 34  | BA    | 112  | G    | P-O5'   | -5.27 | 1.54        | 1.59     |
| 35  | BB    | 176  | A    | N9-C4   | -5.27 | 1.34        | 1.37     |
| 35  | BB    | 286  | U    | O3'-P   | -5.27 | 1.54        | 1.61     |
| 35  | BB    | 488  | G    | C8-N7   | -5.27 | 1.27        | 1.30     |
| 35  | BB    | 675  | A    | O4'-C1' | 5.27  | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 960  | A    | C5-C4   | 5.27  | 1.42        | 1.38     |
| 35  | BB    | 1002 | G    | C8-N7   | 5.27  | 1.34        | 1.30     |
| 35  | BB    | 1515 | A    | C6-N1   | 5.27  | 1.39        | 1.35     |
| 35  | BB    | 2782 | G    | N1-C2   | 5.27  | 1.42        | 1.37     |
| 1   | AA    | 326  | G    | N7-C5   | -5.27 | 1.36        | 1.39     |
| 35  | BB    | 24   | G    | N7-C5   | -5.27 | 1.36        | 1.39     |
| 35  | BB    | 321  | U    | C2'-C1' | -5.27 | 1.47        | 1.53     |
| 35  | BB    | 1220 | G    | C2-N2   | 5.27  | 1.39        | 1.34     |
| 35  | BB    | 1272 | A    | C3'-C2' | 5.27  | 1.58        | 1.52     |
| 35  | BB    | 1578 | U    | P-O5'   | 5.27  | 1.65        | 1.59     |
| 44  | BK    | 18   | ARG  | CD-NE   | 5.27  | 1.55        | 1.46     |
| 1   | AA    | 734  | G    | C6-O6   | -5.26 | 1.19        | 1.24     |
| 1   | AA    | 867  | G    | C2-N3   | 5.26  | 1.36        | 1.32     |
| 1   | AA    | 946  | A    | O4'-C1' | 5.26  | 1.48        | 1.41     |
| 1   | AA    | 968  | A    | N9-C4   | 5.26  | 1.41        | 1.37     |
| 1   | AA    | 1028 | C    | C2-O2   | -5.26 | 1.19        | 1.24     |
| 1   | AA    | 1079 | G    | C5-C6   | -5.26 | 1.37        | 1.42     |
| 1   | AA    | 1434 | A    | C3'-C2' | -5.26 | 1.47        | 1.52     |
| 26  | B1    | 5    | GLU  | CG-CD   | 5.26  | 1.59        | 1.51     |
| 35  | BB    | 997  | G    | C6-O6   | 5.26  | 1.28        | 1.24     |
| 35  | BB    | 2250 | G    | N1-C2   | 5.26  | 1.42        | 1.37     |
| 35  | BB    | 2611 | C    | C4'-C3' | 5.26  | 1.58        | 1.53     |
| 35  | BB    | 2839 | G    | C3'-C2' | 5.26  | 1.58        | 1.52     |
| 1   | AA    | 385  | C    | P-O5'   | -5.26 | 1.54        | 1.59     |
| 1   | AA    | 1318 | A    | C8-N7   | 5.26  | 1.35        | 1.31     |
| 34  | BA    | 51   | G    | N1-C2   | 5.26  | 1.42        | 1.37     |
| 35  | BB    | 1080 | A    | N9-C8   | -5.26 | 1.33        | 1.37     |
| 35  | BB    | 1565 | C    | N3-C4   | 5.26  | 1.37        | 1.33     |
| 35  | BB    | 1583 | A    | C4'-C3' | 5.26  | 1.58        | 1.53     |
| 35  | BB    | 2599 | G    | N7-C5   | 5.26  | 1.42        | 1.39     |
| 1   | AA    | 432  | A    | C6-N1   | 5.26  | 1.39        | 1.35     |
| 1   | AA    | 712  | A    | N3-C4   | -5.26 | 1.31        | 1.34     |
| 1   | AA    | 831  | A    | C5'-C4' | 5.26  | 1.57        | 1.51     |
| 35  | BB    | 350  | G    | C1'-N9  | 5.26  | 1.56        | 1.48     |
| 35  | BB    | 422  | A    | C2-N3   | 5.26  | 1.38        | 1.33     |
| 35  | BB    | 535  | G    | N7-C5   | -5.26 | 1.36        | 1.39     |
| 35  | BB    | 800  | A    | C5'-C4' | 5.26  | 1.57        | 1.51     |
| 35  | BB    | 861  | A    | N7-C5   | -5.26 | 1.36        | 1.39     |
| 35  | BB    | 1688 | U    | C5'-C4' | 5.26  | 1.57        | 1.51     |
| 35  | BB    | 2136 | G    | C2-N3   | 5.26  | 1.36        | 1.32     |
| 35  | BB    | 2491 | U    | C4-C5   | 5.26  | 1.48        | 1.43     |
| 35  | BB    | 2810 | A    | N9-C8   | 5.26  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 40  | BG    | 113  | ASP  | CB-CG   | 5.26  | 1.62        | 1.51     |
| 1   | AA    | 236  | A    | N3-C4   | -5.26 | 1.31        | 1.34     |
| 1   | AA    | 339  | C    | C3'-C2' | -5.26 | 1.47        | 1.52     |
| 1   | AA    | 615  | G    | N1-C2   | 5.26  | 1.42        | 1.37     |
| 1   | AA    | 725  | G    | C5'-C4' | 5.26  | 1.57        | 1.51     |
| 34  | BA    | 49   | C    | C2-N3   | 5.26  | 1.40        | 1.35     |
| 35  | BB    | 989  | G    | N3-C4   | -5.26 | 1.31        | 1.35     |
| 35  | BB    | 1160 | G    | C5'-C4' | 5.26  | 1.57        | 1.51     |
| 35  | BB    | 2409 | G    | C4'-C3' | -5.26 | 1.47        | 1.52     |
| 1   | AA    | 280  | C    | N1-C6   | 5.26  | 1.40        | 1.37     |
| 1   | AA    | 414  | A    | P-O5'   | -5.26 | 1.54        | 1.59     |
| 35  | BB    | 287  | G    | C3'-C2' | 5.26  | 1.58        | 1.52     |
| 35  | BB    | 1341 | G    | C8-N7   | -5.26 | 1.27        | 1.30     |
| 35  | BB    | 1923 | U    | C2-N3   | 5.26  | 1.41        | 1.37     |
| 35  | BB    | 2846 | G    | C3'-C2' | -5.26 | 1.47        | 1.52     |
| 1   | AA    | 460  | A    | C6-N1   | 5.26  | 1.39        | 1.35     |
| 1   | AA    | 768  | A    | C6-N1   | 5.26  | 1.39        | 1.35     |
| 1   | AA    | 771  | G    | N1-C2   | 5.26  | 1.42        | 1.37     |
| 1   | AA    | 857  | C    | C4-N4   | 5.26  | 1.38        | 1.33     |
| 1   | AA    | 1008 | U    | P-O5'   | -5.26 | 1.54        | 1.59     |
| 1   | AA    | 1147 | C    | C2-O2   | 5.26  | 1.29        | 1.24     |
| 9   | AI    | 102  | PHE  | CB-CG   | -5.26 | 1.42        | 1.51     |
| 34  | BA    | 114  | C    | N3-C4   | 5.26  | 1.37        | 1.33     |
| 35  | BB    | 51   | G    | N9-C8   | 5.26  | 1.41        | 1.37     |
| 35  | BB    | 155  | A    | C2'-C1' | -5.26 | 1.47        | 1.53     |
| 35  | BB    | 614  | A    | N9-C4   | -5.26 | 1.34        | 1.37     |
| 35  | BB    | 1048 | A    | N9-C4   | -5.26 | 1.34        | 1.37     |
| 35  | BB    | 1763 | G    | C2-N2   | 5.26  | 1.39        | 1.34     |
| 39  | BF    | 94   | ARG  | NE-CZ   | 5.26  | 1.39        | 1.33     |
| 1   | AA    | 315  | A    | N9-C8   | 5.25  | 1.42        | 1.37     |
| 1   | AA    | 533  | A    | C5-C4   | 5.25  | 1.42        | 1.38     |
| 1   | AA    | 553  | A    | C5-C4   | -5.25 | 1.35        | 1.38     |
| 1   | AA    | 803  | G    | N1-C2   | 5.25  | 1.42        | 1.37     |
| 1   | AA    | 963  | G    | O3'-P   | 5.25  | 1.67        | 1.61     |
| 35  | BB    | 20   | C    | C2-N3   | 5.25  | 1.40        | 1.35     |
| 35  | BB    | 691  | C    | C4-N4   | 5.25  | 1.38        | 1.33     |
| 35  | BB    | 1767 | G    | O3'-P   | -5.25 | 1.54        | 1.61     |
| 1   | AA    | 715  | A    | O4'-C1' | -5.25 | 1.34        | 1.41     |
| 34  | BA    | 51   | G    | C5-C4   | -5.25 | 1.34        | 1.38     |
| 34  | BA    | 104  | A    | C4'-C3' | 5.25  | 1.58        | 1.53     |
| 35  | BB    | 28   | A    | C5'-C4' | 5.25  | 1.57        | 1.51     |
| 35  | BB    | 949  | G    | C1'-N9  | -5.25 | 1.39        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1061 | U    | N3-C4   | 5.25  | 1.43        | 1.38     |
| 35  | BB    | 1726 | C    | N1-C6   | 5.25  | 1.40        | 1.37     |
| 35  | BB    | 1883 | U    | C2-N3   | 5.25  | 1.41        | 1.37     |
| 35  | BB    | 2868 | A    | N9-C8   | -5.25 | 1.33        | 1.37     |
| 1   | AA    | 665  | A    | N9-C4   | 5.25  | 1.41        | 1.37     |
| 1   | AA    | 714  | G    | N9-C8   | 5.25  | 1.41        | 1.37     |
| 1   | AA    | 1322 | C    | O4'-C1' | 5.25  | 1.48        | 1.41     |
| 35  | BB    | 1013 | C    | P-O5'   | 5.25  | 1.65        | 1.59     |
| 35  | BB    | 1991 | U    | C5-C6   | 5.25  | 1.38        | 1.34     |
| 35  | BB    | 2398 | U    | C4-C5   | -5.25 | 1.38        | 1.43     |
| 35  | BB    | 2485 | G    | C5'-C4' | 5.25  | 1.57        | 1.51     |
| 35  | BB    | 2569 | G    | P-O5'   | 5.25  | 1.65        | 1.59     |
| 35  | BB    | 2581 | G    | C6-N1   | 5.25  | 1.43        | 1.39     |
| 35  | BB    | 2856 | A    | C4'-C3' | -5.25 | 1.47        | 1.52     |
| 1   | AA    | 699  | C    | C2-N3   | 5.25  | 1.40        | 1.35     |
| 1   | AA    | 1379 | G    | O3'-P   | -5.25 | 1.54        | 1.61     |
| 1   | AA    | 1398 | A    | C4'-O4' | 5.25  | 1.52        | 1.45     |
| 35  | BB    | 168  | G    | O4'-C1' | -5.25 | 1.34        | 1.41     |
| 35  | BB    | 350  | G    | C6-N1   | 5.25  | 1.43        | 1.39     |
| 35  | BB    | 520  | G    | N7-C5   | -5.25 | 1.36        | 1.39     |
| 35  | BB    | 1067 | A    | C5-C6   | -5.25 | 1.36        | 1.41     |
| 35  | BB    | 1144 | A    | C5-C4   | 5.25  | 1.42        | 1.38     |
| 1   | AA    | 84   | U    | O3'-P   | -5.25 | 1.54        | 1.61     |
| 1   | AA    | 354  | G    | C5'-C4' | 5.25  | 1.57        | 1.51     |
| 1   | AA    | 746  | A    | C4'-C3' | -5.25 | 1.47        | 1.52     |
| 1   | AA    | 1143 | G    | C2-N3   | 5.25  | 1.36        | 1.32     |
| 1   | AA    | 1185 | G    | C5'-C4' | 5.25  | 1.57        | 1.51     |
| 34  | BA    | 117  | G    | C6-O6   | -5.25 | 1.19        | 1.24     |
| 35  | BB    | 23   | G    | N3-C4   | -5.25 | 1.31        | 1.35     |
| 35  | BB    | 292  | U    | O3'-P   | -5.25 | 1.54        | 1.61     |
| 35  | BB    | 658  | U    | C2'-C1' | -5.25 | 1.47        | 1.53     |
| 35  | BB    | 1337 | G    | N3-C4   | -5.25 | 1.31        | 1.35     |
| 35  | BB    | 1742 | U    | O3'-P   | -5.25 | 1.54        | 1.61     |
| 35  | BB    | 2050 | C    | P-O5'   | -5.25 | 1.54        | 1.59     |
| 35  | BB    | 2603 | G    | C2-N2   | 5.25  | 1.39        | 1.34     |
| 35  | BB    | 2700 | A    | N9-C8   | 5.25  | 1.42        | 1.37     |
| 35  | BB    | 2805 | C    | C4-C5   | 5.25  | 1.47        | 1.43     |
| 1   | AA    | 64   | G    | N7-C5   | -5.25 | 1.36        | 1.39     |
| 1   | AA    | 691  | G    | C4'-O4' | 5.25  | 1.52        | 1.45     |
| 35  | BB    | 17   | G    | O4'-C1' | 5.25  | 1.48        | 1.41     |
| 35  | BB    | 410  | G    | C2-N3   | 5.25  | 1.36        | 1.32     |
| 35  | BB    | 498  | G    | N9-C4   | 5.25  | 1.42        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 524  | G    | C5-C6   | -5.25 | 1.37        | 1.42     |
| 35  | BB    | 579  | G    | C5'-C4' | 5.25  | 1.57        | 1.51     |
| 35  | BB    | 793  | A    | C2'-O2' | -5.25 | 1.34        | 1.41     |
| 35  | BB    | 1173 | U    | C5'-C4' | 5.25  | 1.57        | 1.51     |
| 35  | BB    | 1244 | A    | C5'-C4' | 5.25  | 1.57        | 1.51     |
| 45  | BL    | 78   | ARG  | CZ-NH1  | 5.25  | 1.39        | 1.33     |
| 47  | BN    | 26   | GLY  | N-CA    | -5.25 | 1.38        | 1.46     |
| 1   | AA    | 593  | U    | C2-N3   | 5.25  | 1.41        | 1.37     |
| 1   | AA    | 866  | C    | C4-C5   | 5.25  | 1.47        | 1.43     |
| 1   | AA    | 869  | G    | N7-C5   | -5.25 | 1.36        | 1.39     |
| 1   | AA    | 928  | G    | C5-C6   | -5.25 | 1.37        | 1.42     |
| 35  | BB    | 1922 | G    | N9-C4   | -5.25 | 1.33        | 1.38     |
| 35  | BB    | 2782 | G    | N3-C4   | -5.25 | 1.31        | 1.35     |
| 1   | AA    | 20   | U    | N1-C6   | 5.24  | 1.42        | 1.38     |
| 1   | AA    | 1261 | A    | C4'-C3' | 5.24  | 1.58        | 1.53     |
| 1   | AA    | 1459 | G    | N7-C5   | -5.24 | 1.36        | 1.39     |
| 34  | BA    | 86   | G    | O3'-P   | -5.24 | 1.54        | 1.61     |
| 35  | BB    | 78   | U    | P-O5'   | -5.24 | 1.54        | 1.59     |
| 35  | BB    | 275  | C    | N3-C4   | 5.24  | 1.37        | 1.33     |
| 35  | BB    | 468  | G    | C2-N3   | 5.24  | 1.36        | 1.32     |
| 35  | BB    | 597  | G    | C2'-C1' | -5.24 | 1.47        | 1.53     |
| 35  | BB    | 816  | C    | C3'-O3' | 5.24  | 1.49        | 1.42     |
| 35  | BB    | 925  | A    | C5-C4   | 5.24  | 1.42        | 1.38     |
| 35  | BB    | 1494 | A    | N3-C4   | -5.24 | 1.31        | 1.34     |
| 35  | BB    | 1656 | C    | N3-C4   | 5.24  | 1.37        | 1.33     |
| 35  | BB    | 1832 | C    | N3-C4   | 5.24  | 1.37        | 1.33     |
| 35  | BB    | 1985 | C    | N1-C2   | 5.24  | 1.45        | 1.40     |
| 35  | BB    | 2010 | G    | C2-N3   | 5.24  | 1.36        | 1.32     |
| 35  | BB    | 2234 | G    | P-O5'   | -5.24 | 1.54        | 1.59     |
| 35  | BB    | 2562 | U    | C3'-O3' | 5.24  | 1.49        | 1.42     |
| 35  | BB    | 2602 | A    | C6-N1   | 5.24  | 1.39        | 1.35     |
| 35  | BB    | 2643 | G    | C2-N2   | 5.24  | 1.39        | 1.34     |
| 35  | BB    | 2872 | A    | N3-C4   | 5.24  | 1.38        | 1.34     |
| 1   | AA    | 90   | C    | C4-C5   | 5.24  | 1.47        | 1.43     |
| 1   | AA    | 200  | G    | P-O5'   | -5.24 | 1.54        | 1.59     |
| 1   | AA    | 459  | A    | N9-C4   | 5.24  | 1.41        | 1.37     |
| 1   | AA    | 983  | A    | P-O5'   | -5.24 | 1.54        | 1.59     |
| 35  | BB    | 157  | C    | C4-N4   | 5.24  | 1.38        | 1.33     |
| 35  | BB    | 1016 | G    | N1-C2   | 5.24  | 1.42        | 1.37     |
| 35  | BB    | 1357 | C    | C5'-C4' | 5.24  | 1.57        | 1.51     |
| 35  | BB    | 1619 | G    | C2'-C1' | -5.24 | 1.47        | 1.53     |
| 35  | BB    | 2119 | A    | C6-N6   | 5.24  | 1.38        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 666  | G    | N9-C4   | 5.24  | 1.42        | 1.38     |
| 1   | AA    | 693  | G    | P-O5'   | -5.24 | 1.54        | 1.59     |
| 1   | AA    | 756  | C    | C3'-C2' | 5.24  | 1.58        | 1.52     |
| 1   | AA    | 1334 | G    | P-O5'   | 5.24  | 1.65        | 1.59     |
| 4   | AD    | 25   | ARG  | CZ-NH2  | 5.24  | 1.39        | 1.33     |
| 35  | BB    | 245  | G    | N9-C4   | -5.24 | 1.33        | 1.38     |
| 35  | BB    | 358  | U    | C5'-C4' | 5.24  | 1.57        | 1.51     |
| 35  | BB    | 1037 | G    | N1-C2   | 5.24  | 1.42        | 1.37     |
| 35  | BB    | 1046 | A    | C2'-C1' | -5.24 | 1.47        | 1.53     |
| 35  | BB    | 1545 | A    | N3-C4   | -5.24 | 1.31        | 1.34     |
| 35  | BB    | 2147 | A    | N9-C8   | -5.24 | 1.33        | 1.37     |
| 35  | BB    | 2592 | G    | O4'-C1' | -5.24 | 1.34        | 1.41     |
| 1   | AA    | 281  | G    | C3'-C2' | 5.24  | 1.58        | 1.52     |
| 1   | AA    | 284  | C    | C2-N3   | 5.24  | 1.40        | 1.35     |
| 1   | AA    | 555  | U    | N1-C2   | 5.24  | 1.43        | 1.38     |
| 1   | AA    | 735  | C    | N1-C2   | 5.24  | 1.45        | 1.40     |
| 1   | AA    | 1110 | A    | C2-N3   | 5.24  | 1.38        | 1.33     |
| 1   | AA    | 1229 | A    | O4'-C1' | 5.24  | 1.48        | 1.41     |
| 1   | AA    | 1367 | C    | N1-C6   | 5.24  | 1.40        | 1.37     |
| 1   | AA    | 1401 | G    | C8-N7   | 5.24  | 1.34        | 1.30     |
| 35  | BB    | 615  | U    | C2-N3   | 5.24  | 1.41        | 1.37     |
| 35  | BB    | 962  | G    | N9-C4   | -5.24 | 1.33        | 1.38     |
| 35  | BB    | 1267 | U    | P-O5'   | -5.24 | 1.54        | 1.59     |
| 35  | BB    | 1278 | C    | C4-C5   | -5.24 | 1.38        | 1.43     |
| 35  | BB    | 1338 | G    | C2-N3   | 5.24  | 1.36        | 1.32     |
| 35  | BB    | 2127 | G    | C6-O6   | -5.24 | 1.19        | 1.24     |
| 35  | BB    | 2158 | A    | C5'-C4' | 5.24  | 1.57        | 1.51     |
| 35  | BB    | 2600 | A    | P-O5'   | -5.24 | 1.54        | 1.59     |
| 1   | AA    | 17   | U    | C2'-C1' | -5.24 | 1.47        | 1.53     |
| 1   | AA    | 1054 | C    | N3-C4   | 5.24  | 1.37        | 1.33     |
| 35  | BB    | 1133 | A    | C6-N1   | 5.24  | 1.39        | 1.35     |
| 35  | BB    | 1359 | A    | C5'-C4' | 5.24  | 1.57        | 1.51     |
| 35  | BB    | 1977 | A    | C1'-N9  | -5.24 | 1.39        | 1.46     |
| 35  | BB    | 2400 | G    | C6-N1   | 5.24  | 1.43        | 1.39     |
| 1   | AA    | 447  | G    | N7-C5   | -5.24 | 1.36        | 1.39     |
| 35  | BB    | 316  | C    | C1'-N1  | 5.24  | 1.56        | 1.48     |
| 35  | BB    | 939  | G    | O3'-P   | -5.24 | 1.54        | 1.61     |
| 35  | BB    | 1026 | G    | C5-C6   | -5.24 | 1.37        | 1.42     |
| 35  | BB    | 1310 | G    | N1-C2   | 5.24  | 1.42        | 1.37     |
| 35  | BB    | 2030 | A    | C6-N6   | 5.24  | 1.38        | 1.33     |
| 35  | BB    | 2168 | G    | C4'-C3' | -5.24 | 1.47        | 1.52     |
| 35  | BB    | 2359 | C    | C4'-C3' | -5.24 | 1.47        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2468 | A    | O3'-P   | -5.24 | 1.54        | 1.61     |
| 35  | BB    | 2787 | C    | C4-C5   | -5.24 | 1.38        | 1.43     |
| 1   | AA    | 252  | U    | N3-C4   | 5.23  | 1.43        | 1.38     |
| 1   | AA    | 307  | C    | C4-C5   | -5.23 | 1.38        | 1.43     |
| 1   | AA    | 630  | A    | C3'-O3' | -5.23 | 1.34        | 1.42     |
| 1   | AA    | 1303 | C    | N1-C6   | -5.23 | 1.34        | 1.37     |
| 18  | AR    | 47   | ARG  | CZ-NH1  | 5.23  | 1.39        | 1.33     |
| 35  | BB    | 548  | G    | C5-C4   | -5.23 | 1.34        | 1.38     |
| 35  | BB    | 766  | U    | C1'-N1  | 5.23  | 1.56        | 1.48     |
| 35  | BB    | 1909 | C    | C2'-C1' | -5.23 | 1.47        | 1.53     |
| 35  | BB    | 2056 | G    | C2-N2   | 5.23  | 1.39        | 1.34     |
| 35  | BB    | 2564 | A    | N9-C4   | 5.23  | 1.41        | 1.37     |
| 1   | AA    | 309  | A    | C3'-O3' | 5.23  | 1.49        | 1.42     |
| 1   | AA    | 1380 | U    | C4-O4   | 5.23  | 1.27        | 1.23     |
| 1   | AA    | 1460 | C    | N3-C4   | 5.23  | 1.37        | 1.33     |
| 35  | BB    | 1016 | G    | C2'-C1' | -5.23 | 1.47        | 1.53     |
| 35  | BB    | 1093 | G    | C3'-C2' | -5.23 | 1.47        | 1.52     |
| 35  | BB    | 1516 | G    | N3-C4   | -5.23 | 1.31        | 1.35     |
| 35  | BB    | 1770 | G    | C2-N3   | 5.23  | 1.36        | 1.32     |
| 35  | BB    | 2116 | G    | P-O5'   | -5.23 | 1.54        | 1.59     |
| 35  | BB    | 2154 | A    | C6-N6   | 5.23  | 1.38        | 1.33     |
| 35  | BB    | 2361 | G    | O4'-C1' | 5.23  | 1.48        | 1.41     |
| 35  | BB    | 2558 | C    | P-O5'   | -5.23 | 1.54        | 1.59     |
| 35  | BB    | 2813 | A    | C5-C6   | 5.23  | 1.45        | 1.41     |
| 1   | AA    | 267  | C    | C5-C6   | -5.23 | 1.30        | 1.34     |
| 1   | AA    | 281  | G    | N1-C2   | 5.23  | 1.42        | 1.37     |
| 1   | AA    | 1286 | U    | C1'-N1  | 5.23  | 1.56        | 1.48     |
| 1   | AA    | 1372 | U    | C4'-O4' | -5.23 | 1.38        | 1.45     |
| 35  | BB    | 318  | C    | C2'-C1' | -5.23 | 1.47        | 1.53     |
| 35  | BB    | 555  | G    | C2'-C1' | -5.23 | 1.47        | 1.53     |
| 35  | BB    | 610  | C    | C2-N3   | 5.23  | 1.40        | 1.35     |
| 35  | BB    | 714  | U    | N1-C2   | 5.23  | 1.43        | 1.38     |
| 35  | BB    | 800  | A    | N9-C4   | -5.23 | 1.34        | 1.37     |
| 35  | BB    | 1616 | A    | N7-C5   | -5.23 | 1.36        | 1.39     |
| 35  | BB    | 2049 | G    | O3'-P   | 5.23  | 1.67        | 1.61     |
| 35  | BB    | 2309 | A    | N9-C4   | -5.23 | 1.34        | 1.37     |
| 1   | AA    | 570  | G    | C5-C6   | -5.23 | 1.37        | 1.42     |
| 1   | AA    | 1257 | A    | C2-N3   | 5.23  | 1.38        | 1.33     |
| 34  | BA    | 68   | C    | N3-C4   | 5.23  | 1.37        | 1.33     |
| 35  | BB    | 169  | G    | C2'-C1' | -5.23 | 1.47        | 1.53     |
| 35  | BB    | 1179 | G    | N3-C4   | 5.23  | 1.39        | 1.35     |
| 35  | BB    | 1918 | A    | C5-C4   | -5.23 | 1.35        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2095 | A    | C6-N1   | 5.23  | 1.39        | 1.35     |
| 35  | BB    | 2868 | A    | C2-N3   | 5.23  | 1.38        | 1.33     |
| 1   | AA    | 27   | G    | C2-N3   | 5.23  | 1.36        | 1.32     |
| 1   | AA    | 96   | U    | N1-C6   | 5.23  | 1.42        | 1.38     |
| 1   | AA    | 349  | A    | C6-N6   | 5.23  | 1.38        | 1.33     |
| 1   | AA    | 1285 | A    | C5-C6   | 5.23  | 1.45        | 1.41     |
| 4   | AD    | 203  | TYR  | CG-CD2  | 5.23  | 1.46        | 1.39     |
| 35  | BB    | 52   | A    | C4'-C3' | 5.23  | 1.58        | 1.53     |
| 35  | BB    | 521  | U    | C2'-C1' | -5.23 | 1.47        | 1.53     |
| 35  | BB    | 544  | C    | C4-N4   | 5.23  | 1.38        | 1.33     |
| 35  | BB    | 933  | A    | C5'-C4' | 5.23  | 1.57        | 1.51     |
| 35  | BB    | 1376 | C    | C4-N4   | 5.23  | 1.38        | 1.33     |
| 35  | BB    | 1451 | C    | C4'-C3' | -5.23 | 1.47        | 1.52     |
| 35  | BB    | 1842 | G    | C8-N7   | 5.23  | 1.34        | 1.30     |
| 35  | BB    | 2468 | A    | C8-N7   | 5.23  | 1.35        | 1.31     |
| 1   | AA    | 42   | G    | C8-N7   | -5.23 | 1.27        | 1.30     |
| 1   | AA    | 413  | G    | C6-O6   | -5.23 | 1.19        | 1.24     |
| 1   | AA    | 1213 | A    | C5-C4   | -5.23 | 1.35        | 1.38     |
| 1   | AA    | 1408 | A    | C2-N3   | 5.23  | 1.38        | 1.33     |
| 35  | BB    | 997  | G    | C5-C6   | -5.23 | 1.37        | 1.42     |
| 35  | BB    | 2427 | C    | C4'-C3' | -5.23 | 1.47        | 1.52     |
| 1   | AA    | 271  | C    | C4'-C3' | 5.22  | 1.58        | 1.53     |
| 1   | AA    | 478  | A    | C3'-C2' | -5.22 | 1.47        | 1.52     |
| 1   | AA    | 705  | G    | N3-C4   | -5.22 | 1.31        | 1.35     |
| 1   | AA    | 811  | C    | O3'-P   | -5.22 | 1.54        | 1.61     |
| 1   | AA    | 836  | G    | C5'-C4' | 5.22  | 1.57        | 1.51     |
| 1   | AA    | 935  | A    | C6-N6   | 5.22  | 1.38        | 1.33     |
| 1   | AA    | 1318 | A    | C2-N3   | -5.22 | 1.28        | 1.33     |
| 21  | AU    | 18   | PHE  | CB-CG   | 5.22  | 1.60        | 1.51     |
| 34  | BA    | 80   | U    | N1-C6   | -5.22 | 1.33        | 1.38     |
| 34  | BA    | 89   | U    | N3-C4   | 5.22  | 1.43        | 1.38     |
| 35  | BB    | 810  | U    | C5-C6   | 5.22  | 1.38        | 1.34     |
| 35  | BB    | 1023 | U    | C5-C6   | -5.22 | 1.29        | 1.34     |
| 35  | BB    | 2107 | G    | O3'-P   | -5.22 | 1.54        | 1.61     |
| 35  | BB    | 2123 | G    | C5-C4   | 5.22  | 1.42        | 1.38     |
| 35  | BB    | 2348 | U    | O4'-C1' | 5.22  | 1.48        | 1.41     |
| 41  | BH    | 123  | ARG  | NE-CZ   | 5.22  | 1.39        | 1.33     |
| 1   | AA    | 180  | U    | C5-C6   | 5.22  | 1.38        | 1.34     |
| 1   | AA    | 271  | C    | C4-N4   | 5.22  | 1.38        | 1.33     |
| 1   | AA    | 299  | G    | N9-C4   | -5.22 | 1.33        | 1.38     |
| 1   | AA    | 379  | C    | N3-C4   | 5.22  | 1.37        | 1.33     |
| 1   | AA    | 1151 | A    | P-O5'   | -5.22 | 1.54        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1351 | U    | C2-N3   | -5.22 | 1.34        | 1.37     |
| 5   | AE    | 111  | ARG  | CZ-NH1  | 5.22  | 1.39        | 1.33     |
| 35  | BB    | 272  | A    | C8-N7   | -5.22 | 1.27        | 1.31     |
| 35  | BB    | 432  | A    | C6-N6   | 5.22  | 1.38        | 1.33     |
| 35  | BB    | 961  | C    | P-O5'   | -5.22 | 1.54        | 1.59     |
| 35  | BB    | 1283 | G    | C5'-C4' | 5.22  | 1.57        | 1.51     |
| 35  | BB    | 2152 | G    | C3'-C2' | 5.22  | 1.58        | 1.52     |
| 35  | BB    | 2680 | U    | N1-C6   | 5.22  | 1.42        | 1.38     |
| 35  | BB    | 2803 | G    | C2'-C1' | -5.22 | 1.47        | 1.53     |
| 1   | AA    | 885  | G    | N3-C4   | -5.22 | 1.31        | 1.35     |
| 35  | BB    | 666  | A    | O3'-P   | -5.22 | 1.54        | 1.61     |
| 35  | BB    | 1040 | A    | O4'-C1' | -5.22 | 1.34        | 1.41     |
| 35  | BB    | 1356 | G    | N3-C4   | -5.22 | 1.31        | 1.35     |
| 35  | BB    | 1634 | A    | C2'-C1' | -5.22 | 1.47        | 1.53     |
| 1   | AA    | 147  | G    | C3'-O3' | 5.22  | 1.49        | 1.42     |
| 1   | AA    | 412  | A    | P-O5'   | -5.22 | 1.54        | 1.59     |
| 1   | AA    | 671  | G    | O3'-P   | -5.22 | 1.54        | 1.61     |
| 1   | AA    | 694  | A    | C4'-C3' | -5.22 | 1.47        | 1.52     |
| 35  | BB    | 547  | A    | C2'-C1' | -5.22 | 1.47        | 1.53     |
| 35  | BB    | 614  | A    | C6-N6   | 5.22  | 1.38        | 1.33     |
| 35  | BB    | 937  | C    | C5'-C4' | 5.22  | 1.57        | 1.51     |
| 35  | BB    | 1022 | G    | O3'-P   | -5.22 | 1.54        | 1.61     |
| 35  | BB    | 1771 | C    | O3'-P   | -5.22 | 1.54        | 1.61     |
| 35  | BB    | 2176 | A    | N7-C5   | -5.22 | 1.36        | 1.39     |
| 35  | BB    | 2239 | G    | C3'-C2' | 5.22  | 1.58        | 1.52     |
| 35  | BB    | 2430 | A    | C2'-O2' | -5.22 | 1.34        | 1.41     |
| 35  | BB    | 2633 | G    | C6-N1   | 5.22  | 1.43        | 1.39     |
| 36  | BC    | 188  | ARG  | CZ-NH1  | 5.22  | 1.39        | 1.33     |
| 34  | BA    | 48   | U    | C4-O4   | -5.22 | 1.19        | 1.23     |
| 35  | BB    | 93   | G    | C2'-C1' | -5.22 | 1.47        | 1.53     |
| 35  | BB    | 1252 | G    | O3'-P   | -5.22 | 1.54        | 1.61     |
| 35  | BB    | 1287 | A    | C2'-C1' | -5.22 | 1.47        | 1.53     |
| 35  | BB    | 2087 | G    | N9-C8   | -5.22 | 1.34        | 1.37     |
| 35  | BB    | 2269 | G    | N7-C5   | 5.22  | 1.42        | 1.39     |
| 1   | AA    | 577  | G    | C2-N2   | 5.22  | 1.39        | 1.34     |
| 35  | BB    | 3    | U    | C1'-N1  | 5.22  | 1.56        | 1.48     |
| 35  | BB    | 498  | G    | N7-C5   | -5.22 | 1.36        | 1.39     |
| 35  | BB    | 609  | A    | C6-N6   | 5.22  | 1.38        | 1.33     |
| 35  | BB    | 818  | G    | C3'-C2' | -5.22 | 1.47        | 1.52     |
| 35  | BB    | 1687 | G    | N7-C5   | -5.22 | 1.36        | 1.39     |
| 35  | BB    | 2156 | G    | C4'-O4' | 5.22  | 1.52        | 1.45     |
| 35  | BB    | 2182 | U    | O3'-P   | -5.22 | 1.54        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2183 | A    | C6-N1   | 5.22  | 1.39        | 1.35     |
| 35  | BB    | 2341 | G    | O3'-P   | -5.22 | 1.54        | 1.61     |
| 35  | BB    | 2538 | C    | C5'-C4' | 5.22  | 1.57        | 1.51     |
| 35  | BB    | 2687 | U    | C2'-C1' | -5.22 | 1.47        | 1.53     |
| 49  | BP    | 71   | ARG  | CZ-NH2  | 5.22  | 1.39        | 1.33     |
| 1   | AA    | 225  | C    | C5'-C4' | 5.21  | 1.57        | 1.51     |
| 1   | AA    | 300  | A    | C5-C4   | -5.21 | 1.35        | 1.38     |
| 1   | AA    | 597  | G    | C6-O6   | -5.21 | 1.19        | 1.24     |
| 35  | BB    | 324  | A    | C2-N3   | 5.21  | 1.38        | 1.33     |
| 35  | BB    | 329  | G    | C2'-C1' | -5.21 | 1.47        | 1.53     |
| 35  | BB    | 479  | A    | C4'-C3' | 5.21  | 1.58        | 1.53     |
| 35  | BB    | 1348 | C    | C5'-C4' | 5.21  | 1.57        | 1.51     |
| 35  | BB    | 1478 | G    | N3-C4   | 5.21  | 1.39        | 1.35     |
| 35  | BB    | 2054 | A    | C3'-C2' | 5.21  | 1.58        | 1.52     |
| 35  | BB    | 2122 | U    | O3'-P   | -5.21 | 1.54        | 1.61     |
| 35  | BB    | 2457 | U    | P-O5'   | -5.21 | 1.54        | 1.59     |
| 40  | BG    | 2    | ARG  | CD-NE   | 5.21  | 1.55        | 1.46     |
| 1   | AA    | 192  | A    | C8-N7   | -5.21 | 1.27        | 1.31     |
| 1   | AA    | 690  | G    | C3'-O3' | 5.21  | 1.49        | 1.42     |
| 34  | BA    | 42   | C    | O3'-P   | -5.21 | 1.54        | 1.61     |
| 35  | BB    | 230  | G    | C2'-C1' | -5.21 | 1.47        | 1.53     |
| 35  | BB    | 522  | A    | N3-C4   | -5.21 | 1.31        | 1.34     |
| 35  | BB    | 2635 | A    | C6-N1   | 5.21  | 1.39        | 1.35     |
| 1   | AA    | 234  | C    | P-O5'   | -5.21 | 1.54        | 1.59     |
| 1   | AA    | 295  | C    | N1-C2   | 5.21  | 1.45        | 1.40     |
| 1   | AA    | 742  | G    | N7-C5   | -5.21 | 1.36        | 1.39     |
| 1   | AA    | 926  | G    | C8-N7   | -5.21 | 1.27        | 1.30     |
| 35  | BB    | 1624 | U    | C3'-C2' | -5.21 | 1.47        | 1.52     |
| 35  | BB    | 1631 | G    | C8-N7   | -5.21 | 1.27        | 1.30     |
| 35  | BB    | 1856 | U    | P-O5'   | -5.21 | 1.54        | 1.59     |
| 35  | BB    | 2522 | U    | N3-C4   | 5.21  | 1.43        | 1.38     |
| 1   | AA    | 20   | U    | C3'-C2' | -5.21 | 1.47        | 1.52     |
| 1   | AA    | 275  | G    | C5-C4   | 5.21  | 1.42        | 1.38     |
| 35  | BB    | 728  | G    | C5-C4   | 5.21  | 1.42        | 1.38     |
| 35  | BB    | 1745 | A    | P-O5'   | -5.21 | 1.54        | 1.59     |
| 35  | BB    | 2461 | A    | O4'-C1' | 5.21  | 1.48        | 1.41     |
| 1   | AA    | 147  | G    | C4'-O4' | 5.21  | 1.52        | 1.45     |
| 1   | AA    | 1158 | C    | N1-C2   | 5.21  | 1.45        | 1.40     |
| 1   | AA    | 1243 | C    | C5-C6   | -5.21 | 1.30        | 1.34     |
| 35  | BB    | 358  | U    | O4'-C1' | 5.21  | 1.48        | 1.41     |
| 35  | BB    | 439  | A    | C4'-C3' | 5.21  | 1.58        | 1.53     |
| 35  | BB    | 844  | A    | N9-C4   | -5.21 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1156 | A    | C2'-C1' | -5.21 | 1.47        | 1.53     |
| 35  | BB    | 1309 | G    | O4'-C1' | -5.21 | 1.34        | 1.41     |
| 35  | BB    | 1410 | G    | N9-C8   | -5.21 | 1.34        | 1.37     |
| 35  | BB    | 1661 | G    | N9-C4   | 5.21  | 1.42        | 1.38     |
| 35  | BB    | 1845 | G    | C2'-C1' | -5.21 | 1.47        | 1.53     |
| 35  | BB    | 1933 | G    | C8-N7   | 5.21  | 1.34        | 1.30     |
| 35  | BB    | 2515 | C    | C2-N3   | 5.21  | 1.40        | 1.35     |
| 36  | BC    | 166  | ARG  | CZ-NH2  | 5.21  | 1.39        | 1.33     |
| 1   | AA    | 826  | C    | C2-N3   | 5.21  | 1.40        | 1.35     |
| 1   | AA    | 1522 | U    | C2-N3   | 5.21  | 1.41        | 1.37     |
| 35  | BB    | 343  | C    | P-O5'   | -5.21 | 1.54        | 1.59     |
| 35  | BB    | 389  | G    | N7-C5   | -5.21 | 1.36        | 1.39     |
| 35  | BB    | 717  | C    | C4-N4   | 5.21  | 1.38        | 1.33     |
| 35  | BB    | 814  | C    | C4-N4   | 5.21  | 1.38        | 1.33     |
| 35  | BB    | 1837 | C    | N3-C4   | 5.21  | 1.37        | 1.33     |
| 35  | BB    | 1871 | A    | C2-N3   | -5.21 | 1.28        | 1.33     |
| 35  | BB    | 2714 | G    | C3'-C2' | -5.21 | 1.47        | 1.52     |
| 1   | AA    | 31   | G    | C2'-C1' | -5.21 | 1.47        | 1.53     |
| 1   | AA    | 67   | C    | C4-N4   | 5.21  | 1.38        | 1.33     |
| 1   | AA    | 1393 | U    | C4'-C3' | 5.21  | 1.58        | 1.53     |
| 35  | BB    | 2102 | G    | C6-O6   | 5.21  | 1.28        | 1.24     |
| 55  | BW    | 21   | ARG  | NE-CZ   | 5.21  | 1.39        | 1.33     |
| 1   | AA    | 354  | G    | N3-C4   | -5.20 | 1.31        | 1.35     |
| 1   | AA    | 594  | U    | N1-C2   | -5.20 | 1.33        | 1.38     |
| 1   | AA    | 1049 | U    | C4'-O4' | -5.20 | 1.38        | 1.45     |
| 9   | AI    | 118  | ARG  | CZ-NH2  | 5.20  | 1.39        | 1.33     |
| 35  | BB    | 618  | G    | C5-C6   | -5.20 | 1.37        | 1.42     |
| 35  | BB    | 1346 | G    | C1'-N9  | -5.20 | 1.39        | 1.46     |
| 35  | BB    | 1388 | G    | C6-O6   | -5.20 | 1.19        | 1.24     |
| 35  | BB    | 1521 | G    | C2-N2   | 5.20  | 1.39        | 1.34     |
| 35  | BB    | 1815 | A    | P-O5'   | -5.20 | 1.54        | 1.59     |
| 35  | BB    | 1899 | A    | C4'-O4' | -5.20 | 1.38        | 1.45     |
| 35  | BB    | 2333 | A    | C6-N1   | 5.20  | 1.39        | 1.35     |
| 35  | BB    | 2398 | U    | C2'-C1' | -5.20 | 1.47        | 1.53     |
| 51  | BR    | 68   | ARG  | NE-CZ   | 5.20  | 1.39        | 1.33     |
| 1   | AA    | 1238 | A    | C6-N1   | 5.20  | 1.39        | 1.35     |
| 1   | AA    | 1406 | U    | C4'-C3' | -5.20 | 1.47        | 1.52     |
| 35  | BB    | 125  | A    | O3'-P   | -5.20 | 1.54        | 1.61     |
| 35  | BB    | 1409 | U    | C2-N3   | 5.20  | 1.41        | 1.37     |
| 35  | BB    | 1937 | A    | C5-C4   | 5.20  | 1.42        | 1.38     |
| 35  | BB    | 2889 | C    | C5'-C4' | 5.20  | 1.57        | 1.51     |
| 1   | AA    | 1176 | A    | N3-C4   | -5.20 | 1.31        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1399 | C    | C4-C5   | -5.20 | 1.38        | 1.43     |
| 34  | BA    | 46   | A    | P-O5'   | -5.20 | 1.54        | 1.59     |
| 35  | BB    | 592  | A    | C5-C4   | 5.20  | 1.42        | 1.38     |
| 35  | BB    | 1228 | G    | C5'-C4' | -5.20 | 1.45        | 1.51     |
| 35  | BB    | 1333 | G    | C5'-C4' | 5.20  | 1.57        | 1.51     |
| 35  | BB    | 1399 | C    | C5-C6   | 5.20  | 1.38        | 1.34     |
| 35  | BB    | 1995 | U    | C2-N3   | 5.20  | 1.41        | 1.37     |
| 35  | BB    | 2027 | G    | C2-N3   | 5.20  | 1.36        | 1.32     |
| 1   | AA    | 725  | G    | C5-C4   | -5.20 | 1.34        | 1.38     |
| 1   | AA    | 1062 | U    | C5-C6   | 5.20  | 1.38        | 1.34     |
| 1   | AA    | 1171 | A    | N9-C8   | 5.20  | 1.42        | 1.37     |
| 1   | AA    | 1252 | A    | C6-N6   | 5.20  | 1.38        | 1.33     |
| 1   | AA    | 1353 | G    | N7-C5   | -5.20 | 1.36        | 1.39     |
| 1   | AA    | 1405 | G    | N7-C5   | -5.20 | 1.36        | 1.39     |
| 1   | AA    | 1431 | A    | N1-C2   | -5.20 | 1.29        | 1.34     |
| 35  | BB    | 128  | C    | C5-C6   | -5.20 | 1.30        | 1.34     |
| 35  | BB    | 321  | U    | C4-C5   | 5.20  | 1.48        | 1.43     |
| 35  | BB    | 444  | C    | C4'-C3' | 5.20  | 1.58        | 1.53     |
| 35  | BB    | 979  | A    | C8-N7   | 5.20  | 1.35        | 1.31     |
| 35  | BB    | 1057 | A    | N3-C4   | 5.20  | 1.38        | 1.34     |
| 35  | BB    | 1167 | C    | C5-C6   | 5.20  | 1.38        | 1.34     |
| 35  | BB    | 2510 | C    | C4-N4   | 5.20  | 1.38        | 1.33     |
| 35  | BB    | 2596 | U    | C2'-C1' | -5.20 | 1.47        | 1.53     |
| 35  | BB    | 674  | G    | N1-C2   | 5.20  | 1.42        | 1.37     |
| 35  | BB    | 1490 | A    | N1-C2   | 5.20  | 1.39        | 1.34     |
| 35  | BB    | 1976 | U    | N1-C2   | -5.20 | 1.33        | 1.38     |
| 35  | BB    | 2027 | G    | C3'-C2' | 5.20  | 1.58        | 1.52     |
| 35  | BB    | 2179 | C    | C4'-C3' | -5.20 | 1.47        | 1.52     |
| 35  | BB    | 2231 | U    | C2'-C1' | -5.20 | 1.47        | 1.53     |
| 35  | BB    | 2821 | A    | N3-C4   | -5.20 | 1.31        | 1.34     |
| 1   | AA    | 306  | A    | C4'-C3' | -5.20 | 1.47        | 1.52     |
| 1   | AA    | 444  | G    | C1'-N9  | -5.20 | 1.39        | 1.46     |
| 1   | AA    | 829  | G    | N7-C5   | -5.20 | 1.36        | 1.39     |
| 1   | AA    | 1073 | U    | C2'-C1' | -5.20 | 1.47        | 1.53     |
| 1   | AA    | 1137 | C    | C4-C5   | 5.20  | 1.47        | 1.43     |
| 1   | AA    | 1324 | A    | C6-N6   | 5.20  | 1.38        | 1.33     |
| 35  | BB    | 33   | C    | O3'-P   | -5.20 | 1.54        | 1.61     |
| 35  | BB    | 468  | G    | C5-C6   | -5.20 | 1.37        | 1.42     |
| 35  | BB    | 931  | U    | N1-C2   | -5.20 | 1.33        | 1.38     |
| 35  | BB    | 1519 | G    | C5-C4   | 5.20  | 1.42        | 1.38     |
| 35  | BB    | 1756 | G    | C6-O6   | -5.20 | 1.19        | 1.24     |
| 35  | BB    | 2280 | G    | C2-N2   | 5.20  | 1.39        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2737 | G    | N3-C4   | 5.20  | 1.39        | 1.35     |
| 52  | BS    | 2    | GLU  | CA-CB   | 5.20  | 1.65        | 1.53     |
| 1   | AA    | 5    | U    | C3'-C2' | 5.19  | 1.58        | 1.52     |
| 1   | AA    | 1159 | U    | C4-O4   | 5.19  | 1.27        | 1.23     |
| 1   | AA    | 1193 | G    | C2'-O2' | 5.19  | 1.48        | 1.41     |
| 1   | AA    | 1227 | A    | N9-C8   | -5.19 | 1.33        | 1.37     |
| 1   | AA    | 1476 | A    | C6-N1   | 5.19  | 1.39        | 1.35     |
| 35  | BB    | 1319 | C    | C2-N3   | 5.19  | 1.40        | 1.35     |
| 35  | BB    | 1352 | U    | C3'-C2' | -5.19 | 1.47        | 1.52     |
| 35  | BB    | 1365 | A    | O4'-C1' | -5.19 | 1.34        | 1.41     |
| 35  | BB    | 1701 | A    | C2-N3   | -5.19 | 1.28        | 1.33     |
| 44  | BK    | 51   | LYS  | CA-CB   | 5.19  | 1.65        | 1.53     |
| 56  | BY    | 34   | SER  | N-CA    | -5.19 | 1.35        | 1.46     |
| 1   | AA    | 1048 | G    | C1'-N9  | -5.19 | 1.39        | 1.46     |
| 1   | AA    | 1509 | C    | N3-C4   | 5.19  | 1.37        | 1.33     |
| 35  | BB    | 253  | C    | C3'-O3' | 5.19  | 1.49        | 1.42     |
| 35  | BB    | 930  | G    | C5-C4   | -5.19 | 1.34        | 1.38     |
| 35  | BB    | 1437 | C    | C2'-C1' | -5.19 | 1.47        | 1.53     |
| 35  | BB    | 1486 | U    | C4-C5   | 5.19  | 1.48        | 1.43     |
| 35  | BB    | 2078 | C    | C3'-C2' | 5.19  | 1.58        | 1.52     |
| 35  | BB    | 2166 | U    | C3'-O3' | 5.19  | 1.49        | 1.42     |
| 35  | BB    | 2808 | G    | C6-O6   | -5.19 | 1.19        | 1.24     |
| 1   | AA    | 1229 | A    | C6-N1   | 5.19  | 1.39        | 1.35     |
| 1   | AA    | 1532 | U    | C2-N3   | 5.19  | 1.41        | 1.37     |
| 34  | BA    | 7    | G    | C8-N7   | -5.19 | 1.27        | 1.30     |
| 35  | BB    | 11   | C    | C2-O2   | 5.19  | 1.29        | 1.24     |
| 35  | BB    | 991  | C    | N1-C6   | 5.19  | 1.40        | 1.37     |
| 35  | BB    | 1580 | A    | C6-N6   | 5.19  | 1.38        | 1.33     |
| 35  | BB    | 1622 | G    | C3'-O3' | 5.19  | 1.49        | 1.42     |
| 35  | BB    | 2466 | C    | C5'-C4' | 5.19  | 1.57        | 1.51     |
| 1   | AA    | 333  | U    | N1-C6   | -5.19 | 1.33        | 1.38     |
| 12  | AL    | 8    | ARG  | NE-CZ   | 5.19  | 1.39        | 1.33     |
| 35  | BB    | 787  | C    | O4'-C1' | 5.19  | 1.48        | 1.41     |
| 35  | BB    | 1132 | U    | C4-O4   | 5.19  | 1.27        | 1.23     |
| 35  | BB    | 1456 | G    | C5'-C4' | -5.19 | 1.45        | 1.51     |
| 35  | BB    | 1597 | A    | P-O5'   | -5.19 | 1.54        | 1.59     |
| 35  | BB    | 1697 | G    | P-O5'   | 5.19  | 1.65        | 1.59     |
| 35  | BB    | 1954 | G    | C2'-C1' | -5.19 | 1.47        | 1.53     |
| 35  | BB    | 1969 | A    | N7-C5   | -5.19 | 1.36        | 1.39     |
| 1   | AA    | 645  | G    | N3-C4   | 5.19  | 1.39        | 1.35     |
| 1   | AA    | 1231 | G    | C2-N3   | 5.19  | 1.36        | 1.32     |
| 1   | AA    | 1268 | G    | C8-N7   | 5.19  | 1.34        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34  | BA    | 110  | C    | C2'-C1' | -5.19 | 1.47        | 1.53     |
| 35  | BB    | 125  | A    | N3-C4   | -5.19 | 1.31        | 1.34     |
| 35  | BB    | 144  | A    | C4'-O4' | 5.19  | 1.52        | 1.45     |
| 35  | BB    | 222  | A    | C8-N7   | -5.19 | 1.27        | 1.31     |
| 35  | BB    | 309  | A    | C2'-C1' | -5.19 | 1.47        | 1.53     |
| 35  | BB    | 1024 | G    | C5-C4   | 5.19  | 1.42        | 1.38     |
| 35  | BB    | 1044 | C    | C2'-C1' | -5.19 | 1.47        | 1.53     |
| 35  | BB    | 1250 | G    | C2'-C1' | -5.19 | 1.47        | 1.53     |
| 35  | BB    | 1388 | G    | N7-C5   | -5.19 | 1.36        | 1.39     |
| 35  | BB    | 1567 | G    | C2-N3   | 5.19  | 1.36        | 1.32     |
| 35  | BB    | 1734 | G    | O3'-P   | -5.19 | 1.54        | 1.61     |
| 35  | BB    | 2397 | G    | C5-C4   | -5.19 | 1.34        | 1.38     |
| 1   | AA    | 354  | G    | C4'-O4' | 5.19  | 1.52        | 1.45     |
| 1   | AA    | 368  | U    | O3'-P   | -5.19 | 1.54        | 1.61     |
| 1   | AA    | 692  | U    | C4-C5   | -5.19 | 1.38        | 1.43     |
| 1   | AA    | 1179 | A    | C5-C4   | -5.19 | 1.35        | 1.38     |
| 35  | BB    | 376  | G    | C5'-C4' | 5.19  | 1.57        | 1.51     |
| 1   | AA    | 464  | U    | C2'-C1' | -5.18 | 1.47        | 1.53     |
| 1   | AA    | 516  | U    | O4'-C1' | -5.18 | 1.34        | 1.41     |
| 1   | AA    | 616  | G    | C2'-C1' | -5.18 | 1.47        | 1.53     |
| 1   | AA    | 1306 | A    | N3-C4   | -5.18 | 1.31        | 1.34     |
| 33  | B8    | 12   | ARG  | CZ-NH2  | 5.18  | 1.39        | 1.33     |
| 35  | BB    | 23   | G    | C5-C4   | 5.18  | 1.42        | 1.38     |
| 35  | BB    | 185  | G    | C6-N1   | 5.18  | 1.43        | 1.39     |
| 35  | BB    | 241  | A    | N9-C8   | 5.18  | 1.41        | 1.37     |
| 35  | BB    | 454  | A    | C5-C6   | 5.18  | 1.45        | 1.41     |
| 35  | BB    | 726  | G    | C2-N3   | -5.18 | 1.28        | 1.32     |
| 35  | BB    | 834  | G    | O3'-P   | -5.18 | 1.54        | 1.61     |
| 35  | BB    | 1141 | U    | P-O5'   | -5.18 | 1.54        | 1.59     |
| 35  | BB    | 1629 | U    | O4'-C1' | 5.18  | 1.48        | 1.41     |
| 35  | BB    | 1876 | A    | N1-C2   | 5.18  | 1.39        | 1.34     |
| 35  | BB    | 1915 | U    | C5-C6   | 5.18  | 1.38        | 1.34     |
| 35  | BB    | 1925 | C    | C4-N4   | 5.18  | 1.38        | 1.33     |
| 35  | BB    | 1973 | G    | C5-C4   | 5.18  | 1.42        | 1.38     |
| 35  | BB    | 2210 | U    | P-O5'   | -5.18 | 1.54        | 1.59     |
| 35  | BB    | 2519 | U    | C3'-O3' | 5.18  | 1.49        | 1.42     |
| 35  | BB    | 2535 | G    | N1-C2   | 5.18  | 1.41        | 1.37     |
| 35  | BB    | 2701 | U    | P-O5'   | -5.18 | 1.54        | 1.59     |
| 35  | BB    | 2819 | G    | C2'-C1' | -5.18 | 1.47        | 1.53     |
| 1   | AA    | 1314 | C    | N1-C2   | -5.18 | 1.34        | 1.40     |
| 4   | AD    | 127  | ARG  | CD-NE   | 5.18  | 1.55        | 1.46     |
| 10  | AJ    | 47   | GLU  | N-CA    | -5.18 | 1.35        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 508  | A    | C5'-C4' | 5.18  | 1.57        | 1.51     |
| 35  | BB    | 588  | U    | N1-C6   | -5.18 | 1.33        | 1.38     |
| 35  | BB    | 716  | A    | C5'-C4' | -5.18 | 1.45        | 1.51     |
| 35  | BB    | 830  | G    | C8-N7   | 5.18  | 1.34        | 1.30     |
| 35  | BB    | 1637 | A    | C5-C6   | 5.18  | 1.45        | 1.41     |
| 35  | BB    | 1834 | U    | N3-C4   | 5.18  | 1.43        | 1.38     |
| 35  | BB    | 1849 | G    | N7-C5   | -5.18 | 1.36        | 1.39     |
| 35  | BB    | 2282 | G    | O3'-P   | -5.18 | 1.54        | 1.61     |
| 35  | BB    | 2547 | A    | N9-C8   | -5.18 | 1.33        | 1.37     |
| 1   | AA    | 604  | G    | C5'-C4' | 5.18  | 1.57        | 1.51     |
| 34  | BA    | 55   | U    | C2-N3   | 5.18  | 1.41        | 1.37     |
| 34  | BA    | 72   | G    | C2-N3   | 5.18  | 1.36        | 1.32     |
| 35  | BB    | 121  | G    | C1'-N9  | 5.18  | 1.56        | 1.48     |
| 35  | BB    | 1373 | A    | C5'-C4' | 5.18  | 1.57        | 1.51     |
| 35  | BB    | 1678 | A    | N3-C4   | -5.18 | 1.31        | 1.34     |
| 35  | BB    | 1743 | G    | N3-C4   | 5.18  | 1.39        | 1.35     |
| 35  | BB    | 2470 | G    | C2-N3   | 5.18  | 1.36        | 1.32     |
| 35  | BB    | 2580 | U    | C4-O4   | -5.18 | 1.19        | 1.23     |
| 35  | BB    | 2694 | G    | C8-N7   | -5.18 | 1.27        | 1.30     |
| 1   | AA    | 948  | C    | N3-C4   | 5.18  | 1.37        | 1.33     |
| 1   | AA    | 1002 | G    | N3-C4   | -5.18 | 1.31        | 1.35     |
| 34  | BA    | 12   | C    | N1-C2   | -5.18 | 1.34        | 1.40     |
| 35  | BB    | 38   | A    | C3'-C2' | -5.18 | 1.47        | 1.52     |
| 35  | BB    | 690  | G    | O3'-P   | -5.18 | 1.54        | 1.61     |
| 35  | BB    | 917  | A    | O3'-P   | -5.18 | 1.54        | 1.61     |
| 35  | BB    | 1571 | A    | P-O5'   | -5.18 | 1.54        | 1.59     |
| 35  | BB    | 1718 | G    | P-O5'   | 5.18  | 1.65        | 1.59     |
| 35  | BB    | 2136 | G    | C6-N1   | 5.18  | 1.43        | 1.39     |
| 35  | BB    | 2351 | G    | C2-N3   | 5.18  | 1.36        | 1.32     |
| 35  | BB    | 2407 | A    | C2-N3   | -5.18 | 1.28        | 1.33     |
| 35  | BB    | 564  | C    | C4-N4   | 5.18  | 1.38        | 1.33     |
| 35  | BB    | 910  | A    | N3-C4   | -5.18 | 1.31        | 1.34     |
| 35  | BB    | 1327 | A    | C5-C6   | 5.18  | 1.45        | 1.41     |
| 35  | BB    | 2589 | A    | C5'-C4' | 5.18  | 1.57        | 1.51     |
| 35  | BB    | 2879 | A    | N1-C2   | 5.18  | 1.39        | 1.34     |
| 1   | AA    | 371  | A    | C2'-C1' | -5.18 | 1.47        | 1.53     |
| 1   | AA    | 533  | A    | N3-C4   | 5.18  | 1.38        | 1.34     |
| 1   | AA    | 1106 | G    | C5-C6   | -5.18 | 1.37        | 1.42     |
| 5   | AE    | 111  | ARG  | CZ-NH2  | 5.18  | 1.39        | 1.33     |
| 35  | BB    | 39   | G    | C1'-N9  | -5.18 | 1.39        | 1.46     |
| 35  | BB    | 737  | C    | C3'-C2' | -5.18 | 1.47        | 1.52     |
| 35  | BB    | 825  | A    | C6-N1   | 5.18  | 1.39        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 974  | G    | N9-C4   | -5.18 | 1.33        | 1.38     |
| 35  | BB    | 1014 | A    | C6-N6   | 5.18  | 1.38        | 1.33     |
| 35  | BB    | 1542 | U    | C4-O4   | 5.18  | 1.27        | 1.23     |
| 35  | BB    | 1657 | U    | C3'-C2' | -5.18 | 1.47        | 1.52     |
| 35  | BB    | 2297 | A    | C2'-C1' | -5.18 | 1.47        | 1.53     |
| 35  | BB    | 2589 | A    | C3'-C2' | -5.18 | 1.47        | 1.52     |
| 35  | BB    | 2834 | G    | C8-N7   | -5.18 | 1.27        | 1.30     |
| 44  | BK    | 32   | TYR  | CZ-OH   | 5.18  | 1.46        | 1.37     |
| 51  | BR    | 90   | ARG  | NE-CZ   | 5.18  | 1.39        | 1.33     |
| 1   | AA    | 83   | C    | C5'-C4' | 5.17  | 1.57        | 1.51     |
| 1   | AA    | 584  | G    | C6-O6   | 5.17  | 1.28        | 1.24     |
| 1   | AA    | 670  | G    | N1-C2   | 5.17  | 1.41        | 1.37     |
| 1   | AA    | 714  | G    | N1-C2   | 5.17  | 1.41        | 1.37     |
| 1   | AA    | 836  | G    | P-O5'   | -5.17 | 1.54        | 1.59     |
| 1   | AA    | 1119 | C    | C4-N4   | 5.17  | 1.38        | 1.33     |
| 1   | AA    | 1434 | A    | N7-C5   | -5.17 | 1.36        | 1.39     |
| 7   | AG    | 89   | GLU  | CG-CD   | 5.17  | 1.59        | 1.51     |
| 15  | AO    | 71   | ARG  | NE-CZ   | 5.17  | 1.39        | 1.33     |
| 35  | BB    | 365  | U    | P-O5'   | -5.17 | 1.54        | 1.59     |
| 35  | BB    | 563  | A    | C6-N1   | 5.17  | 1.39        | 1.35     |
| 35  | BB    | 1103 | A    | C8-N7   | -5.17 | 1.27        | 1.31     |
| 35  | BB    | 1132 | U    | C2-N3   | 5.17  | 1.41        | 1.37     |
| 35  | BB    | 1950 | G    | P-O5'   | -5.17 | 1.54        | 1.59     |
| 35  | BB    | 1991 | U    | C4'-C3' | -5.17 | 1.47        | 1.52     |
| 35  | BB    | 2097 | A    | C3'-C2' | -5.17 | 1.47        | 1.52     |
| 35  | BB    | 2613 | U    | C1'-N1  | 5.17  | 1.56        | 1.48     |
| 35  | BB    | 2655 | G    | C5'-C4' | 5.17  | 1.57        | 1.51     |
| 35  | BB    | 2718 | G    | N9-C4   | -5.17 | 1.33        | 1.38     |
| 1   | AA    | 734  | G    | C2-N3   | 5.17  | 1.36        | 1.32     |
| 1   | AA    | 1010 | U    | C5-C6   | 5.17  | 1.38        | 1.34     |
| 35  | BB    | 245  | G    | C6-N1   | 5.17  | 1.43        | 1.39     |
| 35  | BB    | 2426 | A    | C6-N6   | 5.17  | 1.38        | 1.33     |
| 41  | BH    | 149  | GLU  | CD-OE2  | 5.17  | 1.31        | 1.25     |
| 1   | AA    | 117  | G    | N7-C5   | -5.17 | 1.36        | 1.39     |
| 1   | AA    | 384  | G    | C5-C4   | 5.17  | 1.42        | 1.38     |
| 1   | AA    | 553  | A    | N7-C5   | -5.17 | 1.36        | 1.39     |
| 1   | AA    | 1148 | U    | N3-C4   | 5.17  | 1.43        | 1.38     |
| 1   | AA    | 1230 | C    | N3-C4   | 5.17  | 1.37        | 1.33     |
| 16  | AP    | 44   | SER  | CB-OG   | 5.17  | 1.49        | 1.42     |
| 34  | BA    | 12   | C    | C5-C6   | -5.17 | 1.30        | 1.34     |
| 35  | BB    | 248  | G    | C4'-C3' | -5.17 | 1.47        | 1.52     |
| 35  | BB    | 833  | A    | P-O5'   | -5.17 | 1.54        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1941 | C    | C1'-N1  | 5.17  | 1.56        | 1.48     |
| 35  | BB    | 2016 | U    | C4-C5   | 5.17  | 1.48        | 1.43     |
| 35  | BB    | 2075 | U    | N1-C2   | -5.17 | 1.33        | 1.38     |
| 35  | BB    | 2752 | C    | C2'-C1' | -5.17 | 1.47        | 1.53     |
| 1   | AA    | 289  | G    | C2'-C1' | -5.17 | 1.47        | 1.53     |
| 1   | AA    | 881  | G    | C8-N7   | 5.17  | 1.34        | 1.30     |
| 35  | BB    | 199  | A    | C2'-C1' | -5.17 | 1.47        | 1.53     |
| 35  | BB    | 1126 | A    | O4'-C1' | -5.17 | 1.34        | 1.41     |
| 35  | BB    | 1903 | G    | C2-N3   | 5.17  | 1.36        | 1.32     |
| 1   | AA    | 853  | C    | C4'-C3' | 5.17  | 1.58        | 1.53     |
| 1   | AA    | 1359 | C    | C2-N3   | 5.17  | 1.39        | 1.35     |
| 19  | AS    | 51   | HIS  | CB-CG   | 5.17  | 1.59        | 1.50     |
| 35  | BB    | 767  | U    | C2-N3   | 5.17  | 1.41        | 1.37     |
| 35  | BB    | 953  | G    | N9-C4   | 5.17  | 1.42        | 1.38     |
| 35  | BB    | 1597 | A    | N3-C4   | 5.17  | 1.38        | 1.34     |
| 35  | BB    | 1901 | A    | P-O5'   | -5.17 | 1.54        | 1.59     |
| 35  | BB    | 2255 | G    | N7-C5   | -5.17 | 1.36        | 1.39     |
| 35  | BB    | 2477 | U    | C4-O4   | 5.17  | 1.27        | 1.23     |
| 1   | AA    | 266  | G    | C6-N1   | 5.17  | 1.43        | 1.39     |
| 1   | AA    | 661  | G    | C2-N3   | 5.17  | 1.36        | 1.32     |
| 1   | AA    | 1223 | C    | C2-O2   | -5.17 | 1.19        | 1.24     |
| 1   | AA    | 1235 | U    | C4'-O4' | -5.17 | 1.38        | 1.45     |
| 1   | AA    | 1297 | G    | N7-C5   | 5.17  | 1.42        | 1.39     |
| 1   | AA    | 1308 | U    | O3'-P   | -5.17 | 1.54        | 1.61     |
| 22  | AV    | 73   | A    | N3-C4   | -5.17 | 1.31        | 1.34     |
| 35  | BB    | 270  | A    | O3'-P   | -5.17 | 1.54        | 1.61     |
| 35  | BB    | 683  | U    | O3'-P   | -5.17 | 1.54        | 1.61     |
| 35  | BB    | 834  | G    | N7-C5   | -5.17 | 1.36        | 1.39     |
| 35  | BB    | 972  | A    | N9-C4   | -5.17 | 1.34        | 1.37     |
| 35  | BB    | 1185 | G    | C2-N3   | -5.17 | 1.28        | 1.32     |
| 35  | BB    | 1269 | A    | C5-C4   | 5.17  | 1.42        | 1.38     |
| 35  | BB    | 1381 | G    | C2'-C1' | -5.17 | 1.47        | 1.53     |
| 35  | BB    | 1587 | G    | C5'-C4' | 5.17  | 1.57        | 1.51     |
| 35  | BB    | 1990 | C    | C2-O2   | 5.17  | 1.29        | 1.24     |
| 35  | BB    | 2028 | U    | C2-O2   | -5.17 | 1.17        | 1.22     |
| 35  | BB    | 2260 | C    | C3'-C2' | 5.17  | 1.58        | 1.52     |
| 44  | BK    | 9    | ASN  | CA-C    | -5.17 | 1.39        | 1.52     |
| 48  | BO    | 36   | TYR  | CE2-CZ  | 5.17  | 1.45        | 1.38     |
| 1   | AA    | 1325 | C    | C3'-O3' | -5.17 | 1.34        | 1.42     |
| 1   | AA    | 1400 | C    | N3-C4   | 5.17  | 1.37        | 1.33     |
| 35  | BB    | 350  | G    | C2'-C1' | -5.17 | 1.47        | 1.53     |
| 35  | BB    | 1385 | A    | C5'-C4' | -5.17 | 1.45        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1400 | U    | C5-C6   | 5.17  | 1.38        | 1.34     |
| 35  | BB    | 1807 | G    | C4'-O4' | -5.17 | 1.38        | 1.45     |
| 1   | AA    | 182  | A    | C6-N1   | 5.16  | 1.39        | 1.35     |
| 1   | AA    | 430  | A    | C4'-C3' | 5.16  | 1.58        | 1.53     |
| 1   | AA    | 482  | A    | C5-C4   | 5.16  | 1.42        | 1.38     |
| 1   | AA    | 631  | C    | C1'-N1  | 5.16  | 1.56        | 1.48     |
| 1   | AA    | 1206 | G    | C2-N2   | 5.16  | 1.39        | 1.34     |
| 1   | AA    | 1207 | G    | C2-N3   | 5.16  | 1.36        | 1.32     |
| 1   | AA    | 1458 | G    | C3'-C2' | 5.16  | 1.58        | 1.52     |
| 35  | BB    | 219  | A    | N3-C4   | -5.16 | 1.31        | 1.34     |
| 35  | BB    | 337  | C    | C3'-C2' | -5.16 | 1.47        | 1.52     |
| 35  | BB    | 403  | U    | C2-N3   | 5.16  | 1.41        | 1.37     |
| 35  | BB    | 607  | U    | C2'-C1' | -5.16 | 1.47        | 1.53     |
| 35  | BB    | 635  | C    | P-O5'   | -5.16 | 1.54        | 1.59     |
| 35  | BB    | 667  | U    | C4'-O4' | -5.16 | 1.38        | 1.45     |
| 35  | BB    | 1654 | A    | C3'-O3' | 5.16  | 1.49        | 1.42     |
| 35  | BB    | 1942 | C    | C4-C5   | -5.16 | 1.38        | 1.43     |
| 35  | BB    | 2586 | U    | C4-C5   | 5.16  | 1.48        | 1.43     |
| 34  | BA    | 117  | G    | C2-N2   | -5.16 | 1.29        | 1.34     |
| 35  | BB    | 2105 | U    | C2'-C1' | -5.16 | 1.47        | 1.53     |
| 35  | BB    | 2246 | G    | C5-C4   | 5.16  | 1.42        | 1.38     |
| 1   | AA    | 705  | G    | C2'-C1' | -5.16 | 1.47        | 1.53     |
| 1   | AA    | 993  | G    | N9-C8   | 5.16  | 1.41        | 1.37     |
| 35  | BB    | 429  | A    | C4'-O4' | 5.16  | 1.52        | 1.45     |
| 35  | BB    | 434  | U    | N1-C6   | -5.16 | 1.33        | 1.38     |
| 35  | BB    | 904  | G    | C5'-C4' | -5.16 | 1.45        | 1.51     |
| 35  | BB    | 1136 | G    | N9-C8   | 5.16  | 1.41        | 1.37     |
| 35  | BB    | 1169 | A    | C6-N6   | 5.16  | 1.38        | 1.33     |
| 35  | BB    | 1734 | G    | C4'-C3' | -5.16 | 1.47        | 1.52     |
| 35  | BB    | 1983 | G    | C6-O6   | -5.16 | 1.19        | 1.24     |
| 35  | BB    | 2414 | G    | C6-N1   | 5.16  | 1.43        | 1.39     |
| 35  | BB    | 2465 | C    | C2-N3   | -5.16 | 1.31        | 1.35     |
| 35  | BB    | 2781 | A    | N9-C4   | -5.16 | 1.34        | 1.37     |
| 1   | AA    | 39   | G    | C4'-O4' | -5.16 | 1.38        | 1.45     |
| 1   | AA    | 187  | G    | C4'-O4' | -5.16 | 1.38        | 1.45     |
| 1   | AA    | 726  | C    | N3-C4   | 5.16  | 1.37        | 1.33     |
| 1   | AA    | 774  | G    | N3-C4   | -5.16 | 1.31        | 1.35     |
| 1   | AA    | 1530 | G    | C2-N2   | 5.16  | 1.39        | 1.34     |
| 34  | BA    | 44   | G    | C2-N3   | 5.16  | 1.36        | 1.32     |
| 35  | BB    | 183  | C    | N3-C4   | 5.16  | 1.37        | 1.33     |
| 35  | BB    | 909  | A    | C6-N6   | 5.16  | 1.38        | 1.33     |
| 35  | BB    | 1336 | A    | C3'-C2' | 5.16  | 1.58        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1488 | C    | C5-C6   | -5.16 | 1.30        | 1.34     |
| 35  | BB    | 1600 | C    | N1-C2   | 5.16  | 1.45        | 1.40     |
| 35  | BB    | 2418 | A    | O3'-P   | -5.16 | 1.54        | 1.61     |
| 1   | AA    | 71   | A    | C2'-C1' | -5.16 | 1.47        | 1.53     |
| 1   | AA    | 1209 | C    | C4'-O4' | 5.16  | 1.52        | 1.45     |
| 35  | BB    | 137  | U    | C5'-C4' | 5.16  | 1.57        | 1.51     |
| 35  | BB    | 1570 | A    | C4'-C3' | 5.16  | 1.58        | 1.53     |
| 35  | BB    | 2287 | A    | C5-C4   | 5.16  | 1.42        | 1.38     |
| 1   | AA    | 429  | U    | C3'-O3' | 5.16  | 1.49        | 1.42     |
| 1   | AA    | 669  | G    | O3'-P   | 5.16  | 1.67        | 1.61     |
| 1   | AA    | 1246 | A    | C3'-C2' | 5.16  | 1.58        | 1.52     |
| 35  | BB    | 1025 | G    | C5-C4   | 5.16  | 1.42        | 1.38     |
| 35  | BB    | 1090 | A    | C5-C6   | -5.16 | 1.36        | 1.41     |
| 35  | BB    | 1627 | G    | N7-C5   | -5.16 | 1.36        | 1.39     |
| 35  | BB    | 1696 | G    | P-O5'   | -5.16 | 1.54        | 1.59     |
| 35  | BB    | 1887 | C    | N3-C4   | 5.16  | 1.37        | 1.33     |
| 35  | BB    | 2169 | A    | C5-C6   | 5.16  | 1.45        | 1.41     |
| 35  | BB    | 2852 | G    | P-O5'   | -5.16 | 1.54        | 1.59     |
| 1   | AA    | 1474 | U    | C4-O4   | 5.15  | 1.27        | 1.23     |
| 30  | B5    | 180  | PHE  | CG-CD1  | 5.15  | 1.46        | 1.38     |
| 35  | BB    | 1186 | G    | N7-C5   | -5.15 | 1.36        | 1.39     |
| 35  | BB    | 1195 | G    | C2-N2   | 5.15  | 1.39        | 1.34     |
| 35  | BB    | 1782 | U    | C4'-C3' | -5.15 | 1.47        | 1.52     |
| 35  | BB    | 2795 | C    | C1'-N1  | 5.15  | 1.56        | 1.48     |
| 55  | BW    | 81   | PRO  | N-CD    | -5.15 | 1.40        | 1.47     |
| 1   | AA    | 388  | G    | C2-N3   | 5.15  | 1.36        | 1.32     |
| 1   | AA    | 847  | G    | C5-C4   | 5.15  | 1.42        | 1.38     |
| 1   | AA    | 849  | G    | C2-N3   | 5.15  | 1.36        | 1.32     |
| 1   | AA    | 1332 | A    | N3-C4   | -5.15 | 1.31        | 1.34     |
| 35  | BB    | 336  | C    | C5'-C4' | 5.15  | 1.57        | 1.51     |
| 35  | BB    | 553  | G    | O3'-P   | -5.15 | 1.54        | 1.61     |
| 35  | BB    | 683  | U    | C5'-C4' | 5.15  | 1.57        | 1.51     |
| 35  | BB    | 802  | A    | C6-N1   | 5.15  | 1.39        | 1.35     |
| 35  | BB    | 1163 | G    | C2-N3   | 5.15  | 1.36        | 1.32     |
| 35  | BB    | 1427 | A    | O4'-C1' | -5.15 | 1.34        | 1.41     |
| 35  | BB    | 1531 | C    | N1-C2   | 5.15  | 1.45        | 1.40     |
| 35  | BB    | 1545 | A    | C2-N3   | -5.15 | 1.28        | 1.33     |
| 35  | BB    | 1625 | C    | N1-C6   | 5.15  | 1.40        | 1.37     |
| 35  | BB    | 1665 | A    | P-O5'   | -5.15 | 1.54        | 1.59     |
| 35  | BB    | 1911 | U    | C2-N3   | 5.15  | 1.41        | 1.37     |
| 35  | BB    | 1934 | C    | C4-N4   | 5.15  | 1.38        | 1.33     |
| 35  | BB    | 2126 | A    | C2'-C1' | -5.15 | 1.47        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2481 | G    | C6-N1   | 5.15  | 1.43        | 1.39     |
| 35  | BB    | 2691 | C    | C4'-O4' | -5.15 | 1.38        | 1.45     |
| 35  | BB    | 2758 | A    | C5'-C4' | 5.15  | 1.57        | 1.51     |
| 35  | BB    | 2879 | A    | C6-N6   | 5.15  | 1.38        | 1.33     |
| 50  | BQ    | 80   | ASN  | CB-CG   | 5.15  | 1.62        | 1.51     |
| 1   | AA    | 615  | G    | C4'-C3' | -5.15 | 1.47        | 1.52     |
| 1   | AA    | 892  | A    | C6-N1   | 5.15  | 1.39        | 1.35     |
| 1   | AA    | 1282 | C    | C5'-C4' | 5.15  | 1.57        | 1.51     |
| 1   | AA    | 1315 | U    | C2-N3   | 5.15  | 1.41        | 1.37     |
| 22  | AV    | 4    | C    | C2-O2   | 5.15  | 1.29        | 1.24     |
| 35  | BB    | 167  | A    | C5-C6   | -5.15 | 1.36        | 1.41     |
| 35  | BB    | 227  | A    | C2'-C1' | -5.15 | 1.47        | 1.53     |
| 35  | BB    | 500  | G    | N9-C4   | -5.15 | 1.33        | 1.38     |
| 35  | BB    | 506  | G    | C5-C4   | -5.15 | 1.34        | 1.38     |
| 35  | BB    | 569  | U    | C4'-C3' | -5.15 | 1.47        | 1.52     |
| 35  | BB    | 660  | C    | C2-N3   | 5.15  | 1.39        | 1.35     |
| 35  | BB    | 2004 | G    | N7-C5   | -5.15 | 1.36        | 1.39     |
| 35  | BB    | 2198 | A    | C4'-C3' | 5.15  | 1.58        | 1.53     |
| 35  | BB    | 2205 | A    | N3-C4   | -5.15 | 1.31        | 1.34     |
| 35  | BB    | 2607 | G    | C1'-N9  | 5.15  | 1.56        | 1.48     |
| 1   | AA    | 193  | C    | C5'-C4' | 5.15  | 1.57        | 1.51     |
| 1   | AA    | 449  | G    | N7-C5   | -5.15 | 1.36        | 1.39     |
| 1   | AA    | 574  | A    | C2'-C1' | -5.15 | 1.47        | 1.53     |
| 1   | AA    | 905  | U    | C2'-C1' | -5.15 | 1.47        | 1.53     |
| 1   | AA    | 1244 | G    | N1-C2   | 5.15  | 1.41        | 1.37     |
| 1   | AA    | 1432 | G    | N9-C8   | -5.15 | 1.34        | 1.37     |
| 35  | BB    | 57   | C    | C4'-O4' | -5.15 | 1.38        | 1.45     |
| 35  | BB    | 892  | A    | C4'-O4' | -5.15 | 1.38        | 1.45     |
| 35  | BB    | 1328 | A    | O4'-C1' | -5.15 | 1.34        | 1.41     |
| 35  | BB    | 1965 | C    | C4'-O4' | -5.15 | 1.38        | 1.45     |
| 55  | BW    | 41   | GLU  | CG-CD   | -5.15 | 1.44        | 1.51     |
| 1   | AA    | 588  | G    | C2'-C1' | -5.15 | 1.47        | 1.53     |
| 1   | AA    | 1181 | G    | C6-O6   | -5.15 | 1.19        | 1.24     |
| 3   | AC    | 36   | PHE  | CG-CD1  | 5.15  | 1.46        | 1.38     |
| 35  | BB    | 75   | G    | C3'-C2' | -5.15 | 1.47        | 1.52     |
| 35  | BB    | 179  | C    | C4-N4   | 5.15  | 1.38        | 1.33     |
| 35  | BB    | 379  | G    | N3-C4   | -5.15 | 1.31        | 1.35     |
| 35  | BB    | 1173 | U    | C5-C6   | 5.15  | 1.38        | 1.34     |
| 35  | BB    | 1486 | U    | C4'-C3' | 5.15  | 1.58        | 1.53     |
| 35  | BB    | 1653 | G    | C8-N7   | -5.15 | 1.27        | 1.30     |
| 35  | BB    | 1970 | A    | C2'-C1' | -5.15 | 1.47        | 1.53     |
| 35  | BB    | 2009 | A    | N1-C2   | -5.15 | 1.29        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2126 | A    | C3'-C2' | 5.15  | 1.58        | 1.52     |
| 35  | BB    | 2206 | C    | C5'-C4' | 5.15  | 1.57        | 1.51     |
| 35  | BB    | 2646 | C    | C4-C5   | -5.15 | 1.38        | 1.43     |
| 35  | BB    | 2744 | G    | C2'-C1' | -5.15 | 1.47        | 1.53     |
| 1   | AA    | 191  | G    | C4'-O4' | 5.15  | 1.52        | 1.45     |
| 35  | BB    | 1936 | A    | C6-N6   | 5.15  | 1.38        | 1.33     |
| 1   | AA    | 17   | U    | C2-N3   | 5.14  | 1.41        | 1.37     |
| 1   | AA    | 201  | G    | C2'-C1' | -5.14 | 1.47        | 1.53     |
| 1   | AA    | 1084 | G    | O5'-C5' | 5.14  | 1.52        | 1.44     |
| 1   | AA    | 1517 | G    | C8-N7   | -5.14 | 1.27        | 1.30     |
| 9   | AI    | 102  | PHE  | CG-CD2  | 5.14  | 1.46        | 1.38     |
| 22  | AV    | 7    | G    | C2'-C1' | -5.14 | 1.47        | 1.53     |
| 34  | BA    | 42   | C    | C4'-O4' | 5.14  | 1.52        | 1.45     |
| 34  | BA    | 75   | G    | C1'-N9  | -5.14 | 1.39        | 1.46     |
| 35  | BB    | 232  | G    | N3-C4   | -5.14 | 1.31        | 1.35     |
| 35  | BB    | 310  | A    | C5'-C4' | 5.14  | 1.57        | 1.51     |
| 35  | BB    | 339  | U    | P-O5'   | -5.14 | 1.54        | 1.59     |
| 35  | BB    | 780  | G    | C2-N2   | 5.14  | 1.39        | 1.34     |
| 35  | BB    | 863  | A    | C2-N3   | 5.14  | 1.38        | 1.33     |
| 35  | BB    | 1253 | A    | C5-C4   | -5.14 | 1.35        | 1.38     |
| 35  | BB    | 1840 | G    | N9-C8   | -5.14 | 1.34        | 1.37     |
| 35  | BB    | 1917 | U    | N1-C6   | 5.14  | 1.42        | 1.38     |
| 35  | BB    | 2376 | A    | C5-C6   | -5.14 | 1.36        | 1.41     |
| 35  | BB    | 2390 | U    | C4-C5   | 5.14  | 1.48        | 1.43     |
| 35  | BB    | 2539 | C    | C4-N4   | 5.14  | 1.38        | 1.33     |
| 35  | BB    | 2623 | G    | C4'-C3' | -5.14 | 1.47        | 1.52     |
| 1   | AA    | 124  | C    | C1'-N1  | 5.14  | 1.56        | 1.48     |
| 1   | AA    | 269  | C    | C2-O2   | 5.14  | 1.29        | 1.24     |
| 1   | AA    | 540  | G    | C2'-C1' | -5.14 | 1.47        | 1.53     |
| 1   | AA    | 862  | C    | N3-C4   | 5.14  | 1.37        | 1.33     |
| 1   | AA    | 988  | G    | C6-O6   | 5.14  | 1.28        | 1.24     |
| 1   | AA    | 1428 | A    | C2'-O2' | -5.14 | 1.34        | 1.41     |
| 19  | AS    | 49   | ALA  | CA-CB   | 5.14  | 1.63        | 1.52     |
| 35  | BB    | 328  | U    | C3'-C2' | 5.14  | 1.58        | 1.52     |
| 35  | BB    | 2441 | U    | C1'-N1  | 5.14  | 1.56        | 1.48     |
| 35  | BB    | 2473 | U    | C5'-C4' | 5.14  | 1.57        | 1.51     |
| 35  | BB    | 2677 | G    | C8-N7   | 5.14  | 1.34        | 1.30     |
| 35  | BB    | 2861 | U    | C4'-O4' | -5.14 | 1.38        | 1.45     |
| 35  | BB    | 2895 | G    | N9-C4   | -5.14 | 1.33        | 1.38     |
| 1   | AA    | 1248 | A    | C5'-C4' | 5.14  | 1.57        | 1.51     |
| 35  | BB    | 975  | A    | C5-C6   | -5.14 | 1.36        | 1.41     |
| 35  | BB    | 1156 | A    | C5-C6   | 5.14  | 1.45        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1355 | G    | C2'-C1' | -5.14 | 1.47        | 1.53     |
| 35  | BB    | 2239 | G    | C5-C4   | 5.14  | 1.42        | 1.38     |
| 35  | BB    | 2617 | U    | O4'-C1' | 5.14  | 1.48        | 1.41     |
| 1   | AA    | 114  | U    | C3'-C2' | 5.14  | 1.58        | 1.52     |
| 1   | AA    | 512  | U    | N1-C6   | 5.14  | 1.42        | 1.38     |
| 1   | AA    | 515  | G    | O3'-P   | -5.14 | 1.54        | 1.61     |
| 1   | AA    | 648  | A    | C4'-O4' | -5.14 | 1.38        | 1.45     |
| 1   | AA    | 693  | G    | C8-N7   | -5.14 | 1.27        | 1.30     |
| 1   | AA    | 1310 | G    | C3'-O3' | 5.14  | 1.49        | 1.42     |
| 1   | AA    | 1383 | C    | N1-C6   | 5.14  | 1.40        | 1.37     |
| 1   | AA    | 1430 | A    | C3'-C2' | 5.14  | 1.58        | 1.52     |
| 34  | BA    | 24   | G    | C2-N3   | 5.14  | 1.36        | 1.32     |
| 35  | BB    | 645  | C    | O3'-P   | -5.14 | 1.54        | 1.61     |
| 35  | BB    | 1175 | A    | O3'-P   | -5.14 | 1.54        | 1.61     |
| 35  | BB    | 1522 | A    | O3'-P   | -5.14 | 1.54        | 1.61     |
| 35  | BB    | 1984 | G    | C8-N7   | 5.14  | 1.34        | 1.30     |
| 39  | BF    | 166  | ARG  | CZ-NH1  | 5.14  | 1.39        | 1.33     |
| 41  | BH    | 116  | ARG  | NE-CZ   | 5.14  | 1.39        | 1.33     |
| 1   | AA    | 374  | A    | C2-N3   | -5.14 | 1.28        | 1.33     |
| 1   | AA    | 523  | A    | C6-N1   | 5.14  | 1.39        | 1.35     |
| 1   | AA    | 1051 | C    | N1-C2   | 5.14  | 1.45        | 1.40     |
| 1   | AA    | 1316 | G    | C3'-C2' | 5.14  | 1.58        | 1.52     |
| 34  | BA    | 98   | G    | C8-N7   | 5.14  | 1.34        | 1.30     |
| 35  | BB    | 637  | A    | C6-N6   | 5.14  | 1.38        | 1.33     |
| 35  | BB    | 1786 | A    | N9-C4   | 5.14  | 1.41        | 1.37     |
| 35  | BB    | 2326 | C    | N3-C4   | 5.14  | 1.37        | 1.33     |
| 35  | BB    | 2411 | A    | C5-C4   | -5.14 | 1.35        | 1.38     |
| 35  | BB    | 2463 | C    | P-O5'   | -5.14 | 1.54        | 1.59     |
| 39  | BF    | 59   | ILE  | CA-CB   | -5.14 | 1.43        | 1.54     |
| 54  | BU    | 85   | ARG  | NE-CZ   | 5.14  | 1.39        | 1.33     |
| 1   | AA    | 730  | G    | C2-N2   | 5.14  | 1.39        | 1.34     |
| 1   | AA    | 856  | C    | C3'-C2' | -5.14 | 1.47        | 1.52     |
| 1   | AA    | 1018 | G    | O4'-C1' | 5.14  | 1.48        | 1.41     |
| 1   | AA    | 1228 | C    | C2-N3   | 5.14  | 1.39        | 1.35     |
| 35  | BB    | 292  | U    | C1'-N1  | 5.14  | 1.56        | 1.48     |
| 35  | BB    | 346  | A    | C6-N6   | 5.14  | 1.38        | 1.33     |
| 35  | BB    | 408  | G    | N1-C2   | -5.14 | 1.33        | 1.37     |
| 35  | BB    | 481  | G    | N9-C8   | -5.14 | 1.34        | 1.37     |
| 35  | BB    | 487  | C    | N1-C6   | 5.14  | 1.40        | 1.37     |
| 35  | BB    | 1134 | A    | N1-C2   | 5.14  | 1.39        | 1.34     |
| 35  | BB    | 1185 | G    | N1-C2   | 5.14  | 1.41        | 1.37     |
| 35  | BB    | 1694 | C    | P-O5'   | 5.14  | 1.64        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1823 | G    | C2-N3   | 5.14  | 1.36        | 1.32     |
| 35  | BB    | 2008 | C    | N1-C6   | 5.14  | 1.40        | 1.37     |
| 35  | BB    | 2796 | U    | C5'-C4' | 5.14  | 1.57        | 1.51     |
| 49  | BP    | 102  | ARG  | NE-CZ   | 5.14  | 1.39        | 1.33     |
| 1   | AA    | 139  | A    | C6-N1   | 5.13  | 1.39        | 1.35     |
| 1   | AA    | 950  | U    | O3'-P   | -5.13 | 1.54        | 1.61     |
| 1   | AA    | 977  | A    | N7-C5   | -5.13 | 1.36        | 1.39     |
| 25  | B0    | 2    | ARG  | CZ-NH1  | 5.13  | 1.39        | 1.33     |
| 35  | BB    | 132  | G    | O4'-C1' | -5.13 | 1.34        | 1.41     |
| 35  | BB    | 315  | G    | N9-C8   | -5.13 | 1.34        | 1.37     |
| 35  | BB    | 1069 | A    | C4'-O4' | 5.13  | 1.52        | 1.45     |
| 35  | BB    | 1342 | A    | C3'-C2' | -5.13 | 1.47        | 1.52     |
| 35  | BB    | 1552 | A    | C3'-O3' | 5.13  | 1.49        | 1.42     |
| 35  | BB    | 1876 | A    | C5-C4   | 5.13  | 1.42        | 1.38     |
| 35  | BB    | 2577 | A    | C3'-C2' | -5.13 | 1.47        | 1.52     |
| 35  | BB    | 35   | G    | C2'-C1' | -5.13 | 1.47        | 1.53     |
| 35  | BB    | 112  | U    | C4'-O4' | -5.13 | 1.38        | 1.45     |
| 35  | BB    | 1147 | A    | P-O5'   | -5.13 | 1.54        | 1.59     |
| 35  | BB    | 1611 | C    | C4-C5   | 5.13  | 1.47        | 1.43     |
| 35  | BB    | 1785 | A    | C5-C6   | 5.13  | 1.45        | 1.41     |
| 1   | AA    | 257  | G    | C4'-C3' | 5.13  | 1.58        | 1.53     |
| 1   | AA    | 744  | C    | C2'-C1' | -5.13 | 1.47        | 1.53     |
| 1   | AA    | 823  | C    | N1-C6   | -5.13 | 1.34        | 1.37     |
| 1   | AA    | 1080 | A    | C3'-O3' | 5.13  | 1.49        | 1.42     |
| 1   | AA    | 1215 | G    | C2-N2   | 5.13  | 1.39        | 1.34     |
| 1   | AA    | 1305 | G    | N9-C8   | -5.13 | 1.34        | 1.37     |
| 35  | BB    | 167  | A    | O3'-P   | -5.13 | 1.54        | 1.61     |
| 35  | BB    | 1151 | A    | C5-C6   | -5.13 | 1.36        | 1.41     |
| 35  | BB    | 1546 | G    | C5'-C4' | 5.13  | 1.57        | 1.51     |
| 35  | BB    | 2272 | U    | C4'-O4' | 5.13  | 1.52        | 1.45     |
| 35  | BB    | 2363 | G    | C8-N7   | -5.13 | 1.27        | 1.30     |
| 35  | BB    | 2863 | C    | C4-C5   | 5.13  | 1.47        | 1.43     |
| 50  | BQ    | 49   | ARG  | CD-NE   | 5.13  | 1.55        | 1.46     |
| 1   | AA    | 440  | C    | C4-N4   | 5.13  | 1.38        | 1.33     |
| 35  | BB    | 197  | A    | C6-N1   | 5.13  | 1.39        | 1.35     |
| 35  | BB    | 1468 | U    | O3'-P   | -5.13 | 1.54        | 1.61     |
| 35  | BB    | 2844 | G    | C2'-O2' | -5.13 | 1.34        | 1.41     |
| 1   | AA    | 404  | G    | C2'-C1' | -5.13 | 1.47        | 1.53     |
| 35  | BB    | 348  | A    | C6-N1   | 5.13  | 1.39        | 1.35     |
| 35  | BB    | 1035 | U    | N1-C2   | -5.13 | 1.33        | 1.38     |
| 35  | BB    | 1473 | G    | C8-N7   | -5.13 | 1.27        | 1.30     |
| 35  | BB    | 1667 | G    | O4'-C1' | 5.13  | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1726 | C    | N1-C2   | -5.13 | 1.35        | 1.40     |
| 35  | BB    | 2013 | A    | C6-N6   | 5.13  | 1.38        | 1.33     |
| 35  | BB    | 2143 | C    | O4'-C1' | -5.13 | 1.34        | 1.41     |
| 35  | BB    | 2305 | U    | C4'-C3' | -5.13 | 1.47        | 1.52     |
| 35  | BB    | 2403 | C    | C2-N3   | 5.13  | 1.39        | 1.35     |
| 1   | AA    | 628  | G    | C4'-C3' | 5.13  | 1.58        | 1.53     |
| 1   | AA    | 1003 | G    | N1-C2   | 5.13  | 1.41        | 1.37     |
| 35  | BB    | 1140 | C    | O3'-P   | -5.13 | 1.54        | 1.61     |
| 35  | BB    | 1431 | A    | C5'-C4' | 5.13  | 1.57        | 1.51     |
| 35  | BB    | 1925 | C    | C5'-C4' | 5.13  | 1.57        | 1.51     |
| 35  | BB    | 2423 | U    | C2'-C1' | -5.13 | 1.47        | 1.53     |
| 35  | BB    | 2598 | A    | C3'-C2' | -5.13 | 1.47        | 1.52     |
| 35  | BB    | 2696 | U    | N1-C2   | -5.13 | 1.33        | 1.38     |
| 1   | AA    | 394  | G    | C6-O6   | -5.12 | 1.19        | 1.24     |
| 1   | AA    | 1220 | G    | C8-N7   | 5.12  | 1.34        | 1.30     |
| 1   | AA    | 1261 | A    | C8-N7   | -5.12 | 1.27        | 1.31     |
| 35  | BB    | 763  | G    | C5'-C4' | 5.12  | 1.57        | 1.51     |
| 35  | BB    | 2361 | G    | C2'-C1' | -5.12 | 1.47        | 1.53     |
| 1   | AA    | 199  | A    | C5-C4   | -5.12 | 1.35        | 1.38     |
| 1   | AA    | 314  | C    | P-O5'   | -5.12 | 1.54        | 1.59     |
| 1   | AA    | 1246 | A    | C4'-C3' | 5.12  | 1.58        | 1.53     |
| 3   | AC    | 178  | ARG  | NE-CZ   | 5.12  | 1.39        | 1.33     |
| 25  | B0    | 17   | ARG  | CZ-NH1  | 5.12  | 1.39        | 1.33     |
| 35  | BB    | 1768 | C    | N3-C4   | 5.12  | 1.37        | 1.33     |
| 35  | BB    | 1969 | A    | C6-N6   | 5.12  | 1.38        | 1.33     |
| 35  | BB    | 2217 | G    | C5'-C4' | 5.12  | 1.57        | 1.51     |
| 35  | BB    | 2314 | A    | C5-C4   | 5.12  | 1.42        | 1.38     |
| 35  | BB    | 2795 | C    | O4'-C1' | -5.12 | 1.34        | 1.41     |
| 38  | BE    | 49   | ARG  | NE-CZ   | 5.12  | 1.39        | 1.33     |
| 1   | AA    | 185  | U    | C3'-C2' | 5.12  | 1.58        | 1.52     |
| 1   | AA    | 526  | C    | C3'-C2' | -5.12 | 1.47        | 1.52     |
| 1   | AA    | 531  | U    | O3'-P   | 5.12  | 1.67        | 1.61     |
| 1   | AA    | 562  | U    | C4-O4   | 5.12  | 1.27        | 1.23     |
| 4   | AD    | 110  | ARG  | NE-CZ   | 5.12  | 1.39        | 1.33     |
| 34  | BA    | 30   | C    | C4-N4   | 5.12  | 1.38        | 1.33     |
| 35  | BB    | 1498 | C    | O3'-P   | -5.12 | 1.55        | 1.61     |
| 35  | BB    | 1789 | A    | N3-C4   | -5.12 | 1.31        | 1.34     |
| 35  | BB    | 2060 | A    | C2'-C1' | -5.12 | 1.47        | 1.53     |
| 35  | BB    | 2215 | C    | N1-C2   | 5.12  | 1.45        | 1.40     |
| 35  | BB    | 2548 | U    | N3-C4   | 5.12  | 1.43        | 1.38     |
| 35  | BB    | 1144 | A    | C6-N6   | 5.12  | 1.38        | 1.33     |
| 35  | BB    | 1535 | A    | C6-N6   | 5.12  | 1.38        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2465 | C    | C4'-O4' | -5.12 | 1.38        | 1.45     |
| 1   | AA    | 156  | C    | C2-N3   | -5.12 | 1.31        | 1.35     |
| 35  | BB    | 388  | G    | C5-C6   | 5.12  | 1.47        | 1.42     |
| 35  | BB    | 745  | G    | C1'-N9  | -5.12 | 1.39        | 1.46     |
| 35  | BB    | 1343 | G    | C2'-C1' | -5.12 | 1.47        | 1.53     |
| 35  | BB    | 1638 | C    | C2'-C1' | -5.12 | 1.47        | 1.53     |
| 35  | BB    | 2020 | A    | C5'-C4' | 5.12  | 1.57        | 1.51     |
| 35  | BB    | 2403 | C    | C4-C5   | -5.12 | 1.38        | 1.43     |
| 35  | BB    | 2434 | A    | C3'-C2' | 5.12  | 1.58        | 1.52     |
| 35  | BB    | 2629 | U    | N1-C2   | 5.12  | 1.43        | 1.38     |
| 35  | BB    | 2776 | A    | C6-N1   | 5.12  | 1.39        | 1.35     |
| 35  | BB    | 2809 | A    | C8-N7   | -5.12 | 1.27        | 1.31     |
| 44  | BK    | 14   | SER  | N-CA    | -5.12 | 1.36        | 1.46     |
| 1   | AA    | 225  | C    | N3-C4   | 5.12  | 1.37        | 1.33     |
| 1   | AA    | 323  | U    | C2-N3   | 5.12  | 1.41        | 1.37     |
| 1   | AA    | 369  | G    | N7-C5   | 5.12  | 1.42        | 1.39     |
| 1   | AA    | 652  | U    | C3'-O3' | 5.12  | 1.49        | 1.42     |
| 1   | AA    | 897  | C    | C2'-C1' | -5.12 | 1.47        | 1.53     |
| 35  | BB    | 321  | U    | C2-N3   | -5.12 | 1.34        | 1.37     |
| 35  | BB    | 340  | A    | C4'-O4' | -5.12 | 1.38        | 1.45     |
| 35  | BB    | 435  | C    | N3-C4   | 5.12  | 1.37        | 1.33     |
| 35  | BB    | 782  | A    | C5-C4   | 5.12  | 1.42        | 1.38     |
| 35  | BB    | 1011 | G    | C8-N7   | -5.12 | 1.27        | 1.30     |
| 35  | BB    | 1096 | A    | C3'-O3' | 5.12  | 1.49        | 1.42     |
| 35  | BB    | 1165 | A    | N7-C5   | -5.12 | 1.36        | 1.39     |
| 35  | BB    | 1295 | C    | C2-O2   | -5.12 | 1.19        | 1.24     |
| 35  | BB    | 1310 | G    | C5-C4   | -5.12 | 1.34        | 1.38     |
| 35  | BB    | 1333 | G    | N7-C5   | -5.12 | 1.36        | 1.39     |
| 35  | BB    | 1879 | C    | C4-N4   | 5.12  | 1.38        | 1.33     |
| 35  | BB    | 2638 | G    | P-O5'   | -5.12 | 1.54        | 1.59     |
| 35  | BB    | 2663 | G    | C8-N7   | 5.12  | 1.34        | 1.30     |
| 1   | AA    | 1193 | G    | C8-N7   | 5.12  | 1.34        | 1.30     |
| 1   | AA    | 1417 | G    | C5-C4   | 5.12  | 1.42        | 1.38     |
| 35  | BB    | 310  | A    | P-O5'   | 5.12  | 1.64        | 1.59     |
| 35  | BB    | 433  | C    | C5-C6   | -5.12 | 1.30        | 1.34     |
| 35  | BB    | 461  | C    | C4-C5   | -5.12 | 1.38        | 1.43     |
| 35  | BB    | 866  | A    | C5-C4   | 5.12  | 1.42        | 1.38     |
| 35  | BB    | 1012 | U    | C2-N3   | 5.12  | 1.41        | 1.37     |
| 35  | BB    | 1096 | A    | C6-N6   | 5.12  | 1.38        | 1.33     |
| 35  | BB    | 1157 | G    | C2-N2   | 5.12  | 1.39        | 1.34     |
| 35  | BB    | 1247 | A    | C5'-C4' | 5.12  | 1.57        | 1.51     |
| 35  | BB    | 1451 | C    | C2'-C1' | -5.12 | 1.47        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1539 | U    | C3'-O3' | 5.12  | 1.49        | 1.42     |
| 35  | BB    | 1817 | G    | C2-N2   | 5.12  | 1.39        | 1.34     |
| 35  | BB    | 1866 | A    | C5-C6   | -5.12 | 1.36        | 1.41     |
| 35  | BB    | 2451 | A    | N7-C5   | 5.12  | 1.42        | 1.39     |
| 35  | BB    | 2708 | G    | C5-C4   | 5.12  | 1.42        | 1.38     |
| 1   | AA    | 306  | A    | N3-C4   | 5.11  | 1.38        | 1.34     |
| 1   | AA    | 865  | A    | C6-N6   | 5.11  | 1.38        | 1.33     |
| 1   | AA    | 1063 | C    | N1-C6   | -5.11 | 1.34        | 1.37     |
| 1   | AA    | 1422 | G    | P-O5'   | -5.11 | 1.54        | 1.59     |
| 1   | AA    | 1432 | G    | C2-N2   | 5.11  | 1.39        | 1.34     |
| 8   | AH    | 1    | SER  | N-CA    | 5.11  | 1.56        | 1.46     |
| 35  | BB    | 667  | U    | C4-O4   | -5.11 | 1.19        | 1.23     |
| 35  | BB    | 804  | A    | N3-C4   | 5.11  | 1.38        | 1.34     |
| 35  | BB    | 1079 | C    | C1'-N1  | 5.11  | 1.56        | 1.48     |
| 35  | BB    | 1280 | G    | N3-C4   | -5.11 | 1.31        | 1.35     |
| 35  | BB    | 1483 | G    | C8-N7   | -5.11 | 1.27        | 1.30     |
| 35  | BB    | 1733 | G    | C2'-C1' | -5.11 | 1.47        | 1.53     |
| 35  | BB    | 1792 | G    | C3'-O3' | -5.11 | 1.34        | 1.42     |
| 35  | BB    | 2758 | A    | C6-N6   | 5.11  | 1.38        | 1.33     |
| 40  | BG    | 54   | ARG  | CD-NE   | 5.11  | 1.55        | 1.46     |
| 1   | AA    | 317  | U    | C5-C6   | 5.11  | 1.38        | 1.34     |
| 1   | AA    | 368  | U    | C2'-C1' | -5.11 | 1.47        | 1.53     |
| 1   | AA    | 1416 | G    | C5-C6   | -5.11 | 1.37        | 1.42     |
| 34  | BA    | 78   | A    | N9-C4   | -5.11 | 1.34        | 1.37     |
| 35  | BB    | 974  | G    | C4'-O4' | -5.11 | 1.39        | 1.45     |
| 35  | BB    | 1546 | G    | C5-C4   | -5.11 | 1.34        | 1.38     |
| 35  | BB    | 1807 | G    | C5-C6   | -5.11 | 1.37        | 1.42     |
| 35  | BB    | 2701 | U    | N3-C4   | 5.11  | 1.43        | 1.38     |
| 35  | BB    | 2792 | A    | C8-N7   | 5.11  | 1.35        | 1.31     |
| 34  | BA    | 111  | U    | C2-N3   | 5.11  | 1.41        | 1.37     |
| 35  | BB    | 963  | U    | C2'-C1' | -5.11 | 1.47        | 1.53     |
| 35  | BB    | 1204 | A    | C3'-C2' | -5.11 | 1.47        | 1.52     |
| 35  | BB    | 1829 | A    | P-O5'   | -5.11 | 1.54        | 1.59     |
| 35  | BB    | 2465 | C    | P-O5'   | -5.11 | 1.54        | 1.59     |
| 1   | AA    | 860  | A    | C2-N3   | 5.11  | 1.38        | 1.33     |
| 1   | AA    | 955  | U    | N3-C4   | 5.11  | 1.43        | 1.38     |
| 1   | AA    | 962  | C    | O4'-C1' | 5.11  | 1.48        | 1.41     |
| 35  | BB    | 649  | G    | C4'-O4' | 5.11  | 1.52        | 1.45     |
| 35  | BB    | 1207 | C    | N3-C4   | 5.11  | 1.37        | 1.33     |
| 35  | BB    | 1326 | U    | C3'-O3' | 5.11  | 1.49        | 1.42     |
| 1   | AA    | 186  | C    | C3'-O3' | 5.11  | 1.49        | 1.42     |
| 1   | AA    | 537  | G    | C6-N1   | 5.11  | 1.43        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 557  | G    | C4'-O4' | -5.11 | 1.39        | 1.45     |
| 1   | AA    | 851  | G    | C5'-C4' | -5.11 | 1.45        | 1.51     |
| 1   | AA    | 1316 | G    | N9-C8   | 5.11  | 1.41        | 1.37     |
| 1   | AA    | 1505 | G    | N1-C2   | 5.11  | 1.41        | 1.37     |
| 35  | BB    | 379  | G    | N7-C5   | -5.11 | 1.36        | 1.39     |
| 35  | BB    | 562  | U    | P-O5'   | -5.11 | 1.54        | 1.59     |
| 35  | BB    | 592  | A    | C2'-O2' | -5.11 | 1.35        | 1.41     |
| 35  | BB    | 829  | A    | C4'-C3' | 5.11  | 1.58        | 1.53     |
| 35  | BB    | 1255 | U    | C2-N3   | 5.11  | 1.41        | 1.37     |
| 35  | BB    | 1313 | U    | N1-C6   | -5.11 | 1.33        | 1.38     |
| 35  | BB    | 1380 | G    | P-O5'   | -5.11 | 1.54        | 1.59     |
| 35  | BB    | 1407 | G    | N9-C4   | -5.11 | 1.33        | 1.38     |
| 35  | BB    | 1740 | G    | C5'-C4' | 5.11  | 1.57        | 1.51     |
| 35  | BB    | 1783 | A    | C5'-C4' | 5.11  | 1.57        | 1.51     |
| 35  | BB    | 1829 | A    | N9-C8   | 5.11  | 1.41        | 1.37     |
| 35  | BB    | 2798 | U    | P-O5'   | -5.11 | 1.54        | 1.59     |
| 1   | AA    | 167  | A    | N3-C4   | -5.11 | 1.31        | 1.34     |
| 1   | AA    | 1087 | G    | C6-O6   | 5.11  | 1.28        | 1.24     |
| 1   | AA    | 1338 | G    | C2-N3   | 5.11  | 1.36        | 1.32     |
| 34  | BA    | 23   | G    | C6-N1   | 5.11  | 1.43        | 1.39     |
| 34  | BA    | 37   | C    | C4'-O4' | 5.11  | 1.52        | 1.45     |
| 34  | BA    | 58   | A    | C3'-C2' | -5.11 | 1.47        | 1.52     |
| 35  | BB    | 172  | A    | C3'-O3' | 5.11  | 1.49        | 1.42     |
| 35  | BB    | 620  | G    | C2-N2   | 5.11  | 1.39        | 1.34     |
| 35  | BB    | 648  | G    | N9-C8   | 5.11  | 1.41        | 1.37     |
| 35  | BB    | 1215 | G    | C8-N7   | 5.11  | 1.34        | 1.30     |
| 35  | BB    | 2045 | C    | N1-C6   | 5.11  | 1.40        | 1.37     |
| 35  | BB    | 2070 | A    | C5-C4   | 5.11  | 1.42        | 1.38     |
| 35  | BB    | 2308 | G    | C3'-C2' | 5.11  | 1.58        | 1.52     |
| 35  | BB    | 2378 | A    | C5'-C4' | 5.11  | 1.57        | 1.51     |
| 56  | BY    | 38   | ARG  | CD-NE   | 5.11  | 1.55        | 1.46     |
| 1   | AA    | 281  | G    | N3-C4   | -5.10 | 1.31        | 1.35     |
| 1   | AA    | 1153 | G    | C5-C4   | 5.10  | 1.42        | 1.38     |
| 29  | B4    | 39   | ASP  | C-N     | 5.10  | 1.44        | 1.34     |
| 35  | BB    | 646  | U    | O3'-P   | 5.10  | 1.67        | 1.61     |
| 1   | AA    | 322  | C    | C4-C5   | 5.10  | 1.47        | 1.43     |
| 1   | AA    | 1377 | A    | C5-C4   | 5.10  | 1.42        | 1.38     |
| 2   | AB    | 211  | LEU  | CA-CB   | 5.10  | 1.65        | 1.53     |
| 9   | AI    | 6    | TYR  | CE1-CZ  | 5.10  | 1.45        | 1.38     |
| 35  | BB    | 137  | U    | C2-O2   | 5.10  | 1.26        | 1.22     |
| 35  | BB    | 334  | C    | O3'-P   | -5.10 | 1.55        | 1.61     |
| 35  | BB    | 1178 | C    | C4-N4   | 5.10  | 1.38        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1342 | A    | C5-C6   | 5.10  | 1.45        | 1.41     |
| 35  | BB    | 1387 | A    | C5-C6   | 5.10  | 1.45        | 1.41     |
| 35  | BB    | 1788 | C    | C2'-C1' | 5.10  | 1.58        | 1.53     |
| 35  | BB    | 1856 | U    | O4'-C1' | 5.10  | 1.48        | 1.41     |
| 35  | BB    | 2704 | C    | C2-O2   | 5.10  | 1.29        | 1.24     |
| 35  | BB    | 2812 | G    | P-O5'   | -5.10 | 1.54        | 1.59     |
| 39  | BF    | 75   | GLY  | CA-C    | 5.10  | 1.60        | 1.51     |
| 35  | BB    | 842  | U    | O4'-C1' | 5.10  | 1.48        | 1.41     |
| 35  | BB    | 851  | C    | C4'-C3' | 5.10  | 1.58        | 1.53     |
| 35  | BB    | 991  | C    | C3'-C2' | 5.10  | 1.58        | 1.52     |
| 35  | BB    | 1080 | A    | P-O5'   | 5.10  | 1.64        | 1.59     |
| 35  | BB    | 1086 | A    | O3'-P   | 5.10  | 1.67        | 1.61     |
| 35  | BB    | 1172 | C    | N3-C4   | 5.10  | 1.37        | 1.33     |
| 35  | BB    | 1368 | G    | C4'-O4' | 5.10  | 1.52        | 1.45     |
| 35  | BB    | 2465 | C    | C4-N4   | 5.10  | 1.38        | 1.33     |
| 53  | BT    | 6    | ARG  | CA-C    | -5.10 | 1.39        | 1.52     |
| 1   | AA    | 682  | G    | C6-N1   | 5.10  | 1.43        | 1.39     |
| 1   | AA    | 1022 | A    | C2'-C1' | -5.10 | 1.47        | 1.53     |
| 1   | AA    | 1222 | G    | C5-C6   | -5.10 | 1.37        | 1.42     |
| 1   | AA    | 1251 | A    | N9-C8   | 5.10  | 1.41        | 1.37     |
| 1   | AA    | 1432 | G    | O3'-P   | -5.10 | 1.55        | 1.61     |
| 34  | BA    | 7    | G    | O4'-C1' | 5.10  | 1.48        | 1.41     |
| 35  | BB    | 469  | G    | O4'-C1' | -5.10 | 1.35        | 1.41     |
| 35  | BB    | 483  | A    | C5'-C4' | 5.10  | 1.57        | 1.51     |
| 35  | BB    | 932  | U    | C2'-C1' | -5.10 | 1.47        | 1.53     |
| 35  | BB    | 1320 | C    | C2-N3   | 5.10  | 1.39        | 1.35     |
| 35  | BB    | 1560 | G    | C8-N7   | -5.10 | 1.27        | 1.30     |
| 35  | BB    | 2332 | C    | C5'-C4' | 5.10  | 1.57        | 1.51     |
| 35  | BB    | 2351 | G    | C2'-C1' | -5.10 | 1.47        | 1.53     |
| 35  | BB    | 2411 | A    | C8-N7   | 5.10  | 1.35        | 1.31     |
| 35  | BB    | 2545 | G    | O3'-P   | -5.10 | 1.55        | 1.61     |
| 35  | BB    | 2658 | C    | C4-N4   | 5.10  | 1.38        | 1.33     |
| 1   | AA    | 346  | G    | N9-C4   | -5.10 | 1.33        | 1.38     |
| 1   | AA    | 577  | G    | N7-C5   | -5.10 | 1.36        | 1.39     |
| 1   | AA    | 1046 | A    | O4'-C1' | -5.10 | 1.35        | 1.41     |
| 1   | AA    | 1521 | C    | N3-C4   | 5.10  | 1.37        | 1.33     |
| 34  | BA    | 29   | A    | C5-C4   | 5.10  | 1.42        | 1.38     |
| 34  | BA    | 109  | A    | P-O5'   | -5.10 | 1.54        | 1.59     |
| 35  | BB    | 103  | A    | C2-N3   | 5.10  | 1.38        | 1.33     |
| 35  | BB    | 263  | G    | P-O5'   | -5.10 | 1.54        | 1.59     |
| 35  | BB    | 1769 | U    | C4'-O4' | 5.10  | 1.52        | 1.45     |
| 35  | BB    | 2721 | A    | N9-C8   | -5.10 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 43  | BJ    | 116  | ARG  | CD-NE   | 5.10  | 1.55        | 1.46     |
| 1   | AA    | 207  | C    | O4'-C1' | -5.10 | 1.35        | 1.41     |
| 1   | AA    | 384  | G    | N9-C8   | -5.10 | 1.34        | 1.37     |
| 1   | AA    | 945  | G    | C5'-C4' | 5.10  | 1.57        | 1.51     |
| 22  | AV    | 70   | C    | O4'-C1' | 5.10  | 1.48        | 1.41     |
| 35  | BB    | 313  | G    | N7-C5   | -5.10 | 1.36        | 1.39     |
| 35  | BB    | 1070 | A    | C6-N6   | 5.10  | 1.38        | 1.33     |
| 35  | BB    | 1755 | A    | C5'-C4' | 5.10  | 1.57        | 1.51     |
| 35  | BB    | 1950 | G    | O3'-P   | -5.10 | 1.55        | 1.61     |
| 1   | AA    | 125  | U    | N1-C6   | 5.09  | 1.42        | 1.38     |
| 1   | AA    | 230  | G    | C2'-C1' | -5.09 | 1.47        | 1.53     |
| 1   | AA    | 641  | U    | N1-C2   | 5.09  | 1.43        | 1.38     |
| 1   | AA    | 822  | U    | C2-N3   | 5.09  | 1.41        | 1.37     |
| 1   | AA    | 1046 | A    | C5-C4   | 5.09  | 1.42        | 1.38     |
| 1   | AA    | 1242 | G    | C2-N3   | 5.09  | 1.36        | 1.32     |
| 4   | AD    | 126  | GLY  | CA-C    | 5.09  | 1.60        | 1.51     |
| 35  | BB    | 298  | G    | C6-N1   | 5.09  | 1.43        | 1.39     |
| 35  | BB    | 554  | U    | C4-O4   | 5.09  | 1.27        | 1.23     |
| 35  | BB    | 711  | G    | C6-N1   | 5.09  | 1.43        | 1.39     |
| 35  | BB    | 1208 | C    | C2-N3   | 5.09  | 1.39        | 1.35     |
| 35  | BB    | 1570 | A    | C5-C6   | -5.09 | 1.36        | 1.41     |
| 35  | BB    | 2237 | G    | C2-N3   | 5.09  | 1.36        | 1.32     |
| 35  | BB    | 2431 | U    | C4-C5   | -5.09 | 1.39        | 1.43     |
| 35  | BB    | 2557 | G    | N9-C4   | -5.09 | 1.33        | 1.38     |
| 35  | BB    | 2715 | C    | O3'-P   | -5.09 | 1.55        | 1.61     |
| 35  | BB    | 2735 | G    | N1-C2   | 5.09  | 1.41        | 1.37     |
| 35  | BB    | 2887 | A    | N3-C4   | -5.09 | 1.31        | 1.34     |
| 1   | AA    | 502  | A    | C6-N6   | 5.09  | 1.38        | 1.33     |
| 1   | AA    | 1294 | G    | C4'-C3' | 5.09  | 1.58        | 1.53     |
| 1   | AA    | 1340 | A    | N9-C8   | 5.09  | 1.41        | 1.37     |
| 1   | AA    | 1397 | C    | O3'-P   | -5.09 | 1.55        | 1.61     |
| 1   | AA    | 1500 | A    | C2-N3   | -5.09 | 1.28        | 1.33     |
| 35  | BB    | 523  | C    | N1-C2   | 5.09  | 1.45        | 1.40     |
| 35  | BB    | 880  | G    | C5-C6   | 5.09  | 1.47        | 1.42     |
| 1   | AA    | 167  | A    | C6-N6   | 5.09  | 1.38        | 1.33     |
| 1   | AA    | 184  | G    | C2-N2   | 5.09  | 1.39        | 1.34     |
| 1   | AA    | 1060 | U    | C2'-C1' | -5.09 | 1.47        | 1.53     |
| 35  | BB    | 141  | G    | C6-N1   | 5.09  | 1.43        | 1.39     |
| 35  | BB    | 226  | A    | N7-C5   | -5.09 | 1.36        | 1.39     |
| 35  | BB    | 265  | A    | N7-C5   | -5.09 | 1.36        | 1.39     |
| 35  | BB    | 403  | U    | C2'-C1' | -5.09 | 1.47        | 1.53     |
| 35  | BB    | 648  | G    | N3-C4   | -5.09 | 1.31        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 856  | G    | N3-C4   | -5.09 | 1.31        | 1.35     |
| 35  | BB    | 1171 | G    | C6-O6   | -5.09 | 1.19        | 1.24     |
| 35  | BB    | 1416 | G    | C5-C4   | 5.09  | 1.42        | 1.38     |
| 35  | BB    | 1586 | A    | C6-N1   | 5.09  | 1.39        | 1.35     |
| 35  | BB    | 2029 | G    | N7-C5   | -5.09 | 1.36        | 1.39     |
| 35  | BB    | 2349 | G    | N9-C8   | 5.09  | 1.41        | 1.37     |
| 36  | BC    | 37   | SER  | CA-CB   | 5.09  | 1.60        | 1.52     |
| 1   | AA    | 24   | U    | N3-C4   | 5.09  | 1.43        | 1.38     |
| 1   | AA    | 984  | C    | N3-C4   | 5.09  | 1.37        | 1.33     |
| 1   | AA    | 1064 | G    | C2'-O2' | -5.09 | 1.35        | 1.41     |
| 1   | AA    | 1503 | A    | N9-C8   | -5.09 | 1.33        | 1.37     |
| 13  | AM    | 24   | VAL  | CB-CG2  | 5.09  | 1.63        | 1.52     |
| 35  | BB    | 638  | G    | C5'-C4' | 5.09  | 1.57        | 1.51     |
| 35  | BB    | 815  | C    | C2'-C1' | -5.09 | 1.47        | 1.53     |
| 35  | BB    | 973  | A    | C8-N7   | -5.09 | 1.27        | 1.31     |
| 35  | BB    | 1348 | C    | P-O5'   | -5.09 | 1.54        | 1.59     |
| 35  | BB    | 1385 | A    | N7-C5   | 5.09  | 1.42        | 1.39     |
| 35  | BB    | 1927 | A    | C8-N7   | 5.09  | 1.35        | 1.31     |
| 35  | BB    | 2336 | A    | C5-C4   | 5.09  | 1.42        | 1.38     |
| 35  | BB    | 2361 | G    | P-O5'   | -5.09 | 1.54        | 1.59     |
| 50  | BQ    | 36   | GLN  | CG-CD   | 5.09  | 1.62        | 1.51     |
| 1   | AA    | 1511 | G    | N7-C5   | 5.09  | 1.42        | 1.39     |
| 1   | AA    | 1528 | U    | C2-N3   | 5.09  | 1.41        | 1.37     |
| 35  | BB    | 531  | C    | O3'-P   | -5.09 | 1.55        | 1.61     |
| 35  | BB    | 854  | C    | C4'-O4' | 5.09  | 1.52        | 1.45     |
| 35  | BB    | 1491 | G    | O3'-P   | -5.09 | 1.55        | 1.61     |
| 35  | BB    | 2736 | A    | C2'-C1' | -5.09 | 1.47        | 1.53     |
| 40  | BG    | 9    | VAL  | N-CA    | -5.09 | 1.36        | 1.46     |
| 1   | AA    | 363  | A    | C2'-C1' | -5.09 | 1.47        | 1.53     |
| 1   | AA    | 409  | U    | C2'-C1' | -5.09 | 1.47        | 1.53     |
| 1   | AA    | 1211 | U    | C5'-C4' | 5.09  | 1.57        | 1.51     |
| 1   | AA    | 1399 | C    | C2'-O2' | 5.09  | 1.48        | 1.41     |
| 1   | AA    | 1399 | C    | N3-C4   | 5.09  | 1.37        | 1.33     |
| 17  | AQ    | 10   | ARG  | CZ-NH2  | 5.09  | 1.39        | 1.33     |
| 35  | BB    | 396  | G    | N3-C4   | 5.09  | 1.39        | 1.35     |
| 35  | BB    | 708  | G    | C5'-C4' | 5.09  | 1.57        | 1.51     |
| 35  | BB    | 1250 | G    | C3'-C2' | -5.09 | 1.47        | 1.52     |
| 35  | BB    | 2000 | C    | C4-C5   | -5.09 | 1.38        | 1.43     |
| 35  | BB    | 2284 | A    | C5-C4   | 5.09  | 1.42        | 1.38     |
| 35  | BB    | 2613 | U    | C4-O4   | 5.09  | 1.27        | 1.23     |
| 35  | BB    | 2724 | U    | N3-C4   | 5.09  | 1.43        | 1.38     |
| 35  | BB    | 2760 | C    | C2-N3   | 5.09  | 1.39        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2872 | A    | N9-C4   | 5.09  | 1.41        | 1.37     |
| 34  | BA    | 111  | U    | C4'-C3' | 5.08  | 1.58        | 1.53     |
| 35  | BB    | 1    | G    | C6-N1   | 5.08  | 1.43        | 1.39     |
| 35  | BB    | 678  | C    | C2'-C1' | -5.08 | 1.47        | 1.53     |
| 35  | BB    | 1621 | U    | C3'-C2' | -5.08 | 1.47        | 1.52     |
| 1   | AA    | 37   | U    | C2'-C1' | 5.08  | 1.58        | 1.53     |
| 1   | AA    | 304  | U    | N1-C6   | 5.08  | 1.42        | 1.38     |
| 1   | AA    | 1331 | G    | O4'-C1' | -5.08 | 1.35        | 1.41     |
| 1   | AA    | 1398 | A    | C2-N3   | 5.08  | 1.38        | 1.33     |
| 35  | BB    | 233  | A    | C3'-C2' | -5.08 | 1.47        | 1.52     |
| 35  | BB    | 1571 | A    | C6-N6   | 5.08  | 1.38        | 1.33     |
| 35  | BB    | 2164 | C    | C5-C6   | 5.08  | 1.38        | 1.34     |
| 35  | BB    | 2474 | U    | C2-N3   | 5.08  | 1.41        | 1.37     |
| 35  | BB    | 2646 | C    | C2-N3   | 5.08  | 1.39        | 1.35     |
| 36  | BC    | 257  | ARG  | CZ-NH1  | 5.08  | 1.39        | 1.33     |
| 55  | BW    | 21   | ARG  | CD-NE   | 5.08  | 1.55        | 1.46     |
| 1   | AA    | 165  | G    | N3-C4   | 5.08  | 1.39        | 1.35     |
| 1   | AA    | 635  | A    | N3-C4   | -5.08 | 1.31        | 1.34     |
| 35  | BB    | 217  | A    | C2'-C1' | -5.08 | 1.47        | 1.53     |
| 35  | BB    | 655  | A    | N9-C4   | 5.08  | 1.40        | 1.37     |
| 35  | BB    | 1056 | G    | C5-C4   | 5.08  | 1.42        | 1.38     |
| 35  | BB    | 1950 | G    | C2-N3   | 5.08  | 1.36        | 1.32     |
| 35  | BB    | 2899 | A    | O3'-P   | -5.08 | 1.55        | 1.61     |
| 54  | BU    | 55   | GLY  | CA-C    | -5.08 | 1.43        | 1.51     |
| 1   | AA    | 169  | C    | N1-C6   | -5.08 | 1.34        | 1.37     |
| 1   | AA    | 1297 | G    | C2-N2   | 5.08  | 1.39        | 1.34     |
| 35  | BB    | 2324 | U    | P-O5'   | -5.08 | 1.54        | 1.59     |
| 1   | AA    | 227  | G    | C2-N3   | -5.08 | 1.28        | 1.32     |
| 1   | AA    | 711  | G    | N7-C5   | -5.08 | 1.36        | 1.39     |
| 1   | AA    | 1005 | A    | C5-C4   | 5.08  | 1.42        | 1.38     |
| 1   | AA    | 1079 | G    | C3'-C2' | -5.08 | 1.47        | 1.52     |
| 34  | BA    | 22   | U    | C4'-O4' | 5.08  | 1.52        | 1.45     |
| 35  | BB    | 205  | G    | O3'-P   | -5.08 | 1.55        | 1.61     |
| 35  | BB    | 413  | C    | N3-C4   | 5.08  | 1.37        | 1.33     |
| 35  | BB    | 800  | A    | C6-N6   | 5.08  | 1.38        | 1.33     |
| 35  | BB    | 1201 | U    | C3'-O3' | 5.08  | 1.49        | 1.42     |
| 35  | BB    | 1221 | C    | N3-C4   | 5.08  | 1.37        | 1.33     |
| 35  | BB    | 1236 | G    | N9-C8   | 5.08  | 1.41        | 1.37     |
| 35  | BB    | 1291 | C    | C1'-N1  | 5.08  | 1.56        | 1.48     |
| 35  | BB    | 2126 | A    | C2-N3   | 5.08  | 1.38        | 1.33     |
| 35  | BB    | 2453 | A    | C2-N3   | 5.08  | 1.38        | 1.33     |
| 35  | BB    | 2740 | A    | N7-C5   | -5.08 | 1.36        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 42   | G    | N9-C8   | -5.08 | 1.34        | 1.37     |
| 1   | AA    | 145  | G    | O4'-C1' | 5.08  | 1.48        | 1.41     |
| 1   | AA    | 240  | G    | N3-C4   | 5.08  | 1.39        | 1.35     |
| 1   | AA    | 443  | C    | C4'-O4' | -5.08 | 1.39        | 1.45     |
| 1   | AA    | 878  | A    | C5-C6   | -5.08 | 1.36        | 1.41     |
| 35  | BB    | 1852 | U    | O3'-P   | -5.08 | 1.55        | 1.61     |
| 35  | BB    | 1878 | G    | C5'-C4' | 5.08  | 1.57        | 1.51     |
| 35  | BB    | 2180 | U    | C4-O4   | 5.08  | 1.27        | 1.23     |
| 1   | AA    | 110  | C    | C2'-C1' | -5.08 | 1.47        | 1.53     |
| 1   | AA    | 335  | C    | C4'-O4' | -5.08 | 1.39        | 1.45     |
| 1   | AA    | 358  | U    | C4-C5   | 5.08  | 1.48        | 1.43     |
| 1   | AA    | 574  | A    | N9-C4   | -5.08 | 1.34        | 1.37     |
| 1   | AA    | 626  | G    | N1-C2   | 5.08  | 1.41        | 1.37     |
| 1   | AA    | 960  | U    | N1-C6   | 5.08  | 1.42        | 1.38     |
| 1   | AA    | 1059 | C    | N3-C4   | 5.08  | 1.37        | 1.33     |
| 1   | AA    | 1277 | C    | N3-C4   | 5.08  | 1.37        | 1.33     |
| 34  | BA    | 108  | A    | C2-N3   | 5.08  | 1.38        | 1.33     |
| 35  | BB    | 501  | A    | N9-C4   | 5.08  | 1.40        | 1.37     |
| 35  | BB    | 599  | A    | C6-N6   | 5.08  | 1.38        | 1.33     |
| 35  | BB    | 1969 | A    | N3-C4   | -5.08 | 1.31        | 1.34     |
| 35  | BB    | 2669 | G    | N1-C2   | 5.08  | 1.41        | 1.37     |
| 55  | BW    | 9    | ARG  | NE-CZ   | 5.08  | 1.39        | 1.33     |
| 1   | AA    | 133  | U    | P-O5'   | -5.07 | 1.54        | 1.59     |
| 1   | AA    | 1432 | G    | N1-C2   | 5.07  | 1.41        | 1.37     |
| 35  | BB    | 800  | A    | C3'-O3' | 5.07  | 1.49        | 1.42     |
| 35  | BB    | 1247 | A    | C4'-O4' | -5.07 | 1.39        | 1.45     |
| 35  | BB    | 1842 | G    | C4'-O4' | 5.07  | 1.52        | 1.45     |
| 35  | BB    | 1920 | C    | P-O5'   | -5.07 | 1.54        | 1.59     |
| 35  | BB    | 2140 | G    | C3'-C2' | 5.07  | 1.58        | 1.52     |
| 35  | BB    | 2235 | G    | C3'-C2' | -5.07 | 1.47        | 1.52     |
| 1   | AA    | 511  | C    | C5'-C4' | 5.07  | 1.57        | 1.51     |
| 3   | AC    | 163  | ARG  | CD-NE   | 5.07  | 1.55        | 1.46     |
| 35  | BB    | 181  | A    | C6-N6   | 5.07  | 1.38        | 1.33     |
| 35  | BB    | 458  | G    | C2'-C1' | -5.07 | 1.47        | 1.53     |
| 35  | BB    | 965  | C    | C3'-O3' | 5.07  | 1.49        | 1.42     |
| 35  | BB    | 1068 | G    | N3-C4   | -5.07 | 1.31        | 1.35     |
| 35  | BB    | 1188 | U    | C2-N3   | 5.07  | 1.41        | 1.37     |
| 35  | BB    | 1360 | G    | C2'-C1' | -5.07 | 1.47        | 1.53     |
| 35  | BB    | 1754 | A    | P-O5'   | -5.07 | 1.54        | 1.59     |
| 35  | BB    | 2152 | G    | C5-C6   | -5.07 | 1.37        | 1.42     |
| 35  | BB    | 2196 | C    | C4-N4   | 5.07  | 1.38        | 1.33     |
| 45  | BL    | 47   | ARG  | NE-CZ   | 5.07  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 135  | C    | C5'-C4' | 5.07  | 1.57        | 1.51     |
| 1   | AA    | 197  | A    | N1-C2   | 5.07  | 1.39        | 1.34     |
| 1   | AA    | 220  | G    | C3'-C2' | -5.07 | 1.47        | 1.52     |
| 1   | AA    | 1031 | C    | C2'-C1' | -5.07 | 1.47        | 1.53     |
| 1   | AA    | 1089 | G    | N9-C8   | -5.07 | 1.34        | 1.37     |
| 1   | AA    | 1152 | A    | C4'-O4' | 5.07  | 1.52        | 1.45     |
| 35  | BB    | 85   | G    | C2'-C1' | 5.07  | 1.58        | 1.53     |
| 35  | BB    | 132  | G    | C2'-C1' | -5.07 | 1.47        | 1.53     |
| 35  | BB    | 546  | U    | O3'-P   | -5.07 | 1.55        | 1.61     |
| 35  | BB    | 633  | A    | N1-C2   | 5.07  | 1.39        | 1.34     |
| 35  | BB    | 764  | A    | C5-C4   | 5.07  | 1.42        | 1.38     |
| 35  | BB    | 1325 | U    | C4-C5   | 5.07  | 1.48        | 1.43     |
| 35  | BB    | 1383 | A    | C1'-N9  | -5.07 | 1.39        | 1.46     |
| 35  | BB    | 1672 | A    | C5-C6   | -5.07 | 1.36        | 1.41     |
| 35  | BB    | 2125 | G    | C8-N7   | 5.07  | 1.33        | 1.30     |
| 35  | BB    | 2592 | G    | P-O5'   | -5.07 | 1.54        | 1.59     |
| 35  | BB    | 2597 | G    | C5-C4   | 5.07  | 1.41        | 1.38     |
| 35  | BB    | 2724 | U    | C2-N3   | 5.07  | 1.41        | 1.37     |
| 35  | BB    | 2811 | G    | P-O5'   | -5.07 | 1.54        | 1.59     |
| 44  | BK    | 108  | ARG  | CZ-NH2  | 5.07  | 1.39        | 1.33     |
| 1   | AA    | 712  | A    | C4'-C3' | -5.07 | 1.47        | 1.52     |
| 35  | BB    | 506  | G    | C1'-N9  | -5.07 | 1.39        | 1.46     |
| 35  | BB    | 1276 | A    | C3'-O3' | 5.07  | 1.49        | 1.42     |
| 1   | AA    | 9    | G    | N3-C4   | -5.07 | 1.31        | 1.35     |
| 1   | AA    | 166  | U    | P-O5'   | -5.07 | 1.54        | 1.59     |
| 1   | AA    | 689  | C    | C4-N4   | 5.07  | 1.38        | 1.33     |
| 1   | AA    | 1487 | G    | N9-C4   | -5.07 | 1.33        | 1.38     |
| 35  | BB    | 366  | C    | C4-N4   | 5.07  | 1.38        | 1.33     |
| 35  | BB    | 464  | U    | N3-C4   | 5.07  | 1.43        | 1.38     |
| 35  | BB    | 643  | A    | N9-C4   | 5.07  | 1.40        | 1.37     |
| 35  | BB    | 1635 | A    | C3'-O3' | 5.07  | 1.49        | 1.42     |
| 35  | BB    | 1970 | A    | C6-N1   | 5.07  | 1.39        | 1.35     |
| 35  | BB    | 2508 | G    | C5'-C4' | 5.07  | 1.57        | 1.51     |
| 1   | AA    | 815  | A    | C8-N7   | 5.07  | 1.35        | 1.31     |
| 1   | AA    | 1007 | U    | O3'-P   | -5.07 | 1.55        | 1.61     |
| 1   | AA    | 1231 | G    | N9-C8   | -5.07 | 1.34        | 1.37     |
| 1   | AA    | 1447 | A    | C2-N3   | 5.07  | 1.38        | 1.33     |
| 35  | BB    | 384  | A    | N7-C5   | -5.07 | 1.36        | 1.39     |
| 35  | BB    | 627  | A    | C4'-C3' | 5.07  | 1.58        | 1.53     |
| 35  | BB    | 642  | U    | C2-N3   | 5.07  | 1.41        | 1.37     |
| 35  | BB    | 1215 | G    | C4'-O4' | -5.07 | 1.39        | 1.45     |
| 35  | BB    | 1222 | U    | C5-C6   | -5.07 | 1.29        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1289 | C    | C5'-C4' | 5.07  | 1.57        | 1.51     |
| 35  | BB    | 1368 | G    | N7-C5   | -5.07 | 1.36        | 1.39     |
| 35  | BB    | 1875 | G    | C2-N2   | 5.07  | 1.39        | 1.34     |
| 35  | BB    | 2417 | C    | N1-C6   | -5.07 | 1.34        | 1.37     |
| 35  | BB    | 2450 | A    | N3-C4   | 5.07  | 1.37        | 1.34     |
| 14  | AN    | 71   | GLY  | CA-C    | -5.06 | 1.43        | 1.51     |
| 34  | BA    | 2    | G    | C6-N1   | 5.06  | 1.43        | 1.39     |
| 35  | BB    | 49   | A    | C6-N1   | 5.06  | 1.39        | 1.35     |
| 35  | BB    | 634  | C    | C4'-C3' | -5.06 | 1.47        | 1.52     |
| 35  | BB    | 1165 | A    | N1-C2   | 5.06  | 1.39        | 1.34     |
| 35  | BB    | 1325 | U    | P-O5'   | -5.06 | 1.54        | 1.59     |
| 35  | BB    | 1623 | G    | C3'-O3' | 5.06  | 1.49        | 1.42     |
| 1   | AA    | 76   | G    | C3'-O3' | -5.06 | 1.35        | 1.42     |
| 1   | AA    | 577  | G    | C2'-C1' | -5.06 | 1.47        | 1.53     |
| 1   | AA    | 727  | G    | N9-C8   | 5.06  | 1.41        | 1.37     |
| 1   | AA    | 1419 | G    | N3-C4   | -5.06 | 1.31        | 1.35     |
| 6   | AF    | 24   | ARG  | NE-CZ   | 5.06  | 1.39        | 1.33     |
| 15  | AO    | 62   | ARG  | NE-CZ   | 5.06  | 1.39        | 1.33     |
| 35  | BB    | 625  | G    | C3'-C2' | -5.06 | 1.47        | 1.52     |
| 35  | BB    | 784  | G    | N1-C2   | 5.06  | 1.41        | 1.37     |
| 35  | BB    | 1142 | A    | C5-C6   | -5.06 | 1.36        | 1.41     |
| 35  | BB    | 1197 | G    | C5-C6   | -5.06 | 1.37        | 1.42     |
| 35  | BB    | 1413 | A    | N9-C8   | -5.06 | 1.33        | 1.37     |
| 35  | BB    | 2009 | A    | N9-C4   | -5.06 | 1.34        | 1.37     |
| 35  | BB    | 2294 | G    | C2'-C1' | 5.06  | 1.58        | 1.53     |
| 35  | BB    | 2354 | C    | C3'-O3' | 5.06  | 1.49        | 1.42     |
| 36  | BC    | 100  | ARG  | NE-CZ   | 5.06  | 1.39        | 1.33     |
| 46  | BM    | 114  | ARG  | NE-CZ   | 5.06  | 1.39        | 1.33     |
| 1   | AA    | 196  | A    | N7-C5   | -5.06 | 1.36        | 1.39     |
| 1   | AA    | 325  | A    | N1-C2   | -5.06 | 1.29        | 1.34     |
| 35  | BB    | 514  | A    | P-O5'   | -5.06 | 1.54        | 1.59     |
| 35  | BB    | 1029 | A    | C5'-C4' | 5.06  | 1.57        | 1.51     |
| 35  | BB    | 1303 | G    | C5'-C4' | 5.06  | 1.57        | 1.51     |
| 35  | BB    | 1511 | G    | C6-O6   | -5.06 | 1.19        | 1.24     |
| 35  | BB    | 2422 | C    | C4'-C3' | 5.06  | 1.58        | 1.53     |
| 35  | BB    | 2765 | A    | C6-N1   | 5.06  | 1.39        | 1.35     |
| 35  | BB    | 2863 | C    | C3'-O3' | 5.06  | 1.49        | 1.42     |
| 1   | AA    | 254  | G    | C5-C6   | 5.06  | 1.47        | 1.42     |
| 1   | AA    | 628  | G    | C5'-C4' | -5.06 | 1.45        | 1.51     |
| 1   | AA    | 689  | C    | C2'-O2' | -5.06 | 1.35        | 1.41     |
| 1   | AA    | 802  | A    | C4'-O4' | 5.06  | 1.52        | 1.45     |
| 1   | AA    | 1051 | C    | C4-C5   | 5.06  | 1.47        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1163 | A    | C5-C6   | -5.06 | 1.36        | 1.41     |
| 1   | AA    | 1417 | G    | P-O5'   | -5.06 | 1.54        | 1.59     |
| 1   | AA    | 1486 | G    | C5-C6   | -5.06 | 1.37        | 1.42     |
| 5   | AE    | 67   | ARG  | NE-CZ   | 5.06  | 1.39        | 1.33     |
| 16  | AP    | 17   | TYR  | CE1-CZ  | 5.06  | 1.45        | 1.38     |
| 19  | AS    | 2    | ARG  | NE-CZ   | 5.06  | 1.39        | 1.33     |
| 22  | AV    | 5    | A    | C8-N7   | 5.06  | 1.35        | 1.31     |
| 35  | BB    | 594  | U    | C3'-O3' | 5.06  | 1.49        | 1.42     |
| 35  | BB    | 960  | A    | N9-C8   | -5.06 | 1.33        | 1.37     |
| 35  | BB    | 969  | G    | C2'-C1' | -5.06 | 1.47        | 1.53     |
| 35  | BB    | 1128 | G    | C2'-C1' | -5.06 | 1.47        | 1.53     |
| 35  | BB    | 1210 | G    | C8-N7   | 5.06  | 1.33        | 1.30     |
| 35  | BB    | 1388 | G    | N1-C2   | 5.06  | 1.41        | 1.37     |
| 35  | BB    | 1570 | A    | N9-C4   | -5.06 | 1.34        | 1.37     |
| 35  | BB    | 1803 | A    | N3-C4   | 5.06  | 1.37        | 1.34     |
| 35  | BB    | 2029 | G    | P-O5'   | 5.06  | 1.64        | 1.59     |
| 35  | BB    | 2054 | A    | C5'-C4' | 5.06  | 1.57        | 1.51     |
| 35  | BB    | 2132 | U    | C2-N3   | 5.06  | 1.41        | 1.37     |
| 35  | BB    | 2573 | C    | C4-C5   | 5.06  | 1.47        | 1.43     |
| 35  | BB    | 2642 | G    | N7-C5   | -5.06 | 1.36        | 1.39     |
| 35  | BB    | 2876 | G    | C5-C6   | -5.06 | 1.37        | 1.42     |
| 1   | AA    | 593  | U    | P-O5'   | -5.06 | 1.54        | 1.59     |
| 1   | AA    | 1127 | G    | N9-C4   | -5.06 | 1.33        | 1.38     |
| 1   | AA    | 1147 | C    | C2-N3   | 5.06  | 1.39        | 1.35     |
| 35  | BB    | 146  | A    | P-O5'   | 5.06  | 1.64        | 1.59     |
| 35  | BB    | 390  | U    | C2-N3   | 5.06  | 1.41        | 1.37     |
| 35  | BB    | 603  | A    | C6-N1   | -5.06 | 1.32        | 1.35     |
| 35  | BB    | 734  | A    | O4'-C1' | 5.06  | 1.48        | 1.41     |
| 35  | BB    | 1124 | G    | O4'-C1' | -5.06 | 1.35        | 1.41     |
| 35  | BB    | 1870 | C    | N3-C4   | 5.06  | 1.37        | 1.33     |
| 35  | BB    | 2535 | G    | C2-N2   | 5.06  | 1.39        | 1.34     |
| 35  | BB    | 2615 | U    | P-O5'   | -5.06 | 1.54        | 1.59     |
| 47  | BN    | 5    | LYS  | CA-C    | -5.06 | 1.39        | 1.52     |
| 1   | AA    | 1178 | G    | C1'-N9  | 5.06  | 1.56        | 1.48     |
| 35  | BB    | 853  | C    | P-O5'   | -5.06 | 1.54        | 1.59     |
| 35  | BB    | 1138 | G    | N3-C4   | -5.06 | 1.31        | 1.35     |
| 35  | BB    | 1546 | G    | C6-O6   | -5.06 | 1.19        | 1.24     |
| 1   | AA    | 330  | C    | P-O5'   | -5.05 | 1.54        | 1.59     |
| 1   | AA    | 1130 | A    | O3'-P   | -5.05 | 1.55        | 1.61     |
| 1   | AA    | 1377 | A    | O3'-P   | 5.05  | 1.67        | 1.61     |
| 35  | BB    | 760  | G    | C5'-C4' | 5.05  | 1.57        | 1.51     |
| 35  | BB    | 1104 | C    | P-O5'   | -5.05 | 1.54        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1202 | G    | C2'-C1' | -5.05 | 1.47        | 1.53     |
| 35  | BB    | 1439 | A    | O4'-C1' | 5.05  | 1.48        | 1.41     |
| 35  | BB    | 1449 | G    | C3'-O3' | 5.05  | 1.49        | 1.42     |
| 35  | BB    | 1834 | U    | N1-C2   | 5.05  | 1.43        | 1.38     |
| 35  | BB    | 2096 | C    | N3-C4   | -5.05 | 1.30        | 1.33     |
| 35  | BB    | 2400 | G    | C4'-C3' | 5.05  | 1.58        | 1.53     |
| 35  | BB    | 2430 | A    | N9-C8   | -5.05 | 1.33        | 1.37     |
| 35  | BB    | 2529 | G    | N7-C5   | -5.05 | 1.36        | 1.39     |
| 35  | BB    | 2655 | G    | C2'-C1' | -5.05 | 1.47        | 1.53     |
| 1   | AA    | 890  | G    | O4'-C1' | -5.05 | 1.35        | 1.41     |
| 1   | AA    | 964  | A    | P-O5'   | -5.05 | 1.54        | 1.59     |
| 35  | BB    | 325  | G    | C2-N2   | 5.05  | 1.39        | 1.34     |
| 35  | BB    | 908  | C    | O4'-C1' | 5.05  | 1.48        | 1.41     |
| 35  | BB    | 1937 | A    | N9-C8   | 5.05  | 1.41        | 1.37     |
| 35  | BB    | 2079 | U    | N1-C6   | -5.05 | 1.33        | 1.38     |
| 35  | BB    | 2192 | U    | N3-C4   | 5.05  | 1.43        | 1.38     |
| 1   | AA    | 127  | G    | O4'-C1' | 5.05  | 1.48        | 1.41     |
| 1   | AA    | 160  | A    | P-O5'   | -5.05 | 1.54        | 1.59     |
| 1   | AA    | 588  | G    | P-O5'   | -5.05 | 1.54        | 1.59     |
| 1   | AA    | 604  | G    | C4'-O4' | -5.05 | 1.39        | 1.45     |
| 1   | AA    | 711  | G    | P-O5'   | -5.05 | 1.54        | 1.59     |
| 34  | BA    | 97   | C    | C3'-O3' | 5.05  | 1.49        | 1.42     |
| 35  | BB    | 164  | C    | C3'-O3' | 5.05  | 1.49        | 1.42     |
| 35  | BB    | 261  | G    | C6-N1   | 5.05  | 1.43        | 1.39     |
| 35  | BB    | 1275 | A    | C2-N3   | 5.05  | 1.38        | 1.33     |
| 35  | BB    | 2091 | C    | C5-C6   | 5.05  | 1.38        | 1.34     |
| 35  | BB    | 2290 | G    | C4'-C3' | 5.05  | 1.58        | 1.53     |
| 35  | BB    | 2430 | A    | N1-C2   | 5.05  | 1.38        | 1.34     |
| 1   | AA    | 65   | A    | C2-N3   | 5.05  | 1.38        | 1.33     |
| 1   | AA    | 253  | A    | C6-N6   | 5.05  | 1.38        | 1.33     |
| 1   | AA    | 371  | A    | P-O5'   | -5.05 | 1.54        | 1.59     |
| 1   | AA    | 422  | C    | C5'-C4' | 5.05  | 1.57        | 1.51     |
| 1   | AA    | 551  | U    | C5'-C4' | 5.05  | 1.57        | 1.51     |
| 1   | AA    | 987  | G    | C3'-C2' | 5.05  | 1.58        | 1.52     |
| 1   | AA    | 1238 | A    | C6-N6   | 5.05  | 1.38        | 1.33     |
| 1   | AA    | 1418 | A    | O3'-P   | -5.05 | 1.55        | 1.61     |
| 1   | AA    | 1485 | U    | C3'-O3' | -5.05 | 1.35        | 1.42     |
| 35  | BB    | 925  | A    | P-O5'   | 5.05  | 1.64        | 1.59     |
| 35  | BB    | 984  | A    | N3-C4   | -5.05 | 1.31        | 1.34     |
| 35  | BB    | 1084 | A    | C3'-C2' | 5.05  | 1.58        | 1.52     |
| 35  | BB    | 1238 | G    | C6-N1   | 5.05  | 1.43        | 1.39     |
| 35  | BB    | 1492 | G    | N9-C8   | 5.05  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1772 | A    | C6-N6   | 5.05  | 1.38        | 1.33     |
| 35  | BB    | 1800 | C    | C2-N3   | 5.05  | 1.39        | 1.35     |
| 35  | BB    | 2460 | U    | C4-C5   | -5.05 | 1.39        | 1.43     |
| 35  | BB    | 2508 | G    | C2'-C1' | -5.05 | 1.47        | 1.53     |
| 46  | BM    | 81   | ARG  | CZ-NH2  | 5.05  | 1.39        | 1.33     |
| 1   | AA    | 539  | A    | C5-C6   | -5.05 | 1.36        | 1.41     |
| 1   | AA    | 558  | G    | N7-C5   | 5.05  | 1.42        | 1.39     |
| 1   | AA    | 597  | G    | C2'-C1' | -5.05 | 1.47        | 1.53     |
| 1   | AA    | 1243 | C    | N1-C6   | -5.05 | 1.34        | 1.37     |
| 35  | BB    | 649  | G    | O4'-C1' | 5.05  | 1.48        | 1.41     |
| 35  | BB    | 1714 | U    | O3'-P   | -5.05 | 1.55        | 1.61     |
| 35  | BB    | 1955 | U    | C4'-O4' | -5.05 | 1.39        | 1.45     |
| 35  | BB    | 2188 | U    | C3'-C2' | -5.05 | 1.47        | 1.52     |
| 35  | BB    | 2880 | C    | P-O5'   | -5.05 | 1.54        | 1.59     |
| 1   | AA    | 95   | C    | C4-N4   | 5.05  | 1.38        | 1.33     |
| 1   | AA    | 201  | G    | P-O5'   | -5.05 | 1.54        | 1.59     |
| 1   | AA    | 259  | G    | C2'-C1' | 5.05  | 1.58        | 1.53     |
| 1   | AA    | 742  | G    | C3'-O3' | 5.05  | 1.49        | 1.42     |
| 1   | AA    | 831  | A    | N3-C4   | -5.05 | 1.31        | 1.34     |
| 1   | AA    | 1502 | A    | O3'-P   | -5.05 | 1.55        | 1.61     |
| 18  | AR    | 31   | TYR  | CZ-OH   | 5.05  | 1.46        | 1.37     |
| 29  | B4    | 27   | ARG  | CZ-NH2  | 5.05  | 1.39        | 1.33     |
| 35  | BB    | 201  | C    | N1-C6   | 5.05  | 1.40        | 1.37     |
| 35  | BB    | 367  | G    | C2-N2   | 5.05  | 1.39        | 1.34     |
| 35  | BB    | 815  | C    | P-OP2   | 5.05  | 1.57        | 1.49     |
| 35  | BB    | 1320 | C    | N1-C6   | -5.05 | 1.34        | 1.37     |
| 35  | BB    | 1745 | A    | N3-C4   | 5.05  | 1.37        | 1.34     |
| 35  | BB    | 2023 | C    | C2'-C1' | -5.05 | 1.47        | 1.53     |
| 35  | BB    | 2070 | A    | N3-C4   | -5.05 | 1.31        | 1.34     |
| 35  | BB    | 2114 | A    | C6-N1   | 5.05  | 1.39        | 1.35     |
| 1   | AA    | 498  | A    | N9-C4   | 5.04  | 1.40        | 1.37     |
| 1   | AA    | 589  | U    | C2'-O2' | -5.04 | 1.35        | 1.41     |
| 1   | AA    | 771  | G    | O3'-P   | -5.04 | 1.55        | 1.61     |
| 1   | AA    | 896  | C    | N3-C4   | 5.04  | 1.37        | 1.33     |
| 1   | AA    | 1415 | G    | C2'-C1' | -5.04 | 1.47        | 1.53     |
| 30  | B5    | 190  | GLU  | CD-OE2  | 5.04  | 1.31        | 1.25     |
| 35  | BB    | 1326 | U    | N1-C2   | 5.04  | 1.43        | 1.38     |
| 35  | BB    | 1910 | G    | C5-C4   | 5.04  | 1.41        | 1.38     |
| 37  | BD    | 83   | ARG  | CZ-NH2  | 5.04  | 1.39        | 1.33     |
| 1   | AA    | 129  | A    | C5-C4   | 5.04  | 1.42        | 1.38     |
| 1   | AA    | 191  | G    | C3'-C2' | 5.04  | 1.58        | 1.52     |
| 1   | AA    | 589  | U    | C4'-C3' | 5.04  | 1.58        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 763  | G    | C2'-C1' | -5.04 | 1.47        | 1.53     |
| 1   | AA    | 1132 | C    | N1-C6   | 5.04  | 1.40        | 1.37     |
| 34  | BA    | 72   | G    | C5'-C4' | 5.04  | 1.57        | 1.51     |
| 35  | BB    | 29   | U    | C2'-O2' | -5.04 | 1.35        | 1.41     |
| 35  | BB    | 360  | U    | C2-N3   | 5.04  | 1.41        | 1.37     |
| 35  | BB    | 466  | A    | O4'-C1' | -5.04 | 1.35        | 1.41     |
| 35  | BB    | 843  | G    | N1-C2   | 5.04  | 1.41        | 1.37     |
| 35  | BB    | 1330 | C    | N3-C4   | 5.04  | 1.37        | 1.33     |
| 35  | BB    | 1341 | G    | C2-N2   | 5.04  | 1.39        | 1.34     |
| 35  | BB    | 1745 | A    | C5-C4   | 5.04  | 1.42        | 1.38     |
| 35  | BB    | 1961 | C    | N1-C2   | -5.04 | 1.35        | 1.40     |
| 35  | BB    | 2121 | G    | N9-C4   | -5.04 | 1.33        | 1.38     |
| 35  | BB    | 2543 | G    | C2-N3   | 5.04  | 1.36        | 1.32     |
| 49  | BP    | 71   | ARG  | NE-CZ   | 5.04  | 1.39        | 1.33     |
| 1   | AA    | 13   | U    | C4'-O4' | -5.04 | 1.39        | 1.45     |
| 1   | AA    | 40   | C    | C4-N4   | 5.04  | 1.38        | 1.33     |
| 1   | AA    | 44   | A    | N3-C4   | -5.04 | 1.31        | 1.34     |
| 1   | AA    | 45   | G    | N9-C8   | -5.04 | 1.34        | 1.37     |
| 1   | AA    | 166  | U    | N3-C4   | 5.04  | 1.43        | 1.38     |
| 1   | AA    | 776  | G    | P-O5'   | -5.04 | 1.54        | 1.59     |
| 1   | AA    | 808  | C    | C5'-C4' | 5.04  | 1.57        | 1.51     |
| 1   | AA    | 814  | A    | C6-N6   | -5.04 | 1.29        | 1.33     |
| 21  | AU    | 23   | GLU  | CD-OE2  | 5.04  | 1.31        | 1.25     |
| 35  | BB    | 87   | U    | C4'-C3' | -5.04 | 1.47        | 1.52     |
| 35  | BB    | 971  | G    | C4'-C3' | -5.04 | 1.47        | 1.52     |
| 35  | BB    | 1422 | G    | N1-C2   | -5.04 | 1.33        | 1.37     |
| 35  | BB    | 1592 | C    | N3-C4   | 5.04  | 1.37        | 1.33     |
| 35  | BB    | 1732 | C    | C3'-C2' | -5.04 | 1.47        | 1.52     |
| 35  | BB    | 2027 | G    | P-O5'   | 5.04  | 1.64        | 1.59     |
| 35  | BB    | 2588 | G    | C5'-C4' | 5.04  | 1.57        | 1.51     |
| 1   | AA    | 393  | A    | C2'-C1' | -5.04 | 1.47        | 1.53     |
| 1   | AA    | 1049 | U    | N3-C4   | 5.04  | 1.43        | 1.38     |
| 4   | AD    | 169  | TRP  | CD2-CE3 | -5.04 | 1.32        | 1.40     |
| 35  | BB    | 1639 | C    | N1-C2   | -5.04 | 1.35        | 1.40     |
| 35  | BB    | 2120 | G    | C6-N1   | -5.04 | 1.36        | 1.39     |
| 35  | BB    | 2483 | C    | C4-C5   | 5.04  | 1.47        | 1.43     |
| 35  | BB    | 2511 | U    | C2-N3   | 5.04  | 1.41        | 1.37     |
| 1   | AA    | 138  | G    | N9-C8   | 5.04  | 1.41        | 1.37     |
| 1   | AA    | 246  | A    | C4'-O4' | 5.04  | 1.52        | 1.45     |
| 1   | AA    | 380  | G    | P-O5'   | -5.04 | 1.54        | 1.59     |
| 1   | AA    | 432  | A    | O4'-C1' | -5.04 | 1.35        | 1.41     |
| 1   | AA    | 500  | G    | C5'-C4' | 5.04  | 1.57        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 646  | G    | C5-C4   | 5.04  | 1.41        | 1.38     |
| 1   | AA    | 1024 | G    | N9-C8   | -5.04 | 1.34        | 1.37     |
| 22  | AV    | 67   | G    | C6-N1   | 5.04  | 1.43        | 1.39     |
| 35  | BB    | 407  | G    | N3-C4   | 5.04  | 1.39        | 1.35     |
| 35  | BB    | 688  | U    | C2-N3   | 5.04  | 1.41        | 1.37     |
| 35  | BB    | 796  | C    | N3-C4   | 5.04  | 1.37        | 1.33     |
| 35  | BB    | 1099 | G    | C2-N2   | -5.04 | 1.29        | 1.34     |
| 35  | BB    | 1558 | C    | C4'-O4' | -5.04 | 1.39        | 1.45     |
| 35  | BB    | 1701 | A    | O3'-P   | -5.04 | 1.55        | 1.61     |
| 35  | BB    | 1800 | C    | C5-C6   | 5.04  | 1.38        | 1.34     |
| 35  | BB    | 2064 | C    | P-O5'   | -5.04 | 1.54        | 1.59     |
| 35  | BB    | 2439 | A    | N7-C5   | -5.04 | 1.36        | 1.39     |
| 35  | BB    | 2594 | C    | C3'-C2' | -5.04 | 1.47        | 1.52     |
| 35  | BB    | 2755 | C    | C3'-C2' | 5.04  | 1.58        | 1.52     |
| 36  | BC    | 41   | GLY  | CA-C    | -5.04 | 1.43        | 1.51     |
| 44  | BK    | 30   | ARG  | CZ-NH1  | 5.04  | 1.39        | 1.33     |
| 2   | AB    | 64   | GLY  | CA-C    | -5.04 | 1.43        | 1.51     |
| 35  | BB    | 1094 | U    | C2-N3   | 5.04  | 1.41        | 1.37     |
| 35  | BB    | 1536 | C    | O3'-P   | -5.04 | 1.55        | 1.61     |
| 35  | BB    | 2201 | G    | N7-C5   | -5.04 | 1.36        | 1.39     |
| 35  | BB    | 2713 | U    | C3'-O3' | -5.04 | 1.35        | 1.42     |
| 55  | BW    | 7    | GLU  | CA-C    | -5.04 | 1.39        | 1.52     |
| 1   | AA    | 1310 | G    | C8-N7   | 5.04  | 1.33        | 1.30     |
| 11  | AK    | 43   | TRP  | CA-CB   | 5.04  | 1.65        | 1.53     |
| 35  | BB    | 124  | G    | C2-N3   | 5.04  | 1.36        | 1.32     |
| 35  | BB    | 563  | A    | C6-N6   | 5.04  | 1.38        | 1.33     |
| 35  | BB    | 771  | G    | N1-C2   | 5.04  | 1.41        | 1.37     |
| 35  | BB    | 799  | G    | C2'-C1' | -5.04 | 1.47        | 1.53     |
| 35  | BB    | 1131 | G    | N3-C4   | -5.04 | 1.31        | 1.35     |
| 35  | BB    | 1195 | G    | O4'-C1' | 5.04  | 1.48        | 1.41     |
| 35  | BB    | 1287 | A    | C8-N7   | -5.04 | 1.28        | 1.31     |
| 35  | BB    | 1416 | G    | O3'-P   | -5.04 | 1.55        | 1.61     |
| 35  | BB    | 1438 | U    | N3-C4   | 5.04  | 1.43        | 1.38     |
| 35  | BB    | 1884 | G    | N1-C2   | 5.04  | 1.41        | 1.37     |
| 35  | BB    | 2347 | C    | N3-C4   | 5.04  | 1.37        | 1.33     |
| 35  | BB    | 2433 | A    | C6-N6   | 5.04  | 1.38        | 1.33     |
| 35  | BB    | 2500 | U    | C4'-C3' | -5.04 | 1.47        | 1.52     |
| 35  | BB    | 2731 | G    | P-O5'   | -5.04 | 1.54        | 1.59     |
| 35  | BB    | 2770 | G    | P-O5'   | -5.04 | 1.54        | 1.59     |
| 1   | AA    | 163  | C    | N1-C6   | -5.03 | 1.34        | 1.37     |
| 1   | AA    | 505  | G    | N9-C4   | -5.03 | 1.33        | 1.38     |
| 1   | AA    | 628  | G    | N7-C5   | -5.03 | 1.36        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 1221 | G    | C3'-C2' | -5.03 | 1.47        | 1.52     |
| 1   | AA    | 1301 | U    | C1'-N1  | 5.03  | 1.56        | 1.48     |
| 35  | BB    | 1374 | G    | C3'-C2' | -5.03 | 1.47        | 1.52     |
| 35  | BB    | 1408 | G    | O5'-C5' | -5.03 | 1.34        | 1.42     |
| 35  | BB    | 1870 | C    | C5'-C4' | 5.03  | 1.57        | 1.51     |
| 35  | BB    | 2291 | U    | C1'-N1  | -5.03 | 1.39        | 1.46     |
| 35  | BB    | 2292 | U    | C5-C6   | 5.03  | 1.38        | 1.34     |
| 35  | BB    | 2343 | U    | N3-C4   | 5.03  | 1.43        | 1.38     |
| 35  | BB    | 2699 | C    | C4-C5   | 5.03  | 1.47        | 1.43     |
| 48  | BO    | 86   | GLY  | CA-C    | -5.03 | 1.43        | 1.51     |
| 5   | AE    | 17   | VAL  | CB-CG2  | 5.03  | 1.63        | 1.52     |
| 35  | BB    | 170  | U    | N1-C6   | 5.03  | 1.42        | 1.38     |
| 35  | BB    | 1134 | A    | C5-C6   | 5.03  | 1.45        | 1.41     |
| 35  | BB    | 1424 | G    | N1-C2   | 5.03  | 1.41        | 1.37     |
| 35  | BB    | 1474 | U    | O3'-P   | -5.03 | 1.55        | 1.61     |
| 35  | BB    | 1695 | G    | C4'-O4' | 5.03  | 1.52        | 1.45     |
| 35  | BB    | 2280 | G    | C2'-O2' | -5.03 | 1.35        | 1.41     |
| 1   | AA    | 118  | U    | N1-C6   | 5.03  | 1.42        | 1.38     |
| 1   | AA    | 456  | A    | P-O5'   | -5.03 | 1.54        | 1.59     |
| 1   | AA    | 607  | A    | N7-C5   | -5.03 | 1.36        | 1.39     |
| 1   | AA    | 611  | C    | C4-N4   | 5.03  | 1.38        | 1.33     |
| 1   | AA    | 1112 | C    | C2'-C1' | -5.03 | 1.47        | 1.53     |
| 34  | BA    | 10   | G    | C3'-C2' | 5.03  | 1.58        | 1.52     |
| 35  | BB    | 313  | G    | N1-C2   | 5.03  | 1.41        | 1.37     |
| 35  | BB    | 431  | U    | N1-C2   | 5.03  | 1.43        | 1.38     |
| 35  | BB    | 532  | A    | C2'-C1' | -5.03 | 1.47        | 1.53     |
| 35  | BB    | 588  | U    | O4'-C1' | -5.03 | 1.35        | 1.41     |
| 35  | BB    | 742  | A    | C3'-C2' | -5.03 | 1.47        | 1.52     |
| 35  | BB    | 1254 | A    | N3-C4   | 5.03  | 1.37        | 1.34     |
| 35  | BB    | 1337 | G    | N9-C4   | -5.03 | 1.33        | 1.38     |
| 35  | BB    | 1817 | G    | C5-C6   | -5.03 | 1.37        | 1.42     |
| 35  | BB    | 1848 | A    | C5-C4   | 5.03  | 1.42        | 1.38     |
| 35  | BB    | 2145 | C    | C4-C5   | -5.03 | 1.39        | 1.43     |
| 35  | BB    | 2427 | C    | P-O5'   | 5.03  | 1.64        | 1.59     |
| 35  | BB    | 2735 | G    | N3-C4   | 5.03  | 1.39        | 1.35     |
| 1   | AA    | 404  | G    | P-O5'   | 5.03  | 1.64        | 1.59     |
| 34  | BA    | 115  | A    | N9-C4   | 5.03  | 1.40        | 1.37     |
| 35  | BB    | 997  | G    | O3'-P   | -5.03 | 1.55        | 1.61     |
| 35  | BB    | 1333 | G    | C2'-C1' | -5.03 | 1.47        | 1.53     |
| 35  | BB    | 1584 | U    | C3'-C2' | 5.03  | 1.58        | 1.52     |
| 35  | BB    | 2741 | A    | C3'-C2' | -5.03 | 1.47        | 1.52     |
| 1   | AA    | 230  | G    | C5-C6   | 5.03  | 1.47        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 426  | U    | C2-O2   | 5.03  | 1.26        | 1.22     |
| 1   | AA    | 851  | G    | C6-N1   | -5.03 | 1.36        | 1.39     |
| 1   | AA    | 1005 | A    | C6-N6   | 5.03  | 1.38        | 1.33     |
| 1   | AA    | 1085 | U    | P-O5'   | -5.03 | 1.54        | 1.59     |
| 1   | AA    | 1358 | U    | O4'-C1' | -5.03 | 1.35        | 1.41     |
| 35  | BB    | 323  | C    | C2'-C1' | -5.03 | 1.47        | 1.53     |
| 35  | BB    | 501  | A    | C5-C6   | -5.03 | 1.36        | 1.41     |
| 35  | BB    | 774  | G    | N7-C5   | -5.03 | 1.36        | 1.39     |
| 35  | BB    | 1127 | A    | C6-N1   | 5.03  | 1.39        | 1.35     |
| 35  | BB    | 1361 | G    | C2'-C1' | -5.03 | 1.47        | 1.53     |
| 35  | BB    | 1622 | G    | C6-N1   | 5.03  | 1.43        | 1.39     |
| 35  | BB    | 2215 | C    | O3'-P   | -5.03 | 1.55        | 1.61     |
| 35  | BB    | 2530 | A    | N1-C2   | 5.03  | 1.38        | 1.34     |
| 1   | AA    | 86   | G    | O4'-C1' | 5.03  | 1.48        | 1.41     |
| 1   | AA    | 172  | A    | N9-C4   | -5.03 | 1.34        | 1.37     |
| 1   | AA    | 319  | G    | C2-N3   | 5.03  | 1.36        | 1.32     |
| 1   | AA    | 951  | G    | C5-C4   | 5.03  | 1.41        | 1.38     |
| 1   | AA    | 1451 | U    | C3'-C2' | 5.03  | 1.58        | 1.52     |
| 1   | AA    | 1466 | C    | P-O5'   | 5.03  | 1.64        | 1.59     |
| 22  | AV    | 69   | G    | N7-C5   | -5.03 | 1.36        | 1.39     |
| 34  | BA    | 87   | U    | N3-C4   | 5.03  | 1.43        | 1.38     |
| 35  | BB    | 645  | C    | C3'-C2' | -5.03 | 1.47        | 1.52     |
| 35  | BB    | 995  | C    | C3'-C2' | 5.03  | 1.58        | 1.52     |
| 35  | BB    | 1589 | U    | P-O5'   | 5.03  | 1.64        | 1.59     |
| 35  | BB    | 1699 | G    | C6-N1   | 5.03  | 1.43        | 1.39     |
| 35  | BB    | 1744 | A    | O3'-P   | -5.03 | 1.55        | 1.61     |
| 35  | BB    | 2168 | G    | C3'-O3' | 5.03  | 1.49        | 1.42     |
| 1   | AA    | 47   | C    | N3-C4   | 5.02  | 1.37        | 1.33     |
| 1   | AA    | 600  | A    | C8-N7   | 5.02  | 1.35        | 1.31     |
| 1   | AA    | 1012 | A    | N9-C4   | 5.02  | 1.40        | 1.37     |
| 34  | BA    | 5    | U    | N1-C2   | 5.02  | 1.43        | 1.38     |
| 35  | BB    | 1032 | A    | C2'-C1' | -5.02 | 1.47        | 1.53     |
| 53  | BT    | 52   | GLU  | CD-OE1  | 5.02  | 1.31        | 1.25     |
| 1   | AA    | 163  | C    | C4'-O4' | 5.02  | 1.52        | 1.45     |
| 1   | AA    | 531  | U    | C5-C6   | 5.02  | 1.38        | 1.34     |
| 1   | AA    | 624  | C    | C3'-C2' | -5.02 | 1.47        | 1.52     |
| 1   | AA    | 939  | G    | N9-C4   | -5.02 | 1.33        | 1.38     |
| 1   | AA    | 1049 | U    | C1'-N1  | 5.02  | 1.56        | 1.48     |
| 1   | AA    | 1056 | U    | C4-C5   | 5.02  | 1.48        | 1.43     |
| 1   | AA    | 1231 | G    | C2'-C1' | -5.02 | 1.47        | 1.53     |
| 1   | AA    | 1449 | C    | N3-C4   | -5.02 | 1.30        | 1.33     |
| 13  | AM    | 92   | ARG  | NE-CZ   | 5.02  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 157  | C    | C2-N3   | -5.02 | 1.31        | 1.35     |
| 35  | BB    | 235  | U    | N3-C4   | 5.02  | 1.43        | 1.38     |
| 35  | BB    | 274  | C    | O4'-C1' | 5.02  | 1.48        | 1.41     |
| 35  | BB    | 495  | G    | C5'-C4' | 5.02  | 1.57        | 1.51     |
| 35  | BB    | 738  | G    | N9-C8   | 5.02  | 1.41        | 1.37     |
| 35  | BB    | 1284 | A    | N9-C4   | 5.02  | 1.40        | 1.37     |
| 35  | BB    | 1877 | A    | C5-C4   | 5.02  | 1.42        | 1.38     |
| 35  | BB    | 2555 | U    | C1'-N1  | 5.02  | 1.56        | 1.48     |
| 35  | BB    | 2590 | A    | N9-C8   | -5.02 | 1.33        | 1.37     |
| 35  | BB    | 19   | A    | C4'-C3' | -5.02 | 1.47        | 1.52     |
| 35  | BB    | 586  | A    | O4'-C1' | -5.02 | 1.35        | 1.41     |
| 35  | BB    | 1541 | C    | C2'-C1' | -5.02 | 1.47        | 1.53     |
| 1   | AA    | 120  | A    | C8-N7   | -5.02 | 1.28        | 1.31     |
| 1   | AA    | 125  | U    | P-O5'   | -5.02 | 1.54        | 1.59     |
| 1   | AA    | 432  | A    | O3'-P   | -5.02 | 1.55        | 1.61     |
| 1   | AA    | 661  | G    | N9-C4   | 5.02  | 1.42        | 1.38     |
| 1   | AA    | 949  | A    | C6-N1   | 5.02  | 1.39        | 1.35     |
| 1   | AA    | 1454 | G    | C6-N1   | 5.02  | 1.43        | 1.39     |
| 1   | AA    | 1457 | G    | C6-N1   | 5.02  | 1.43        | 1.39     |
| 13  | AM    | 1    | ALA  | N-CA    | 5.02  | 1.56        | 1.46     |
| 34  | BA    | 8    | C    | C2'-C1' | -5.02 | 1.47        | 1.53     |
| 35  | BB    | 36   | G    | C4'-C3' | -5.02 | 1.47        | 1.52     |
| 35  | BB    | 240  | C    | C4-C5   | 5.02  | 1.47        | 1.43     |
| 35  | BB    | 380  | G    | C1'-N9  | -5.02 | 1.39        | 1.46     |
| 35  | BB    | 594  | U    | O5'-C5' | 5.02  | 1.52        | 1.44     |
| 35  | BB    | 855  | G    | C5'-C4' | 5.02  | 1.57        | 1.51     |
| 35  | BB    | 1428 | C    | C4-N4   | 5.02  | 1.38        | 1.33     |
| 35  | BB    | 1678 | A    | C5-C4   | -5.02 | 1.35        | 1.38     |
| 35  | BB    | 2358 | A    | N9-C8   | 5.02  | 1.41        | 1.37     |
| 36  | BC    | 225  | ASN  | CG-ND2  | 5.02  | 1.45        | 1.32     |
| 1   | AA    | 406  | G    | C2-N3   | 5.02  | 1.36        | 1.32     |
| 1   | AA    | 903  | G    | C8-N7   | -5.02 | 1.27        | 1.30     |
| 1   | AA    | 1089 | G    | N9-C4   | -5.02 | 1.33        | 1.38     |
| 1   | AA    | 1208 | C    | P-O5'   | -5.02 | 1.54        | 1.59     |
| 1   | AA    | 1262 | C    | N3-C4   | 5.02  | 1.37        | 1.33     |
| 1   | AA    | 1277 | C    | O4'-C1' | -5.02 | 1.35        | 1.41     |
| 5   | AE    | 141  | ASP  | CB-CG   | 5.02  | 1.62        | 1.51     |
| 35  | BB    | 224  | U    | C4'-C3' | -5.02 | 1.47        | 1.52     |
| 35  | BB    | 469  | G    | N3-C4   | -5.02 | 1.31        | 1.35     |
| 35  | BB    | 763  | G    | C1'-N9  | -5.02 | 1.39        | 1.46     |
| 35  | BB    | 1467 | U    | C4-C5   | 5.02  | 1.48        | 1.43     |
| 35  | BB    | 1729 | U    | C4'-O4' | -5.02 | 1.39        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2019 | A    | C5'-C4' | 5.02  | 1.57        | 1.51     |
| 35  | BB    | 2086 | U    | C1'-N1  | 5.02  | 1.56        | 1.48     |
| 35  | BB    | 2377 | A    | C6-N6   | 5.02  | 1.38        | 1.33     |
| 35  | BB    | 2480 | C    | C4-N4   | 5.02  | 1.38        | 1.33     |
| 1   | AA    | 418  | C    | O3'-P   | -5.02 | 1.55        | 1.61     |
| 1   | AA    | 1333 | A    | C6-N1   | 5.02  | 1.39        | 1.35     |
| 35  | BB    | 42   | A    | C2-N3   | 5.02  | 1.38        | 1.33     |
| 35  | BB    | 45   | G    | N1-C2   | 5.02  | 1.41        | 1.37     |
| 35  | BB    | 327  | G    | N3-C4   | -5.02 | 1.31        | 1.35     |
| 35  | BB    | 333  | G    | O3'-P   | -5.02 | 1.55        | 1.61     |
| 35  | BB    | 798  | G    | O3'-P   | -5.02 | 1.55        | 1.61     |
| 35  | BB    | 1303 | G    | C4'-O4' | -5.02 | 1.39        | 1.45     |
| 35  | BB    | 1567 | G    | O3'-P   | -5.02 | 1.55        | 1.61     |
| 35  | BB    | 2446 | G    | C6-O6   | -5.02 | 1.19        | 1.24     |
| 1   | AA    | 72   | A    | N3-C4   | -5.01 | 1.31        | 1.34     |
| 1   | AA    | 113  | G    | C6-N1   | 5.01  | 1.43        | 1.39     |
| 1   | AA    | 240  | G    | N9-C4   | -5.01 | 1.33        | 1.38     |
| 1   | AA    | 244  | U    | O3'-P   | -5.01 | 1.55        | 1.61     |
| 1   | AA    | 405  | U    | N3-C4   | 5.01  | 1.43        | 1.38     |
| 1   | AA    | 537  | G    | C3'-C2' | -5.01 | 1.47        | 1.52     |
| 1   | AA    | 937  | A    | O3'-P   | -5.01 | 1.55        | 1.61     |
| 1   | AA    | 1088 | G    | N9-C8   | -5.01 | 1.34        | 1.37     |
| 35  | BB    | 5    | A    | N7-C5   | -5.01 | 1.36        | 1.39     |
| 35  | BB    | 188  | G    | C5-C6   | 5.01  | 1.47        | 1.42     |
| 35  | BB    | 610  | C    | C5'-C4' | 5.01  | 1.57        | 1.51     |
| 35  | BB    | 1205 | A    | C5-C4   | -5.01 | 1.35        | 1.38     |
| 35  | BB    | 1399 | C    | N3-C4   | 5.01  | 1.37        | 1.33     |
| 35  | BB    | 2153 | C    | C4-C5   | -5.01 | 1.39        | 1.43     |
| 35  | BB    | 2167 | U    | C2-N3   | 5.01  | 1.41        | 1.37     |
| 35  | BB    | 2175 | C    | N3-C4   | 5.01  | 1.37        | 1.33     |
| 35  | BB    | 2205 | A    | O3'-P   | -5.01 | 1.55        | 1.61     |
| 35  | BB    | 2315 | G    | C2-N2   | 5.01  | 1.39        | 1.34     |
| 35  | BB    | 2451 | A    | C5-C4   | 5.01  | 1.42        | 1.38     |
| 35  | BB    | 2486 | C    | C4'-O4' | 5.01  | 1.52        | 1.45     |
| 37  | BD    | 46   | ARG  | CZ-NH1  | 5.01  | 1.39        | 1.33     |
| 1   | AA    | 146  | G    | N1-C2   | 5.01  | 1.41        | 1.37     |
| 1   | AA    | 324  | G    | C6-N1   | 5.01  | 1.43        | 1.39     |
| 1   | AA    | 953  | G    | C6-N1   | 5.01  | 1.43        | 1.39     |
| 1   | AA    | 1227 | A    | C5'-C4' | 5.01  | 1.57        | 1.51     |
| 34  | BA    | 71   | C    | N1-C6   | -5.01 | 1.34        | 1.37     |
| 35  | BB    | 1139 | G    | C2-N2   | -5.01 | 1.29        | 1.34     |
| 35  | BB    | 1907 | G    | N1-C2   | 5.01  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2076 | U    | C4'-C3' | 5.01  | 1.58        | 1.53     |
| 35  | BB    | 2338 | C    | C4-C5   | 5.01  | 1.47        | 1.43     |
| 1   | AA    | 64   | G    | C6-O6   | 5.01  | 1.28        | 1.24     |
| 1   | AA    | 834  | U    | C2-N3   | 5.01  | 1.41        | 1.37     |
| 1   | AA    | 1249 | C    | N3-C4   | 5.01  | 1.37        | 1.33     |
| 8   | AH    | 85   | TYR  | CG-CD1  | 5.01  | 1.45        | 1.39     |
| 35  | BB    | 71   | A    | O4'-C1' | 5.01  | 1.48        | 1.41     |
| 35  | BB    | 276  | U    | C3'-C2' | 5.01  | 1.58        | 1.52     |
| 35  | BB    | 673  | C    | C2-N3   | 5.01  | 1.39        | 1.35     |
| 35  | BB    | 1993 | U    | N1-C6   | 5.01  | 1.42        | 1.38     |
| 35  | BB    | 2538 | C    | C2-N3   | 5.01  | 1.39        | 1.35     |
| 35  | BB    | 2646 | C    | C2'-C1' | -5.01 | 1.47        | 1.53     |
| 35  | BB    | 2714 | G    | C2-N3   | 5.01  | 1.36        | 1.32     |
| 35  | BB    | 2726 | A    | C8-N7   | -5.01 | 1.28        | 1.31     |
| 47  | BN    | 22   | ARG  | NE-CZ   | 5.01  | 1.39        | 1.33     |
| 1   | AA    | 141  | G    | N1-C2   | -5.01 | 1.33        | 1.37     |
| 1   | AA    | 689  | C    | C4'-C3' | -5.01 | 1.47        | 1.52     |
| 1   | AA    | 1012 | A    | N3-C4   | -5.01 | 1.31        | 1.34     |
| 1   | AA    | 1381 | U    | C2-N3   | -5.01 | 1.34        | 1.37     |
| 34  | BA    | 31   | C    | C4'-C3' | -5.01 | 1.47        | 1.52     |
| 35  | BB    | 101  | A    | N3-C4   | 5.01  | 1.37        | 1.34     |
| 35  | BB    | 364  | C    | C4-N4   | 5.01  | 1.38        | 1.33     |
| 35  | BB    | 1113 | U    | C4-C5   | 5.01  | 1.48        | 1.43     |
| 35  | BB    | 1320 | C    | C3'-C2' | -5.01 | 1.47        | 1.52     |
| 35  | BB    | 1583 | A    | C8-N7   | -5.01 | 1.28        | 1.31     |
| 35  | BB    | 2120 | G    | O5'-C5' | 5.01  | 1.52        | 1.44     |
| 35  | BB    | 2204 | G    | N9-C4   | -5.01 | 1.33        | 1.38     |
| 35  | BB    | 2461 | A    | C6-N6   | 5.01  | 1.38        | 1.33     |
| 35  | BB    | 2491 | U    | O4'-C1' | 5.01  | 1.48        | 1.41     |
| 1   | AA    | 408  | A    | C4'-O4' | -5.01 | 1.39        | 1.45     |
| 4   | AD    | 145  | ARG  | NE-CZ   | 5.01  | 1.39        | 1.33     |
| 35  | BB    | 800  | A    | N1-C2   | -5.01 | 1.29        | 1.34     |
| 35  | BB    | 1730 | C    | C2-N3   | -5.01 | 1.31        | 1.35     |
| 35  | BB    | 1827 | U    | C2-N3   | 5.01  | 1.41        | 1.37     |
| 1   | AA    | 269  | C    | C4-N4   | 5.01  | 1.38        | 1.33     |
| 1   | AA    | 423  | G    | C8-N7   | 5.01  | 1.33        | 1.30     |
| 1   | AA    | 986  | U    | N1-C6   | 5.01  | 1.42        | 1.38     |
| 1   | AA    | 1502 | A    | N1-C2   | -5.01 | 1.29        | 1.34     |
| 7   | AG    | 95   | ARG  | CZ-NH2  | 5.01  | 1.39        | 1.33     |
| 35  | BB    | 4    | U    | C2'-O2' | 5.01  | 1.48        | 1.41     |
| 35  | BB    | 347  | A    | C4'-C3' | 5.01  | 1.58        | 1.53     |
| 35  | BB    | 905  | A    | N9-C4   | 5.01  | 1.40        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 1249 | U    | C2'-C1' | -5.01 | 1.47        | 1.53     |
| 35  | BB    | 1569 | A    | C6-N1   | 5.01  | 1.39        | 1.35     |
| 35  | BB    | 2126 | A    | N7-C5   | -5.01 | 1.36        | 1.39     |
| 35  | BB    | 2315 | G    | C2-N3   | 5.01  | 1.36        | 1.32     |
| 35  | BB    | 2547 | A    | C2-N3   | 5.01  | 1.38        | 1.33     |
| 35  | BB    | 2849 | U    | O4'-C1' | -5.01 | 1.35        | 1.41     |
| 1   | AA    | 1170 | A    | O4'-C1' | -5.00 | 1.35        | 1.41     |
| 1   | AA    | 1214 | C    | C1'-N1  | 5.00  | 1.56        | 1.48     |
| 1   | AA    | 1473 | G    | N9-C4   | -5.00 | 1.33        | 1.38     |
| 35  | BB    | 1479 | G    | N9-C8   | 5.00  | 1.41        | 1.37     |
| 35  | BB    | 2862 | G    | O3'-P   | -5.00 | 1.55        | 1.61     |
| 1   | AA    | 285  | C    | C2-O2   | -5.00 | 1.20        | 1.24     |
| 1   | AA    | 431  | A    | C5-C6   | 5.00  | 1.45        | 1.41     |
| 1   | AA    | 431  | A    | N1-C2   | 5.00  | 1.38        | 1.34     |
| 1   | AA    | 816  | A    | N1-C2   | -5.00 | 1.29        | 1.34     |
| 1   | AA    | 1262 | C    | O3'-P   | -5.00 | 1.55        | 1.61     |
| 1   | AA    | 1411 | C    | N1-C6   | 5.00  | 1.40        | 1.37     |
| 35  | BB    | 423  | A    | O3'-P   | -5.00 | 1.55        | 1.61     |
| 35  | BB    | 581  | C    | P-O5'   | -5.00 | 1.54        | 1.59     |
| 35  | BB    | 589  | U    | C2-O2   | 5.00  | 1.26        | 1.22     |
| 35  | BB    | 633  | A    | P-O5'   | -5.00 | 1.54        | 1.59     |
| 35  | BB    | 766  | U    | N3-C4   | 5.00  | 1.43        | 1.38     |
| 35  | BB    | 826  | U    | N1-C6   | 5.00  | 1.42        | 1.38     |
| 35  | BB    | 2812 | G    | C5'-C4' | 5.00  | 1.57        | 1.51     |
| 35  | BB    | 2839 | G    | C2'-C1' | -5.00 | 1.47        | 1.53     |
| 35  | BB    | 2879 | A    | C5-C6   | -5.00 | 1.36        | 1.41     |
| 1   | AA    | 16   | A    | N9-C4   | -5.00 | 1.34        | 1.37     |
| 1   | AA    | 130  | A    | C2-N3   | 5.00  | 1.38        | 1.33     |
| 1   | AA    | 422  | C    | P-O5'   | -5.00 | 1.54        | 1.59     |
| 1   | AA    | 1069 | C    | C3'-C2' | -5.00 | 1.47        | 1.52     |
| 1   | AA    | 1465 | A    | C6-N1   | -5.00 | 1.32        | 1.35     |
| 35  | BB    | 14   | A    | C3'-C2' | -5.00 | 1.47        | 1.52     |
| 35  | BB    | 41   | C    | C1'-N1  | 5.00  | 1.56        | 1.48     |
| 35  | BB    | 175  | G    | C2-N3   | 5.00  | 1.36        | 1.32     |
| 35  | BB    | 233  | A    | N1-C2   | 5.00  | 1.38        | 1.34     |
| 35  | BB    | 251  | A    | C5'-C4' | -5.00 | 1.45        | 1.51     |
| 35  | BB    | 389  | G    | N3-C4   | -5.00 | 1.31        | 1.35     |
| 35  | BB    | 410  | G    | N3-C4   | -5.00 | 1.31        | 1.35     |
| 35  | BB    | 429  | A    | C2'-C1' | -5.00 | 1.47        | 1.53     |
| 35  | BB    | 1685 | C    | C2-N3   | 5.00  | 1.39        | 1.35     |
| 35  | BB    | 1836 | C    | C5'-C4' | 5.00  | 1.57        | 1.51     |
| 35  | BB    | 2221 | G    | P-O5'   | -5.00 | 1.54        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | BB    | 2522 | U    | C2'-C1' | -5.00 | 1.47        | 1.53     |
| 35  | BB    | 2613 | U    | C4-C5   | 5.00  | 1.48        | 1.43     |

All (26300) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1   | AA    | 753  | A    | N1-C6-N6  | 30.52  | 136.91      | 118.60   |
| 35  | BB    | 666  | A    | N1-C6-N6  | 26.10  | 134.26      | 118.60   |
| 35  | BB    | 533  | G    | N1-C6-O6  | 25.90  | 135.44      | 119.90   |
| 1   | AA    | 242  | G    | C5-C6-O6  | -25.60 | 113.24      | 128.60   |
| 35  | BB    | 1014 | A    | N1-C6-N6  | 25.57  | 133.94      | 118.60   |
| 1   | AA    | 977  | A    | N1-C6-N6  | 25.54  | 133.92      | 118.60   |
| 35  | BB    | 1566 | A    | N1-C6-N6  | 25.23  | 133.74      | 118.60   |
| 1   | AA    | 1507 | A    | N1-C6-N6  | 24.69  | 133.41      | 118.60   |
| 35  | BB    | 1347 | A    | N1-C6-N6  | 24.39  | 133.23      | 118.60   |
| 35  | BB    | 315  | G    | N1-C6-O6  | 24.16  | 134.40      | 119.90   |
| 1   | AA    | 293  | G    | N1-C6-O6  | 24.08  | 134.35      | 119.90   |
| 35  | BB    | 1358 | G    | C5-C6-O6  | -23.83 | 114.30      | 128.60   |
| 35  | BB    | 2119 | A    | N1-C6-N6  | 23.80  | 132.88      | 118.60   |
| 1   | AA    | 85   | U    | P-O3'-C3' | 23.75  | 148.21      | 119.70   |
| 35  | BB    | 272  | A    | N1-C6-N6  | 23.55  | 132.73      | 118.60   |
| 1   | AA    | 1111 | A    | N1-C6-N6  | 23.52  | 132.71      | 118.60   |
| 35  | BB    | 730  | A    | N1-C6-N6  | 23.46  | 132.68      | 118.60   |
| 35  | BB    | 1622 | G    | N1-C6-O6  | 23.36  | 133.92      | 119.90   |
| 35  | BB    | 217  | A    | N1-C6-N6  | 23.08  | 132.45      | 118.60   |
| 1   | AA    | 1396 | A    | N1-C6-N6  | 23.03  | 132.42      | 118.60   |
| 1   | AA    | 164  | G    | C5-C6-O6  | -22.97 | 114.82      | 128.60   |
| 35  | BB    | 647  | G    | N1-C6-O6  | 22.95  | 133.67      | 119.90   |
| 22  | AV    | 73   | A    | N1-C6-N6  | 22.87  | 132.32      | 118.60   |
| 35  | BB    | 2426 | A    | N1-C6-N6  | 22.86  | 132.32      | 118.60   |
| 35  | BB    | 1193 | G    | C5-C6-O6  | -22.70 | 114.98      | 128.60   |
| 35  | BB    | 1622 | G    | C5-C6-O6  | -22.61 | 115.03      | 128.60   |
| 1   | AA    | 164  | G    | N1-C6-O6  | 22.56  | 133.44      | 119.90   |
| 1   | AA    | 262  | A    | N1-C6-N6  | 22.47  | 132.08      | 118.60   |
| 35  | BB    | 2042 | A    | N1-C6-N6  | 22.46  | 132.08      | 118.60   |
| 35  | BB    | 261  | G    | C5-C6-O6  | -22.42 | 115.15      | 128.60   |
| 1   | AA    | 1418 | A    | N1-C6-N6  | 22.40  | 132.04      | 118.60   |
| 35  | BB    | 1659 | G    | C5-C6-O6  | -22.34 | 115.19      | 128.60   |
| 35  | BB    | 2731 | G    | N1-C6-O6  | 22.34  | 133.30      | 119.90   |
| 35  | BB    | 2013 | A    | N1-C6-N6  | 22.31  | 131.99      | 118.60   |
| 1   | AA    | 369  | G    | N1-C6-O6  | 22.27  | 133.26      | 119.90   |
| 35  | BB    | 1676 | A    | N1-C6-N6  | 22.25  | 131.95      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 34  | BA    | 115  | A    | N1-C6-N6  | 22.23  | 131.94      | 118.60   |
| 35  | BB    | 881  | G    | N1-C6-O6  | 22.22  | 133.23      | 119.90   |
| 1   | AA    | 242  | G    | N1-C6-O6  | 22.19  | 133.21      | 119.90   |
| 35  | BB    | 800  | A    | N1-C6-N6  | 22.18  | 131.91      | 118.60   |
| 35  | BB    | 1936 | A    | N1-C6-N6  | 22.13  | 131.88      | 118.60   |
| 1   | AA    | 1276 | G    | N1-C6-O6  | 22.10  | 133.16      | 119.90   |
| 1   | AA    | 1012 | A    | N1-C6-N6  | 22.09  | 131.85      | 118.60   |
| 35  | BB    | 2132 | U    | P-O3'-C3' | 22.00  | 146.10      | 119.70   |
| 35  | BB    | 2037 | A    | N1-C6-N6  | 21.92  | 131.75      | 118.60   |
| 35  | BB    | 896  | A    | N1-C6-N6  | 21.90  | 131.74      | 118.60   |
| 1   | AA    | 1251 | A    | N1-C6-N6  | 21.82  | 131.69      | 118.60   |
| 35  | BB    | 123  | G    | N1-C6-O6  | 21.80  | 132.98      | 119.90   |
| 35  | BB    | 738  | G    | C5-C6-O6  | -21.80 | 115.52      | 128.60   |
| 1   | AA    | 263  | A    | N1-C6-N6  | 21.75  | 131.65      | 118.60   |
| 35  | BB    | 2201 | G    | N1-C6-O6  | 21.74  | 132.95      | 119.90   |
| 35  | BB    | 1193 | G    | N1-C6-O6  | 21.74  | 132.94      | 119.90   |
| 35  | BB    | 1659 | G    | N1-C6-O6  | 21.74  | 132.94      | 119.90   |
| 35  | BB    | 2217 | G    | C5-C6-O6  | -21.70 | 115.58      | 128.60   |
| 35  | BB    | 2471 | A    | N1-C6-N6  | 21.66  | 131.59      | 118.60   |
| 1   | AA    | 718  | A    | N1-C6-N6  | 21.62  | 131.57      | 118.60   |
| 1   | AA    | 192  | A    | N1-C6-N6  | 21.58  | 131.55      | 118.60   |
| 1   | AA    | 881  | G    | N1-C6-O6  | 21.31  | 132.69      | 119.90   |
| 35  | BB    | 647  | G    | C5-C6-O6  | -21.31 | 115.82      | 128.60   |
| 35  | BB    | 261  | G    | N1-C6-O6  | 21.30  | 132.68      | 119.90   |
| 35  | BB    | 131  | A    | N1-C6-N6  | 21.22  | 131.33      | 118.60   |
| 35  | BB    | 788  | A    | N1-C6-N6  | 21.14  | 131.29      | 118.60   |
| 35  | BB    | 2134 | A    | N1-C6-N6  | 21.14  | 131.28      | 118.60   |
| 1   | AA    | 1493 | A    | N1-C6-N6  | 21.13  | 131.28      | 118.60   |
| 35  | BB    | 2003 | A    | N1-C6-N6  | 21.13  | 131.28      | 118.60   |
| 35  | BB    | 738  | G    | N1-C6-O6  | 21.12  | 132.57      | 119.90   |
| 34  | BA    | 102  | G    | C5-C6-O6  | -21.07 | 115.96      | 128.60   |
| 34  | BA    | 102  | G    | N1-C6-O6  | 21.03  | 132.52      | 119.90   |
| 35  | BB    | 515  | A    | N1-C6-N6  | 21.00  | 131.20      | 118.60   |
| 1   | AA    | 1196 | A    | N1-C6-N6  | 20.99  | 131.19      | 118.60   |
| 1   | AA    | 369  | G    | C5-C6-O6  | -20.98 | 116.01      | 128.60   |
| 1   | AA    | 765  | G    | N1-C6-O6  | 20.93  | 132.46      | 119.90   |
| 35  | BB    | 2852 | G    | N1-C6-O6  | 20.91  | 132.45      | 119.90   |
| 34  | BA    | 29   | A    | N1-C6-N6  | 20.90  | 131.14      | 118.60   |
| 35  | BB    | 1246 | A    | N1-C6-N6  | 20.90  | 131.14      | 118.60   |
| 35  | BB    | 1387 | A    | N1-C6-N6  | 20.82  | 131.09      | 118.60   |
| 1   | AA    | 1077 | G    | C5-C6-O6  | -20.81 | 116.11      | 128.60   |
| 35  | BB    | 2446 | G    | N1-C6-O6  | 20.80  | 132.38      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1   | AA    | 781  | A    | N1-C6-N6  | 20.78  | 131.07      | 118.60   |
| 35  | BB    | 354  | A    | N1-C6-N6  | 20.77  | 131.06      | 118.60   |
| 1   | AA    | 205  | A    | N1-C6-N6  | 20.77  | 131.06      | 118.60   |
| 35  | BB    | 379  | G    | N1-C6-O6  | 20.65  | 132.29      | 119.90   |
| 1   | AA    | 975  | A    | N1-C6-N6  | 20.64  | 130.98      | 118.60   |
| 35  | BB    | 1424 | G    | C5-C6-O6  | -20.64 | 116.22      | 128.60   |
| 1   | AA    | 278  | G    | N1-C6-O6  | 20.63  | 132.28      | 119.90   |
| 35  | BB    | 315  | G    | C5-C6-O6  | -20.59 | 116.25      | 128.60   |
| 1   | AA    | 1252 | A    | N1-C6-N6  | 20.55  | 130.93      | 118.60   |
| 35  | BB    | 637  | A    | N1-C6-N6  | 20.55  | 130.93      | 118.60   |
| 35  | BB    | 1504 | A    | N1-C6-N6  | 20.54  | 130.93      | 118.60   |
| 1   | AA    | 1016 | A    | N1-C6-N6  | 20.49  | 130.90      | 118.60   |
| 35  | BB    | 1054 | A    | N1-C6-N6  | 20.49  | 130.89      | 118.60   |
| 35  | BB    | 1593 | A    | N1-C6-N6  | 20.27  | 130.76      | 118.60   |
| 35  | BB    | 533  | G    | C5-C6-O6  | -20.27 | 116.44      | 128.60   |
| 35  | BB    | 583  | G    | C5-C6-O6  | -20.21 | 116.47      | 128.60   |
| 35  | BB    | 1525 | A    | N1-C6-N6  | 20.21  | 130.73      | 118.60   |
| 35  | BB    | 2585 | U    | P-O3'-C3' | 20.18  | 143.91      | 119.70   |
| 35  | BB    | 2217 | G    | N1-C6-O6  | 20.18  | 132.00      | 119.90   |
| 35  | BB    | 190  | A    | N1-C6-N6  | 20.14  | 130.69      | 118.60   |
| 35  | BB    | 1697 | G    | N1-C6-O6  | 20.09  | 131.95      | 119.90   |
| 35  | BB    | 2340 | A    | N1-C6-N6  | 20.09  | 130.65      | 118.60   |
| 1   | AA    | 994  | A    | N1-C6-N6  | 20.08  | 130.65      | 118.60   |
| 34  | BA    | 45   | A    | N1-C6-N6  | 20.08  | 130.65      | 118.60   |
| 1   | AA    | 907  | A    | N1-C6-N6  | 20.07  | 130.64      | 118.60   |
| 35  | BB    | 2323 | G    | N1-C6-O6  | 20.05  | 131.93      | 119.90   |
| 35  | BB    | 1434 | A    | N1-C6-N6  | 20.04  | 130.63      | 118.60   |
| 35  | BB    | 2869 | G    | C5-C6-O6  | -20.01 | 116.59      | 128.60   |
| 1   | AA    | 1087 | G    | N1-C6-O6  | 20.01  | 131.91      | 119.90   |
| 35  | BB    | 160  | A    | N1-C6-N6  | 19.98  | 130.59      | 118.60   |
| 35  | BB    | 1296 | G    | N1-C6-O6  | 19.98  | 131.89      | 119.90   |
| 35  | BB    | 2446 | G    | C5-C6-O6  | -19.97 | 116.62      | 128.60   |
| 1   | AA    | 432  | A    | N1-C6-N6  | 19.96  | 130.57      | 118.60   |
| 1   | AA    | 1019 | A    | N1-C6-N6  | 19.95  | 130.57      | 118.60   |
| 35  | BB    | 123  | G    | C5-C6-O6  | -19.91 | 116.65      | 128.60   |
| 1   | AA    | 179  | A    | N1-C6-N6  | 19.89  | 130.53      | 118.60   |
| 35  | BB    | 1634 | A    | N1-C6-N6  | 19.88  | 130.53      | 118.60   |
| 35  | BB    | 1089 | A    | N1-C6-N6  | 19.88  | 130.53      | 118.60   |
| 34  | BA    | 96   | G    | C5-C6-O6  | -19.87 | 116.68      | 128.60   |
| 35  | BB    | 2835 | A    | N1-C6-N6  | 19.84  | 130.50      | 118.60   |
| 22  | AV    | 69   | G    | N1-C6-O6  | 19.80  | 131.78      | 119.90   |
| 35  | BB    | 2024 | G    | N1-C6-O6  | 19.77  | 131.76      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1519 | G    | N1-C6-O6   | 19.76  | 131.76      | 119.90   |
| 35  | BB    | 833  | A    | N1-C6-N6   | 19.74  | 130.44      | 118.60   |
| 35  | BB    | 2530 | A    | N1-C6-N6   | 19.74  | 130.44      | 118.60   |
| 34  | BA    | 112  | G    | C5-C6-O6   | -19.71 | 116.78      | 128.60   |
| 1   | AA    | 499  | A    | N1-C6-N6   | 19.70  | 130.42      | 118.60   |
| 35  | BB    | 2675 | A    | N1-C6-N6   | 19.65  | 130.39      | 118.60   |
| 22  | AV    | 69   | G    | C5-C6-O6   | -19.59 | 116.85      | 128.60   |
| 1   | AA    | 98   | A    | N1-C6-N6   | 19.58  | 130.35      | 118.60   |
| 34  | BA    | 34   | A    | N1-C6-N6   | 19.57  | 130.34      | 118.60   |
| 1   | AA    | 1373 | G    | C5-C6-O6   | -19.55 | 116.87      | 128.60   |
| 1   | AA    | 441  | A    | N1-C6-N6   | 19.49  | 130.29      | 118.60   |
| 1   | AA    | 1276 | G    | C5-C6-O6   | -19.47 | 116.92      | 128.60   |
| 1   | AA    | 303  | A    | N1-C6-N6   | 19.44  | 130.26      | 118.60   |
| 35  | BB    | 503  | A    | N1-C6-N6   | 19.42  | 130.25      | 118.60   |
| 1   | AA    | 710  | G    | N1-C6-O6   | 19.37  | 131.52      | 119.90   |
| 35  | BB    | 75   | G    | N1-C6-O6   | 19.35  | 131.51      | 119.90   |
| 35  | BB    | 324  | A    | N1-C6-N6   | 19.34  | 130.21      | 118.60   |
| 1   | AA    | 75   | G    | N1-C6-O6   | 19.34  | 131.50      | 119.90   |
| 35  | BB    | 1000 | A    | N1-C6-N6   | 19.33  | 130.20      | 118.60   |
| 1   | AA    | 31   | G    | N1-C6-O6   | 19.33  | 131.50      | 119.90   |
| 34  | BA    | 96   | G    | N1-C6-O6   | 19.30  | 131.48      | 119.90   |
| 34  | BA    | 71   | C    | C6-N1-C2   | -19.27 | 112.59      | 120.30   |
| 1   | AA    | 1429 | A    | N1-C6-N6   | 19.25  | 130.15      | 118.60   |
| 35  | BB    | 2572 | A    | N1-C6-N6   | 19.24  | 130.15      | 118.60   |
| 1   | AA    | 1101 | A    | N1-C6-N6   | 19.18  | 130.11      | 118.60   |
| 35  | BB    | 2763 | G    | N1-C6-O6   | 19.18  | 131.41      | 119.90   |
| 35  | BB    | 677  | A    | N1-C6-N6   | 19.15  | 130.09      | 118.60   |
| 35  | BB    | 1831 | G    | C5-C6-O6   | -19.13 | 117.12      | 128.60   |
| 1   | AA    | 1043 | G    | N1-C6-O6   | 19.05  | 131.33      | 119.90   |
| 34  | BA    | 109  | A    | N1-C6-N6   | 19.05  | 130.03      | 118.60   |
| 1   | AA    | 314  | C    | O4'-C1'-N1 | 19.02  | 123.42      | 108.20   |
| 1   | AA    | 902  | G    | N1-C6-O6   | 19.01  | 131.31      | 119.90   |
| 1   | AA    | 1431 | A    | N1-C6-N6   | 19.01  | 130.00      | 118.60   |
| 35  | BB    | 2136 | G    | N1-C6-O6   | 18.95  | 131.27      | 119.90   |
| 35  | BB    | 1215 | G    | C5-C6-O6   | -18.93 | 117.25      | 128.60   |
| 35  | BB    | 1385 | A    | N1-C6-N6   | 18.92  | 129.95      | 118.60   |
| 1   | AA    | 484  | G    | N1-C6-O6   | 18.92  | 131.25      | 119.90   |
| 35  | BB    | 969  | G    | N1-C6-O6   | 18.91  | 131.25      | 119.90   |
| 35  | BB    | 2158 | A    | N1-C6-N6   | 18.91  | 129.94      | 118.60   |
| 35  | BB    | 910  | A    | N1-C6-N6   | 18.84  | 129.90      | 118.60   |
| 35  | BB    | 977  | G    | N1-C6-O6   | 18.84  | 131.20      | 119.90   |
| 35  | BB    | 347  | A    | N1-C6-N6   | 18.82  | 129.89      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1701 | A    | N1-C6-N6   | 18.82  | 129.89      | 118.60   |
| 1   | AA    | 240  | G    | N1-C6-O6   | 18.81  | 131.18      | 119.90   |
| 35  | BB    | 907  | G    | N1-C6-O6   | 18.79  | 131.17      | 119.90   |
| 35  | BB    | 843  | G    | N1-C6-O6   | 18.77  | 131.16      | 119.90   |
| 35  | BB    | 2162 | G    | N1-C6-O6   | 18.77  | 131.16      | 119.90   |
| 1   | AA    | 16   | A    | N1-C6-N6   | 18.70  | 129.82      | 118.60   |
| 1   | AA    | 1401 | G    | N1-C6-O6   | 18.69  | 131.12      | 119.90   |
| 1   | AA    | 424  | G    | N1-C6-O6   | 18.68  | 131.11      | 119.90   |
| 35  | BB    | 332  | A    | N1-C6-N6   | 18.67  | 129.81      | 118.60   |
| 35  | BB    | 1642 | G    | N1-C6-O6   | 18.61  | 131.06      | 119.90   |
| 1   | AA    | 1144 | G    | N1-C6-O6   | 18.59  | 131.06      | 119.90   |
| 1   | AA    | 519  | C    | N3-C4-C5   | -18.59 | 114.47      | 121.90   |
| 35  | BB    | 1388 | G    | C5-C6-O6   | -18.58 | 117.45      | 128.60   |
| 35  | BB    | 1374 | G    | N1-C6-O6   | 18.56  | 131.04      | 119.90   |
| 35  | BB    | 1051 | G    | N1-C6-O6   | 18.55  | 131.03      | 119.90   |
| 1   | AA    | 1092 | A    | N1-C6-N6   | 18.52  | 129.71      | 118.60   |
| 35  | BB    | 1831 | G    | N1-C6-O6   | 18.51  | 131.01      | 119.90   |
| 35  | BB    | 1875 | G    | C5-C6-O6   | -18.51 | 117.49      | 128.60   |
| 35  | BB    | 2377 | A    | N1-C6-N6   | 18.50  | 129.70      | 118.60   |
| 1   | AA    | 279  | A    | N1-C6-N6   | 18.49  | 129.69      | 118.60   |
| 35  | BB    | 2717 | C    | C6-N1-C2   | -18.48 | 112.91      | 120.30   |
| 1   | AA    | 493  | A    | N1-C6-N6   | 18.46  | 129.68      | 118.60   |
| 1   | AA    | 1509 | C    | N3-C4-N4   | 18.45  | 130.91      | 118.00   |
| 1   | AA    | 948  | C    | N3-C4-C5   | -18.44 | 114.52      | 121.90   |
| 35  | BB    | 1358 | G    | N1-C6-O6   | 18.44  | 130.96      | 119.90   |
| 1   | AA    | 1077 | G    | N1-C6-O6   | 18.43  | 130.96      | 119.90   |
| 35  | BB    | 1609 | A    | N1-C6-N6   | 18.43  | 129.66      | 118.60   |
| 1   | AA    | 181  | A    | N1-C6-N6   | 18.43  | 129.66      | 118.60   |
| 1   | AA    | 190  | A    | N1-C6-N6   | 18.38  | 129.63      | 118.60   |
| 1   | AA    | 327  | A    | N1-C6-N6   | 18.37  | 129.62      | 118.60   |
| 35  | BB    | 327  | G    | N1-C6-O6   | 18.37  | 130.92      | 119.90   |
| 35  | BB    | 2628 | C    | O4'-C1'-N1 | 18.35  | 122.88      | 108.20   |
| 1   | AA    | 675  | A    | N1-C6-N6   | 18.33  | 129.60      | 118.60   |
| 1   | AA    | 189  | A    | N1-C6-N6   | 18.32  | 129.59      | 118.60   |
| 35  | BB    | 1237 | A    | N1-C6-N6   | 18.31  | 129.58      | 118.60   |
| 35  | BB    | 2006 | C    | N3-C4-C5   | -18.27 | 114.59      | 121.90   |
| 35  | BB    | 2468 | A    | C4-C5-C6   | 18.27  | 126.13      | 117.00   |
| 1   | AA    | 1408 | A    | N1-C6-N6   | 18.26  | 129.56      | 118.60   |
| 35  | BB    | 494  | G    | C5-C6-O6   | -18.25 | 117.65      | 128.60   |
| 1   | AA    | 168  | G    | N1-C6-O6   | 18.21  | 130.83      | 119.90   |
| 35  | BB    | 918  | A    | N1-C6-N6   | 18.20  | 129.52      | 118.60   |
| 35  | BB    | 1144 | A    | N1-C6-N6   | 18.19  | 129.51      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2764 | A    | N1-C6-N6   | 18.18  | 129.50      | 118.60   |
| 35  | BB    | 2812 | G    | C5-C6-O6   | -18.17 | 117.70      | 128.60   |
| 35  | BB    | 1085 | A    | N1-C6-N6   | 18.16  | 129.50      | 118.60   |
| 1   | AA    | 964  | A    | N1-C6-N6   | 18.14  | 129.48      | 118.60   |
| 35  | BB    | 1713 | A    | N1-C6-N6   | 18.12  | 129.47      | 118.60   |
| 35  | BB    | 80   | G    | N1-C6-O6   | 18.08  | 130.75      | 119.90   |
| 35  | BB    | 2691 | C    | O4'-C1'-N1 | 18.07  | 122.66      | 108.20   |
| 1   | AA    | 1285 | A    | N1-C6-N6   | 18.06  | 129.44      | 118.60   |
| 1   | AA    | 1433 | A    | N1-C6-N6   | 18.06  | 129.44      | 118.60   |
| 35  | BB    | 203  | A    | N1-C6-N6   | 18.06  | 129.43      | 118.60   |
| 35  | BB    | 2781 | A    | N1-C6-N6   | 18.05  | 129.43      | 118.60   |
| 35  | BB    | 2899 | A    | N1-C6-N6   | 18.05  | 129.43      | 118.60   |
| 35  | BB    | 2191 | A    | N1-C6-N6   | 18.02  | 129.41      | 118.60   |
| 1   | AA    | 993  | G    | C5-C6-O6   | -18.01 | 117.79      | 128.60   |
| 35  | BB    | 2029 | G    | C5-C6-O6   | -18.00 | 117.80      | 128.60   |
| 35  | BB    | 1469 | A    | C5-C6-N1   | -17.98 | 108.71      | 117.70   |
| 1   | AA    | 833  | G    | N1-C6-O6   | 17.98  | 130.69      | 119.90   |
| 1   | AA    | 1226 | C    | P-O3'-C3'  | 17.98  | 141.27      | 119.70   |
| 1   | AA    | 1482 | G    | N1-C6-O6   | 17.96  | 130.67      | 119.90   |
| 35  | BB    | 722  | A    | N1-C6-N6   | 17.92  | 129.35      | 118.60   |
| 35  | BB    | 2682 | A    | N1-C6-N6   | 17.91  | 129.34      | 118.60   |
| 35  | BB    | 699  | A    | C4-C5-C6   | 17.89  | 125.95      | 117.00   |
| 35  | BB    | 2402 | U    | P-O3'-C3'  | 17.89  | 141.17      | 119.70   |
| 35  | BB    | 326  | G    | C6-C5-N7   | -17.88 | 119.67      | 130.40   |
| 1   | AA    | 44   | A    | N1-C2-N3   | 17.87  | 138.23      | 129.30   |
| 1   | AA    | 604  | G    | N1-C6-O6   | 17.86  | 130.62      | 119.90   |
| 1   | AA    | 645  | G    | N1-C6-O6   | 17.86  | 130.62      | 119.90   |
| 1   | AA    | 167  | A    | N1-C6-N6   | 17.85  | 129.31      | 118.60   |
| 35  | BB    | 2027 | G    | N1-C6-O6   | 17.84  | 130.60      | 119.90   |
| 35  | BB    | 2883 | A    | N1-C6-N6   | 17.83  | 129.30      | 118.60   |
| 35  | BB    | 1548 | A    | N1-C6-N6   | 17.82  | 129.29      | 118.60   |
| 35  | BB    | 721  | A    | N1-C6-N6   | 17.81  | 129.29      | 118.60   |
| 35  | BB    | 2497 | A    | N1-C6-N6   | 17.81  | 129.29      | 118.60   |
| 35  | BB    | 739  | A    | N1-C6-N6   | 17.80  | 129.28      | 118.60   |
| 1   | AA    | 227  | G    | N1-C6-O6   | 17.78  | 130.57      | 119.90   |
| 35  | BB    | 2734 | A    | N1-C6-N6   | 17.77  | 129.26      | 118.60   |
| 35  | BB    | 1641 | A    | N1-C6-N6   | 17.75  | 129.25      | 118.60   |
| 35  | BB    | 2325 | G    | N1-C6-O6   | 17.75  | 130.55      | 119.90   |
| 35  | BB    | 2447 | G    | C5-C6-O6   | -17.75 | 117.95      | 128.60   |
| 35  | BB    | 2857 | G    | N1-C6-O6   | 17.75  | 130.55      | 119.90   |
| 1   | AA    | 1039 | G    | C5-C6-O6   | -17.74 | 117.96      | 128.60   |
| 35  | BB    | 626  | A    | N1-C6-N6   | 17.74  | 129.24      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2241 | A    | N1-C6-N6   | 17.71  | 129.22      | 118.60   |
| 35  | BB    | 480  | A    | N1-C6-N6   | 17.69  | 129.21      | 118.60   |
| 1   | AA    | 1422 | G    | C5-C6-O6   | -17.68 | 118.00      | 128.60   |
| 35  | BB    | 2225 | A    | N1-C6-N6   | 17.67  | 129.20      | 118.60   |
| 35  | BB    | 734  | A    | N1-C6-N6   | 17.66  | 129.19      | 118.60   |
| 1   | AA    | 15   | G    | O4'-C1'-N9 | 17.65  | 122.32      | 108.20   |
| 35  | BB    | 1810 | A    | N1-C6-N6   | 17.65  | 129.19      | 118.60   |
| 35  | BB    | 1663 | G    | C5-C6-O6   | -17.64 | 118.01      | 128.60   |
| 1   | AA    | 627  | G    | N1-C6-O6   | 17.62  | 130.47      | 119.90   |
| 1   | AA    | 201  | G    | N1-C6-O6   | 17.61  | 130.47      | 119.90   |
| 35  | BB    | 1927 | A    | N1-C6-N6   | 17.61  | 129.17      | 118.60   |
| 34  | BA    | 33   | G    | N1-C6-O6   | 17.61  | 130.46      | 119.90   |
| 35  | BB    | 1928 | A    | N1-C6-N6   | 17.59  | 129.15      | 118.60   |
| 35  | BB    | 1598 | A    | N1-C6-N6   | 17.58  | 129.15      | 118.60   |
| 35  | BB    | 2019 | A    | N1-C6-N6   | 17.58  | 129.15      | 118.60   |
| 1   | AA    | 645  | G    | C5-C6-O6   | -17.58 | 118.05      | 128.60   |
| 35  | BB    | 1226 | A    | N1-C6-N6   | 17.57  | 129.15      | 118.60   |
| 35  | BB    | 1735 | A    | N1-C6-N6   | 17.51  | 129.11      | 118.60   |
| 35  | BB    | 2146 | C    | N3-C4-C5   | -17.50 | 114.90      | 121.90   |
| 1   | AA    | 142  | G    | N1-C6-O6   | 17.49  | 130.39      | 119.90   |
| 35  | BB    | 2536 | G    | N1-C6-O6   | 17.48  | 130.39      | 119.90   |
| 35  | BB    | 1424 | G    | N1-C6-O6   | 17.47  | 130.38      | 119.90   |
| 1   | AA    | 933  | G    | N1-C6-O6   | 17.47  | 130.38      | 119.90   |
| 35  | BB    | 2635 | A    | N1-C6-N6   | 17.46  | 129.07      | 118.60   |
| 35  | BB    | 2275 | C    | N3-C4-C5   | -17.44 | 114.92      | 121.90   |
| 1   | AA    | 240  | G    | C5-C6-O6   | -17.43 | 118.14      | 128.60   |
| 35  | BB    | 1389 | G    | N1-C6-O6   | 17.43  | 130.36      | 119.90   |
| 35  | BB    | 2765 | A    | N1-C6-N6   | 17.41  | 129.05      | 118.60   |
| 1   | AA    | 50   | A    | N1-C6-N6   | 17.41  | 129.04      | 118.60   |
| 35  | BB    | 621  | A    | N1-C6-N6   | 17.41  | 129.04      | 118.60   |
| 35  | BB    | 471  | A    | N1-C6-N6   | 17.40  | 129.04      | 118.60   |
| 35  | BB    | 1590 | A    | N1-C6-N6   | 17.39  | 129.04      | 118.60   |
| 1   | AA    | 673  | A    | N1-C6-N6   | 17.39  | 129.03      | 118.60   |
| 34  | BA    | 33   | G    | C5-C6-O6   | -17.38 | 118.17      | 128.60   |
| 35  | BB    | 1862 | G    | N1-C6-O6   | 17.36  | 130.32      | 119.90   |
| 35  | BB    | 2358 | A    | N1-C6-N6   | 17.35  | 129.01      | 118.60   |
| 1   | AA    | 527  | G    | O4'-C1'-N9 | 17.34  | 122.07      | 108.20   |
| 35  | BB    | 380  | G    | C8-N9-C4   | -17.34 | 99.46       | 106.40   |
| 35  | BB    | 1284 | A    | N1-C6-N6   | 17.34  | 129.00      | 118.60   |
| 1   | AA    | 328  | C    | P-O3'-C3'  | 17.34  | 140.50      | 119.70   |
| 1   | AA    | 1035 | A    | N1-C6-N6   | 17.34  | 129.00      | 118.60   |
| 1   | AA    | 132  | C    | O4'-C1'-N1 | 17.32  | 122.06      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1   | AA    | 918  | A    | N1-C6-N6  | 17.32  | 128.99      | 118.60   |
| 35  | BB    | 2731 | G    | C5-C6-O6  | -17.31 | 118.22      | 128.60   |
| 35  | BB    | 1839 | G    | C5-C6-O6  | -17.31 | 118.22      | 128.60   |
| 1   | AA    | 59   | A    | C4-C5-C6  | 17.31  | 125.65      | 117.00   |
| 35  | BB    | 2625 | G    | C5-C6-O6  | -17.30 | 118.22      | 128.60   |
| 1   | AA    | 1482 | G    | C5-C6-O6  | -17.30 | 118.22      | 128.60   |
| 35  | BB    | 258  | G    | C5-C6-O6  | -17.29 | 118.22      | 128.60   |
| 1   | AA    | 968  | A    | N1-C6-N6  | 17.27  | 128.96      | 118.60   |
| 35  | BB    | 2529 | G    | C5-C6-O6  | -17.27 | 118.24      | 128.60   |
| 34  | BA    | 15   | A    | N1-C6-N6  | 17.26  | 128.95      | 118.60   |
| 1   | AA    | 1266 | G    | C8-N9-C4  | -17.25 | 99.50       | 106.40   |
| 35  | BB    | 2886 | A    | N1-C6-N6  | 17.25  | 128.95      | 118.60   |
| 35  | BB    | 697  | G    | C5-C6-O6  | -17.24 | 118.26      | 128.60   |
| 1   | AA    | 1422 | G    | N1-C6-O6  | 17.24  | 130.24      | 119.90   |
| 35  | BB    | 844  | A    | N1-C6-N6  | 17.20  | 128.92      | 118.60   |
| 35  | BB    | 2837 | A    | N1-C6-N6  | 17.20  | 128.92      | 118.60   |
| 35  | BB    | 482  | A    | N1-C6-N6  | 17.19  | 128.91      | 118.60   |
| 1   | AA    | 1166 | G    | N1-C6-O6  | 17.18  | 130.21      | 119.90   |
| 1   | AA    | 1370 | G    | N1-C6-O6  | 17.18  | 130.21      | 119.90   |
| 35  | BB    | 488  | G    | N1-C6-O6  | 17.17  | 130.20      | 119.90   |
| 35  | BB    | 718  | A    | N1-C6-N6  | 17.15  | 128.89      | 118.60   |
| 35  | BB    | 2323 | G    | C5-C6-O6  | -17.15 | 118.31      | 128.60   |
| 35  | BB    | 890  | C    | P-O3'-C3' | 17.14  | 140.27      | 119.70   |
| 1   | AA    | 539  | A    | N1-C6-N6  | 17.14  | 128.88      | 118.60   |
| 35  | BB    | 2516 | A    | N1-C6-N6  | 17.14  | 128.88      | 118.60   |
| 35  | BB    | 2444 | G    | N1-C6-O6  | 17.13  | 130.18      | 119.90   |
| 35  | BB    | 2094 | A    | N1-C6-N6  | 17.12  | 128.87      | 118.60   |
| 1   | AA    | 777  | A    | N1-C6-N6  | 17.11  | 128.86      | 118.60   |
| 1   | AA    | 376  | G    | N1-C6-O6  | 17.10  | 130.16      | 119.90   |
| 35  | BB    | 2083 | G    | C8-N9-C4  | -17.10 | 99.56       | 106.40   |
| 1   | AA    | 1373 | G    | N1-C6-O6  | 17.07  | 130.14      | 119.90   |
| 34  | BA    | 27   | C    | C6-N1-C2  | -17.07 | 113.47      | 120.30   |
| 35  | BB    | 1953 | A    | N1-C6-N6  | 17.04  | 128.82      | 118.60   |
| 35  | BB    | 2336 | A    | P-O3'-C3' | 17.03  | 140.14      | 119.70   |
| 35  | BB    | 2198 | A    | N1-C6-N6  | 17.01  | 128.81      | 118.60   |
| 35  | BB    | 2335 | A    | N1-C6-N6  | 17.00  | 128.80      | 118.60   |
| 1   | AA    | 993  | G    | N1-C6-O6  | 16.99  | 130.09      | 119.90   |
| 1   | AA    | 888  | G    | N1-C6-O6  | 16.98  | 130.09      | 119.90   |
| 35  | BB    | 1342 | A    | N1-C6-N6  | 16.97  | 128.78      | 118.60   |
| 35  | BB    | 745  | G    | N1-C6-O6  | 16.96  | 130.08      | 119.90   |
| 35  | BB    | 439  | A    | N1-C6-N6  | 16.96  | 128.78      | 118.60   |
| 1   | AA    | 1456 | A    | N1-C6-N6  | 16.95  | 128.77      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 505  | A    | N1-C6-N6   | 16.94  | 128.76      | 118.60   |
| 35  | BB    | 1690 | A    | O4'-C1'-N9 | 16.94  | 121.75      | 108.20   |
| 35  | BB    | 1524 | G    | N1-C2-N3   | -16.92 | 113.75      | 123.90   |
| 35  | BB    | 142  | A    | N1-C6-N6   | 16.92  | 128.75      | 118.60   |
| 35  | BB    | 2627 | G    | N1-C6-O6   | 16.92  | 130.05      | 119.90   |
| 35  | BB    | 256  | A    | N1-C6-N6   | 16.92  | 128.75      | 118.60   |
| 35  | BB    | 881  | G    | C5-C6-O6   | -16.90 | 118.46      | 128.60   |
| 35  | BB    | 1322 | A    | N1-C6-N6   | 16.90  | 128.74      | 118.60   |
| 35  | BB    | 901  | C    | N3-C4-C5   | -16.88 | 115.15      | 121.90   |
| 35  | BB    | 960  | A    | N1-C6-N6   | 16.88  | 128.73      | 118.60   |
| 35  | BB    | 2363 | G    | N1-C6-O6   | 16.88  | 130.03      | 119.90   |
| 35  | BB    | 2156 | G    | N1-C6-O6   | 16.88  | 130.03      | 119.90   |
| 35  | BB    | 2488 | G    | N1-C6-O6   | 16.87  | 130.02      | 119.90   |
| 35  | BB    | 1352 | U    | O4'-C1'-N1 | 16.86  | 121.69      | 108.20   |
| 1   | AA    | 881  | G    | C5-C6-O6   | -16.86 | 118.48      | 128.60   |
| 1   | AA    | 1128 | C    | C6-N1-C2   | -16.86 | 113.56      | 120.30   |
| 35  | BB    | 410  | G    | N1-C6-O6   | 16.85  | 130.01      | 119.90   |
| 35  | BB    | 2289 | G    | N1-C6-O6   | 16.83  | 130.00      | 119.90   |
| 1   | AA    | 983  | A    | N1-C6-N6   | 16.83  | 128.70      | 118.60   |
| 35  | BB    | 2136 | G    | C5-C6-O6   | -16.82 | 118.51      | 128.60   |
| 35  | BB    | 2030 | A    | N1-C6-N6   | 16.82  | 128.69      | 118.60   |
| 35  | BB    | 2459 | A    | N1-C6-N6   | 16.81  | 128.69      | 118.60   |
| 35  | BB    | 2281 | A    | N1-C2-N3   | 16.81  | 137.71      | 129.30   |
| 1   | AA    | 100  | G    | N1-C6-O6   | 16.81  | 129.99      | 119.90   |
| 35  | BB    | 638  | G    | N1-C6-O6   | 16.78  | 129.97      | 119.90   |
| 35  | BB    | 1900 | A    | N1-C6-N6   | 16.77  | 128.66      | 118.60   |
| 35  | BB    | 707  | G    | N1-C6-O6   | 16.76  | 129.96      | 119.90   |
| 35  | BB    | 715  | A    | N1-C6-N6   | 16.76  | 128.66      | 118.60   |
| 35  | BB    | 748  | G    | N1-C6-O6   | 16.76  | 129.96      | 119.90   |
| 1   | AA    | 45   | G    | N1-C6-O6   | 16.75  | 129.95      | 119.90   |
| 1   | AA    | 616  | G    | C8-N9-C4   | -16.73 | 99.71       | 106.40   |
| 1   | AA    | 243  | A    | N1-C6-N6   | 16.73  | 128.64      | 118.60   |
| 35  | BB    | 91   | A    | N1-C6-N6   | 16.70  | 128.62      | 118.60   |
| 35  | BB    | 2418 | A    | N1-C6-N6   | 16.66  | 128.60      | 118.60   |
| 35  | BB    | 2378 | A    | C4-C5-C6   | 16.65  | 125.32      | 117.00   |
| 35  | BB    | 900  | A    | O4'-C1'-N9 | 16.64  | 121.52      | 108.20   |
| 35  | BB    | 633  | A    | N1-C6-N6   | 16.64  | 128.59      | 118.60   |
| 35  | BB    | 1875 | G    | N1-C6-O6   | 16.61  | 129.87      | 119.90   |
| 35  | BB    | 2114 | A    | N1-C6-N6   | 16.61  | 128.57      | 118.60   |
| 34  | BA    | 50   | A    | N1-C6-N6   | 16.61  | 128.56      | 118.60   |
| 35  | BB    | 859  | G    | N1-C6-O6   | 16.60  | 129.86      | 119.90   |
| 34  | BA    | 117  | G    | N1-C6-O6   | 16.59  | 129.85      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1551 | A    | P-O3'-C3'  | 16.58  | 139.60      | 119.70   |
| 35  | BB    | 990  | A    | C5-C6-N1   | -16.58 | 109.41      | 117.70   |
| 35  | BB    | 2872 | A    | N1-C6-N6   | 16.58  | 128.55      | 118.60   |
| 1   | AA    | 1036 | A    | N1-C6-N6   | 16.58  | 128.55      | 118.60   |
| 35  | BB    | 2632 | A    | N1-C6-N6   | 16.58  | 128.55      | 118.60   |
| 35  | BB    | 1448 | G    | N1-C6-O6   | 16.56  | 129.84      | 119.90   |
| 1   | AA    | 1055 | A    | N1-C6-N6   | 16.55  | 128.53      | 118.60   |
| 35  | BB    | 2875 | C    | C6-N1-C2   | -16.55 | 113.68      | 120.30   |
| 1   | AA    | 60   | A    | N1-C6-N6   | 16.54  | 128.53      | 118.60   |
| 35  | BB    | 1456 | G    | N1-C6-O6   | 16.54  | 129.83      | 119.90   |
| 35  | BB    | 886  | A    | P-O3'-C3'  | 16.54  | 139.54      | 119.70   |
| 35  | BB    | 2852 | G    | C5-C6-O6   | -16.53 | 118.68      | 128.60   |
| 1   | AA    | 1507 | A    | C5-C6-N6   | -16.52 | 110.48      | 123.70   |
| 35  | BB    | 2602 | A    | N1-C6-N6   | 16.52  | 128.51      | 118.60   |
| 35  | BB    | 2448 | A    | N1-C6-N6   | 16.51  | 128.50      | 118.60   |
| 1   | AA    | 1244 | G    | N1-C6-O6   | 16.50  | 129.80      | 119.90   |
| 1   | AA    | 304  | U    | O4'-C1'-N1 | 16.50  | 121.40      | 108.20   |
| 35  | BB    | 1542 | U    | O4'-C1'-N1 | 16.50  | 121.40      | 108.20   |
| 35  | BB    | 781  | A    | C5-C6-N1   | -16.49 | 109.45      | 117.70   |
| 35  | BB    | 13   | A    | N1-C6-N6   | 16.48  | 128.49      | 118.60   |
| 35  | BB    | 1791 | A    | N1-C6-N6   | 16.47  | 128.48      | 118.60   |
| 35  | BB    | 2097 | A    | N1-C6-N6   | 16.46  | 128.48      | 118.60   |
| 35  | BB    | 954  | G    | N1-C6-O6   | 16.44  | 129.77      | 119.90   |
| 1   | AA    | 411  | A    | C5-C6-N1   | -16.43 | 109.48      | 117.70   |
| 35  | BB    | 972  | A    | C4-C5-C6   | 16.43  | 125.22      | 117.00   |
| 4   | AD    | 25   | ARG  | NE-CZ-NH1  | 16.41  | 128.51      | 120.30   |
| 35  | BB    | 2383 | G    | N1-C6-O6   | 16.40  | 129.74      | 119.90   |
| 35  | BB    | 843  | G    | C5-C6-O6   | -16.40 | 118.76      | 128.60   |
| 34  | BA    | 58   | A    | N1-C6-N6   | 16.40  | 128.44      | 118.60   |
| 1   | AA    | 1244 | G    | C5-C6-O6   | -16.39 | 118.76      | 128.60   |
| 35  | BB    | 2450 | A    | N1-C6-N6   | 16.39  | 128.43      | 118.60   |
| 35  | BB    | 996  | A    | N1-C6-N6   | 16.38  | 128.43      | 118.60   |
| 35  | BB    | 2375 | G    | N1-C6-O6   | 16.38  | 129.73      | 119.90   |
| 1   | AA    | 1480 | A    | N1-C6-N6   | 16.37  | 128.42      | 118.60   |
| 35  | BB    | 271  | G    | C5-C6-O6   | -16.36 | 118.78      | 128.60   |
| 35  | BB    | 2478 | A    | N1-C6-N6   | 16.36  | 128.42      | 118.60   |
| 34  | BA    | 30   | C    | N3-C4-N4   | 16.36  | 129.45      | 118.00   |
| 1   | AA    | 1257 | A    | N1-C6-N6   | 16.35  | 128.41      | 118.60   |
| 35  | BB    | 1682 | G    | N1-C6-O6   | 16.35  | 129.71      | 119.90   |
| 1   | AA    | 923  | A    | N1-C6-N6   | 16.33  | 128.40      | 118.60   |
| 35  | BB    | 538  | A    | N1-C6-N6   | 16.33  | 128.40      | 118.60   |
| 35  | BB    | 2360 | G    | C5-C6-O6   | -16.31 | 118.81      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 987  | G    | C4-C5-C6   | 16.30  | 128.58      | 118.80   |
| 1   | AA    | 435  | A    | N1-C6-N6   | 16.29  | 128.38      | 118.60   |
| 1   | AA    | 293  | G    | C5-C6-O6   | -16.27 | 118.84      | 128.60   |
| 35  | BB    | 716  | A    | C4-C5-C6   | 16.26  | 125.13      | 117.00   |
| 1   | AA    | 1284 | C    | P-O3'-C3'  | 16.25  | 139.20      | 119.70   |
| 1   | AA    | 431  | A    | N1-C6-N6   | 16.24  | 128.34      | 118.60   |
| 35  | BB    | 1994 | C    | O4'-C1'-N1 | 16.23  | 121.18      | 108.20   |
| 35  | BB    | 1462 | C    | O4'-C1'-N1 | 16.23  | 121.18      | 108.20   |
| 35  | BB    | 1527 | G    | N1-C6-O6   | 16.23  | 129.64      | 119.90   |
| 1   | AA    | 1065 | U    | P-O3'-C3'  | 16.20  | 139.14      | 119.70   |
| 1   | AA    | 1312 | G    | N1-C6-O6   | 16.20  | 129.62      | 119.90   |
| 1   | AA    | 667  | G    | N1-C6-O6   | 16.20  | 129.62      | 119.90   |
| 1   | AA    | 411  | A    | N1-C6-N6   | 16.19  | 128.32      | 118.60   |
| 1   | AA    | 1280 | A    | N1-C6-N6   | 16.19  | 128.31      | 118.60   |
| 35  | BB    | 1519 | G    | C5-C6-O6   | -16.18 | 118.89      | 128.60   |
| 35  | BB    | 483  | A    | O4'-C1'-N9 | 16.18  | 121.14      | 108.20   |
| 35  | BB    | 1241 | A    | N1-C6-N6   | 16.17  | 128.30      | 118.60   |
| 35  | BB    | 2318 | G    | N1-C6-O6   | 16.17  | 129.60      | 119.90   |
| 1   | AA    | 48   | C    | N3-C4-C5   | -16.16 | 115.44      | 121.90   |
| 35  | BB    | 194  | G    | N1-C6-O6   | 16.16  | 129.59      | 119.90   |
| 35  | BB    | 1694 | C    | N3-C4-C5   | -16.16 | 115.44      | 121.90   |
| 35  | BB    | 879  | G    | C5-C6-O6   | -16.15 | 118.91      | 128.60   |
| 35  | BB    | 182  | A    | C4-C5-C6   | 16.14  | 125.07      | 117.00   |
| 35  | BB    | 1309 | G    | N1-C6-O6   | 16.14  | 129.58      | 119.90   |
| 35  | BB    | 2115 | G    | C5-C6-O6   | -16.14 | 118.92      | 128.60   |
| 35  | BB    | 2284 | A    | N1-C6-N6   | 16.14  | 128.28      | 118.60   |
| 35  | BB    | 2588 | G    | N1-C6-O6   | 16.14  | 129.58      | 119.90   |
| 1   | AA    | 227  | G    | C5-C6-O6   | -16.12 | 118.93      | 128.60   |
| 35  | BB    | 2763 | G    | C5-C6-O6   | -16.11 | 118.93      | 128.60   |
| 35  | BB    | 1456 | G    | C5-C6-O6   | -16.11 | 118.93      | 128.60   |
| 35  | BB    | 752  | A    | N1-C6-N6   | 16.11  | 128.26      | 118.60   |
| 1   | AA    | 1434 | A    | N1-C2-N3   | 16.11  | 137.35      | 129.30   |
| 30  | B5    | 180  | PHE  | CB-CG-CD1  | 16.11  | 132.07      | 120.80   |
| 35  | BB    | 1444 | G    | C5-C6-O6   | -16.10 | 118.94      | 128.60   |
| 35  | BB    | 948  | C    | O4'-C1'-N1 | 16.09  | 121.07      | 108.20   |
| 1   | AA    | 577  | G    | N1-C6-O6   | 16.09  | 129.55      | 119.90   |
| 35  | BB    | 2123 | G    | C5-C6-O6   | -16.07 | 118.95      | 128.60   |
| 1   | AA    | 1446 | A    | N1-C6-N6   | 16.07  | 128.24      | 118.60   |
| 1   | AA    | 1401 | G    | C5-C6-O6   | -16.05 | 118.97      | 128.60   |
| 1   | AA    | 16   | A    | C5-C6-N1   | -16.05 | 109.67      | 117.70   |
| 1   | AA    | 331  | G    | C5-C6-O6   | -16.05 | 118.97      | 128.60   |
| 1   | AA    | 1357 | A    | N1-C6-N6   | 16.05  | 128.23      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1089 | A    | C5-C6-N6   | -16.04 | 110.87      | 123.70   |
| 1   | AA    | 746  | A    | N1-C6-N6   | 16.02  | 128.21      | 118.60   |
| 35  | BB    | 2049 | G    | C5-C6-O6   | -16.02 | 118.99      | 128.60   |
| 35  | BB    | 2211 | A    | N1-C6-N6   | 16.01  | 128.21      | 118.60   |
| 35  | BB    | 2183 | A    | N1-C6-N6   | 16.01  | 128.21      | 118.60   |
| 1   | AA    | 364  | A    | N1-C6-N6   | 16.01  | 128.20      | 118.60   |
| 35  | BB    | 2432 | A    | N1-C6-N6   | 16.01  | 128.20      | 118.60   |
| 35  | BB    | 1354 | A    | N1-C6-N6   | 16.00  | 128.20      | 118.60   |
| 35  | BB    | 417  | C    | N3-C4-C5   | -16.00 | 115.50      | 121.90   |
| 35  | BB    | 165  | A    | N1-C6-N6   | 15.99  | 128.20      | 118.60   |
| 35  | BB    | 1213 | A    | N1-C6-N6   | 15.99  | 128.19      | 118.60   |
| 35  | BB    | 716  | A    | C5-C6-N1   | -15.98 | 109.71      | 117.70   |
| 35  | BB    | 1839 | G    | N1-C6-O6   | 15.98  | 129.49      | 119.90   |
| 35  | BB    | 1526 | C    | N3-C4-C5   | -15.98 | 115.51      | 121.90   |
| 1   | AA    | 671  | G    | C5-C6-O6   | -15.97 | 119.02      | 128.60   |
| 1   | AA    | 604  | G    | C5-C6-O6   | -15.97 | 119.02      | 128.60   |
| 1   | AA    | 902  | G    | C5-C6-O6   | -15.96 | 119.02      | 128.60   |
| 35  | BB    | 1037 | G    | N1-C6-O6   | 15.96  | 129.47      | 119.90   |
| 35  | BB    | 1967 | C    | N3-C4-C5   | -15.95 | 115.52      | 121.90   |
| 35  | BB    | 1419 | A    | N1-C6-N6   | 15.94  | 128.16      | 118.60   |
| 1   | AA    | 640  | A    | N1-C6-N6   | 15.93  | 128.16      | 118.60   |
| 28  | B3    | 51   | ARG  | NE-CZ-NH2  | 15.93  | 128.26      | 120.30   |
| 1   | AA    | 377  | G    | C5-C6-O6   | -15.93 | 119.05      | 128.60   |
| 35  | BB    | 95   | A    | N1-C6-N6   | 15.92  | 128.15      | 118.60   |
| 35  | BB    | 575  | A    | N1-C6-N6   | 15.92  | 128.15      | 118.60   |
| 1   | AA    | 386  | C    | C6-N1-C2   | -15.91 | 113.93      | 120.30   |
| 1   | AA    | 702  | A    | N1-C6-N6   | 15.90  | 128.14      | 118.60   |
| 35  | BB    | 1975 | G    | N1-C6-O6   | 15.88  | 129.43      | 119.90   |
| 35  | BB    | 151  | C    | N3-C4-C5   | -15.85 | 115.56      | 121.90   |
| 35  | BB    | 2175 | C    | O4'-C1'-N1 | 15.84  | 120.87      | 108.20   |
| 1   | AA    | 162  | A    | N1-C6-N6   | 15.84  | 128.10      | 118.60   |
| 1   | AA    | 909  | A    | N1-C6-N6   | 15.84  | 128.10      | 118.60   |
| 35  | BB    | 818  | G    | C5-C6-O6   | -15.83 | 119.10      | 128.60   |
| 35  | BB    | 805  | G    | N1-C6-O6   | 15.83  | 129.40      | 119.90   |
| 35  | BB    | 2826 | A    | N1-C6-N6   | 15.82  | 128.09      | 118.60   |
| 1   | AA    | 817  | C    | C6-N1-C2   | -15.82 | 113.97      | 120.30   |
| 1   | AA    | 1453 | G    | O4'-C1'-N9 | 15.81  | 120.85      | 108.20   |
| 35  | BB    | 2414 | G    | N1-C6-O6   | 15.81  | 129.39      | 119.90   |
| 1   | AA    | 384  | G    | C5-C6-O6   | -15.81 | 119.11      | 128.60   |
| 1   | AA    | 400  | C    | N3-C4-N4   | 15.81  | 129.06      | 118.00   |
| 35  | BB    | 2531 | A    | N1-C6-N6   | 15.80  | 128.08      | 118.60   |
| 35  | BB    | 1669 | A    | N1-C6-N6   | 15.80  | 128.08      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1350 | C    | O4'-C1'-N1 | 15.79  | 120.83      | 108.20   |
| 35  | BB    | 727  | A    | N1-C6-N6   | 15.79  | 128.07      | 118.60   |
| 34  | BA    | 112  | G    | N1-C6-O6   | 15.78  | 129.37      | 119.90   |
| 1   | AA    | 1087 | G    | C5-C6-O6   | -15.78 | 119.13      | 128.60   |
| 35  | BB    | 947  | A    | N1-C6-N6   | 15.78  | 128.07      | 118.60   |
| 35  | BB    | 2812 | G    | N1-C6-O6   | 15.78  | 129.37      | 119.90   |
| 35  | BB    | 2170 | A    | N1-C6-N6   | 15.76  | 128.06      | 118.60   |
| 1   | AA    | 1067 | A    | N1-C6-N6   | 15.76  | 128.05      | 118.60   |
| 35  | BB    | 551  | G    | C5-C6-O6   | -15.76 | 119.15      | 128.60   |
| 35  | BB    | 1029 | A    | N1-C6-N6   | 15.76  | 128.05      | 118.60   |
| 1   | AA    | 946  | A    | N1-C6-N6   | 15.75  | 128.05      | 118.60   |
| 35  | BB    | 2434 | A    | N1-C6-N6   | 15.75  | 128.05      | 118.60   |
| 1   | AA    | 1022 | A    | C8-N9-C4   | -15.74 | 99.50       | 105.80   |
| 1   | AA    | 1150 | A    | N1-C6-N6   | 15.74  | 128.04      | 118.60   |
| 35  | BB    | 1766 | G    | N1-C6-O6   | 15.74  | 129.34      | 119.90   |
| 35  | BB    | 1868 | C    | O4'-C1'-N1 | 15.73  | 120.78      | 108.20   |
| 35  | BB    | 1984 | G    | N1-C6-O6   | 15.73  | 129.34      | 119.90   |
| 1   | AA    | 320  | A    | N1-C6-N6   | 15.72  | 128.03      | 118.60   |
| 1   | AA    | 1218 | C    | C6-N1-C2   | -15.72 | 114.01      | 120.30   |
| 35  | BB    | 1371 | G    | N1-C6-O6   | 15.72  | 129.33      | 119.90   |
| 1   | AA    | 1299 | A    | C4-C5-C6   | 15.71  | 124.86      | 117.00   |
| 35  | BB    | 1575 | C    | O4'-C1'-N1 | 15.71  | 120.77      | 108.20   |
| 35  | BB    | 2766 | A    | N1-C6-N6   | 15.71  | 128.03      | 118.60   |
| 1   | AA    | 851  | G    | N1-C6-O6   | 15.70  | 129.32      | 119.90   |
| 35  | BB    | 863  | A    | N1-C6-N6   | 15.70  | 128.02      | 118.60   |
| 35  | BB    | 1048 | A    | N1-C6-N6   | 15.70  | 128.02      | 118.60   |
| 35  | BB    | 1296 | G    | C5-C6-O6   | -15.69 | 119.18      | 128.60   |
| 1   | AA    | 116  | A    | N1-C6-N6   | 15.69  | 128.01      | 118.60   |
| 35  | BB    | 730  | A    | C5-C6-N6   | -15.68 | 111.16      | 123.70   |
| 35  | BB    | 1134 | A    | N1-C6-N6   | 15.67  | 128.00      | 118.60   |
| 35  | BB    | 1544 | A    | N1-C6-N6   | 15.67  | 128.00      | 118.60   |
| 1   | AA    | 353  | A    | N1-C6-N6   | 15.66  | 128.00      | 118.60   |
| 35  | BB    | 1754 | A    | N1-C6-N6   | 15.66  | 128.00      | 118.60   |
| 1   | AA    | 377  | G    | N1-C6-O6   | 15.66  | 129.30      | 119.90   |
| 35  | BB    | 210  | C    | O4'-C1'-N1 | 15.66  | 120.73      | 108.20   |
| 1   | AA    | 404  | G    | N1-C6-O6   | 15.66  | 129.29      | 119.90   |
| 1   | AA    | 649  | A    | N1-C6-N6   | 15.65  | 127.99      | 118.60   |
| 35  | BB    | 194  | G    | C5-C6-O6   | -15.65 | 119.21      | 128.60   |
| 35  | BB    | 2633 | G    | N1-C6-O6   | 15.65  | 129.29      | 119.90   |
| 35  | BB    | 648  | G    | N1-C6-O6   | 15.64  | 129.29      | 119.90   |
| 35  | BB    | 1520 | U    | O4'-C1'-N1 | 15.64  | 120.71      | 108.20   |
| 28  | B3    | 12   | ARG  | NE-CZ-NH2  | -15.64 | 112.48      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 990  | A    | N1-C6-N6   | 15.64  | 127.98      | 118.60   |
| 35  | BB    | 1603 | A    | N1-C6-N6   | 15.64  | 127.98      | 118.60   |
| 35  | BB    | 2031 | A    | N1-C6-N6   | 15.64  | 127.98      | 118.60   |
| 35  | BB    | 2102 | G    | N1-C6-O6   | 15.64  | 129.28      | 119.90   |
| 35  | BB    | 1050 | A    | N1-C6-N6   | 15.62  | 127.97      | 118.60   |
| 35  | BB    | 2516 | A    | C8-N9-C4   | -15.62 | 99.55       | 105.80   |
| 35  | BB    | 1144 | A    | C5-C6-N1   | -15.61 | 109.89      | 117.70   |
| 1   | AA    | 784  | A    | N1-C6-N6   | 15.61  | 127.97      | 118.60   |
| 1   | AA    | 315  | A    | N1-C6-N6   | 15.61  | 127.97      | 118.60   |
| 35  | BB    | 330  | A    | N1-C6-N6   | 15.61  | 127.96      | 118.60   |
| 1   | AA    | 121  | U    | O4'-C1'-N1 | 15.60  | 120.68      | 108.20   |
| 1   | AA    | 424  | G    | C5-C6-N1   | -15.60 | 103.70      | 111.50   |
| 1   | AA    | 1055 | A    | C8-N9-C4   | -15.60 | 99.56       | 105.80   |
| 35  | BB    | 443  | A    | N1-C6-N6   | 15.60  | 127.96      | 118.60   |
| 1   | AA    | 1418 | A    | C5-C6-N1   | -15.60 | 109.90      | 117.70   |
| 35  | BB    | 2115 | G    | N1-C6-O6   | 15.60  | 129.26      | 119.90   |
| 34  | BA    | 115  | A    | C5-C6-N6   | -15.60 | 111.22      | 123.70   |
| 1   | AA    | 197  | A    | N1-C6-N6   | 15.59  | 127.95      | 118.60   |
| 35  | BB    | 101  | A    | N1-C6-N6   | 15.59  | 127.95      | 118.60   |
| 35  | BB    | 1032 | A    | N1-C6-N6   | 15.59  | 127.95      | 118.60   |
| 1   | AA    | 1465 | A    | N1-C6-N6   | 15.59  | 127.95      | 118.60   |
| 1   | AA    | 142  | G    | C5-C6-O6   | -15.58 | 119.25      | 128.60   |
| 35  | BB    | 1429 | G    | N1-C6-O6   | 15.58  | 129.25      | 119.90   |
| 35  | BB    | 2882 | A    | N1-C6-N6   | 15.57  | 127.94      | 118.60   |
| 35  | BB    | 809  | G    | N1-C6-O6   | 15.57  | 129.24      | 119.90   |
| 35  | BB    | 2369 | A    | N1-C6-N6   | 15.57  | 127.94      | 118.60   |
| 35  | BB    | 1429 | G    | C5-C6-O6   | -15.56 | 119.26      | 128.60   |
| 1   | AA    | 819  | A    | C8-N9-C4   | -15.56 | 99.58       | 105.80   |
| 35  | BB    | 2235 | G    | C5-C6-O6   | -15.55 | 119.27      | 128.60   |
| 35  | BB    | 2542 | A    | N1-C6-N6   | 15.55  | 127.93      | 118.60   |
| 35  | BB    | 1246 | A    | C5-C6-N1   | -15.54 | 109.93      | 117.70   |
| 34  | BA    | 52   | A    | N1-C6-N6   | 15.53  | 127.92      | 118.60   |
| 1   | AA    | 1514 | G    | C5-C6-O6   | -15.53 | 119.28      | 128.60   |
| 35  | BB    | 1572 | A    | N1-C6-N6   | 15.53  | 127.92      | 118.60   |
| 35  | BB    | 196  | A    | N1-C6-N6   | 15.53  | 127.92      | 118.60   |
| 47  | BN    | 86   | ARG  | NE-CZ-NH2  | -15.53 | 112.54      | 120.30   |
| 1   | AA    | 1413 | A    | O4'-C1'-N9 | 15.52  | 120.62      | 108.20   |
| 1   | AA    | 68   | G    | C5-C6-O6   | -15.52 | 119.29      | 128.60   |
| 35  | BB    | 352  | A    | N1-C6-N6   | 15.51  | 127.91      | 118.60   |
| 1   | AA    | 747  | A    | N1-C6-N6   | 15.51  | 127.91      | 118.60   |
| 35  | BB    | 291  | G    | N1-C6-O6   | 15.51  | 129.21      | 119.90   |
| 35  | BB    | 771  | G    | N1-C6-O6   | 15.51  | 129.21      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2147 | A    | N1-C6-N6   | 15.51  | 127.90      | 118.60   |
| 35  | BB    | 1007 | C    | N3-C4-N4   | 15.50  | 128.85      | 118.00   |
| 35  | BB    | 2199 | A    | N1-C6-N6   | 15.50  | 127.90      | 118.60   |
| 1   | AA    | 325  | A    | N1-C6-N6   | 15.50  | 127.90      | 118.60   |
| 1   | AA    | 393  | A    | N1-C6-N6   | 15.50  | 127.90      | 118.60   |
| 1   | AA    | 869  | G    | N1-C6-O6   | 15.49  | 129.19      | 119.90   |
| 35  | BB    | 260  | G    | C5-C6-O6   | -15.49 | 119.31      | 128.60   |
| 35  | BB    | 622  | G    | N1-C6-O6   | 15.49  | 129.19      | 119.90   |
| 35  | BB    | 2434 | A    | C5-C6-N1   | -15.49 | 109.96      | 117.70   |
| 35  | BB    | 2294 | G    | C8-N9-C4   | -15.48 | 100.21      | 106.40   |
| 35  | BB    | 2318 | G    | C5-C6-O6   | -15.48 | 119.31      | 128.60   |
| 35  | BB    | 1475 | G    | N1-C6-O6   | 15.47  | 129.19      | 119.90   |
| 35  | BB    | 531  | C    | N3-C4-N4   | 15.46  | 128.83      | 118.00   |
| 35  | BB    | 1328 | A    | N1-C6-N6   | 15.47  | 127.88      | 118.60   |
| 1   | AA    | 410  | G    | O4'-C1'-N9 | 15.46  | 120.57      | 108.20   |
| 35  | BB    | 1759 | A    | N1-C6-N6   | 15.46  | 127.88      | 118.60   |
| 35  | BB    | 1780 | A    | N1-C6-N6   | 15.45  | 127.87      | 118.60   |
| 35  | BB    | 2375 | G    | C5-C6-O6   | -15.46 | 119.33      | 128.60   |
| 35  | BB    | 2327 | A    | N1-C6-N6   | 15.45  | 127.87      | 118.60   |
| 35  | BB    | 2247 | A    | O4'-C1'-N9 | 15.45  | 120.56      | 108.20   |
| 1   | AA    | 1155 | A    | N1-C6-N6   | 15.44  | 127.86      | 118.60   |
| 35  | BB    | 1496 | A    | C8-N9-C4   | -15.42 | 99.63       | 105.80   |
| 1   | AA    | 149  | A    | C4-C5-C6   | 15.41  | 124.71      | 117.00   |
| 1   | AA    | 1497 | G    | N1-C6-O6   | 15.41  | 129.15      | 119.90   |
| 35  | BB    | 1805 | A    | N1-C6-N6   | 15.41  | 127.85      | 118.60   |
| 22  | AV    | 73   | A    | C5-C6-N6   | -15.40 | 111.38      | 123.70   |
| 35  | BB    | 1969 | A    | N1-C6-N6   | 15.40  | 127.84      | 118.60   |
| 34  | BA    | 118  | C    | N3-C4-C5   | -15.40 | 115.74      | 121.90   |
| 1   | AA    | 1068 | G    | N1-C6-O6   | 15.39  | 129.13      | 119.90   |
| 1   | AA    | 53   | A    | N1-C6-N6   | 15.39  | 127.83      | 118.60   |
| 35  | BB    | 989  | G    | N1-C6-O6   | 15.38  | 129.13      | 119.90   |
| 35  | BB    | 1206 | G    | N1-C6-O6   | 15.38  | 129.13      | 119.90   |
| 35  | BB    | 1566 | A    | C5-C6-N1   | -15.38 | 110.01      | 117.70   |
| 35  | BB    | 1676 | A    | C5-C6-N1   | -15.38 | 110.01      | 117.70   |
| 35  | BB    | 1828 | G    | N1-C6-O6   | 15.38  | 129.13      | 119.90   |
| 35  | BB    | 1020 | A    | N1-C6-N6   | 15.37  | 127.82      | 118.60   |
| 1   | AA    | 1151 | A    | N1-C6-N6   | 15.36  | 127.82      | 118.60   |
| 1   | AA    | 1287 | A    | N1-C6-N6   | 15.36  | 127.82      | 118.60   |
| 35  | BB    | 233  | A    | N1-C6-N6   | 15.36  | 127.82      | 118.60   |
| 1   | AA    | 1409 | C    | N3-C4-C5   | -15.36 | 115.76      | 121.90   |
| 35  | BB    | 2287 | A    | N1-C6-N6   | 15.36  | 127.81      | 118.60   |
| 35  | BB    | 2288 | A    | N1-C6-N6   | 15.36  | 127.81      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1828 | G    | C5-C6-O6   | -15.35 | 119.39      | 128.60   |
| 35  | BB    | 1819 | A    | N1-C6-N6   | 15.34  | 127.81      | 118.60   |
| 35  | BB    | 1238 | G    | N1-C6-O6   | 15.34  | 129.10      | 119.90   |
| 35  | BB    | 2642 | G    | C8-N9-C4   | -15.34 | 100.26      | 106.40   |
| 35  | BB    | 372  | G    | C5-C6-O6   | -15.33 | 119.40      | 128.60   |
| 35  | BB    | 207  | A    | N1-C6-N6   | 15.33  | 127.80      | 118.60   |
| 1   | AA    | 544  | G    | N1-C6-O6   | 15.32  | 129.09      | 119.90   |
| 36  | BC    | 202  | ARG  | NE-CZ-NH1  | 15.32  | 127.96      | 120.30   |
| 1   | AA    | 635  | A    | N1-C6-N6   | 15.31  | 127.79      | 118.60   |
| 35  | BB    | 660  | C    | C6-N1-C2   | -15.31 | 114.18      | 120.30   |
| 35  | BB    | 2126 | A    | N1-C6-N6   | 15.31  | 127.78      | 118.60   |
| 47  | BN    | 64   | ARG  | NE-CZ-NH1  | 15.31  | 127.95      | 120.30   |
| 1   | AA    | 250  | A    | N1-C6-N6   | 15.30  | 127.78      | 118.60   |
| 35  | BB    | 2241 | A    | C4-C5-C6   | 15.30  | 124.65      | 117.00   |
| 35  | BB    | 379  | G    | C5-C6-O6   | -15.29 | 119.42      | 128.60   |
| 35  | BB    | 298  | G    | N1-C6-O6   | 15.28  | 129.07      | 119.90   |
| 1   | AA    | 1318 | A    | N1-C6-N6   | 15.28  | 127.77      | 118.60   |
| 1   | AA    | 532  | A    | N1-C6-N6   | 15.27  | 127.76      | 118.60   |
| 35  | BB    | 75   | G    | C5-N7-C8   | 15.27  | 111.93      | 104.30   |
| 35  | BB    | 1910 | G    | O4'-C1'-N9 | 15.27  | 120.42      | 108.20   |
| 35  | BB    | 477  | A    | N1-C6-N6   | 15.27  | 127.76      | 118.60   |
| 35  | BB    | 1376 | C    | O4'-C1'-N1 | 15.27  | 120.41      | 108.20   |
| 35  | BB    | 2381 | A    | N1-C6-N6   | 15.27  | 127.76      | 118.60   |
| 35  | BB    | 1515 | A    | N1-C6-N6   | 15.26  | 127.75      | 118.60   |
| 35  | BB    | 1978 | A    | N1-C6-N6   | 15.26  | 127.75      | 118.60   |
| 35  | BB    | 1197 | G    | C5-C6-O6   | -15.25 | 119.45      | 128.60   |
| 1   | AA    | 941  | G    | N1-C6-O6   | 15.24  | 129.05      | 119.90   |
| 35  | BB    | 1530 | G    | N1-C6-O6   | 15.24  | 129.04      | 119.90   |
| 1   | AA    | 1185 | G    | N1-C6-O6   | 15.23  | 129.04      | 119.90   |
| 35  | BB    | 38   | A    | N1-C6-N6   | 15.23  | 127.74      | 118.60   |
| 35  | BB    | 861  | A    | C8-N9-C4   | 15.22  | 111.89      | 105.80   |
| 35  | BB    | 1989 | G    | C8-N9-C4   | -15.22 | 100.31      | 106.40   |
| 35  | BB    | 1074 | G    | N1-C6-O6   | 15.22  | 129.03      | 119.90   |
| 35  | BB    | 2024 | G    | C5-C6-O6   | -15.22 | 119.47      | 128.60   |
| 35  | BB    | 2396 | G    | C5-C6-O6   | -15.21 | 119.47      | 128.60   |
| 35  | BB    | 212  | G    | N1-C6-O6   | 15.20  | 129.02      | 119.90   |
| 35  | BB    | 1807 | G    | C5-C6-O6   | -15.20 | 119.48      | 128.60   |
| 35  | BB    | 752  | A    | C5-C6-N1   | -15.18 | 110.11      | 117.70   |
| 35  | BB    | 1750 | G    | C5-C6-O6   | -15.17 | 119.50      | 128.60   |
| 1   | AA    | 451  | A    | N1-C6-N6   | 15.16  | 127.69      | 118.60   |
| 35  | BB    | 1882 | U    | C5-C4-O4   | -15.16 | 116.80      | 125.90   |
| 35  | BB    | 2625 | G    | N1-C6-O6   | 15.16  | 129.00      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 1072 | G    | N1-C6-O6   | 15.15  | 128.99      | 119.90   |
| 35  | BB    | 466  | A    | N1-C6-N6   | 15.15  | 127.69      | 118.60   |
| 35  | BB    | 781  | A    | C4-C5-C6   | 15.15  | 124.57      | 117.00   |
| 1   | AA    | 1215 | G    | C8-N9-C4   | -15.14 | 100.34      | 106.40   |
| 1   | AA    | 1441 | A    | N1-C6-N6   | 15.13  | 127.68      | 118.60   |
| 1   | AA    | 1163 | A    | N1-C2-N3   | -15.12 | 121.74      | 129.30   |
| 35  | BB    | 1491 | G    | N1-C6-O6   | 15.12  | 128.97      | 119.90   |
| 35  | BB    | 2275 | C    | C2-N3-C4   | 15.12  | 127.46      | 119.90   |
| 35  | BB    | 2005 | A    | N1-C6-N6   | 15.12  | 127.67      | 118.60   |
| 35  | BB    | 1445 | G    | C5-C6-O6   | -15.11 | 119.53      | 128.60   |
| 35  | BB    | 1853 | A    | N1-C6-N6   | 15.11  | 127.66      | 118.60   |
| 1   | AA    | 1175 | G    | N1-C6-O6   | 15.10  | 128.96      | 119.90   |
| 1   | AA    | 77   | A    | N1-C6-N6   | 15.09  | 127.65      | 118.60   |
| 35  | BB    | 2004 | G    | N1-C6-O6   | 15.09  | 128.95      | 119.90   |
| 35  | BB    | 2538 | C    | N3-C4-N4   | 15.08  | 128.56      | 118.00   |
| 1   | AA    | 1185 | G    | C5-C6-O6   | -15.08 | 119.55      | 128.60   |
| 35  | BB    | 680  | C    | N3-C4-N4   | 15.08  | 128.56      | 118.00   |
| 1   | AA    | 310  | G    | N1-C6-O6   | 15.08  | 128.94      | 119.90   |
| 1   | AA    | 546  | A    | N1-C2-N3   | 15.07  | 136.83      | 129.30   |
| 35  | BB    | 2641 | G    | N1-C6-O6   | 15.06  | 128.94      | 119.90   |
| 35  | BB    | 2729 | G    | N1-C6-O6   | 15.06  | 128.94      | 119.90   |
| 1   | AA    | 1269 | A    | N1-C6-N6   | 15.05  | 127.63      | 118.60   |
| 35  | BB    | 2588 | G    | C5-C6-O6   | -15.04 | 119.58      | 128.60   |
| 35  | BB    | 974  | G    | N1-C6-O6   | 15.04  | 128.92      | 119.90   |
| 1   | AA    | 105  | G    | N1-C6-O6   | 15.03  | 128.92      | 119.90   |
| 35  | BB    | 322  | A    | N1-C6-N6   | 15.03  | 127.62      | 118.60   |
| 34  | BA    | 61   | G    | C5-C6-O6   | -15.03 | 119.58      | 128.60   |
| 35  | BB    | 362  | A    | N1-C6-N6   | 15.02  | 127.61      | 118.60   |
| 1   | AA    | 1514 | G    | N1-C6-O6   | 15.01  | 128.91      | 119.90   |
| 35  | BB    | 1674 | G    | N1-C6-O6   | 15.01  | 128.91      | 119.90   |
| 1   | AA    | 839  | C    | N3-C4-N4   | 15.01  | 128.50      | 118.00   |
| 1   | AA    | 1138 | G    | C8-N9-C4   | -15.00 | 100.40      | 106.40   |
| 35  | BB    | 2406 | A    | N1-C6-N6   | 15.00  | 127.60      | 118.60   |
| 1   | AA    | 729  | A    | N1-C6-N6   | 15.00  | 127.60      | 118.60   |
| 1   | AA    | 990  | C    | N3-C4-N4   | 14.99  | 128.50      | 118.00   |
| 35  | BB    | 1289 | C    | O4'-C1'-N1 | 14.99  | 120.19      | 108.20   |
| 35  | BB    | 1282 | U    | O4'-C1'-N1 | 14.98  | 120.19      | 108.20   |
| 34  | BA    | 117  | G    | P-O3'-C3'  | 14.98  | 137.67      | 119.70   |
| 35  | BB    | 2487 | G    | C5-C6-O6   | -14.98 | 119.61      | 128.60   |
| 19  | AS    | 31   | ARG  | NE-CZ-NH1  | 14.97  | 127.78      | 120.30   |
| 1   | AA    | 1508 | A    | N1-C6-N6   | 14.97  | 127.58      | 118.60   |
| 34  | BA    | 117  | G    | C5-C6-O6   | -14.97 | 119.62      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 41  | BH    | 25   | TYR  | CB-CG-CD2  | -14.96 | 112.02      | 121.00   |
| 1   | AA    | 321  | A    | N1-C6-N6   | 14.96  | 127.58      | 118.60   |
| 35  | BB    | 2366 | A    | N1-C6-N6   | 14.96  | 127.58      | 118.60   |
| 35  | BB    | 2553 | G    | N1-C6-O6   | 14.96  | 128.88      | 119.90   |
| 35  | BB    | 1889 | A    | N1-C6-N6   | 14.95  | 127.57      | 118.60   |
| 1   | AA    | 1469 | C    | O4'-C1'-N1 | 14.94  | 120.15      | 108.20   |
| 1   | AA    | 1489 | G    | C5-C6-O6   | -14.94 | 119.64      | 128.60   |
| 35  | BB    | 1482 | G    | N1-C6-O6   | 14.94  | 128.86      | 119.90   |
| 35  | BB    | 9    | G    | O4'-C1'-N9 | 14.93  | 120.14      | 108.20   |
| 35  | BB    | 829  | A    | N1-C6-N6   | 14.93  | 127.56      | 118.60   |
| 1   | AA    | 1396 | A    | C5-C6-N6   | -14.92 | 111.76      | 123.70   |
| 35  | BB    | 350  | G    | N1-C6-O6   | 14.92  | 128.85      | 119.90   |
| 35  | BB    | 2085 | U    | O4'-C1'-N1 | 14.91  | 120.12      | 108.20   |
| 35  | BB    | 2753 | A    | N9-C4-C5   | 14.91  | 111.76      | 105.80   |
| 35  | BB    | 1773 | A    | N1-C6-N6   | 14.90  | 127.54      | 118.60   |
| 35  | BB    | 907  | G    | C5-C6-O6   | -14.89 | 119.66      | 128.60   |
| 35  | BB    | 60   | G    | C5-C6-O6   | -14.88 | 119.67      | 128.60   |
| 35  | BB    | 1058 | U    | O4'-C1'-N1 | 14.88  | 120.11      | 108.20   |
| 35  | BB    | 1248 | G    | N1-C6-O6   | 14.88  | 128.83      | 119.90   |
| 34  | BA    | 85   | G    | N1-C6-O6   | 14.88  | 128.83      | 119.90   |
| 1   | AA    | 45   | G    | C5-C6-O6   | -14.88 | 119.67      | 128.60   |
| 1   | AA    | 601  | G    | C5-C6-O6   | -14.87 | 119.68      | 128.60   |
| 1   | AA    | 711  | G    | N1-C6-O6   | 14.87  | 128.82      | 119.90   |
| 35  | BB    | 1077 | A    | N1-C6-N6   | 14.87  | 127.52      | 118.60   |
| 1   | AA    | 797  | C    | O4'-C1'-N1 | 14.87  | 120.09      | 108.20   |
| 1   | AA    | 1513 | A    | N1-C6-N6   | 14.87  | 127.52      | 118.60   |
| 35  | BB    | 2776 | A    | C4-C5-C6   | 14.86  | 124.43      | 117.00   |
| 35  | BB    | 1177 | G    | N1-C6-O6   | 14.85  | 128.81      | 119.90   |
| 35  | BB    | 804  | A    | N1-C6-N6   | 14.85  | 127.51      | 118.60   |
| 1   | AA    | 79   | G    | N1-C6-O6   | 14.84  | 128.81      | 119.90   |
| 35  | BB    | 214  | G    | N1-C6-O6   | 14.84  | 128.81      | 119.90   |
| 35  | BB    | 2467 | C    | N3-C4-C5   | -14.84 | 115.96      | 121.90   |
| 1   | AA    | 338  | A    | N1-C6-N6   | 14.83  | 127.50      | 118.60   |
| 35  | BB    | 1403 | A    | N1-C6-N6   | 14.83  | 127.50      | 118.60   |
| 35  | BB    | 429  | A    | N1-C6-N6   | 14.83  | 127.50      | 118.60   |
| 35  | BB    | 272  | A    | C5-C6-N1   | -14.82 | 110.29      | 117.70   |
| 1   | AA    | 1021 | A    | N1-C6-N6   | 14.82  | 127.49      | 118.60   |
| 35  | BB    | 1088 | A    | O4'-C1'-N9 | 14.82  | 120.05      | 108.20   |
| 1   | AA    | 911  | U    | C6-N1-C2   | 14.81  | 129.89      | 121.00   |
| 1   | AA    | 466  | A    | N1-C6-N6   | 14.80  | 127.48      | 118.60   |
| 35  | BB    | 2899 | A    | C5-C6-N1   | -14.80 | 110.30      | 117.70   |
| 1   | AA    | 947  | G    | N1-C6-O6   | 14.80  | 128.78      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 61   | C    | N3-C4-C5   | -14.79 | 115.98      | 121.90   |
| 35  | BB    | 500  | G    | N1-C6-O6   | 14.79  | 128.77      | 119.90   |
| 35  | BB    | 2066 | C    | N3-C4-C5   | -14.79 | 115.98      | 121.90   |
| 35  | BB    | 9    | G    | N1-C6-O6   | 14.79  | 128.77      | 119.90   |
| 35  | BB    | 473  | G    | N1-C6-O6   | 14.79  | 128.77      | 119.90   |
| 35  | BB    | 797  | G    | C5-C6-O6   | -14.79 | 119.73      | 128.60   |
| 35  | BB    | 2057 | G    | N1-C6-O6   | 14.79  | 128.77      | 119.90   |
| 35  | BB    | 575  | A    | C5-C6-N6   | -14.78 | 111.87      | 123.70   |
| 35  | BB    | 2468 | A    | N1-C6-N6   | 14.78  | 127.47      | 118.60   |
| 35  | BB    | 2235 | G    | N1-C6-O6   | 14.78  | 128.77      | 119.90   |
| 35  | BB    | 2020 | A    | N1-C6-N6   | 14.78  | 127.47      | 118.60   |
| 35  | BB    | 2089 | C    | N3-C4-C5   | -14.78 | 115.99      | 121.90   |
| 35  | BB    | 1006 | C    | N3-C4-C5   | -14.77 | 115.99      | 121.90   |
| 39  | BF    | 91   | ARG  | NE-CZ-NH2  | -14.77 | 112.92      | 120.30   |
| 35  | BB    | 41   | C    | N3-C4-N4   | 14.77  | 128.34      | 118.00   |
| 35  | BB    | 181  | A    | N1-C6-N6   | 14.77  | 127.46      | 118.60   |
| 35  | BB    | 1529 | G    | C4-C5-N7   | 14.76  | 116.70      | 110.80   |
| 35  | BB    | 1823 | G    | N1-C2-N3   | -14.76 | 115.05      | 123.90   |
| 35  | BB    | 60   | G    | N1-C6-O6   | 14.75  | 128.75      | 119.90   |
| 31  | B6    | 21   | ARG  | NE-CZ-NH1  | -14.75 | 112.93      | 120.30   |
| 1   | AA    | 19   | A    | N1-C6-N6   | 14.74  | 127.44      | 118.60   |
| 1   | AA    | 141  | G    | N1-C6-O6   | 14.74  | 128.74      | 119.90   |
| 35  | BB    | 2597 | G    | C5-C6-O6   | -14.73 | 119.76      | 128.60   |
| 39  | BF    | 6    | TYR  | CB-CG-CD2  | -14.73 | 112.16      | 121.00   |
| 35  | BB    | 893  | C    | O4'-C1'-N1 | 14.72  | 119.98      | 108.20   |
| 35  | BB    | 1711 | A    | N1-C6-N6   | 14.72  | 127.44      | 118.60   |
| 35  | BB    | 1005 | C    | O4'-C1'-N1 | 14.72  | 119.97      | 108.20   |
| 1   | AA    | 865  | A    | N1-C6-N6   | 14.71  | 127.42      | 118.60   |
| 39  | BF    | 6    | TYR  | CB-CG-CD1  | 14.71  | 129.82      | 121.00   |
| 1   | AA    | 1256 | A    | N1-C6-N6   | 14.70  | 127.42      | 118.60   |
| 35  | BB    | 2639 | A    | N1-C6-N6   | 14.70  | 127.42      | 118.60   |
| 1   | AA    | 141  | G    | C5-C6-O6   | -14.70 | 119.78      | 128.60   |
| 35  | BB    | 1719 | G    | O4'-C1'-N9 | 14.69  | 119.95      | 108.20   |
| 35  | BB    | 1333 | G    | N1-C6-O6   | 14.69  | 128.72      | 119.90   |
| 35  | BB    | 1077 | A    | C5-C6-N1   | -14.69 | 110.36      | 117.70   |
| 35  | BB    | 1311 | G    | N1-C6-O6   | 14.69  | 128.71      | 119.90   |
| 35  | BB    | 2227 | A    | N9-C4-C5   | 14.68  | 111.67      | 105.80   |
| 1   | AA    | 1233 | G    | N1-C6-O6   | 14.68  | 128.71      | 119.90   |
| 1   | AA    | 181  | A    | C5-C6-N1   | -14.68 | 110.36      | 117.70   |
| 35  | BB    | 1772 | A    | N1-C6-N6   | 14.68  | 127.41      | 118.60   |
| 35  | BB    | 2663 | G    | C6-C5-N7   | -14.68 | 121.59      | 130.40   |
| 35  | BB    | 1635 | A    | N1-C6-N6   | 14.67  | 127.40      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1112 | G    | N1-C6-O6   | 14.67  | 128.70      | 119.90   |
| 35  | BB    | 181  | A    | O4'-C1'-N9 | 14.66  | 119.93      | 108.20   |
| 35  | BB    | 421  | C    | C6-N1-C2   | -14.66 | 114.44      | 120.30   |
| 1   | AA    | 1347 | G    | N1-C6-O6   | 14.66  | 128.69      | 119.90   |
| 35  | BB    | 83   | A    | N9-C4-C5   | 14.66  | 111.66      | 105.80   |
| 35  | BB    | 2846 | G    | N1-C6-O6   | 14.65  | 128.69      | 119.90   |
| 35  | BB    | 1094 | U    | O4'-C1'-N1 | 14.65  | 119.92      | 108.20   |
| 35  | BB    | 260  | G    | N1-C6-O6   | 14.65  | 128.69      | 119.90   |
| 35  | BB    | 2630 | G    | C5-C6-O6   | -14.65 | 119.81      | 128.60   |
| 35  | BB    | 510  | C    | O4'-C1'-N1 | 14.64  | 119.91      | 108.20   |
| 35  | BB    | 959  | A    | N1-C2-N3   | -14.64 | 121.98      | 129.30   |
| 1   | AA    | 422  | C    | N3-C4-C5   | -14.64 | 116.05      | 121.90   |
| 1   | AA    | 595  | A    | N1-C6-N6   | 14.64  | 127.38      | 118.60   |
| 35  | BB    | 1465 | G    | C5-C6-O6   | -14.63 | 119.82      | 128.60   |
| 35  | BB    | 1210 | G    | N1-C6-O6   | 14.63  | 128.68      | 119.90   |
| 34  | BA    | 56   | G    | C8-N9-C4   | -14.62 | 100.55      | 106.40   |
| 35  | BB    | 2863 | C    | O4'-C1'-N1 | 14.62  | 119.90      | 108.20   |
| 35  | BB    | 654  | A    | N1-C6-N6   | 14.62  | 127.37      | 118.60   |
| 35  | BB    | 1076 | C    | O4'-C1'-N1 | 14.62  | 119.89      | 108.20   |
| 35  | BB    | 1804 | C    | C5-C6-N1   | 14.61  | 128.31      | 121.00   |
| 35  | BB    | 1935 | G    | C5-C6-O6   | -14.61 | 119.83      | 128.60   |
| 35  | BB    | 680  | C    | C5-C4-N4   | -14.61 | 109.97      | 120.20   |
| 35  | BB    | 1528 | A    | N1-C6-N6   | 14.60  | 127.36      | 118.60   |
| 1   | AA    | 1102 | A    | N1-C6-N6   | 14.59  | 127.36      | 118.60   |
| 1   | AA    | 1521 | C    | O4'-C1'-N1 | 14.59  | 119.87      | 108.20   |
| 1   | AA    | 269  | C    | O4'-C1'-N1 | 14.59  | 119.87      | 108.20   |
| 1   | AA    | 286  | C    | O4'-C1'-N1 | 14.59  | 119.87      | 108.20   |
| 1   | AA    | 1288 | A    | C8-N9-C4   | -14.59 | 99.97       | 105.80   |
| 35  | BB    | 2665 | A    | N1-C6-N6   | 14.59  | 127.35      | 118.60   |
| 1   | AA    | 1331 | G    | N1-C6-O6   | 14.58  | 128.65      | 119.90   |
| 35  | BB    | 371  | A    | N1-C6-N6   | 14.58  | 127.35      | 118.60   |
| 35  | BB    | 404  | A    | N1-C6-N6   | 14.58  | 127.35      | 118.60   |
| 35  | BB    | 2809 | A    | N1-C6-N6   | 14.58  | 127.35      | 118.60   |
| 35  | BB    | 1797 | G    | N1-C2-N3   | -14.57 | 115.16      | 123.90   |
| 35  | BB    | 215  | G    | C5-C6-O6   | -14.57 | 119.86      | 128.60   |
| 1   | AA    | 1180 | A    | N1-C6-N6   | 14.56  | 127.34      | 118.60   |
| 35  | BB    | 948  | C    | N3-C4-N4   | 14.55  | 128.18      | 118.00   |
| 35  | BB    | 2394 | C    | N3-C4-C5   | -14.55 | 116.08      | 121.90   |
| 35  | BB    | 1818 | U    | O4'-C1'-N1 | 14.54  | 119.83      | 108.20   |
| 40  | BG    | 108  | PHE  | CB-CG-CD2  | 14.54  | 130.98      | 120.80   |
| 35  | BB    | 1013 | C    | C6-N1-C2   | 14.54  | 126.12      | 120.30   |
| 35  | BB    | 764  | A    | N1-C6-N6   | 14.53  | 127.32      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 848  | C    | O4'-C1'-N1 | 14.53  | 119.82      | 108.20   |
| 35  | BB    | 2772 | C    | O4'-C1'-N1 | 14.53  | 119.82      | 108.20   |
| 35  | BB    | 528  | A    | N1-C6-N6   | 14.53  | 127.32      | 118.60   |
| 1   | AA    | 313  | A    | N1-C6-N6   | 14.52  | 127.31      | 118.60   |
| 35  | BB    | 1034 | G    | N1-C6-O6   | 14.50  | 128.60      | 119.90   |
| 35  | BB    | 2106 | U    | O4'-C1'-N1 | 14.49  | 119.79      | 108.20   |
| 35  | BB    | 2813 | A    | N1-C6-N6   | 14.49  | 127.29      | 118.60   |
| 1   | AA    | 575  | G    | C5-C6-O6   | -14.49 | 119.91      | 128.60   |
| 35  | BB    | 859  | G    | C5-C6-O6   | -14.48 | 119.91      | 128.60   |
| 1   | AA    | 1219 | A    | N1-C6-N6   | 14.48  | 127.29      | 118.60   |
| 35  | BB    | 1998 | A    | N1-C6-N6   | 14.48  | 127.29      | 118.60   |
| 35  | BB    | 2430 | A    | C4-C5-C6   | 14.48  | 124.24      | 117.00   |
| 35  | BB    | 2867 | G    | N1-C2-N3   | -14.47 | 115.22      | 123.90   |
| 1   | AA    | 59   | A    | C4-C5-N7   | -14.47 | 103.47      | 110.70   |
| 1   | AA    | 563  | A    | N1-C6-N6   | 14.46  | 127.28      | 118.60   |
| 35  | BB    | 1465 | G    | N1-C6-O6   | 14.46  | 128.57      | 119.90   |
| 35  | BB    | 1593 | A    | C5-C6-N6   | -14.46 | 112.13      | 123.70   |
| 35  | BB    | 1994 | C    | N3-C4-N4   | 14.46  | 128.12      | 118.00   |
| 39  | BF    | 21   | TYR  | CB-CG-CD1  | -14.46 | 112.33      | 121.00   |
| 1   | AA    | 1455 | G    | N1-C6-O6   | 14.45  | 128.57      | 119.90   |
| 35  | BB    | 943  | A    | C4-C5-C6   | 14.45  | 124.23      | 117.00   |
| 35  | BB    | 1096 | A    | N1-C6-N6   | 14.45  | 127.27      | 118.60   |
| 35  | BB    | 682  | G    | N1-C6-O6   | 14.45  | 128.57      | 119.90   |
| 1   | AA    | 897  | C    | N3-C4-C5   | -14.45 | 116.12      | 121.90   |
| 35  | BB    | 213  | A    | N1-C6-N6   | 14.45  | 127.27      | 118.60   |
| 35  | BB    | 1470 | A    | N1-C6-N6   | 14.45  | 127.27      | 118.60   |
| 1   | AA    | 1043 | G    | C5-C6-O6   | -14.44 | 119.94      | 128.60   |
| 1   | AA    | 1096 | C    | O4'-C1'-N1 | 14.44  | 119.75      | 108.20   |
| 35  | BB    | 2294 | G    | N9-C4-C5   | 14.44  | 111.18      | 105.40   |
| 35  | BB    | 1309 | G    | C5-C6-O6   | -14.44 | 119.94      | 128.60   |
| 35  | BB    | 597  | G    | N7-C8-N9   | -14.44 | 105.88      | 113.10   |
| 35  | BB    | 1737 | G    | C4-C5-N7   | 14.43  | 116.57      | 110.80   |
| 1   | AA    | 1248 | A    | N1-C6-N6   | 14.43  | 127.26      | 118.60   |
| 25  | B0    | 49   | ARG  | NE-CZ-NH2  | 14.43  | 127.52      | 120.30   |
| 35  | BB    | 2088 | A    | N1-C6-N6   | 14.43  | 127.26      | 118.60   |
| 35  | BB    | 2435 | A    | N1-C6-N6   | 14.42  | 127.25      | 118.60   |
| 35  | BB    | 1414 | C    | O4'-C1'-N1 | 14.42  | 119.74      | 108.20   |
| 35  | BB    | 1597 | A    | N1-C6-N6   | 14.42  | 127.25      | 118.60   |
| 35  | BB    | 63   | A    | N1-C6-N6   | 14.42  | 127.25      | 118.60   |
| 35  | BB    | 1067 | A    | N1-C6-N6   | 14.42  | 127.25      | 118.60   |
| 35  | BB    | 2792 | A    | N1-C6-N6   | 14.41  | 127.25      | 118.60   |
| 35  | BB    | 406  | G    | N1-C6-O6   | 14.41  | 128.55      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1290 | C    | N3-C4-N4   | 14.41  | 128.09      | 118.00   |
| 35  | BB    | 2543 | G    | C5-C6-O6   | -14.41 | 119.95      | 128.60   |
| 1   | AA    | 184  | G    | C5-C6-O6   | -14.41 | 119.95      | 128.60   |
| 35  | BB    | 1682 | G    | C5-C6-O6   | -14.41 | 119.96      | 128.60   |
| 35  | BB    | 645  | C    | N3-C4-C5   | -14.40 | 116.14      | 121.90   |
| 35  | BB    | 2543 | G    | N1-C6-O6   | 14.40  | 128.54      | 119.90   |
| 1   | AA    | 286  | C    | N3-C4-N4   | 14.40  | 128.08      | 118.00   |
| 35  | BB    | 1574 | C    | N3-C4-C5   | -14.40 | 116.14      | 121.90   |
| 35  | BB    | 1627 | G    | N1-C6-O6   | 14.40  | 128.54      | 119.90   |
| 1   | AA    | 838  | G    | N1-C6-O6   | 14.40  | 128.54      | 119.90   |
| 35  | BB    | 442  | G    | N1-C6-O6   | 14.39  | 128.54      | 119.90   |
| 35  | BB    | 1073 | A    | N1-C6-N6   | 14.39  | 127.24      | 118.60   |
| 1   | AA    | 1447 | A    | N1-C6-N6   | 14.39  | 127.23      | 118.60   |
| 1   | AA    | 1020 | G    | N1-C6-O6   | 14.39  | 128.53      | 119.90   |
| 35  | BB    | 1143 | A    | C4-C5-C6   | 14.38  | 124.19      | 117.00   |
| 35  | BB    | 1144 | A    | C4-C5-C6   | 14.38  | 124.19      | 117.00   |
| 35  | BB    | 2766 | A    | C4-C5-C6   | 14.38  | 124.19      | 117.00   |
| 35  | BB    | 1333 | G    | C4-C5-C6   | 14.38  | 127.43      | 118.80   |
| 35  | BB    | 2095 | A    | C6-C5-N7   | -14.38 | 122.23      | 132.30   |
| 1   | AA    | 974  | A    | C4-C5-C6   | 14.38  | 124.19      | 117.00   |
| 34  | BA    | 42   | C    | N3-C4-C5   | -14.38 | 116.15      | 121.90   |
| 1   | AA    | 794  | A    | C8-N9-C4   | -14.37 | 100.05      | 105.80   |
| 35  | BB    | 1272 | A    | N1-C6-N6   | 14.37  | 127.22      | 118.60   |
| 35  | BB    | 63   | A    | N9-C4-C5   | 14.37  | 111.55      | 105.80   |
| 35  | BB    | 2137 | U    | O4'-C1'-N1 | 14.36  | 119.69      | 108.20   |
| 1   | AA    | 771  | G    | C5-C6-O6   | -14.36 | 119.98      | 128.60   |
| 35  | BB    | 186  | G    | N1-C6-O6   | 14.36  | 128.51      | 119.90   |
| 35  | BB    | 1215 | G    | N1-C6-O6   | 14.35  | 128.51      | 119.90   |
| 35  | BB    | 1534 | U    | C2-N3-C4   | -14.34 | 118.39      | 127.00   |
| 1   | AA    | 79   | G    | C5-C6-O6   | -14.34 | 120.00      | 128.60   |
| 35  | BB    | 1626 | A    | N1-C6-N6   | 14.34  | 127.21      | 118.60   |
| 1   | AA    | 1508 | A    | O4'-C1'-N9 | 14.34  | 119.67      | 108.20   |
| 34  | BA    | 104  | A    | N1-C6-N6   | 14.34  | 127.20      | 118.60   |
| 35  | BB    | 64   | A    | C4-C5-C6   | 14.34  | 124.17      | 117.00   |
| 35  | BB    | 2642 | G    | N1-C6-O6   | 14.34  | 128.50      | 119.90   |
| 35  | BB    | 2162 | G    | C5-C6-O6   | -14.33 | 120.00      | 128.60   |
| 35  | BB    | 157  | C    | N3-C4-N4   | 14.33  | 128.03      | 118.00   |
| 35  | BB    | 1690 | A    | N1-C6-N6   | 14.33  | 127.20      | 118.60   |
| 35  | BB    | 278  | A    | N1-C2-N3   | -14.33 | 122.14      | 129.30   |
| 35  | BB    | 80   | G    | C5-C6-O6   | -14.32 | 120.00      | 128.60   |
| 35  | BB    | 648  | G    | C5-C6-O6   | -14.32 | 120.00      | 128.60   |
| 35  | BB    | 1744 | A    | N1-C6-N6   | 14.32  | 127.19      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1862 | G    | C5-C6-O6   | -14.32 | 120.01      | 128.60   |
| 1   | AA    | 676  | A    | N1-C6-N6   | 14.32  | 127.19      | 118.60   |
| 35  | BB    | 1168 | G    | N1-C6-O6   | 14.32  | 128.49      | 119.90   |
| 1   | AA    | 792  | A    | N1-C6-N6   | 14.31  | 127.19      | 118.60   |
| 18  | AR    | 50   | TYR  | CB-CG-CD1  | -14.30 | 112.42      | 121.00   |
| 35  | BB    | 2627 | G    | C5-C6-O6   | -14.30 | 120.02      | 128.60   |
| 35  | BB    | 189  | G    | N3-C2-N2   | 14.30  | 129.91      | 119.90   |
| 1   | AA    | 753  | A    | C5-C6-N6   | -14.30 | 112.26      | 123.70   |
| 1   | AA    | 1184 | G    | N1-C6-O6   | 14.29  | 128.48      | 119.90   |
| 34  | BA    | 110  | C    | O4'-C1'-N1 | 14.29  | 119.63      | 108.20   |
| 35  | BB    | 454  | A    | N1-C6-N6   | 14.29  | 127.18      | 118.60   |
| 35  | BB    | 1977 | A    | N1-C6-N6   | 14.29  | 127.18      | 118.60   |
| 35  | BB    | 71   | A    | N1-C6-N6   | 14.29  | 127.17      | 118.60   |
| 35  | BB    | 1746 | A    | O4'-C1'-N9 | 14.29  | 119.63      | 108.20   |
| 35  | BB    | 2776 | A    | C5-C6-N1   | -14.29 | 110.56      | 117.70   |
| 35  | BB    | 49   | A    | N1-C6-N6   | 14.29  | 127.17      | 118.60   |
| 1   | AA    | 51   | A    | N1-C6-N6   | 14.28  | 127.17      | 118.60   |
| 35  | BB    | 238  | C    | O4'-C1'-N1 | 14.28  | 119.62      | 108.20   |
| 1   | AA    | 278  | G    | C5-C6-O6   | -14.27 | 120.04      | 128.60   |
| 35  | BB    | 2884 | U    | O4'-C1'-N1 | 14.27  | 119.62      | 108.20   |
| 1   | AA    | 969  | A    | N1-C6-N6   | 14.26  | 127.16      | 118.60   |
| 35  | BB    | 195  | A    | N1-C6-N6   | 14.26  | 127.16      | 118.60   |
| 35  | BB    | 2538 | C    | C5-C4-N4   | -14.26 | 110.22      | 120.20   |
| 35  | BB    | 76   | C    | O4'-C1'-N1 | 14.26  | 119.60      | 108.20   |
| 35  | BB    | 1871 | A    | N1-C6-N6   | 14.26  | 127.15      | 118.60   |
| 35  | BB    | 2201 | G    | C5-C6-O6   | -14.26 | 120.05      | 128.60   |
| 1   | AA    | 668  | G    | N7-C8-N9   | -14.25 | 105.97      | 113.10   |
| 35  | BB    | 410  | G    | C5-C6-O6   | -14.25 | 120.05      | 128.60   |
| 35  | BB    | 2600 | A    | N1-C6-N6   | 14.25  | 127.15      | 118.60   |
| 1   | AA    | 32   | A    | N1-C6-N6   | 14.25  | 127.15      | 118.60   |
| 35  | BB    | 818  | G    | N1-C6-O6   | 14.24  | 128.45      | 119.90   |
| 35  | BB    | 2848 | G    | N1-C6-O6   | 14.24  | 128.44      | 119.90   |
| 35  | BB    | 1490 | A    | N9-C4-C5   | 14.24  | 111.50      | 105.80   |
| 1   | AA    | 970  | C    | N3-C4-C5   | -14.23 | 116.21      | 121.90   |
| 35  | BB    | 2013 | A    | C2-N3-C4   | -14.23 | 103.48      | 110.60   |
| 1   | AA    | 581  | G    | C5-C6-O6   | -14.23 | 120.06      | 128.60   |
| 1   | AA    | 629  | A    | N1-C6-N6   | 14.22  | 127.13      | 118.60   |
| 35  | BB    | 2278 | A    | N1-C6-N6   | 14.22  | 127.13      | 118.60   |
| 1   | AA    | 1410 | A    | N1-C6-N6   | 14.22  | 127.13      | 118.60   |
| 1   | AA    | 1453 | G    | N1-C6-O6   | 14.21  | 128.43      | 119.90   |
| 1   | AA    | 490  | C    | O4'-C1'-N1 | 14.21  | 119.57      | 108.20   |
| 35  | BB    | 1723 | G    | C5-C6-O6   | -14.21 | 120.08      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 82   | G    | N1-C6-O6   | 14.20  | 128.42      | 119.90   |
| 35  | BB    | 1946 | U    | O4'-C1'-N1 | 14.20  | 119.56      | 108.20   |
| 35  | BB    | 190  | A    | C5-C6-N6   | -14.20 | 112.34      | 123.70   |
| 35  | BB    | 258  | G    | N1-C6-O6   | 14.20  | 128.42      | 119.90   |
| 35  | BB    | 1533 | C    | C5-C6-N1   | 14.19  | 128.10      | 121.00   |
| 35  | BB    | 2267 | A    | N1-C6-N6   | 14.19  | 127.11      | 118.60   |
| 35  | BB    | 717  | C    | O4'-C1'-N1 | 14.18  | 119.55      | 108.20   |
| 35  | BB    | 1084 | A    | N1-C6-N6   | 14.18  | 127.11      | 118.60   |
| 35  | BB    | 1526 | C    | N3-C4-N4   | 14.18  | 127.93      | 118.00   |
| 35  | BB    | 2899 | A    | C4-C5-C6   | 14.18  | 124.09      | 117.00   |
| 1   | AA    | 851  | G    | C5-C6-O6   | -14.18 | 120.09      | 128.60   |
| 35  | BB    | 1418 | G    | N1-C6-O6   | 14.18  | 128.41      | 119.90   |
| 35  | BB    | 2642 | G    | C5-C6-O6   | -14.18 | 120.09      | 128.60   |
| 1   | AA    | 486  | U    | O4'-C1'-N1 | 14.17  | 119.54      | 108.20   |
| 1   | AA    | 1328 | C    | O4'-C1'-N1 | 14.17  | 119.54      | 108.20   |
| 1   | AA    | 181  | A    | C4-C5-C6   | 14.17  | 124.09      | 117.00   |
| 35  | BB    | 1967 | C    | N3-C4-N4   | 14.17  | 127.92      | 118.00   |
| 1   | AA    | 368  | U    | O4'-C1'-N1 | 14.17  | 119.54      | 108.20   |
| 1   | AA    | 765  | G    | C5-C6-O6   | -14.17 | 120.10      | 128.60   |
| 1   | AA    | 1288 | A    | N1-C6-N6   | 14.17  | 127.10      | 118.60   |
| 35  | BB    | 285  | G    | N1-C6-O6   | 14.17  | 128.40      | 119.90   |
| 35  | BB    | 2349 | G    | N1-C6-O6   | 14.16  | 128.40      | 119.90   |
| 1   | AA    | 887  | G    | N1-C6-O6   | 14.16  | 128.40      | 119.90   |
| 1   | AA    | 1044 | A    | N1-C6-N6   | 14.16  | 127.10      | 118.60   |
| 35  | BB    | 136  | G    | N1-C6-O6   | 14.16  | 128.40      | 119.90   |
| 35  | BB    | 2072 | C    | C6-N1-C2   | -14.16 | 114.64      | 120.30   |
| 35  | BB    | 825  | A    | N1-C6-N6   | 14.16  | 127.09      | 118.60   |
| 35  | BB    | 122  | G    | N1-C6-O6   | 14.15  | 128.39      | 119.90   |
| 35  | BB    | 1660 | G    | C5-C6-O6   | -14.15 | 120.11      | 128.60   |
| 35  | BB    | 2582 | G    | N1-C6-O6   | 14.15  | 128.39      | 119.90   |
| 35  | BB    | 2227 | A    | N1-C6-N6   | 14.15  | 127.09      | 118.60   |
| 35  | BB    | 175  | G    | C5-C6-O6   | -14.15 | 120.11      | 128.60   |
| 35  | BB    | 2702 | G    | N1-C6-O6   | 14.15  | 128.39      | 119.90   |
| 1   | AA    | 198  | G    | C5-C6-O6   | -14.14 | 120.11      | 128.60   |
| 35  | BB    | 1903 | G    | C5-C6-O6   | -14.14 | 120.11      | 128.60   |
| 35  | BB    | 1678 | A    | N1-C6-N6   | 14.14  | 127.08      | 118.60   |
| 35  | BB    | 602  | A    | N1-C6-N6   | 14.14  | 127.08      | 118.60   |
| 35  | BB    | 2601 | C    | P-O3'-C3'  | 14.13  | 136.66      | 119.70   |
| 1   | AA    | 1398 | A    | N1-C6-N6   | 14.13  | 127.08      | 118.60   |
| 1   | AA    | 1057 | G    | C5-C6-O6   | -14.12 | 120.13      | 128.60   |
| 1   | AA    | 34   | C    | O4'-C1'-N1 | 14.12  | 119.49      | 108.20   |
| 35  | BB    | 484  | C    | N3-C4-C5   | -14.12 | 116.25      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 361  | G    | N1-C6-O6   | 14.11  | 128.37      | 119.90   |
| 34  | BA    | 39   | A    | N1-C6-N6   | 14.11  | 127.07      | 118.60   |
| 35  | BB    | 758  | C    | C6-N1-C2   | -14.11 | 114.66      | 120.30   |
| 35  | BB    | 1467 | U    | O4'-C1'-N1 | 14.11  | 119.49      | 108.20   |
| 35  | BB    | 212  | G    | C5-C6-O6   | -14.11 | 120.14      | 128.60   |
| 35  | BB    | 748  | G    | C5-C6-O6   | -14.11 | 120.14      | 128.60   |
| 36  | BC    | 257  | ARG  | NE-CZ-NH1  | 14.10  | 127.35      | 120.30   |
| 1   | AA    | 1310 | G    | C5-C6-O6   | -14.10 | 120.14      | 128.60   |
| 35  | BB    | 1274 | A    | N1-C2-N3   | -14.09 | 122.25      | 129.30   |
| 35  | BB    | 818  | G    | N3-C2-N2   | 14.09  | 129.76      | 119.90   |
| 1   | AA    | 214  | C    | N3-C4-C5   | -14.08 | 116.27      | 121.90   |
| 1   | AA    | 726  | C    | O4'-C1'-N1 | 14.08  | 119.47      | 108.20   |
| 35  | BB    | 1808 | A    | C8-N9-C4   | -14.08 | 100.17      | 105.80   |
| 1   | AA    | 715  | A    | N1-C6-N6   | 14.08  | 127.05      | 118.60   |
| 35  | BB    | 1231 | U    | N3-C4-O4   | 14.08  | 129.25      | 119.40   |
| 1   | AA    | 346  | G    | N1-C6-O6   | 14.07  | 128.34      | 119.90   |
| 1   | AA    | 493  | A    | C5-C6-N6   | -14.07 | 112.44      | 123.70   |
| 1   | AA    | 1012 | A    | C5-C6-N6   | -14.07 | 112.44      | 123.70   |
| 1   | AA    | 1350 | A    | N1-C6-N6   | 14.06  | 127.04      | 118.60   |
| 1   | AA    | 263  | A    | C5-C6-N1   | -14.06 | 110.67      | 117.70   |
| 35  | BB    | 841  | G    | N1-C6-O6   | 14.05  | 128.33      | 119.90   |
| 35  | BB    | 2119 | A    | C5-C6-N1   | -14.05 | 110.67      | 117.70   |
| 35  | BB    | 180  | G    | N1-C6-O6   | 14.05  | 128.33      | 119.90   |
| 1   | AA    | 688  | G    | C5-C6-N1   | -14.05 | 104.47      | 111.50   |
| 35  | BB    | 2487 | G    | N1-C6-O6   | 14.05  | 128.33      | 119.90   |
| 35  | BB    | 1663 | G    | N1-C6-O6   | 14.05  | 128.33      | 119.90   |
| 1   | AA    | 698  | G    | N1-C6-O6   | 14.05  | 128.33      | 119.90   |
| 35  | BB    | 2686 | G    | C5-C6-O6   | -14.05 | 120.17      | 128.60   |
| 35  | BB    | 695  | G    | N1-C6-O6   | 14.04  | 128.33      | 119.90   |
| 35  | BB    | 10   | A    | N1-C6-N6   | 14.04  | 127.02      | 118.60   |
| 35  | BB    | 1708 | C    | O4'-C1'-N1 | 14.04  | 119.43      | 108.20   |
| 35  | BB    | 1934 | C    | N3-C4-N4   | 14.04  | 127.83      | 118.00   |
| 35  | BB    | 2867 | G    | N3-C2-N2   | 14.03  | 129.72      | 119.90   |
| 1   | AA    | 915  | A    | N1-C6-N6   | 14.02  | 127.01      | 118.60   |
| 1   | AA    | 1491 | G    | N1-C6-O6   | 14.02  | 128.31      | 119.90   |
| 35  | BB    | 1249 | U    | O4'-C1'-N1 | 14.02  | 119.42      | 108.20   |
| 1   | AA    | 766  | A    | N1-C6-N6   | 14.02  | 127.01      | 118.60   |
| 34  | BA    | 79   | G    | N1-C6-O6   | 14.01  | 128.31      | 119.90   |
| 35  | BB    | 572  | A    | O4'-C1'-N9 | 14.01  | 119.41      | 108.20   |
| 1   | AA    | 1398 | A    | C5-N7-C8   | 14.01  | 110.91      | 103.90   |
| 47  | BN    | 94   | TYR  | CB-CG-CD2  | -14.01 | 112.59      | 121.00   |
| 1   | AA    | 356  | A    | N1-C6-N6   | 14.01  | 127.00      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 258  | G    | N1-C6-O6   | 14.00  | 128.30      | 119.90   |
| 35  | BB    | 1685 | C    | N3-C4-C5   | -14.00 | 116.30      | 121.90   |
| 35  | BB    | 656  | G    | N1-C6-O6   | 14.00  | 128.30      | 119.90   |
| 1   | AA    | 345  | C    | N3-C4-C5   | -14.00 | 116.30      | 121.90   |
| 1   | AA    | 868  | C    | C6-N1-C2   | -14.00 | 114.70      | 120.30   |
| 1   | AA    | 22   | G    | N1-C6-O6   | 14.00  | 128.30      | 119.90   |
| 1   | AA    | 470  | C    | O4'-C1'-N1 | 14.00  | 119.40      | 108.20   |
| 1   | AA    | 524  | G    | N1-C6-O6   | 14.00  | 128.30      | 119.90   |
| 35  | BB    | 19   | A    | N1-C6-N6   | 14.00  | 127.00      | 118.60   |
| 1   | AA    | 532  | A    | C4-C5-C6   | 13.99  | 124.00      | 117.00   |
| 34  | BA    | 118  | C    | N3-C4-N4   | 13.99  | 127.80      | 118.00   |
| 35  | BB    | 1797 | G    | C2-N3-C4   | 13.99  | 118.89      | 111.90   |
| 1   | AA    | 1254 | A    | N1-C6-N6   | 13.99  | 126.99      | 118.60   |
| 1   | AA    | 1233 | G    | C5-C6-O6   | -13.98 | 120.21      | 128.60   |
| 1   | AA    | 581  | G    | N1-C6-O6   | 13.98  | 128.29      | 119.90   |
| 34  | BA    | 13   | G    | N1-C6-O6   | 13.98  | 128.29      | 119.90   |
| 35  | BB    | 63   | A    | C4-C5-C6   | 13.97  | 123.99      | 117.00   |
| 35  | BB    | 2366 | A    | C5-C6-N6   | -13.97 | 112.52      | 123.70   |
| 35  | BB    | 520  | G    | N1-C6-O6   | 13.97  | 128.28      | 119.90   |
| 1   | AA    | 529  | G    | N1-C2-N3   | -13.96 | 115.52      | 123.90   |
| 1   | AA    | 1204 | A    | N1-C6-N6   | 13.96  | 126.98      | 118.60   |
| 35  | BB    | 73   | A    | N1-C6-N6   | 13.96  | 126.98      | 118.60   |
| 35  | BB    | 2550 | G    | N1-C6-O6   | 13.95  | 128.27      | 119.90   |
| 35  | BB    | 1651 | G    | C5-C6-O6   | -13.95 | 120.23      | 128.60   |
| 1   | AA    | 477  | C    | O4'-C1'-N1 | 13.95  | 119.36      | 108.20   |
| 35  | BB    | 1619 | G    | C5-C6-O6   | -13.94 | 120.24      | 128.60   |
| 35  | BB    | 1550 | C    | C6-N1-C2   | -13.93 | 114.73      | 120.30   |
| 35  | BB    | 2631 | G    | C4-C5-N7   | 13.93  | 116.37      | 110.80   |
| 1   | AA    | 168  | G    | C5-C6-O6   | -13.93 | 120.24      | 128.60   |
| 1   | AA    | 1344 | C    | O4'-C1'-N1 | 13.93  | 119.34      | 108.20   |
| 35  | BB    | 384  | A    | N1-C6-N6   | 13.93  | 126.96      | 118.60   |
| 35  | BB    | 1493 | C    | N3-C4-C5   | -13.92 | 116.33      | 121.90   |
| 35  | BB    | 1475 | G    | C5-C6-O6   | -13.92 | 120.25      | 128.60   |
| 1   | AA    | 1359 | C    | O4'-C1'-N1 | 13.91  | 119.33      | 108.20   |
| 35  | BB    | 1994 | C    | N3-C4-C5   | -13.91 | 116.33      | 121.90   |
| 1   | AA    | 1158 | C    | O4'-C1'-N1 | 13.91  | 119.33      | 108.20   |
| 1   | AA    | 319  | G    | N1-C6-O6   | 13.91  | 128.24      | 119.90   |
| 1   | AA    | 648  | A    | N1-C6-N6   | 13.91  | 126.94      | 118.60   |
| 35  | BB    | 2471 | A    | C5-C6-N1   | -13.90 | 110.75      | 117.70   |
| 35  | BB    | 751  | A    | N1-C6-N6   | 13.90  | 126.94      | 118.60   |
| 1   | AA    | 1042 | A    | N1-C6-N6   | 13.90  | 126.94      | 118.60   |
| 35  | BB    | 877  | A    | N9-C4-C5   | 13.90  | 111.36      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 726  | G    | O4'-C1'-N9 | 13.89  | 119.31      | 108.20   |
| 1   | AA    | 390  | U    | O4'-C1'-N1 | 13.89  | 119.31      | 108.20   |
| 35  | BB    | 1697 | G    | C5-C6-O6   | -13.89 | 120.27      | 128.60   |
| 35  | BB    | 236  | C    | O4'-C1'-N1 | 13.88  | 119.31      | 108.20   |
| 1   | AA    | 611  | C    | N3-C4-C5   | -13.88 | 116.35      | 121.90   |
| 35  | BB    | 1409 | U    | O4'-C1'-N1 | 13.88  | 119.30      | 108.20   |
| 1   | AA    | 1031 | C    | N3-C4-C5   | -13.87 | 116.35      | 121.90   |
| 35  | BB    | 257  | C    | O4'-C1'-N1 | 13.88  | 119.30      | 108.20   |
| 35  | BB    | 1374 | G    | C5-C6-O6   | -13.88 | 120.27      | 128.60   |
| 35  | BB    | 890  | C    | O4'-C1'-N1 | 13.87  | 119.30      | 108.20   |
| 1   | AA    | 495  | A    | C4-C5-C6   | 13.87  | 123.93      | 117.00   |
| 35  | BB    | 1055 | G    | O4'-C1'-N9 | 13.87  | 119.30      | 108.20   |
| 1   | AA    | 814  | A    | P-O3'-C3'  | 13.87  | 136.34      | 119.70   |
| 35  | BB    | 2634 | A    | C4-C5-C6   | 13.86  | 123.93      | 117.00   |
| 35  | BB    | 1833 | C    | N3-C4-N4   | 13.86  | 127.70      | 118.00   |
| 29  | B4    | 20   | TYR  | CB-CG-CD1  | -13.86 | 112.69      | 121.00   |
| 35  | BB    | 272  | A    | C4-C5-C6   | 13.85  | 123.93      | 117.00   |
| 1   | AA    | 418  | C    | O4'-C1'-N1 | 13.85  | 119.28      | 108.20   |
| 1   | AA    | 194  | C    | O4'-C1'-N1 | 13.85  | 119.28      | 108.20   |
| 1   | AA    | 66   | A    | C5-C6-N1   | -13.84 | 110.78      | 117.70   |
| 35  | BB    | 1684 | G    | C8-N9-C4   | -13.84 | 100.86      | 106.40   |
| 1   | AA    | 496  | A    | N1-C6-N6   | 13.84  | 126.90      | 118.60   |
| 35  | BB    | 2357 | G    | N1-C6-O6   | 13.83  | 128.20      | 119.90   |
| 35  | BB    | 2630 | G    | N1-C6-O6   | 13.83  | 128.20      | 119.90   |
| 35  | BB    | 2658 | C    | C5-C4-N4   | -13.83 | 110.52      | 120.20   |
| 35  | BB    | 784  | G    | N1-C6-O6   | 13.82  | 128.19      | 119.90   |
| 35  | BB    | 19   | A    | N1-C2-N3   | 13.82  | 136.21      | 129.30   |
| 1   | AA    | 1060 | U    | C5-C4-O4   | -13.81 | 117.61      | 125.90   |
| 35  | BB    | 1609 | A    | C5-C6-N1   | -13.81 | 110.79      | 117.70   |
| 1   | AA    | 1029 | U    | C5-C6-N1   | 13.81  | 129.60      | 122.70   |
| 1   | AA    | 1509 | C    | C5-C4-N4   | -13.81 | 110.53      | 120.20   |
| 35  | BB    | 2821 | A    | N1-C6-N6   | 13.81  | 126.88      | 118.60   |
| 35  | BB    | 1452 | G    | C5-C6-O6   | -13.80 | 120.32      | 128.60   |
| 1   | AA    | 415  | A    | N1-C6-N6   | 13.80  | 126.88      | 118.60   |
| 1   | AA    | 59   | A    | C5-N7-C8   | 13.80  | 110.80      | 103.90   |
| 35  | BB    | 61   | C    | O4'-C1'-N1 | 13.79  | 119.24      | 108.20   |
| 35  | BB    | 477  | A    | C5-C6-N1   | -13.79 | 110.80      | 117.70   |
| 1   | AA    | 285  | C    | O4'-C1'-N1 | 13.79  | 119.23      | 108.20   |
| 1   | AA    | 925  | G    | C5-C6-O6   | -13.79 | 120.32      | 128.60   |
| 1   | AA    | 1281 | C    | N3-C4-C5   | -13.79 | 116.38      | 121.90   |
| 35  | BB    | 157  | C    | C5-C4-N4   | -13.79 | 110.55      | 120.20   |
| 35  | BB    | 1989 | G    | N1-C6-O6   | 13.78  | 128.17      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 1139 | G    | N1-C6-O6   | 13.78  | 128.17      | 119.90   |
| 35  | BB    | 2516 | A    | C5-C6-N1   | -13.78 | 110.81      | 117.70   |
| 1   | AA    | 753  | A    | C5-C6-N1   | -13.78 | 110.81      | 117.70   |
| 35  | BB    | 1238 | G    | C5-C6-O6   | -13.78 | 120.33      | 128.60   |
| 1   | AA    | 422  | C    | C6-N1-C2   | -13.77 | 114.79      | 120.30   |
| 35  | BB    | 1250 | G    | N1-C6-O6   | 13.77  | 128.16      | 119.90   |
| 35  | BB    | 924  | G    | O4'-C1'-N9 | 13.76  | 119.21      | 108.20   |
| 1   | AA    | 174  | A    | C2-N3-C4   | -13.76 | 103.72      | 110.60   |
| 35  | BB    | 742  | A    | N1-C6-N6   | 13.76  | 126.86      | 118.60   |
| 1   | AA    | 1303 | C    | N3-C4-C5   | -13.76 | 116.40      | 121.90   |
| 35  | BB    | 558  | U    | O4'-C1'-N1 | 13.75  | 119.20      | 108.20   |
| 1   | AA    | 371  | A    | C5-N7-C8   | 13.73  | 110.77      | 103.90   |
| 1   | AA    | 635  | A    | O4'-C1'-N9 | 13.73  | 119.18      | 108.20   |
| 1   | AA    | 661  | G    | C5-C6-O6   | -13.73 | 120.36      | 128.60   |
| 23  | AX    | 19   | A    | N1-C6-N6   | 13.73  | 126.84      | 118.60   |
| 35  | BB    | 2331 | G    | N1-C6-O6   | 13.73  | 128.14      | 119.90   |
| 35  | BB    | 275  | C    | O4'-C1'-N1 | 13.73  | 119.18      | 108.20   |
| 35  | BB    | 2413 | G    | N1-C6-O6   | 13.73  | 128.14      | 119.90   |
| 1   | AA    | 136  | C    | C6-N1-C2   | -13.73 | 114.81      | 120.30   |
| 35  | BB    | 508  | A    | C4-C5-C6   | 13.72  | 123.86      | 117.00   |
| 1   | AA    | 774  | G    | C2-N3-C4   | 13.72  | 118.76      | 111.90   |
| 35  | BB    | 1175 | A    | C5-C6-N1   | -13.72 | 110.84      | 117.70   |
| 35  | BB    | 1563 | U    | O4'-C1'-N1 | 13.72  | 119.17      | 108.20   |
| 35  | BB    | 1751 | U    | O4'-C1'-N1 | 13.72  | 119.17      | 108.20   |
| 35  | BB    | 2851 | A    | N1-C6-N6   | 13.71  | 126.83      | 118.60   |
| 1   | AA    | 218  | U    | O4'-C1'-N1 | 13.71  | 119.17      | 108.20   |
| 1   | AA    | 1370 | G    | C5-C6-O6   | -13.71 | 120.38      | 128.60   |
| 35  | BB    | 2134 | A    | C5-C6-N6   | -13.71 | 112.73      | 123.70   |
| 1   | AA    | 810  | C    | O4'-C1'-N1 | 13.70  | 119.16      | 108.20   |
| 35  | BB    | 1269 | A    | N1-C6-N6   | 13.70  | 126.82      | 118.60   |
| 35  | BB    | 2270 | A    | N1-C6-N6   | 13.70  | 126.82      | 118.60   |
| 35  | BB    | 1916 | A    | N1-C6-N6   | 13.69  | 126.82      | 118.60   |
| 1   | AA    | 366  | A    | N9-C4-C5   | 13.69  | 111.28      | 105.80   |
| 35  | BB    | 579  | G    | N1-C6-O6   | 13.68  | 128.11      | 119.90   |
| 1   | AA    | 968  | A    | C5-C6-N1   | -13.68 | 110.86      | 117.70   |
| 35  | BB    | 1579 | A    | N1-C6-N6   | 13.68  | 126.81      | 118.60   |
| 1   | AA    | 241  | G    | N1-C6-O6   | 13.68  | 128.11      | 119.90   |
| 35  | BB    | 2061 | G    | N1-C6-O6   | 13.68  | 128.10      | 119.90   |
| 1   | AA    | 363  | A    | N1-C6-N6   | 13.67  | 126.80      | 118.60   |
| 22  | AV    | 2    | G    | N1-C6-O6   | 13.66  | 128.10      | 119.90   |
| 35  | BB    | 659  | G    | C5-C6-O6   | -13.66 | 120.40      | 128.60   |
| 35  | BB    | 711  | G    | N3-C2-N2   | 13.66  | 129.46      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2003 | A    | C5-C6-N6   | -13.66 | 112.77      | 123.70   |
| 35  | BB    | 2402 | U    | O4'-C1'-N1 | 13.66  | 119.13      | 108.20   |
| 1   | AA    | 1219 | A    | C5-C6-N6   | -13.66 | 112.78      | 123.70   |
| 1   | AA    | 1152 | A    | N1-C6-N6   | 13.65  | 126.79      | 118.60   |
| 35  | BB    | 2363 | G    | C5-C6-O6   | -13.65 | 120.41      | 128.60   |
| 1   | AA    | 1534 | A    | C4-C5-C6   | 13.65  | 123.83      | 117.00   |
| 1   | AA    | 1179 | A    | C4-C5-C6   | 13.65  | 123.83      | 117.00   |
| 35  | BB    | 1248 | G    | C5-C6-O6   | -13.65 | 120.41      | 128.60   |
| 35  | BB    | 2464 | G    | O4'-C1'-N9 | 13.65  | 119.12      | 108.20   |
| 1   | AA    | 1292 | G    | O4'-C1'-N9 | 13.65  | 119.12      | 108.20   |
| 35  | BB    | 1262 | A    | N1-C6-N6   | 13.65  | 126.79      | 118.60   |
| 1   | AA    | 6    | G    | C5-C6-O6   | -13.64 | 120.41      | 128.60   |
| 34  | BA    | 79   | G    | C5-C6-O6   | -13.64 | 120.42      | 128.60   |
| 35  | BB    | 1281 | G    | N1-C6-O6   | 13.64  | 128.09      | 119.90   |
| 35  | BB    | 1720 | U    | O4'-C1'-N1 | 13.64  | 119.11      | 108.20   |
| 1   | AA    | 184  | G    | N1-C6-O6   | 13.64  | 128.08      | 119.90   |
| 1   | AA    | 235  | C    | C6-N1-C2   | -13.64 | 114.84      | 120.30   |
| 35  | BB    | 700  | G    | N1-C6-O6   | 13.64  | 128.08      | 119.90   |
| 35  | BB    | 1933 | G    | C5-C6-O6   | -13.64 | 120.42      | 128.60   |
| 35  | BB    | 1371 | G    | O4'-C1'-N9 | 13.63  | 119.11      | 108.20   |
| 35  | BB    | 1616 | A    | C5-C6-N6   | -13.63 | 112.80      | 123.70   |
| 35  | BB    | 605  | G    | C8-N9-C4   | 13.63  | 111.85      | 106.40   |
| 37  | BD    | 83   | ARG  | NE-CZ-NH1  | -13.62 | 113.49      | 120.30   |
| 35  | BB    | 752  | A    | C4-C5-C6   | 13.62  | 123.81      | 117.00   |
| 35  | BB    | 1569 | A    | C4-C5-C6   | 13.62  | 123.81      | 117.00   |
| 35  | BB    | 1920 | C    | N3-C4-N4   | 13.62  | 127.54      | 118.00   |
| 35  | BB    | 2415 | G    | N1-C6-O6   | 13.62  | 128.07      | 119.90   |
| 35  | BB    | 300  | A    | C4-C5-C6   | 13.62  | 123.81      | 117.00   |
| 35  | BB    | 2400 | G    | N1-C6-O6   | 13.62  | 128.07      | 119.90   |
| 35  | BB    | 946  | C    | O4'-C1'-N1 | 13.62  | 119.09      | 108.20   |
| 35  | BB    | 1088 | A    | N1-C6-N6   | 13.62  | 126.77      | 118.60   |
| 35  | BB    | 638  | G    | C5-C6-O6   | -13.61 | 120.43      | 128.60   |
| 35  | BB    | 1960 | A    | N1-C6-N6   | 13.62  | 126.77      | 118.60   |
| 35  | BB    | 2808 | G    | N1-C2-N3   | -13.61 | 115.73      | 123.90   |
| 35  | BB    | 2084 | C    | N3-C4-N4   | 13.60  | 127.52      | 118.00   |
| 22  | AV    | 3    | G    | C6-C5-N7   | -13.60 | 122.24      | 130.40   |
| 35  | BB    | 670  | A    | N1-C6-N6   | 13.59  | 126.76      | 118.60   |
| 35  | BB    | 2222 | C    | O4'-C1'-N1 | 13.59  | 119.08      | 108.20   |
| 1   | AA    | 1124 | G    | N1-C6-O6   | 13.59  | 128.05      | 119.90   |
| 35  | BB    | 1143 | A    | N1-C6-N6   | 13.59  | 126.75      | 118.60   |
| 1   | AA    | 869  | G    | C5-C6-O6   | -13.59 | 120.45      | 128.60   |
| 35  | BB    | 1749 | A    | N1-C2-N3   | 13.59  | 136.09      | 129.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2168 | G    | N1-C6-O6   | 13.59  | 128.05      | 119.90   |
| 1   | AA    | 451  | A    | C4-C5-C6   | 13.58  | 123.79      | 117.00   |
| 1   | AA    | 1475 | G    | N1-C6-O6   | 13.58  | 128.05      | 119.90   |
| 1   | AA    | 927  | G    | N1-C6-O6   | 13.58  | 128.05      | 119.90   |
| 1   | AA    | 1443 | C    | O4'-C1'-N1 | 13.58  | 119.06      | 108.20   |
| 1   | AA    | 82   | G    | C5-C6-O6   | -13.58 | 120.45      | 128.60   |
| 35  | BB    | 809  | G    | C5-C6-O6   | -13.57 | 120.46      | 128.60   |
| 35  | BB    | 2156 | G    | C5-C6-O6   | -13.57 | 120.46      | 128.60   |
| 1   | AA    | 174  | A    | C5-C6-N1   | -13.57 | 110.92      | 117.70   |
| 1   | AA    | 554  | A    | N1-C6-N6   | 13.57  | 126.74      | 118.60   |
| 1   | AA    | 1094 | G    | C5-C6-O6   | -13.57 | 120.46      | 128.60   |
| 35  | BB    | 2655 | G    | C5-C6-O6   | -13.57 | 120.46      | 128.60   |
| 1   | AA    | 495  | A    | N1-C6-N6   | 13.56  | 126.74      | 118.60   |
| 35  | BB    | 446  | G    | N3-C2-N2   | 13.56  | 129.39      | 119.90   |
| 35  | BB    | 921  | C    | C5-C6-N1   | 13.55  | 127.78      | 121.00   |
| 35  | BB    | 2776 | A    | N1-C6-N6   | 13.55  | 126.73      | 118.60   |
| 35  | BB    | 89   | A    | N1-C6-N6   | 13.55  | 126.73      | 118.60   |
| 35  | BB    | 597  | G    | N9-C4-C5   | 13.55  | 110.82      | 105.40   |
| 35  | BB    | 1014 | A    | C5-C6-N6   | -13.55 | 112.86      | 123.70   |
| 35  | BB    | 2006 | C    | C2-N3-C4   | 13.55  | 126.68      | 119.90   |
| 1   | AA    | 1051 | C    | N3-C4-N4   | 13.55  | 127.48      | 118.00   |
| 1   | AA    | 1333 | A    | N1-C6-N6   | 13.55  | 126.73      | 118.60   |
| 1   | AA    | 355  | C    | N3-C4-N4   | 13.55  | 127.48      | 118.00   |
| 35  | BB    | 1055 | G    | C5-C6-O6   | -13.54 | 120.47      | 128.60   |
| 1   | AA    | 1434 | A    | N1-C6-N6   | 13.54  | 126.72      | 118.60   |
| 35  | BB    | 1445 | G    | N1-C6-O6   | 13.54  | 128.02      | 119.90   |
| 35  | BB    | 2037 | A    | C5-C6-N1   | -13.53 | 110.94      | 117.70   |
| 35  | BB    | 574  | A    | N1-C6-N6   | 13.52  | 126.72      | 118.60   |
| 35  | BB    | 2524 | G    | C8-N9-C4   | -13.52 | 100.99      | 106.40   |
| 1   | AA    | 1157 | A    | N1-C6-N6   | 13.52  | 126.71      | 118.60   |
| 1   | AA    | 1111 | A    | C5-C6-N6   | -13.52 | 112.89      | 123.70   |
| 35  | BB    | 1250 | G    | C5-C6-O6   | -13.51 | 120.50      | 128.60   |
| 1   | AA    | 1031 | C    | N3-C4-N4   | 13.51  | 127.45      | 118.00   |
| 35  | BB    | 1334 | G    | O4'-C1'-N9 | 13.50  | 119.00      | 108.20   |
| 35  | BB    | 368  | A    | O4'-C1'-N9 | 13.50  | 119.00      | 108.20   |
| 35  | BB    | 2027 | G    | C5-C6-O6   | -13.50 | 120.50      | 128.60   |
| 35  | BB    | 318  | C    | O4'-C1'-N1 | 13.49  | 119.00      | 108.20   |
| 35  | BB    | 2475 | C    | N3-C4-C5   | -13.49 | 116.50      | 121.90   |
| 1   | AA    | 274  | A    | N1-C6-N6   | 13.49  | 126.69      | 118.60   |
| 35  | BB    | 456  | C    | N3-C4-C5   | -13.49 | 116.50      | 121.90   |
| 35  | BB    | 2084 | C    | C5-C4-N4   | -13.49 | 110.76      | 120.20   |
| 35  | BB    | 1679 | A    | N1-C6-N6   | 13.48  | 126.69      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 574  | A    | N1-C6-N6   | 13.48  | 126.69      | 118.60   |
| 1   | AA    | 1251 | A    | C5-C6-N1   | -13.48 | 110.96      | 117.70   |
| 35  | BB    | 2256 | G    | C5-C6-O6   | -13.48 | 120.51      | 128.60   |
| 35  | BB    | 1762 | A    | N1-C6-N6   | 13.48  | 126.69      | 118.60   |
| 1   | AA    | 808  | C    | N3-C4-C5   | -13.47 | 116.51      | 121.90   |
| 1   | AA    | 355  | C    | C2-N3-C4   | 13.47  | 126.64      | 119.90   |
| 35  | BB    | 1370 | C    | N3-C4-C5   | -13.47 | 116.51      | 121.90   |
| 35  | BB    | 2049 | G    | N1-C6-O6   | 13.47  | 127.98      | 119.90   |
| 35  | BB    | 2634 | A    | N1-C6-N6   | 13.47  | 126.68      | 118.60   |
| 35  | BB    | 1021 | A    | N1-C6-N6   | 13.47  | 126.68      | 118.60   |
| 35  | BB    | 1962 | C    | N3-C4-C5   | -13.47 | 116.51      | 121.90   |
| 35  | BB    | 1327 | A    | N1-C6-N6   | 13.47  | 126.68      | 118.60   |
| 35  | BB    | 2685 | G    | C5-C6-O6   | -13.46 | 120.52      | 128.60   |
| 1   | AA    | 278  | G    | N3-C2-N2   | 13.46  | 129.32      | 119.90   |
| 1   | AA    | 987  | G    | N1-C6-O6   | 13.46  | 127.98      | 119.90   |
| 34  | BA    | 98   | G    | N1-C6-O6   | 13.46  | 127.97      | 119.90   |
| 35  | BB    | 900  | A    | P-O3'-C3'  | -13.46 | 103.55      | 119.70   |
| 35  | BB    | 1766 | G    | C5-C6-O6   | -13.46 | 120.52      | 128.60   |
| 35  | BB    | 420  | C    | N3-C4-C5   | -13.45 | 116.52      | 121.90   |
| 35  | BB    | 2101 | A    | N1-C6-N6   | 13.45  | 126.67      | 118.60   |
| 1   | AA    | 129  | A    | C8-N9-C4   | -13.45 | 100.42      | 105.80   |
| 35  | BB    | 494  | G    | N1-C6-O6   | 13.45  | 127.97      | 119.90   |
| 1   | AA    | 469  | C    | O4'-C1'-N1 | 13.44  | 118.95      | 108.20   |
| 35  | BB    | 1821 | A    | N1-C6-N6   | 13.44  | 126.66      | 118.60   |
| 35  | BB    | 2371 | G    | N1-C6-O6   | 13.44  | 127.96      | 119.90   |
| 35  | BB    | 1936 | A    | C5-C6-N1   | -13.43 | 110.98      | 117.70   |
| 1   | AA    | 1466 | C    | O4'-C1'-N1 | 13.43  | 118.95      | 108.20   |
| 35  | BB    | 2178 | C    | O4'-C1'-N1 | 13.43  | 118.94      | 108.20   |
| 35  | BB    | 1984 | G    | C5-C6-O6   | -13.43 | 120.54      | 128.60   |
| 1   | AA    | 943  | U    | C5-C6-N1   | 13.43  | 129.41      | 122.70   |
| 35  | BB    | 1230 | A    | C4-C5-C6   | 13.43  | 123.71      | 117.00   |
| 1   | AA    | 781  | A    | C4-C5-C6   | 13.42  | 123.71      | 117.00   |
| 35  | BB    | 2481 | G    | C5-C6-O6   | -13.42 | 120.55      | 128.60   |
| 35  | BB    | 458  | G    | C6-C5-N7   | -13.42 | 122.35      | 130.40   |
| 35  | BB    | 1750 | G    | O4'-C1'-N9 | 13.42  | 118.93      | 108.20   |
| 35  | BB    | 1320 | C    | C6-N1-C2   | -13.41 | 114.94      | 120.30   |
| 1   | AA    | 1191 | A    | C4-C5-C6   | 13.41  | 123.70      | 117.00   |
| 35  | BB    | 1718 | G    | N1-C6-O6   | 13.41  | 127.94      | 119.90   |
| 35  | BB    | 1824 | G    | C2-N3-C4   | 13.41  | 118.61      | 111.90   |
| 1   | AA    | 1417 | G    | C5-C6-O6   | -13.41 | 120.56      | 128.60   |
| 1   | AA    | 628  | G    | N1-C6-O6   | 13.40  | 127.94      | 119.90   |
| 35  | BB    | 2797 | U    | O4'-C1'-N1 | 13.40  | 118.92      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 48  | BO    | 7    | ARG  | NE-CZ-NH2  | -13.40 | 113.60      | 120.30   |
| 34  | BA    | 53   | A    | N1-C6-N6   | 13.39  | 126.64      | 118.60   |
| 35  | BB    | 215  | G    | N1-C6-O6   | 13.39  | 127.94      | 119.90   |
| 35  | BB    | 1422 | G    | N1-C6-O6   | 13.39  | 127.93      | 119.90   |
| 35  | BB    | 2719 | G    | N1-C6-O6   | 13.39  | 127.93      | 119.90   |
| 1   | AA    | 1169 | A    | N1-C6-N6   | 13.38  | 126.63      | 118.60   |
| 35  | BB    | 2058 | A    | C8-N9-C4   | -13.38 | 100.45      | 105.80   |
| 1   | AA    | 31   | G    | C5-C6-O6   | -13.38 | 120.57      | 128.60   |
| 35  | BB    | 351  | C    | N3-C4-C5   | -13.38 | 116.55      | 121.90   |
| 35  | BB    | 2742 | G    | N1-C6-O6   | 13.38  | 127.93      | 119.90   |
| 1   | AA    | 775  | G    | O4'-C1'-N9 | 13.37  | 118.89      | 108.20   |
| 34  | BA    | 9    | G    | C5-C6-O6   | -13.37 | 120.58      | 128.60   |
| 35  | BB    | 2200 | C    | O4'-C1'-N1 | 13.36  | 118.89      | 108.20   |
| 35  | BB    | 2328 | A    | N1-C6-N6   | 13.36  | 126.62      | 118.60   |
| 35  | BB    | 173  | A    | N1-C6-N6   | 13.36  | 126.61      | 118.60   |
| 1   | AA    | 731  | G    | N1-C6-O6   | 13.35  | 127.91      | 119.90   |
| 35  | BB    | 2421 | G    | C5-C6-N1   | -13.35 | 104.82      | 111.50   |
| 1   | AA    | 818  | G    | C5-C6-O6   | -13.35 | 120.59      | 128.60   |
| 35  | BB    | 1134 | A    | C4-C5-C6   | 13.35  | 123.67      | 117.00   |
| 1   | AA    | 823  | C    | O4'-C1'-N1 | 13.34  | 118.87      | 108.20   |
| 1   | AA    | 1480 | A    | C4-C5-N7   | -13.34 | 104.03      | 110.70   |
| 35  | BB    | 218  | A    | N1-C6-N6   | 13.34  | 126.61      | 118.60   |
| 35  | BB    | 441  | U    | O4'-C1'-N1 | 13.34  | 118.87      | 108.20   |
| 35  | BB    | 1975 | G    | C4-C5-N7   | 13.34  | 116.14      | 110.80   |
| 1   | AA    | 128  | G    | C5-C6-O6   | -13.34 | 120.60      | 128.60   |
| 1   | AA    | 142  | G    | C8-N9-C4   | -13.34 | 101.07      | 106.40   |
| 35  | BB    | 2069 | G    | N1-C6-O6   | 13.34  | 127.90      | 119.90   |
| 35  | BB    | 2392 | A    | N1-C6-N6   | 13.34  | 126.60      | 118.60   |
| 35  | BB    | 473  | G    | C2-N3-C4   | -13.33 | 105.23      | 111.90   |
| 35  | BB    | 820  | A    | N1-C6-N6   | 13.33  | 126.60      | 118.60   |
| 35  | BB    | 1633 | G    | N1-C6-O6   | 13.33  | 127.90      | 119.90   |
| 1   | AA    | 1268 | G    | N1-C6-O6   | 13.33  | 127.90      | 119.90   |
| 35  | BB    | 764  | A    | C5-C6-N1   | -13.33 | 111.03      | 117.70   |
| 1   | AA    | 519  | C    | O4'-C1'-N1 | 13.33  | 118.86      | 108.20   |
| 1   | AA    | 584  | G    | N1-C6-O6   | 13.33  | 127.90      | 119.90   |
| 35  | BB    | 309  | A    | N9-C4-C5   | 13.33  | 111.13      | 105.80   |
| 35  | BB    | 2407 | A    | C5-C6-N1   | -13.33 | 111.04      | 117.70   |
| 1   | AA    | 371  | A    | N7-C8-N9   | -13.32 | 107.14      | 113.80   |
| 35  | BB    | 1095 | A    | N1-C6-N6   | 13.32  | 126.59      | 118.60   |
| 1   | AA    | 1385 | G    | N1-C6-O6   | 13.32  | 127.89      | 119.90   |
| 35  | BB    | 1207 | C    | O4'-C1'-N1 | 13.32  | 118.85      | 108.20   |
| 35  | BB    | 2830 | C    | N3-C4-C5   | -13.32 | 116.57      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1882 | U    | N3-C4-O4   | 13.31  | 128.72      | 119.40   |
| 35  | BB    | 1257 | C    | O4'-C1'-N1 | 13.31  | 118.85      | 108.20   |
| 1   | AA    | 628  | G    | O4'-C1'-N9 | 13.31  | 118.85      | 108.20   |
| 1   | AA    | 1353 | G    | N1-C2-N3   | -13.31 | 115.92      | 123.90   |
| 1   | AA    | 542  | G    | O4'-C1'-N9 | 13.30  | 118.84      | 108.20   |
| 35  | BB    | 1090 | A    | N1-C6-N6   | 13.30  | 126.58      | 118.60   |
| 1   | AA    | 1004 | A    | N1-C6-N6   | 13.30  | 126.58      | 118.60   |
| 35  | BB    | 2015 | A    | N9-C4-C5   | 13.30  | 111.12      | 105.80   |
| 35  | BB    | 2760 | C    | N3-C4-C5   | -13.30 | 116.58      | 121.90   |
| 34  | BA    | 19   | C    | N3-C4-C5   | -13.30 | 116.58      | 121.90   |
| 35  | BB    | 477  | A    | C5-N7-C8   | 13.30  | 110.55      | 103.90   |
| 22  | AV    | 4    | C    | N3-C4-N4   | 13.29  | 127.31      | 118.00   |
| 35  | BB    | 2095 | A    | N1-C6-N6   | 13.29  | 126.58      | 118.60   |
| 35  | BB    | 662  | G    | N1-C6-O6   | 13.29  | 127.87      | 119.90   |
| 35  | BB    | 1968 | G    | N1-C6-O6   | 13.29  | 127.87      | 119.90   |
| 1   | AA    | 507  | C    | N3-C4-N4   | 13.29  | 127.30      | 118.00   |
| 35  | BB    | 2281 | A    | N1-C6-N6   | 13.28  | 126.57      | 118.60   |
| 35  | BB    | 2602 | A    | C4-C5-C6   | 13.28  | 123.64      | 117.00   |
| 54  | BU    | 84   | PHE  | CB-CG-CD2  | -13.28 | 111.50      | 120.80   |
| 1   | AA    | 673  | A    | C5-C6-N6   | -13.28 | 113.08      | 123.70   |
| 1   | AA    | 1210 | C    | N3-C4-C5   | -13.28 | 116.59      | 121.90   |
| 35  | BB    | 844  | A    | C5-C6-N1   | -13.28 | 111.06      | 117.70   |
| 35  | BB    | 1654 | A    | N1-C6-N6   | 13.28  | 126.56      | 118.60   |
| 35  | BB    | 2084 | C    | O4'-C1'-N1 | 13.28  | 118.82      | 108.20   |
| 35  | BB    | 760  | G    | C5-C6-O6   | -13.27 | 120.64      | 128.60   |
| 1   | AA    | 914  | A    | N1-C6-N6   | 13.27  | 126.56      | 118.60   |
| 35  | BB    | 753  | A    | N1-C6-N6   | 13.27  | 126.56      | 118.60   |
| 1   | AA    | 106  | C    | O4'-C1'-N1 | 13.26  | 118.81      | 108.20   |
| 35  | BB    | 478  | A    | N1-C6-N6   | 13.26  | 126.56      | 118.60   |
| 35  | BB    | 480  | A    | C5-C6-N6   | -13.26 | 113.09      | 123.70   |
| 44  | BK    | 49   | ARG  | NE-CZ-NH2  | -13.25 | 113.67      | 120.30   |
| 1   | AA    | 364  | A    | C5-C6-N1   | -13.25 | 111.07      | 117.70   |
| 1   | AA    | 575  | G    | N1-C6-O6   | 13.25  | 127.85      | 119.90   |
| 31  | B6    | 19   | ARG  | NE-CZ-NH2  | 13.25  | 126.93      | 120.30   |
| 35  | BB    | 1020 | A    | C2-N3-C4   | -13.25 | 103.97      | 110.60   |
| 35  | BB    | 2829 | A    | N1-C6-N6   | 13.25  | 126.55      | 118.60   |
| 35  | BB    | 2095 | A    | C5-C6-N1   | -13.25 | 111.07      | 117.70   |
| 35  | BB    | 2536 | G    | C5-C6-O6   | -13.25 | 120.65      | 128.60   |
| 1   | AA    | 171  | A    | N1-C6-N6   | 13.24  | 126.55      | 118.60   |
| 1   | AA    | 909  | A    | C4-C5-C6   | 13.24  | 123.62      | 117.00   |
| 35  | BB    | 104  | A    | N7-C8-N9   | -13.24 | 107.18      | 113.80   |
| 34  | BA    | 78   | A    | N1-C6-N6   | 13.24  | 126.54      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 201  | G    | C5-C6-O6   | -13.24 | 120.66      | 128.60   |
| 35  | BB    | 250  | G    | C8-N9-C4   | 13.24  | 111.69      | 106.40   |
| 35  | BB    | 1054 | A    | C4-C5-C6   | 13.24  | 123.62      | 117.00   |
| 1   | AA    | 728  | A    | C4-C5-C6   | 13.23  | 123.61      | 117.00   |
| 1   | AA    | 355  | C    | N3-C4-C5   | -13.23 | 116.61      | 121.90   |
| 35  | BB    | 1806 | C    | N3-C4-C5   | -13.23 | 116.61      | 121.90   |
| 1   | AA    | 600  | A    | N1-C6-N6   | 13.22  | 126.53      | 118.60   |
| 35  | BB    | 2043 | C    | N3-C4-C5   | -13.22 | 116.61      | 121.90   |
| 35  | BB    | 651  | G    | O4'-C1'-N9 | 13.22  | 118.77      | 108.20   |
| 1   | AA    | 27   | G    | O4'-C1'-N9 | 13.21  | 118.77      | 108.20   |
| 35  | BB    | 878  | A    | N1-C6-N6   | 13.21  | 126.53      | 118.60   |
| 1   | AA    | 606  | G    | N1-C6-O6   | 13.21  | 127.83      | 119.90   |
| 34  | BA    | 15   | A    | C4-C5-C6   | 13.21  | 123.61      | 117.00   |
| 35  | BB    | 398  | C    | O4'-C1'-N1 | 13.21  | 118.77      | 108.20   |
| 35  | BB    | 1637 | A    | N7-C8-N9   | -13.21 | 107.19      | 113.80   |
| 35  | BB    | 1536 | C    | C6-N1-C2   | -13.21 | 115.02      | 120.30   |
| 35  | BB    | 2011 | U    | O4'-C1'-N1 | 13.21  | 118.77      | 108.20   |
| 1   | AA    | 404  | G    | O4'-C1'-N9 | 13.21  | 118.77      | 108.20   |
| 35  | BB    | 2350 | C    | N3-C4-C5   | -13.21 | 116.62      | 121.90   |
| 35  | BB    | 1212 | G    | N1-C6-O6   | 13.20  | 127.82      | 119.90   |
| 35  | BB    | 346  | A    | N1-C6-N6   | 13.20  | 126.52      | 118.60   |
| 35  | BB    | 497  | A    | N1-C6-N6   | 13.20  | 126.52      | 118.60   |
| 1   | AA    | 128  | G    | N1-C6-O6   | 13.20  | 127.82      | 119.90   |
| 35  | BB    | 1956 | U    | O4'-C1'-N1 | 13.20  | 118.76      | 108.20   |
| 35  | BB    | 2549 | G    | O4'-C1'-N9 | 13.20  | 118.76      | 108.20   |
| 35  | BB    | 2618 | G    | N1-C6-O6   | 13.20  | 127.82      | 119.90   |
| 45  | BL    | 126  | ARG  | NE-CZ-NH1  | 13.19  | 126.90      | 120.30   |
| 1   | AA    | 325  | A    | C5-C6-N1   | -13.19 | 111.11      | 117.70   |
| 35  | BB    | 622  | G    | C5-C6-O6   | -13.19 | 120.69      | 128.60   |
| 35  | BB    | 127  | A    | C6-N1-C2   | -13.18 | 110.69      | 118.60   |
| 35  | BB    | 795  | C    | C6-N1-C2   | -13.18 | 115.03      | 120.30   |
| 35  | BB    | 989  | G    | C5-C6-O6   | -13.18 | 120.69      | 128.60   |
| 1   | AA    | 1207 | G    | C5-C6-O6   | -13.18 | 120.69      | 128.60   |
| 35  | BB    | 2582 | G    | C5-C6-O6   | -13.18 | 120.69      | 128.60   |
| 1   | AA    | 1163 | A    | O4'-C1'-N9 | 13.17  | 118.74      | 108.20   |
| 35  | BB    | 2215 | C    | O4'-C1'-N1 | 13.17  | 118.74      | 108.20   |
| 35  | BB    | 415  | A    | N1-C6-N6   | 13.17  | 126.50      | 118.60   |
| 35  | BB    | 671  | C    | C5-C6-N1   | 13.17  | 127.59      | 121.00   |
| 35  | BB    | 503  | A    | C4-C5-C6   | 13.16  | 123.58      | 117.00   |
| 35  | BB    | 855  | G    | N9-C4-C5   | -13.16 | 100.13      | 105.40   |
| 35  | BB    | 1448 | G    | C5-C6-O6   | -13.16 | 120.70      | 128.60   |
| 34  | BA    | 68   | C    | O4'-C1'-N1 | 13.15  | 118.72      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 34  | BA    | 49   | C    | C5-C6-N1   | 13.15  | 127.57      | 121.00   |
| 1   | AA    | 1278 | G    | C5-C6-O6   | -13.14 | 120.72      | 128.60   |
| 35  | BB    | 309  | A    | N1-C6-N6   | 13.14  | 126.48      | 118.60   |
| 1   | AA    | 1444 | U    | O4'-C1'-N1 | 13.14  | 118.71      | 108.20   |
| 35  | BB    | 1631 | G    | N1-C6-O6   | 13.14  | 127.78      | 119.90   |
| 35  | BB    | 1672 | A    | C4-C5-C6   | 13.13  | 123.56      | 117.00   |
| 35  | BB    | 1651 | G    | N1-C6-O6   | 13.12  | 127.77      | 119.90   |
| 35  | BB    | 866  | A    | N1-C6-N6   | 13.12  | 126.47      | 118.60   |
| 1   | AA    | 728  | A    | C5-C6-N1   | -13.11 | 111.14      | 117.70   |
| 35  | BB    | 2361 | G    | C5-C6-O6   | -13.11 | 120.73      | 128.60   |
| 18  | AR    | 56   | ARG  | NE-CZ-NH1  | 13.11  | 126.86      | 120.30   |
| 22  | AV    | 70   | C    | O4'-C1'-N1 | 13.11  | 118.69      | 108.20   |
| 35  | BB    | 374  | A    | N1-C6-N6   | 13.11  | 126.47      | 118.60   |
| 35  | BB    | 1590 | A    | C5-C6-N6   | -13.11 | 113.21      | 123.70   |
| 35  | BB    | 2814 | A    | N1-C6-N6   | 13.11  | 126.47      | 118.60   |
| 35  | BB    | 2759 | G    | N1-C6-O6   | 13.11  | 127.77      | 119.90   |
| 1   | AA    | 143  | A    | O4'-C1'-N9 | 13.11  | 118.69      | 108.20   |
| 1   | AA    | 376  | G    | C5-C6-O6   | -13.11 | 120.74      | 128.60   |
| 35  | BB    | 2543 | G    | N3-C2-N2   | 13.10  | 129.07      | 119.90   |
| 1   | AA    | 1015 | G    | N1-C6-O6   | 13.10  | 127.76      | 119.90   |
| 22  | AV    | 67   | G    | N1-C6-O6   | 13.10  | 127.76      | 119.90   |
| 35  | BB    | 502  | A    | N1-C6-N6   | 13.09  | 126.45      | 118.60   |
| 34  | BA    | 46   | A    | N9-C4-C5   | -13.09 | 100.56      | 105.80   |
| 35  | BB    | 1478 | G    | N1-C6-O6   | 13.09  | 127.75      | 119.90   |
| 1   | AA    | 777  | A    | C2-N3-C4   | -13.09 | 104.06      | 110.60   |
| 35  | BB    | 978  | G    | C5-C6-O6   | -13.09 | 120.75      | 128.60   |
| 50  | BQ    | 27   | ARG  | NE-CZ-NH2  | -13.09 | 113.76      | 120.30   |
| 35  | BB    | 147  | C    | N3-C4-C5   | -13.08 | 116.67      | 121.90   |
| 35  | BB    | 900  | A    | N1-C6-N6   | 13.08  | 126.45      | 118.60   |
| 35  | BB    | 1168 | G    | N3-C2-N2   | 13.08  | 129.06      | 119.90   |
| 35  | BB    | 1831 | G    | O4'-C1'-N9 | 13.08  | 118.67      | 108.20   |
| 1   | AA    | 352  | C    | C2-N3-C4   | 13.08  | 126.44      | 119.90   |
| 1   | AA    | 547  | A    | N1-C6-N6   | 13.08  | 126.45      | 118.60   |
| 35  | BB    | 2877 | G    | C5-C6-O6   | -13.08 | 120.75      | 128.60   |
| 35  | BB    | 172  | A    | O4'-C1'-N9 | 13.08  | 118.66      | 108.20   |
| 35  | BB    | 1501 | G    | C5-C6-O6   | -13.08 | 120.75      | 128.60   |
| 35  | BB    | 2870 | C    | N3-C4-N4   | 13.08  | 127.16      | 118.00   |
| 35  | BB    | 1195 | G    | C5-C6-O6   | -13.07 | 120.75      | 128.60   |
| 35  | BB    | 2315 | G    | O4'-C1'-N9 | 13.07  | 118.66      | 108.20   |
| 1   | AA    | 25   | C    | O4'-C1'-N1 | 13.07  | 118.66      | 108.20   |
| 35  | BB    | 1517 | G    | N1-C6-O6   | -13.07 | 112.06      | 119.90   |
| 35  | BB    | 1009 | A    | N1-C6-N6   | 13.07  | 126.44      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 174  | A    | N1-C2-N3   | 13.07  | 135.83      | 129.30   |
| 35  | BB    | 2740 | A    | N1-C6-N6   | 13.07  | 126.44      | 118.60   |
| 35  | BB    | 2842 | G    | N1-C6-O6   | 13.07  | 127.74      | 119.90   |
| 1   | AA    | 86   | G    | N1-C6-O6   | 13.06  | 127.73      | 119.90   |
| 35  | BB    | 2054 | A    | N1-C6-N6   | 13.06  | 126.44      | 118.60   |
| 1   | AA    | 1110 | A    | C4-C5-C6   | 13.06  | 123.53      | 117.00   |
| 1   | AA    | 857  | C    | O4'-C1'-N1 | 13.06  | 118.64      | 108.20   |
| 1   | AA    | 761  | G    | N1-C6-O6   | 13.05  | 127.73      | 119.90   |
| 35  | BB    | 2090 | A    | N1-C6-N6   | 13.05  | 126.43      | 118.60   |
| 35  | BB    | 2032 | G    | C5-C6-O6   | -13.05 | 120.77      | 128.60   |
| 1   | AA    | 986  | U    | O4'-C1'-N1 | 13.04  | 118.64      | 108.20   |
| 39  | BF    | 21   | TYR  | CB-CG-CD2  | 13.04  | 128.83      | 121.00   |
| 35  | BB    | 1541 | C    | O4'-C1'-N1 | 13.04  | 118.63      | 108.20   |
| 1   | AA    | 847  | G    | N9-C4-C5   | -13.04 | 100.18      | 105.40   |
| 35  | BB    | 533  | G    | N3-C2-N2   | 13.04  | 129.03      | 119.90   |
| 35  | BB    | 702  | U    | O4'-C1'-N1 | 13.04  | 118.63      | 108.20   |
| 35  | BB    | 2503 | A    | N1-C6-N6   | 13.04  | 126.42      | 118.60   |
| 35  | BB    | 1804 | C    | C6-N1-C2   | -13.03 | 115.09      | 120.30   |
| 35  | BB    | 2214 | C    | N3-C4-N4   | 13.03  | 127.12      | 118.00   |
| 35  | BB    | 897  | C    | O4'-C1'-N1 | 13.03  | 118.63      | 108.20   |
| 35  | BB    | 1322 | A    | C5-C6-N1   | -13.03 | 111.18      | 117.70   |
| 1   | AA    | 880  | C    | C6-N1-C2   | -13.03 | 115.09      | 120.30   |
| 35  | BB    | 442  | G    | C5-C6-O6   | -13.03 | 120.78      | 128.60   |
| 1   | AA    | 503  | C    | O4'-C1'-N1 | 13.02  | 118.62      | 108.20   |
| 35  | BB    | 877  | A    | C8-N9-C4   | -13.02 | 100.59      | 105.80   |
| 35  | BB    | 771  | G    | C5-C6-O6   | -13.02 | 120.79      | 128.60   |
| 35  | BB    | 507  | A    | N1-C6-N6   | 13.02  | 126.41      | 118.60   |
| 35  | BB    | 1901 | A    | C8-N9-C4   | -13.02 | 100.59      | 105.80   |
| 35  | BB    | 175  | G    | N1-C6-O6   | 13.01  | 127.71      | 119.90   |
| 1   | AA    | 120  | A    | N1-C6-N6   | 13.01  | 126.41      | 118.60   |
| 1   | AA    | 839  | C    | C5-C4-N4   | -13.01 | 111.09      | 120.20   |
| 35  | BB    | 659  | G    | N1-C6-O6   | 13.01  | 127.71      | 119.90   |
| 35  | BB    | 1509 | A    | N1-C6-N6   | 13.01  | 126.40      | 118.60   |
| 35  | BB    | 2414 | G    | C5-C6-O6   | -13.00 | 120.80      | 128.60   |
| 35  | BB    | 2439 | A    | N1-C6-N6   | 13.00  | 126.40      | 118.60   |
| 35  | BB    | 1160 | G    | N1-C6-O6   | 13.00  | 127.70      | 119.90   |
| 35  | BB    | 670  | A    | C5-C6-N1   | -12.99 | 111.20      | 117.70   |
| 35  | BB    | 1534 | U    | N1-C2-N3   | 12.99  | 122.70      | 114.90   |
| 35  | BB    | 66   | C    | N3-C4-C5   | -12.99 | 116.70      | 121.90   |
| 35  | BB    | 2820 | A    | C4-C5-C6   | 12.99  | 123.50      | 117.00   |
| 35  | BB    | 971  | G    | O4'-C1'-N9 | 12.99  | 118.59      | 108.20   |
| 35  | BB    | 841  | G    | C5-C6-O6   | -12.99 | 120.81      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 829  | G    | C5-C6-O6   | -12.98 | 120.81      | 128.60   |
| 1   | AA    | 833  | G    | C5-C6-O6   | -12.98 | 120.81      | 128.60   |
| 1   | AA    | 1516 | G    | N1-C6-O6   | 12.98  | 127.69      | 119.90   |
| 35  | BB    | 559  | G    | C5-C6-O6   | -12.98 | 120.81      | 128.60   |
| 35  | BB    | 660  | C    | C5-C6-N1   | 12.98  | 127.49      | 121.00   |
| 35  | BB    | 733  | G    | C5-C6-O6   | -12.98 | 120.81      | 128.60   |
| 35  | BB    | 1112 | G    | C5-C6-O6   | -12.98 | 120.81      | 128.60   |
| 35  | BB    | 1791 | A    | C5-C6-N6   | -12.98 | 113.31      | 123.70   |
| 35  | BB    | 1987 | A    | O4'-C1'-N9 | 12.98  | 118.58      | 108.20   |
| 40  | BG    | 2    | ARG  | NE-CZ-NH2  | 12.98  | 126.79      | 120.30   |
| 35  | BB    | 48   | G    | C5-C6-O6   | -12.98 | 120.81      | 128.60   |
| 35  | BB    | 520  | G    | C5-C6-O6   | -12.97 | 120.81      | 128.60   |
| 35  | BB    | 1973 | G    | N3-C2-N2   | 12.97  | 128.98      | 119.90   |
| 35  | BB    | 1662 | U    | O4'-C1'-N1 | 12.97  | 118.58      | 108.20   |
| 35  | BB    | 1854 | A    | N1-C6-N6   | 12.97  | 126.38      | 118.60   |
| 35  | BB    | 1646 | C    | O4'-C1'-N1 | 12.97  | 118.58      | 108.20   |
| 35  | BB    | 2764 | A    | C5-C6-N1   | -12.97 | 111.22      | 117.70   |
| 35  | BB    | 1116 | G    | C5-C6-O6   | -12.97 | 120.82      | 128.60   |
| 35  | BB    | 1502 | A    | N1-C6-N6   | 12.96  | 126.38      | 118.60   |
| 1   | AA    | 577  | G    | C5-C6-O6   | -12.96 | 120.82      | 128.60   |
| 35  | BB    | 1510 | G    | C5-C6-O6   | -12.96 | 120.83      | 128.60   |
| 35  | BB    | 368  | A    | N1-C6-N6   | 12.96  | 126.37      | 118.60   |
| 35  | BB    | 1392 | A    | N1-C6-N6   | 12.96  | 126.37      | 118.60   |
| 35  | BB    | 2520 | C    | N3-C4-C5   | -12.96 | 116.72      | 121.90   |
| 35  | BB    | 283  | G    | N1-C6-O6   | 12.95  | 127.67      | 119.90   |
| 35  | BB    | 2885 | G    | C5-C6-O6   | -12.95 | 120.83      | 128.60   |
| 35  | BB    | 265  | A    | N1-C6-N6   | 12.95  | 126.37      | 118.60   |
| 35  | BB    | 2348 | U    | O4'-C1'-N1 | 12.95  | 118.56      | 108.20   |
| 35  | BB    | 1126 | A    | N1-C2-N3   | -12.95 | 122.83      | 129.30   |
| 35  | BB    | 1051 | G    | C5-C6-O6   | -12.94 | 120.84      | 128.60   |
| 35  | BB    | 1482 | G    | C4-C5-C6   | 12.94  | 126.56      | 118.80   |
| 1   | AA    | 927  | G    | O4'-C1'-N9 | 12.94  | 118.55      | 108.20   |
| 35  | BB    | 1808 | A    | N1-C6-N6   | 12.93  | 126.36      | 118.60   |
| 1   | AA    | 311  | C    | O4'-C1'-N1 | 12.93  | 118.55      | 108.20   |
| 1   | AA    | 1427 | C    | C4-C5-C6   | 12.93  | 123.86      | 117.40   |
| 35  | BB    | 1592 | C    | O4'-C1'-N1 | 12.93  | 118.54      | 108.20   |
| 35  | BB    | 2061 | G    | N3-C2-N2   | 12.93  | 128.95      | 119.90   |
| 35  | BB    | 961  | C    | O4'-C1'-N1 | 12.92  | 118.54      | 108.20   |
| 35  | BB    | 2550 | G    | C6-C5-N7   | -12.91 | 122.65      | 130.40   |
| 35  | BB    | 656  | G    | C5-C6-N1   | -12.91 | 105.04      | 111.50   |
| 8   | AH    | 83   | ARG  | NE-CZ-NH2  | -12.91 | 113.84      | 120.30   |
| 35  | BB    | 592  | A    | N1-C2-N3   | 12.91  | 135.75      | 129.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 903  | G    | C5-C6-O6   | -12.91 | 120.86      | 128.60   |
| 35  | BB    | 115  | C    | O4'-C1'-N1 | 12.91  | 118.53      | 108.20   |
| 35  | BB    | 727  | A    | N1-C2-N3   | 12.90  | 135.75      | 129.30   |
| 35  | BB    | 909  | A    | N1-C6-N6   | 12.90  | 126.34      | 118.60   |
| 35  | BB    | 2289 | G    | C5-C6-O6   | -12.90 | 120.86      | 128.60   |
| 1   | AA    | 223  | A    | N1-C6-N6   | 12.90  | 126.34      | 118.60   |
| 35  | BB    | 1390 | U    | O4'-C1'-N1 | 12.90  | 118.52      | 108.20   |
| 35  | BB    | 1757 | A    | O4'-C1'-N9 | 12.90  | 118.52      | 108.20   |
| 34  | BA    | 98   | G    | C5-C6-O6   | -12.90 | 120.86      | 128.60   |
| 35  | BB    | 737  | C    | O4'-C1'-N1 | 12.90  | 118.52      | 108.20   |
| 35  | BB    | 164  | C    | N3-C4-C5   | -12.89 | 116.74      | 121.90   |
| 35  | BB    | 583  | G    | N1-C6-O6   | 12.89  | 127.64      | 119.90   |
| 35  | BB    | 2433 | A    | N1-C6-N6   | 12.89  | 126.34      | 118.60   |
| 35  | BB    | 131  | A    | O4'-C1'-N9 | 12.89  | 118.51      | 108.20   |
| 35  | BB    | 2232 | C    | C5-C4-N4   | -12.89 | 111.18      | 120.20   |
| 35  | BB    | 2843 | G    | N1-C6-O6   | 12.89  | 127.64      | 119.90   |
| 1   | AA    | 990  | C    | N3-C4-C5   | -12.89 | 116.75      | 121.90   |
| 35  | BB    | 6    | A    | C4-C5-C6   | 12.89  | 123.44      | 117.00   |
| 35  | BB    | 2286 | G    | N1-C6-O6   | 12.89  | 127.63      | 119.90   |
| 35  | BB    | 2365 | G    | N1-C6-O6   | 12.88  | 127.63      | 119.90   |
| 1   | AA    | 289  | G    | C5-C6-N1   | 12.88  | 117.94      | 111.50   |
| 35  | BB    | 666  | A    | C5-C6-N6   | -12.88 | 113.39      | 123.70   |
| 35  | BB    | 106  | C    | O4'-C1'-N1 | 12.88  | 118.50      | 108.20   |
| 35  | BB    | 1504 | A    | C5-C6-N6   | -12.88 | 113.39      | 123.70   |
| 35  | BB    | 1696 | G    | C5-C6-O6   | -12.88 | 120.87      | 128.60   |
| 1   | AA    | 819  | A    | N1-C6-N6   | 12.88  | 126.33      | 118.60   |
| 35  | BB    | 1627 | G    | C5-C6-O6   | -12.88 | 120.87      | 128.60   |
| 35  | BB    | 1909 | C    | O4'-C1'-N1 | 12.87  | 118.50      | 108.20   |
| 1   | AA    | 544  | G    | C5-C6-O6   | -12.87 | 120.88      | 128.60   |
| 36  | BC    | 61   | TYR  | CB-CG-CD2  | -12.87 | 113.28      | 121.00   |
| 35  | BB    | 1515 | A    | C4-C5-C6   | 12.87  | 123.43      | 117.00   |
| 35  | BB    | 2103 | C    | O4'-C1'-N1 | 12.86  | 118.49      | 108.20   |
| 1   | AA    | 1192 | C    | N3-C4-C5   | -12.85 | 116.76      | 121.90   |
| 35  | BB    | 1478 | G    | C4-C5-N7   | -12.85 | 105.66      | 110.80   |
| 1   | AA    | 542  | G    | N1-C6-O6   | 12.85  | 127.61      | 119.90   |
| 35  | BB    | 2095 | A    | C4-C5-C6   | 12.85  | 123.42      | 117.00   |
| 35  | BB    | 1810 | A    | O4'-C1'-N9 | 12.85  | 118.48      | 108.20   |
| 35  | BB    | 332  | A    | C5-C6-N6   | -12.84 | 113.43      | 123.70   |
| 35  | BB    | 1270 | C    | O4'-C1'-N1 | 12.84  | 118.47      | 108.20   |
| 35  | BB    | 1514 | G    | N1-C6-O6   | 12.84  | 127.60      | 119.90   |
| 1   | AA    | 222  | C    | N3-C4-C5   | -12.83 | 116.77      | 121.90   |
| 47  | BN    | 8    | ARG  | NE-CZ-NH2  | -12.83 | 113.88      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 496  | A    | C5-C6-N1   | -12.83 | 111.29      | 117.70   |
| 1   | AA    | 308  | C    | N3-C4-C5   | -12.82 | 116.77      | 121.90   |
| 1   | AA    | 16   | A    | C4-C5-C6   | 12.82  | 123.41      | 117.00   |
| 35  | BB    | 44   | A    | N1-C6-N6   | 12.82  | 126.29      | 118.60   |
| 35  | BB    | 1195 | G    | N1-C6-O6   | 12.82  | 127.59      | 119.90   |
| 1   | AA    | 666  | G    | N1-C6-O6   | 12.82  | 127.59      | 119.90   |
| 35  | BB    | 99   | U    | O4'-C1'-N1 | 12.82  | 118.46      | 108.20   |
| 1   | AA    | 46   | G    | O4'-C1'-N9 | 12.82  | 118.45      | 108.20   |
| 1   | AA    | 207  | C    | O4'-C1'-N1 | 12.82  | 118.45      | 108.20   |
| 35  | BB    | 933  | A    | P-O3'-C3'  | 12.81  | 135.08      | 119.70   |
| 1   | AA    | 1314 | C    | N3-C4-N4   | 12.81  | 126.97      | 118.00   |
| 35  | BB    | 832  | U    | O4'-C1'-N1 | 12.81  | 118.45      | 108.20   |
| 35  | BB    | 1050 | A    | C5-C6-N1   | -12.81 | 111.29      | 117.70   |
| 35  | BB    | 2838 | G    | C5-C6-O6   | -12.81 | 120.91      | 128.60   |
| 1   | AA    | 1405 | G    | N1-C6-O6   | 12.80  | 127.58      | 119.90   |
| 35  | BB    | 858  | G    | N1-C6-O6   | 12.80  | 127.58      | 119.90   |
| 35  | BB    | 2432 | A    | C5-N7-C8   | 12.80  | 110.30      | 103.90   |
| 35  | BB    | 1531 | C    | C5-C6-N1   | 12.80  | 127.40      | 121.00   |
| 1   | AA    | 1260 | G    | C5-C6-O6   | -12.80 | 120.92      | 128.60   |
| 34  | BA    | 113  | C    | O4'-C1'-N1 | 12.80  | 118.44      | 108.20   |
| 35  | BB    | 781  | A    | N1-C6-N6   | 12.80  | 126.28      | 118.60   |
| 35  | BB    | 1126 | A    | N1-C6-N6   | 12.80  | 126.28      | 118.60   |
| 35  | BB    | 2676 | C    | N3-C4-C5   | -12.80 | 116.78      | 121.90   |
| 1   | AA    | 1241 | G    | C2-N3-C4   | 12.79  | 118.30      | 111.90   |
| 35  | BB    | 2481 | G    | N1-C6-O6   | 12.79  | 127.58      | 119.90   |
| 1   | AA    | 441  | A    | C5-C6-N6   | -12.79 | 113.47      | 123.70   |
| 1   | AA    | 105  | G    | N1-C2-N3   | -12.79 | 116.22      | 123.90   |
| 35  | BB    | 1347 | A    | C5-C6-N6   | -12.79 | 113.47      | 123.70   |
| 1   | AA    | 953  | G    | N1-C6-O6   | 12.79  | 127.57      | 119.90   |
| 35  | BB    | 124  | G    | C5-N7-C8   | 12.79  | 110.69      | 104.30   |
| 1   | AA    | 362  | G    | C5-C6-O6   | -12.78 | 120.93      | 128.60   |
| 1   | AA    | 489  | C    | O4'-C1'-N1 | 12.78  | 118.43      | 108.20   |
| 1   | AA    | 596  | A    | N1-C6-N6   | 12.78  | 126.27      | 118.60   |
| 1   | AA    | 132  | C    | N3-C4-C5   | -12.78 | 116.79      | 121.90   |
| 35  | BB    | 277  | G    | N9-C4-C5   | -12.78 | 100.29      | 105.40   |
| 1   | AA    | 1499 | A    | C5-N7-C8   | 12.78  | 110.29      | 103.90   |
| 35  | BB    | 846  | U    | O4'-C1'-N1 | 12.78  | 118.42      | 108.20   |
| 34  | BA    | 85   | G    | C5-C6-O6   | -12.78 | 120.93      | 128.60   |
| 35  | BB    | 1728 | C    | N3-C4-C5   | -12.78 | 116.79      | 121.90   |
| 35  | BB    | 2053 | G    | C5-C6-O6   | -12.78 | 120.93      | 128.60   |
| 35  | BB    | 602  | A    | C4-C5-C6   | 12.77  | 123.39      | 117.00   |
| 35  | BB    | 677  | A    | C5-C6-N6   | -12.77 | 113.48      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 639  | G    | C5-C6-O6   | -12.77 | 120.94      | 128.60   |
| 1   | AA    | 834  | U    | N1-C2-O2   | -12.77 | 113.86      | 122.80   |
| 35  | BB    | 2364 | C    | O4'-C1'-N1 | 12.77  | 118.42      | 108.20   |
| 1   | AA    | 817  | C    | N3-C4-C5   | -12.77 | 116.79      | 121.90   |
| 1   | AA    | 1305 | G    | N1-C6-O6   | 12.77  | 127.56      | 119.90   |
| 22  | AV    | 4    | C    | C5-C4-N4   | -12.77 | 111.26      | 120.20   |
| 35  | BB    | 1006 | C    | O4'-C1'-N1 | 12.76  | 118.41      | 108.20   |
| 1   | AA    | 1322 | C    | C5-C6-N1   | 12.76  | 127.38      | 121.00   |
| 35  | BB    | 1792 | G    | N1-C6-O6   | 12.76  | 127.56      | 119.90   |
| 35  | BB    | 148  | U    | N3-C4-C5   | -12.76 | 106.95      | 114.60   |
| 35  | BB    | 671  | C    | O4'-C1'-N1 | 12.76  | 118.41      | 108.20   |
| 1   | AA    | 443  | C    | N3-C4-N4   | 12.75  | 126.93      | 118.00   |
| 25  | B0    | 26   | ARG  | NE-CZ-NH2  | -12.75 | 113.92      | 120.30   |
| 34  | BA    | 118  | C    | O4'-C1'-N1 | 12.75  | 118.40      | 108.20   |
| 34  | BA    | 24   | G    | C5-C6-O6   | -12.75 | 120.95      | 128.60   |
| 1   | AA    | 737  | C    | N3-C4-C5   | -12.75 | 116.80      | 121.90   |
| 35  | BB    | 2704 | C    | N3-C4-C5   | -12.75 | 116.80      | 121.90   |
| 35  | BB    | 2726 | A    | N1-C6-N6   | 12.75  | 126.25      | 118.60   |
| 1   | AA    | 1210 | C    | N3-C4-N4   | 12.74  | 126.92      | 118.00   |
| 35  | BB    | 182  | A    | C4-C5-N7   | -12.74 | 104.33      | 110.70   |
| 35  | BB    | 2694 | G    | N1-C6-O6   | 12.74  | 127.55      | 119.90   |
| 1   | AA    | 400  | C    | C5-C4-N4   | -12.74 | 111.28      | 120.20   |
| 22  | AV    | 39   | G    | C8-N9-C4   | -12.74 | 101.30      | 106.40   |
| 35  | BB    | 2654 | A    | N1-C6-N6   | 12.74  | 126.24      | 118.60   |
| 35  | BB    | 1686 | C    | O4'-C1'-N1 | 12.74  | 118.39      | 108.20   |
| 35  | BB    | 2675 | A    | C5-C6-N1   | -12.73 | 111.33      | 117.70   |
| 1   | AA    | 190  | A    | C5-C6-N1   | -12.73 | 111.33      | 117.70   |
| 18  | AR    | 63   | TYR  | CB-CG-CD2  | -12.73 | 113.36      | 121.00   |
| 34  | BA    | 76   | G    | N1-C6-O6   | 12.73  | 127.54      | 119.90   |
| 1   | AA    | 395  | C    | N3-C4-N4   | 12.73  | 126.91      | 118.00   |
| 1   | AA    | 517  | G    | N1-C6-O6   | 12.73  | 127.54      | 119.90   |
| 1   | AA    | 1134 | G    | C5-C6-O6   | -12.73 | 120.96      | 128.60   |
| 35  | BB    | 2709 | G    | N1-C6-O6   | 12.73  | 127.53      | 119.90   |
| 1   | AA    | 682  | G    | N1-C6-O6   | 12.72  | 127.53      | 119.90   |
| 35  | BB    | 630  | G    | N1-C6-O6   | 12.72  | 127.53      | 119.90   |
| 1   | AA    | 1365 | G    | C5-C6-O6   | -12.72 | 120.97      | 128.60   |
| 35  | BB    | 1056 | G    | O4'-C1'-N9 | 12.72  | 118.38      | 108.20   |
| 1   | AA    | 180  | U    | O4'-C1'-N1 | 12.72  | 118.37      | 108.20   |
| 34  | BA    | 61   | G    | N1-C6-O6   | 12.72  | 127.53      | 119.90   |
| 1   | AA    | 465  | A    | N1-C6-N6   | 12.71  | 126.23      | 118.60   |
| 1   | AA    | 653  | U    | O4'-C1'-N1 | 12.71  | 118.37      | 108.20   |
| 1   | AA    | 1456 | A    | O4'-C1'-N9 | 12.71  | 118.37      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2486 | C    | O4'-C1'-N1 | 12.71  | 118.36      | 108.20   |
| 35  | BB    | 2359 | C    | O4'-C1'-N1 | 12.70  | 118.36      | 108.20   |
| 35  | BB    | 597  | G    | C4-C5-N7   | -12.70 | 105.72      | 110.80   |
| 1   | AA    | 974  | A    | N1-C6-N6   | 12.70  | 126.22      | 118.60   |
| 1   | AA    | 1144 | G    | C5-C6-O6   | -12.70 | 120.98      | 128.60   |
| 30  | B5    | 180  | PHE  | CB-CG-CD2  | -12.70 | 111.91      | 120.80   |
| 35  | BB    | 1147 | A    | N1-C6-N6   | 12.70  | 126.22      | 118.60   |
| 35  | BB    | 1672 | A    | N1-C6-N6   | 12.69  | 126.22      | 118.60   |
| 51  | BR    | 80   | ARG  | NE-CZ-NH1  | -12.69 | 113.95      | 120.30   |
| 35  | BB    | 94   | A    | N1-C6-N6   | 12.69  | 126.22      | 118.60   |
| 35  | BB    | 1135 | C    | O4'-C1'-N1 | 12.69  | 118.35      | 108.20   |
| 35  | BB    | 2349 | G    | C5-C6-O6   | -12.69 | 120.98      | 128.60   |
| 1   | AA    | 111  | G    | C5-C6-O6   | -12.69 | 120.99      | 128.60   |
| 35  | BB    | 1768 | C    | O4'-C1'-N1 | 12.69  | 118.35      | 108.20   |
| 35  | BB    | 1824 | G    | N1-C2-N3   | -12.69 | 116.29      | 123.90   |
| 1   | AA    | 880  | C    | O4'-C1'-N1 | 12.68  | 118.35      | 108.20   |
| 1   | AA    | 918  | A    | O4'-C1'-N9 | 12.68  | 118.34      | 108.20   |
| 35  | BB    | 2152 | G    | P-O3'-C3'  | 12.68  | 134.92      | 119.70   |
| 35  | BB    | 2682 | A    | C4-C5-N7   | -12.68 | 104.36      | 110.70   |
| 1   | AA    | 858  | G    | N3-C2-N2   | 12.68  | 128.78      | 119.90   |
| 1   | AA    | 1384 | C    | O4'-C1'-N1 | 12.68  | 118.34      | 108.20   |
| 35  | BB    | 1328 | A    | C5-C6-N1   | -12.68 | 111.36      | 117.70   |
| 35  | BB    | 951  | C    | O4'-C1'-N1 | 12.67  | 118.34      | 108.20   |
| 35  | BB    | 1187 | G    | C8-N9-C4   | -12.67 | 101.33      | 106.40   |
| 35  | BB    | 1146 | C    | O4'-C1'-N1 | 12.67  | 118.33      | 108.20   |
| 35  | BB    | 2142 | A    | C8-N9-C4   | -12.67 | 100.73      | 105.80   |
| 35  | BB    | 2498 | C    | N3-C4-C5   | -12.67 | 116.83      | 121.90   |
| 1   | AA    | 1001 | C    | O4'-C1'-N1 | 12.66  | 118.33      | 108.20   |
| 35  | BB    | 616  | A    | N1-C6-N6   | 12.66  | 126.20      | 118.60   |
| 1   | AA    | 655  | A    | N1-C6-N6   | 12.66  | 126.20      | 118.60   |
| 35  | BB    | 298  | G    | C6-C5-N7   | -12.66 | 122.80      | 130.40   |
| 35  | BB    | 2359 | C    | N3-C4-N4   | 12.66  | 126.86      | 118.00   |
| 35  | BB    | 2815 | C    | O4'-C1'-N1 | 12.66  | 118.33      | 108.20   |
| 35  | BB    | 364  | C    | O4'-C1'-N1 | 12.66  | 118.33      | 108.20   |
| 35  | BB    | 1444 | G    | N1-C6-O6   | 12.66  | 127.50      | 119.90   |
| 35  | BB    | 2578 | G    | N1-C6-O6   | 12.66  | 127.49      | 119.90   |
| 1   | AA    | 206  | C    | N3-C4-N4   | 12.65  | 126.86      | 118.00   |
| 35  | BB    | 1757 | A    | N1-C6-N6   | 12.65  | 126.19      | 118.60   |
| 35  | BB    | 1823 | G    | N3-C2-N2   | 12.65  | 128.76      | 119.90   |
| 32  | B7    | 13   | PHE  | CB-CG-CD1  | -12.65 | 111.95      | 120.80   |
| 35  | BB    | 35   | G    | C8-N9-C4   | -12.65 | 101.34      | 106.40   |
| 1   | AA    | 984  | C    | N3-C4-N4   | 12.64  | 126.85      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1   | AA    | 1209 | C    | O4'-C1'-N1  | 12.64  | 118.31      | 108.20   |
| 35  | BB    | 1836 | C    | N3-C4-C5    | -12.64 | 116.84      | 121.90   |
| 35  | BB    | 2704 | C    | N3-C4-N4    | 12.64  | 126.85      | 118.00   |
| 1   | AA    | 908  | A    | C5-C6-N1    | -12.64 | 111.38      | 117.70   |
| 1   | AA    | 983  | A    | C8-N9-C4    | -12.64 | 100.75      | 105.80   |
| 35  | BB    | 2211 | A    | C5-C6-N1    | -12.64 | 111.38      | 117.70   |
| 35  | BB    | 2809 | A    | O4'-C1'-N9  | 12.64  | 118.31      | 108.20   |
| 8   | AH    | 65   | PHE  | CB-CG-CD1   | -12.63 | 111.96      | 120.80   |
| 35  | BB    | 2892 | G    | N1-C6-O6    | 12.63  | 127.48      | 119.90   |
| 1   | AA    | 1082 | A    | N1-C6-N6    | 12.63  | 126.18      | 118.60   |
| 35  | BB    | 1081 | U    | C5'-C4'-C3' | 12.62  | 136.20      | 116.00   |
| 35  | BB    | 1987 | A    | N1-C6-N6    | 12.63  | 126.18      | 118.60   |
| 35  | BB    | 2488 | G    | O4'-C1'-N9  | 12.62  | 118.30      | 108.20   |
| 1   | AA    | 468  | A    | C5-C6-N6    | -12.62 | 113.60      | 123.70   |
| 1   | AA    | 977  | A    | C5-C6-N6    | -12.62 | 113.61      | 123.70   |
| 1   | AA    | 332  | G    | C5-C6-O6    | -12.62 | 121.03      | 128.60   |
| 1   | AA    | 1407 | C    | C6-N1-C2    | 12.62  | 125.35      | 120.30   |
| 35  | BB    | 271  | G    | N1-C6-O6    | 12.61  | 127.47      | 119.90   |
| 22  | AV    | 26   | A    | N1-C6-N6    | 12.61  | 126.17      | 118.60   |
| 1   | AA    | 246  | A    | N1-C2-N3    | 12.61  | 135.60      | 129.30   |
| 35  | BB    | 936  | A    | C5-N7-C8    | 12.61  | 110.20      | 103.90   |
| 1   | AA    | 1511 | G    | N1-C6-O6    | 12.60  | 127.46      | 119.90   |
| 35  | BB    | 359  | G    | O4'-C1'-N9  | 12.60  | 118.28      | 108.20   |
| 35  | BB    | 1452 | G    | N1-C6-O6    | 12.60  | 127.46      | 119.90   |
| 1   | AA    | 1531 | A    | N1-C6-N6    | 12.60  | 126.16      | 118.60   |
| 1   | AA    | 184  | G    | O4'-C1'-N9  | 12.59  | 118.27      | 108.20   |
| 1   | AA    | 1365 | G    | N3-C2-N2    | 12.59  | 128.71      | 119.90   |
| 35  | BB    | 1175 | A    | N1-C6-N6    | 12.59  | 126.16      | 118.60   |
| 35  | BB    | 2053 | G    | N1-C6-O6    | 12.59  | 127.45      | 119.90   |
| 35  | BB    | 1953 | A    | C5-C6-N1    | -12.59 | 111.41      | 117.70   |
| 35  | BB    | 2550 | G    | C5-C6-O6    | -12.59 | 121.05      | 128.60   |
| 1   | AA    | 301  | G    | N1-C6-O6    | 12.58  | 127.45      | 119.90   |
| 1   | AA    | 815  | A    | O4'-C1'-N9  | 12.58  | 118.27      | 108.20   |
| 35  | BB    | 644  | A    | N1-C6-N6    | 12.58  | 126.15      | 118.60   |
| 35  | BB    | 2325 | G    | C5-C6-O6    | -12.58 | 121.05      | 128.60   |
| 1   | AA    | 1057 | G    | N3-C2-N2    | 12.58  | 128.71      | 119.90   |
| 35  | BB    | 188  | G    | C4-C5-N7    | -12.58 | 105.77      | 110.80   |
| 1   | AA    | 98   | A    | C4-C5-C6    | 12.58  | 123.29      | 117.00   |
| 1   | AA    | 746  | A    | C5-C6-N6    | -12.58 | 113.64      | 123.70   |
| 35  | BB    | 2480 | C    | O4'-C1'-N1  | 12.57  | 118.26      | 108.20   |
| 1   | AA    | 200  | G    | N1-C6-O6    | 12.57  | 127.44      | 119.90   |
| 35  | BB    | 2901 | C    | O4'-C1'-N1  | 12.57  | 118.26      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1618 | A    | N1-C6-N6   | 12.57  | 126.14      | 118.60   |
| 1   | AA    | 52   | C    | O4'-C1'-N1 | 12.56  | 118.25      | 108.20   |
| 1   | AA    | 438  | U    | O4'-C1'-N1 | 12.56  | 118.25      | 108.20   |
| 1   | AA    | 688  | G    | C4-C5-C6   | 12.56  | 126.34      | 118.80   |
| 1   | AA    | 953  | G    | C5-C6-O6   | -12.56 | 121.06      | 128.60   |
| 35  | BB    | 2638 | G    | C5-C6-O6   | -12.56 | 121.06      | 128.60   |
| 1   | AA    | 1325 | C    | N3-C4-C5   | -12.56 | 116.88      | 121.90   |
| 35  | BB    | 2870 | C    | N3-C4-C5   | -12.56 | 116.88      | 121.90   |
| 1   | AA    | 1279 | G    | C8-N9-C4   | -12.56 | 101.38      | 106.40   |
| 35  | BB    | 125  | A    | N1-C6-N6   | 12.56  | 126.13      | 118.60   |
| 1   | AA    | 361  | G    | C5-C6-O6   | -12.56 | 121.07      | 128.60   |
| 1   | AA    | 688  | G    | C4-C5-N7   | -12.55 | 105.78      | 110.80   |
| 1   | AA    | 10   | A    | N1-C6-N6   | 12.55  | 126.13      | 118.60   |
| 1   | AA    | 140  | U    | C5-C6-N1   | 12.55  | 128.97      | 122.70   |
| 1   | AA    | 1434 | A    | O4'-C1'-N9 | 12.55  | 118.24      | 108.20   |
| 1   | AA    | 760  | G    | C4-C5-N7   | -12.54 | 105.78      | 110.80   |
| 1   | AA    | 976  | G    | C5-C6-O6   | -12.55 | 121.07      | 128.60   |
| 1   | AA    | 1267 | C    | N3-C4-C5   | -12.54 | 116.88      | 121.90   |
| 35  | BB    | 70   | G    | N1-C6-O6   | 12.54  | 127.42      | 119.90   |
| 35  | BB    | 1646 | C    | N3-C4-C5   | -12.54 | 116.88      | 121.90   |
| 35  | BB    | 488  | G    | C5-C6-O6   | -12.54 | 121.08      | 128.60   |
| 35  | BB    | 2252 | G    | C5-C6-N1   | -12.54 | 105.23      | 111.50   |
| 1   | AA    | 203  | G    | O4'-C1'-N9 | 12.53  | 118.23      | 108.20   |
| 1   | AA    | 1207 | G    | N9-C4-C5   | -12.53 | 100.39      | 105.40   |
| 1   | AA    | 449  | G    | C6-C5-N7   | -12.53 | 122.88      | 130.40   |
| 1   | AA    | 80   | A    | N1-C6-N6   | 12.53  | 126.12      | 118.60   |
| 1   | AA    | 1315 | U    | O4'-C1'-N1 | 12.53  | 118.22      | 108.20   |
| 35  | BB    | 1389 | G    | C5-C6-O6   | -12.53 | 121.08      | 128.60   |
| 1   | AA    | 922  | G    | C4-C5-N7   | 12.53  | 115.81      | 110.80   |
| 1   | AA    | 779  | C    | O4'-C1'-N1 | 12.52  | 118.22      | 108.20   |
| 1   | AA    | 254  | G    | N1-C6-O6   | 12.52  | 127.41      | 119.90   |
| 35  | BB    | 1306 | C    | O4'-C1'-N1 | 12.52  | 118.22      | 108.20   |
| 35  | BB    | 1723 | G    | N1-C6-O6   | 12.52  | 127.41      | 119.90   |
| 35  | BB    | 2357 | G    | N1-C2-N3   | -12.52 | 116.39      | 123.90   |
| 35  | BB    | 298  | G    | N3-C4-N9   | 12.52  | 133.51      | 126.00   |
| 1   | AA    | 931  | C    | O4'-C1'-N1 | 12.51  | 118.21      | 108.20   |
| 35  | BB    | 2476 | A    | O4'-C1'-N9 | 12.51  | 118.21      | 108.20   |
| 1   | AA    | 1019 | A    | C5-C6-N1   | -12.51 | 111.44      | 117.70   |
| 1   | AA    | 1452 | C    | N3-C4-C5   | -12.51 | 116.90      | 121.90   |
| 31  | B6    | 39   | ARG  | NE-CZ-NH1  | 12.51  | 126.56      | 120.30   |
| 35  | BB    | 1077 | A    | C6-C5-N7   | -12.51 | 123.54      | 132.30   |
| 35  | BB    | 127  | A    | N1-C6-N6   | 12.51  | 126.10      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 299  | A    | C4-C5-C6   | 12.51  | 123.25      | 117.00   |
| 35  | BB    | 635  | C    | O4'-C1'-N1 | 12.51  | 118.20      | 108.20   |
| 22  | AV    | 6    | C    | C6-N1-C2   | -12.50 | 115.30      | 120.30   |
| 35  | BB    | 685  | A    | N1-C6-N6   | 12.50  | 126.10      | 118.60   |
| 1   | AA    | 266  | G    | N1-C6-O6   | 12.50  | 127.40      | 119.90   |
| 35  | BB    | 1450 | G    | N1-C6-O6   | 12.50  | 127.40      | 119.90   |
| 1   | AA    | 1280 | A    | N1-C2-N3   | 12.49  | 135.55      | 129.30   |
| 1   | AA    | 1470 | U    | O4'-C1'-N1 | 12.49  | 118.19      | 108.20   |
| 1   | AA    | 1516 | G    | C5-C6-O6   | -12.49 | 121.11      | 128.60   |
| 1   | AA    | 1290 | G    | N1-C6-O6   | 12.49  | 127.39      | 119.90   |
| 34  | BA    | 90   | C    | O4'-C1'-N1 | 12.49  | 118.19      | 108.20   |
| 35  | BB    | 2021 | C    | N3-C4-N4   | 12.49  | 126.74      | 118.00   |
| 35  | BB    | 2575 | C    | N3-C4-N4   | 12.49  | 126.74      | 118.00   |
| 1   | AA    | 357  | G    | C6-C5-N7   | -12.48 | 122.91      | 130.40   |
| 1   | AA    | 642  | A    | C4-C5-C6   | 12.48  | 123.24      | 117.00   |
| 1   | AA    | 1022 | A    | N1-C6-N6   | 12.48  | 126.09      | 118.60   |
| 1   | AA    | 1275 | A    | N1-C6-N6   | 12.48  | 126.09      | 118.60   |
| 35  | BB    | 1165 | A    | O4'-C1'-N9 | 12.48  | 118.19      | 108.20   |
| 35  | BB    | 1724 | G    | C5-C6-O6   | -12.48 | 121.11      | 128.60   |
| 35  | BB    | 2044 | C    | N3-C4-C5   | -12.48 | 116.91      | 121.90   |
| 1   | AA    | 299  | G    | N1-C6-O6   | 12.48  | 127.39      | 119.90   |
| 1   | AA    | 985  | C    | O4'-C1'-N1 | 12.48  | 118.18      | 108.20   |
| 35  | BB    | 599  | A    | N1-C6-N6   | 12.48  | 126.09      | 118.60   |
| 35  | BB    | 1047 | G    | C5-C6-O6   | -12.48 | 121.11      | 128.60   |
| 35  | BB    | 2190 | G    | O4'-C1'-N9 | 12.48  | 118.18      | 108.20   |
| 35  | BB    | 1957 | C    | N3-C4-N4   | 12.47  | 126.73      | 118.00   |
| 35  | BB    | 2706 | A    | N1-C6-N6   | 12.47  | 126.08      | 118.60   |
| 35  | BB    | 2748 | A    | N1-C6-N6   | 12.47  | 126.08      | 118.60   |
| 35  | BB    | 1123 | C    | N3-C4-N4   | 12.47  | 126.73      | 118.00   |
| 35  | BB    | 1346 | G    | O4'-C1'-N9 | 12.47  | 118.18      | 108.20   |
| 1   | AA    | 1142 | G    | N1-C6-O6   | 12.47  | 127.38      | 119.90   |
| 35  | BB    | 412  | A    | N1-C6-N6   | 12.46  | 126.08      | 118.60   |
| 1   | AA    | 1110 | A    | C5-C6-N1   | -12.46 | 111.47      | 117.70   |
| 35  | BB    | 1039 | A    | N1-C6-N6   | 12.46  | 126.08      | 118.60   |
| 47  | BN    | 90   | ARG  | NE-CZ-NH1  | 12.46  | 126.53      | 120.30   |
| 1   | AA    | 1493 | A    | C5-C6-N6   | -12.46 | 113.74      | 123.70   |
| 35  | BB    | 1966 | A    | C4-C5-C6   | 12.46  | 123.23      | 117.00   |
| 35  | BB    | 127  | A    | C5-C6-N6   | -12.45 | 113.74      | 123.70   |
| 43  | BJ    | 44   | TYR  | CB-CG-CD2  | -12.45 | 113.53      | 121.00   |
| 35  | BB    | 1344 | U    | O4'-C1'-N1 | 12.45  | 118.16      | 108.20   |
| 35  | BB    | 2488 | G    | C5-C6-O6   | -12.45 | 121.13      | 128.60   |
| 35  | BB    | 2378 | A    | C5-C6-N1   | -12.45 | 111.48      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2758 | A    | N9-C4-C5   | -12.45 | 100.82      | 105.80   |
| 1   | AA    | 905  | U    | O4'-C1'-N1 | 12.45  | 118.16      | 108.20   |
| 1   | AA    | 967  | C    | O4'-C1'-N1 | 12.45  | 118.16      | 108.20   |
| 1   | AA    | 1177 | G    | N1-C6-O6   | 12.45  | 127.37      | 119.90   |
| 35  | BB    | 1460 | U    | O4'-C1'-N1 | 12.45  | 118.16      | 108.20   |
| 1   | AA    | 117  | G    | C5-C6-O6   | -12.44 | 121.14      | 128.60   |
| 1   | AA    | 814  | A    | N1-C6-N6   | 12.44  | 126.07      | 118.60   |
| 35  | BB    | 2791 | G    | N1-C6-O6   | 12.44  | 127.36      | 119.90   |
| 1   | AA    | 143  | A    | N1-C6-N6   | 12.43  | 126.06      | 118.60   |
| 1   | AA    | 485  | U    | C6-N1-C2   | 12.43  | 128.46      | 121.00   |
| 35  | BB    | 2658 | C    | N3-C4-N4   | 12.43  | 126.70      | 118.00   |
| 35  | BB    | 762  | U    | O4'-C1'-N1 | 12.43  | 118.14      | 108.20   |
| 35  | BB    | 1054 | A    | C5-C6-N1   | -12.42 | 111.49      | 117.70   |
| 35  | BB    | 2583 | G    | N1-C6-O6   | 12.42  | 127.35      | 119.90   |
| 1   | AA    | 382  | A    | N1-C6-N6   | 12.42  | 126.05      | 118.60   |
| 35  | BB    | 707  | G    | C5-C6-O6   | -12.42 | 121.15      | 128.60   |
| 1   | AA    | 141  | G    | N3-C4-C5   | -12.42 | 122.39      | 128.60   |
| 35  | BB    | 795  | C    | N3-C4-N4   | 12.41  | 126.69      | 118.00   |
| 35  | BB    | 1587 | G    | C8-N9-C4   | -12.41 | 101.44      | 106.40   |
| 35  | BB    | 507  | A    | N9-C4-C5   | 12.41  | 110.76      | 105.80   |
| 35  | BB    | 478  | A    | O4'-C1'-N9 | 12.41  | 118.12      | 108.20   |
| 1   | AA    | 374  | A    | C5-C6-N1   | -12.40 | 111.50      | 117.70   |
| 35  | BB    | 500  | G    | C4-C5-N7   | -12.40 | 105.84      | 110.80   |
| 35  | BB    | 676  | A    | N1-C6-N6   | 12.40  | 126.04      | 118.60   |
| 1   | AA    | 1296 | C    | C6-N1-C2   | 12.40  | 125.26      | 120.30   |
| 35  | BB    | 292  | U    | O4'-C1'-N1 | 12.40  | 118.12      | 108.20   |
| 35  | BB    | 625  | G    | O4'-C1'-N9 | 12.40  | 118.12      | 108.20   |
| 21  | AU    | 18   | PHE  | CB-CG-CD2  | 12.39  | 129.48      | 120.80   |
| 35  | BB    | 656  | G    | C4-C5-C6   | 12.39  | 126.24      | 118.80   |
| 35  | BB    | 856  | G    | C5-C6-O6   | -12.39 | 121.16      | 128.60   |
| 1   | AA    | 117  | G    | N1-C6-O6   | 12.39  | 127.33      | 119.90   |
| 22  | AV    | 21   | A    | N1-C6-N6   | 12.39  | 126.03      | 118.60   |
| 35  | BB    | 2722 | G    | N1-C6-O6   | 12.39  | 127.33      | 119.90   |
| 1   | AA    | 64   | G    | C6-C5-N7   | -12.39 | 122.97      | 130.40   |
| 35  | BB    | 450  | G    | O4'-C1'-N9 | 12.39  | 118.11      | 108.20   |
| 35  | BB    | 1920 | C    | O4'-C1'-N1 | 12.39  | 118.11      | 108.20   |
| 1   | AA    | 1206 | G    | N1-C6-O6   | 12.38  | 127.33      | 119.90   |
| 35  | BB    | 1271 | G    | C5-C6-O6   | -12.38 | 121.17      | 128.60   |
| 35  | BB    | 164  | C    | O4'-C1'-N1 | 12.38  | 118.11      | 108.20   |
| 35  | BB    | 713  | G    | C5-C6-O6   | -12.38 | 121.17      | 128.60   |
| 35  | BB    | 2709 | G    | C5-C6-O6   | -12.38 | 121.17      | 128.60   |
| 1   | AA    | 199  | A    | N1-C6-N6   | 12.37  | 126.02      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 34  | BA    | 21   | G    | N1-C6-O6   | 12.37  | 127.32      | 119.90   |
| 35  | BB    | 13   | A    | P-O3'-C3'  | 12.37  | 134.54      | 119.70   |
| 35  | BB    | 293  | U    | C5-C6-N1   | 12.37  | 128.89      | 122.70   |
| 35  | BB    | 327  | G    | C5-C6-O6   | -12.37 | 121.18      | 128.60   |
| 35  | BB    | 666  | A    | C5-C6-N1   | -12.37 | 111.51      | 117.70   |
| 35  | BB    | 1027 | A    | N1-C6-N6   | 12.37  | 126.02      | 118.60   |
| 35  | BB    | 1569 | A    | C5-C6-N1   | -12.37 | 111.52      | 117.70   |
| 35  | BB    | 1748 | C    | N3-C4-C5   | -12.37 | 116.95      | 121.90   |
| 35  | BB    | 2184 | A    | O4'-C1'-N9 | 12.37  | 118.09      | 108.20   |
| 1   | AA    | 713  | G    | C2-N3-C4   | 12.36  | 118.08      | 111.90   |
| 1   | AA    | 760  | G    | C5-N7-C8   | 12.36  | 110.48      | 104.30   |
| 35  | BB    | 317  | G    | N1-C6-O6   | 12.36  | 127.32      | 119.90   |
| 35  | BB    | 745  | G    | C5-C6-O6   | -12.36 | 121.18      | 128.60   |
| 1   | AA    | 1222 | G    | C8-N9-C4   | -12.36 | 101.46      | 106.40   |
| 35  | BB    | 5    | A    | C4-C5-C6   | 12.36  | 123.18      | 117.00   |
| 35  | BB    | 26   | G    | N1-C6-O6   | 12.36  | 127.31      | 119.90   |
| 1   | AA    | 661  | G    | N1-C6-O6   | 12.36  | 127.31      | 119.90   |
| 35  | BB    | 838  | C    | O4'-C1'-N1 | 12.36  | 118.08      | 108.20   |
| 51  | BR    | 84   | ARG  | NE-CZ-NH2  | 12.36  | 126.48      | 120.30   |
| 1   | AA    | 792  | A    | C5-C6-N1   | -12.36 | 111.52      | 117.70   |
| 35  | BB    | 2138 | G    | C5-C6-O6   | -12.35 | 121.19      | 128.60   |
| 35  | BB    | 521  | U    | O4'-C1'-N1 | 12.35  | 118.08      | 108.20   |
| 22  | AV    | 9    | A    | N1-C6-N6   | 12.35  | 126.01      | 118.60   |
| 35  | BB    | 261  | G    | C4-C5-N7   | 12.34  | 115.74      | 110.80   |
| 35  | BB    | 2070 | A    | O4'-C1'-N9 | 12.34  | 118.08      | 108.20   |
| 1   | AA    | 271  | C    | N3-C4-N4   | 12.34  | 126.64      | 118.00   |
| 35  | BB    | 2180 | U    | C2-N3-C4   | -12.34 | 119.59      | 127.00   |
| 1   | AA    | 1100 | C    | N3-C4-C5   | -12.34 | 116.96      | 121.90   |
| 35  | BB    | 978  | G    | N1-C6-O6   | 12.34  | 127.31      | 119.90   |
| 1   | AA    | 1326 | U    | O4'-C1'-N1 | 12.34  | 118.07      | 108.20   |
| 35  | BB    | 2112 | G    | C5-C6-O6   | -12.34 | 121.20      | 128.60   |
| 35  | BB    | 19   | A    | C2-N3-C4   | -12.33 | 104.43      | 110.60   |
| 35  | BB    | 773  | U    | C2-N3-C4   | -12.33 | 119.60      | 127.00   |
| 35  | BB    | 2380 | C    | O4'-C1'-N1 | 12.33  | 118.06      | 108.20   |
| 1   | AA    | 491  | G    | C2-N3-C4   | 12.33  | 118.06      | 111.90   |
| 35  | BB    | 1297 | C    | N3-C4-N4   | 12.33  | 126.63      | 118.00   |
| 35  | BB    | 1177 | G    | C5-C6-O6   | -12.32 | 121.21      | 128.60   |
| 35  | BB    | 1252 | G    | N1-C6-O6   | 12.32  | 127.29      | 119.90   |
| 1   | AA    | 671  | G    | N1-C6-O6   | 12.32  | 127.29      | 119.90   |
| 1   | AA    | 552  | U    | O4'-C1'-N1 | 12.32  | 118.06      | 108.20   |
| 35  | BB    | 2390 | U    | O4'-C1'-N1 | 12.32  | 118.06      | 108.20   |
| 35  | BB    | 2573 | C    | N3-C2-O2   | -12.32 | 113.28      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 131  | A    | C5-C6-N6   | -12.32 | 113.85      | 123.70   |
| 35  | BB    | 1674 | G    | C5-C6-O6   | -12.32 | 121.21      | 128.60   |
| 1   | AA    | 487  | A    | N1-C6-N6   | 12.31  | 125.99      | 118.60   |
| 35  | BB    | 1493 | C    | N3-C4-N4   | 12.31  | 126.62      | 118.00   |
| 1   | AA    | 1395 | C    | C6-N1-C2   | 12.31  | 125.22      | 120.30   |
| 1   | AA    | 1044 | A    | C5-C6-N6   | -12.31 | 113.85      | 123.70   |
| 35  | BB    | 2043 | C    | C6-N1-C2   | -12.31 | 115.38      | 120.30   |
| 39  | BF    | 19   | PHE  | CB-CG-CD2  | 12.31  | 129.42      | 120.80   |
| 1   | AA    | 557  | G    | O4'-C1'-N9 | 12.31  | 118.05      | 108.20   |
| 1   | AA    | 1432 | G    | C5-C6-O6   | -12.31 | 121.22      | 128.60   |
| 35  | BB    | 93   | G    | C5-C6-O6   | -12.31 | 121.21      | 128.60   |
| 35  | BB    | 701  | G    | N1-C6-O6   | 12.31  | 127.28      | 119.90   |
| 35  | BB    | 88   | G    | N1-C2-N3   | -12.30 | 116.52      | 123.90   |
| 35  | BB    | 1548 | A    | C5-C6-N6   | -12.30 | 113.86      | 123.70   |
| 35  | BB    | 2490 | G    | N1-C6-O6   | 12.31  | 127.28      | 119.90   |
| 35  | BB    | 2697 | G    | N1-C6-O6   | 12.31  | 127.28      | 119.90   |
| 35  | BB    | 1928 | A    | C4-C5-C6   | 12.30  | 123.15      | 117.00   |
| 1   | AA    | 576  | C    | N3-C4-C5   | -12.30 | 116.98      | 121.90   |
| 35  | BB    | 2874 | C    | O4'-C1'-N1 | 12.30  | 118.04      | 108.20   |
| 35  | BB    | 1920 | C    | C5-C4-N4   | -12.30 | 111.59      | 120.20   |
| 1   | AA    | 332  | G    | N1-C6-O6   | 12.30  | 127.28      | 119.90   |
| 1   | AA    | 520  | A    | N1-C6-N6   | 12.29  | 125.98      | 118.60   |
| 1   | AA    | 825  | A    | C8-N9-C4   | -12.29 | 100.88      | 105.80   |
| 1   | AA    | 1238 | A    | C4-C5-N7   | -12.29 | 104.55      | 110.70   |
| 1   | AA    | 604  | G    | C4-C5-N7   | 12.29  | 115.72      | 110.80   |
| 1   | AA    | 1196 | A    | C5-C6-N6   | -12.29 | 113.87      | 123.70   |
| 35  | BB    | 793  | A    | N1-C6-N6   | 12.29  | 125.97      | 118.60   |
| 35  | BB    | 879  | G    | N1-C6-O6   | 12.28  | 127.27      | 119.90   |
| 35  | BB    | 348  | A    | N1-C6-N6   | 12.28  | 125.97      | 118.60   |
| 35  | BB    | 695  | G    | C5-C6-O6   | -12.28 | 121.23      | 128.60   |
| 35  | BB    | 2156 | G    | O4'-C1'-N9 | 12.28  | 118.03      | 108.20   |
| 35  | BB    | 2505 | G    | N1-C6-O6   | 12.28  | 127.27      | 119.90   |
| 35  | BB    | 2618 | G    | C5-C6-O6   | -12.28 | 121.23      | 128.60   |
| 1   | AA    | 384  | G    | N1-C6-O6   | 12.28  | 127.27      | 119.90   |
| 1   | AA    | 1434 | A    | C4-C5-C6   | 12.28  | 123.14      | 117.00   |
| 35  | BB    | 887  | U    | C6-N1-C2   | -12.28 | 113.63      | 121.00   |
| 35  | BB    | 1290 | C    | N3-C4-C5   | -12.28 | 116.99      | 121.90   |
| 35  | BB    | 2224 | G    | N9-C4-C5   | 12.28  | 110.31      | 105.40   |
| 1   | AA    | 673  | A    | O4'-C1'-N9 | 12.28  | 118.02      | 108.20   |
| 1   | AA    | 1513 | A    | C5-C6-N6   | -12.28 | 113.88      | 123.70   |
| 35  | BB    | 2101 | A    | C5-C6-N1   | -12.27 | 111.56      | 117.70   |
| 1   | AA    | 487  | A    | C4-C5-N7   | -12.27 | 104.57      | 110.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 688  | G    | N9-C4-C5   | 12.27  | 110.31      | 105.40   |
| 1   | AA    | 1022 | A    | N9-C4-C5   | 12.27  | 110.71      | 105.80   |
| 35  | BB    | 1819 | A    | C5-C6-N6   | -12.27 | 113.88      | 123.70   |
| 35  | BB    | 2665 | A    | C4-C5-C6   | 12.27  | 123.14      | 117.00   |
| 35  | BB    | 93   | G    | N1-C6-O6   | 12.27  | 127.26      | 119.90   |
| 35  | BB    | 143  | C    | O4'-C1'-N1 | 12.27  | 118.01      | 108.20   |
| 1   | AA    | 1268 | G    | C5-C6-O6   | -12.26 | 121.24      | 128.60   |
| 16  | AP    | 35   | ARG  | NE-CZ-NH1  | 12.26  | 126.43      | 120.30   |
| 22  | AV    | 51   | A    | N1-C6-N6   | 12.26  | 125.96      | 118.60   |
| 35  | BB    | 2224 | G    | C8-N9-C4   | -12.26 | 101.50      | 106.40   |
| 35  | BB    | 2515 | C    | N3-C4-C5   | -12.26 | 117.00      | 121.90   |
| 1   | AA    | 1051 | C    | C5-C4-N4   | -12.26 | 111.62      | 120.20   |
| 35  | BB    | 2467 | C    | C2-N3-C4   | 12.25  | 126.03      | 119.90   |
| 1   | AA    | 572  | A    | N1-C6-N6   | 12.25  | 125.95      | 118.60   |
| 35  | BB    | 1935 | G    | O4'-C1'-N9 | 12.25  | 118.00      | 108.20   |
| 35  | BB    | 2553 | G    | C5-C6-O6   | -12.25 | 121.25      | 128.60   |
| 35  | BB    | 247  | G    | N1-C6-O6   | 12.24  | 127.25      | 119.90   |
| 35  | BB    | 314  | C    | N3-C4-C5   | -12.24 | 117.00      | 121.90   |
| 35  | BB    | 2012 | G    | N1-C6-O6   | 12.24  | 127.24      | 119.90   |
| 35  | BB    | 2407 | A    | N1-C6-N6   | 12.24  | 125.94      | 118.60   |
| 9   | AI    | 98   | ARG  | NE-CZ-NH2  | -12.24 | 114.18      | 120.30   |
| 34  | BA    | 36   | C    | O4'-C1'-N1 | 12.23  | 117.99      | 108.20   |
| 35  | BB    | 911  | A    | O4'-C1'-N9 | 12.23  | 117.99      | 108.20   |
| 35  | BB    | 1637 | A    | N1-C6-N6   | 12.23  | 125.94      | 118.60   |
| 35  | BB    | 2676 | C    | C2-N3-C4   | 12.23  | 126.02      | 119.90   |
| 35  | BB    | 1857 | G    | N1-C6-O6   | 12.23  | 127.24      | 119.90   |
| 35  | BB    | 2018 | G    | N1-C6-O6   | 12.23  | 127.24      | 119.90   |
| 1   | AA    | 815  | A    | N1-C6-N6   | 12.23  | 125.94      | 118.60   |
| 1   | AA    | 384  | G    | N7-C8-N9   | 12.23  | 119.21      | 113.10   |
| 1   | AA    | 499  | A    | C5-C6-N6   | -12.23 | 113.92      | 123.70   |
| 22  | AV    | 5    | A    | O4'-C1'-N9 | 12.23  | 117.98      | 108.20   |
| 1   | AA    | 1284 | C    | O4'-C1'-N1 | 12.22  | 117.98      | 108.20   |
| 35  | BB    | 214  | G    | C5-C6-O6   | -12.22 | 121.27      | 128.60   |
| 35  | BB    | 2227 | A    | C4-C5-N7   | -12.22 | 104.59      | 110.70   |
| 1   | AA    | 1002 | G    | N1-C6-O6   | 12.22  | 127.23      | 119.90   |
| 35  | BB    | 2406 | A    | C8-N9-C4   | -12.22 | 100.91      | 105.80   |
| 1   | AA    | 1164 | G    | N1-C6-O6   | 12.22  | 127.23      | 119.90   |
| 35  | BB    | 1106 | G    | C5-C6-O6   | -12.22 | 121.27      | 128.60   |
| 1   | AA    | 321  | A    | C4-C5-C6   | 12.22  | 123.11      | 117.00   |
| 35  | BB    | 507  | A    | C5-C6-N6   | -12.22 | 113.92      | 123.70   |
| 35  | BB    | 2415 | G    | C5-C6-O6   | -12.21 | 121.27      | 128.60   |
| 1   | AA    | 1230 | C    | N3-C4-N4   | 12.21  | 126.55      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2065 | C    | N3-C4-C5   | -12.21 | 117.02      | 121.90   |
| 1   | AA    | 767  | A    | N1-C6-N6   | 12.21  | 125.93      | 118.60   |
| 1   | AA    | 935  | A    | N1-C6-N6   | 12.21  | 125.93      | 118.60   |
| 35  | BB    | 951  | C    | N3-C4-N4   | 12.21  | 126.55      | 118.00   |
| 35  | BB    | 2478 | A    | C5-C6-N1   | -12.21 | 111.59      | 117.70   |
| 1   | AA    | 820  | U    | N3-C4-O4   | 12.21  | 127.94      | 119.40   |
| 35  | BB    | 2835 | A    | C5-C6-N6   | -12.21 | 113.94      | 123.70   |
| 35  | BB    | 803  | U    | O4'-C1'-N1 | 12.20  | 117.96      | 108.20   |
| 1   | AA    | 925  | G    | N9-C4-C5   | -12.20 | 100.52      | 105.40   |
| 35  | BB    | 1384 | A    | N1-C6-N6   | 12.20  | 125.92      | 118.60   |
| 35  | BB    | 341  | C    | C5-C4-N4   | -12.19 | 111.66      | 120.20   |
| 1   | AA    | 1101 | A    | C5-C6-N1   | -12.19 | 111.61      | 117.70   |
| 1   | AA    | 1164 | G    | N1-C2-N3   | -12.19 | 116.58      | 123.90   |
| 35  | BB    | 146  | A    | N1-C6-N6   | 12.19  | 125.91      | 118.60   |
| 35  | BB    | 363  | G    | N1-C6-O6   | 12.19  | 127.21      | 119.90   |
| 35  | BB    | 1034 | G    | O4'-C1'-N9 | 12.19  | 117.95      | 108.20   |
| 35  | BB    | 2434 | A    | C4-C5-C6   | 12.19  | 123.09      | 117.00   |
| 35  | BB    | 1936 | A    | C4-C5-C6   | 12.18  | 123.09      | 117.00   |
| 1   | AA    | 1462 | C    | C5-C4-N4   | -12.18 | 111.68      | 120.20   |
| 35  | BB    | 2145 | C    | C2-N1-C1'  | 12.17  | 132.19      | 118.80   |
| 1   | AA    | 1439 | G    | C5-C6-O6   | -12.17 | 121.30      | 128.60   |
| 1   | AA    | 758  | C    | N3-C4-N4   | 12.17  | 126.52      | 118.00   |
| 1   | AA    | 1116 | U    | O4'-C1'-N1 | 12.17  | 117.93      | 108.20   |
| 1   | AA    | 1094 | G    | N1-C6-O6   | 12.16  | 127.20      | 119.90   |
| 35  | BB    | 1183 | U    | O4'-C1'-N1 | 12.16  | 117.93      | 108.20   |
| 35  | BB    | 2294 | G    | C4-C5-N7   | -12.16 | 105.94      | 110.80   |
| 35  | BB    | 2726 | A    | C5-C6-N1   | -12.16 | 111.62      | 117.70   |
| 18  | AR    | 47   | ARG  | NE-CZ-NH1  | 12.16  | 126.38      | 120.30   |
| 21  | AU    | 17   | ARG  | NE-CZ-NH2  | -12.16 | 114.22      | 120.30   |
| 35  | BB    | 2234 | G    | C6-N1-C2   | 12.16  | 132.39      | 125.10   |
| 22  | AV    | 14   | A    | N1-C6-N6   | 12.15  | 125.89      | 118.60   |
| 35  | BB    | 497  | A    | O4'-C1'-N9 | 12.15  | 117.92      | 108.20   |
| 35  | BB    | 2004 | G    | C5-C6-O6   | -12.15 | 121.31      | 128.60   |
| 1   | AA    | 205  | A    | C5-C6-N1   | -12.14 | 111.63      | 117.70   |
| 35  | BB    | 1153 | C    | C6-N1-C2   | -12.14 | 115.44      | 120.30   |
| 35  | BB    | 2512 | C    | N3-C4-N4   | 12.14  | 126.50      | 118.00   |
| 1   | AA    | 295  | C    | C6-N1-C2   | -12.13 | 115.45      | 120.30   |
| 1   | AA    | 693  | G    | N1-C6-O6   | 12.13  | 127.18      | 119.90   |
| 34  | BA    | 75   | G    | N1-C2-N3   | -12.13 | 116.62      | 123.90   |
| 35  | BB    | 1555 | G    | N1-C6-O6   | 12.13  | 127.18      | 119.90   |
| 35  | BB    | 1668 | A    | N1-C6-N6   | 12.13  | 125.88      | 118.60   |
| 35  | BB    | 950  | G    | O4'-C1'-N9 | 12.13  | 117.90      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1383 | A    | N1-C6-N6   | 12.13  | 125.88      | 118.60   |
| 35  | BB    | 281  | C    | N3-C4-C5   | -12.12 | 117.05      | 121.90   |
| 35  | BB    | 1653 | G    | N1-C6-O6   | 12.12  | 127.17      | 119.90   |
| 35  | BB    | 1276 | A    | N1-C6-N6   | 12.12  | 125.87      | 118.60   |
| 1   | AA    | 765  | G    | O4'-C1'-N9 | 12.12  | 117.90      | 108.20   |
| 21  | AU    | 34   | ARG  | NE-CZ-NH2  | -12.12 | 114.24      | 120.30   |
| 35  | BB    | 2485 | G    | N1-C6-O6   | 12.12  | 127.17      | 119.90   |
| 35  | BB    | 2256 | G    | N1-C6-O6   | 12.11  | 127.17      | 119.90   |
| 1   | AA    | 15   | G    | C5-C6-O6   | -12.11 | 121.33      | 128.60   |
| 1   | AA    | 968  | A    | C2-N3-C4   | -12.11 | 104.55      | 110.60   |
| 1   | AA    | 1028 | C    | C2-N3-C4   | 12.11  | 125.95      | 119.90   |
| 35  | BB    | 1756 | G    | N1-C6-O6   | 12.11  | 127.17      | 119.90   |
| 35  | BB    | 2050 | C    | N3-C4-N4   | 12.11  | 126.48      | 118.00   |
| 35  | BB    | 2721 | A    | N1-C6-N6   | 12.11  | 125.86      | 118.60   |
| 35  | BB    | 2260 | C    | N3-C4-C5   | -12.11 | 117.06      | 121.90   |
| 35  | BB    | 2666 | C    | N3-C4-C5   | -12.11 | 117.06      | 121.90   |
| 1   | AA    | 537  | G    | C5-C6-O6   | -12.10 | 121.34      | 128.60   |
| 35  | BB    | 1571 | A    | N1-C2-N3   | 12.10  | 135.35      | 129.30   |
| 35  | BB    | 2842 | G    | C5-C6-O6   | -12.10 | 121.34      | 128.60   |
| 1   | AA    | 880  | C    | N3-C4-C5   | -12.10 | 117.06      | 121.90   |
| 35  | BB    | 2228 | G    | N1-C6-O6   | 12.10  | 127.16      | 119.90   |
| 1   | AA    | 896  | C    | O4'-C1'-N1 | 12.10  | 117.88      | 108.20   |
| 13  | AM    | 89   | ARG  | NE-CZ-NH2  | -12.10 | 114.25      | 120.30   |
| 1   | AA    | 1302 | C    | N3-C2-O2   | -12.09 | 113.44      | 121.90   |
| 35  | BB    | 1531 | C    | C6-N1-C2   | -12.09 | 115.47      | 120.30   |
| 35  | BB    | 2648 | G    | C6-C5-N7   | -12.09 | 123.15      | 130.40   |
| 1   | AA    | 1048 | G    | N1-C6-O6   | 12.09  | 127.15      | 119.90   |
| 35  | BB    | 1912 | A    | N1-C6-N6   | 12.08  | 125.85      | 118.60   |
| 35  | BB    | 772  | C    | N3-C4-C5   | -12.08 | 117.07      | 121.90   |
| 35  | BB    | 795  | C    | C5-C6-N1   | 12.07  | 127.04      | 121.00   |
| 35  | BB    | 2572 | A    | C5-C6-N1   | -12.07 | 111.66      | 117.70   |
| 1   | AA    | 113  | G    | N3-C4-C5   | 12.07  | 134.64      | 128.60   |
| 35  | BB    | 2875 | C    | O4'-C1'-N1 | 12.07  | 117.86      | 108.20   |
| 35  | BB    | 2268 | A    | N9-C4-C5   | 12.07  | 110.63      | 105.80   |
| 1   | AA    | 200  | G    | C5-C6-O6   | -12.07 | 121.36      | 128.60   |
| 35  | BB    | 453  | A    | C2-N3-C4   | -12.06 | 104.57      | 110.60   |
| 35  | BB    | 1705 | A    | N1-C6-N6   | 12.06  | 125.84      | 118.60   |
| 35  | BB    | 1018 | U    | O4'-C1'-N1 | 12.06  | 117.85      | 108.20   |
| 35  | BB    | 1572 | A    | C5-C6-N6   | -12.06 | 114.05      | 123.70   |
| 35  | BB    | 1845 | G    | C5-C6-O6   | -12.06 | 121.36      | 128.60   |
| 35  | BB    | 1197 | G    | N1-C6-O6   | 12.05  | 127.13      | 119.90   |
| 1   | AA    | 299  | G    | N3-C2-N2   | 12.05  | 128.34      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 174  | U    | O4'-C1'-N1 | 12.05  | 117.84      | 108.20   |
| 35  | BB    | 2412 | A    | O4'-C1'-N9 | 12.05  | 117.84      | 108.20   |
| 35  | BB    | 493  | G    | C8-N9-C4   | -12.05 | 101.58      | 106.40   |
| 1   | AA    | 308  | C    | O4'-C1'-N1 | 12.05  | 117.84      | 108.20   |
| 1   | AA    | 1334 | G    | N1-C6-O6   | 12.05  | 127.13      | 119.90   |
| 1   | AA    | 1352 | C    | O4'-C1'-N1 | 12.04  | 117.83      | 108.20   |
| 2   | AB    | 29   | PHE  | CB-CG-CD1  | -12.04 | 112.37      | 120.80   |
| 35  | BB    | 23   | G    | N1-C6-O6   | 12.04  | 127.13      | 119.90   |
| 35  | BB    | 1515 | A    | C5-C6-N1   | -12.04 | 111.68      | 117.70   |
| 35  | BB    | 2079 | U    | O4'-C1'-N1 | 12.04  | 117.83      | 108.20   |
| 35  | BB    | 2483 | C    | O4'-C1'-N1 | 12.04  | 117.83      | 108.20   |
| 1   | AA    | 282  | A    | N1-C2-N3   | 12.04  | 135.32      | 129.30   |
| 1   | AA    | 495  | A    | C5-C6-N1   | -12.04 | 111.68      | 117.70   |
| 35  | BB    | 178  | G    | C4-C5-N7   | 12.04  | 115.61      | 110.80   |
| 35  | BB    | 267  | C    | O4'-C1'-N1 | 12.04  | 117.83      | 108.20   |
| 35  | BB    | 424  | G    | N1-C6-O6   | 12.03  | 127.12      | 119.90   |
| 1   | AA    | 796  | C    | N3-C4-C5   | -12.03 | 117.09      | 121.90   |
| 35  | BB    | 2227 | A    | C4-C5-C6   | 12.03  | 123.02      | 117.00   |
| 35  | BB    | 148  | U    | C4-C5-C6   | 12.03  | 126.92      | 119.70   |
| 35  | BB    | 1007 | C    | C5-C4-N4   | -12.03 | 111.78      | 120.20   |
| 35  | BB    | 1404 | C    | O4'-C1'-N1 | 12.03  | 117.82      | 108.20   |
| 35  | BB    | 1976 | U    | O4'-C1'-N1 | 12.03  | 117.82      | 108.20   |
| 35  | BB    | 2848 | G    | C5-C6-O6   | -12.03 | 121.38      | 128.60   |
| 13  | AM    | 22   | TYR  | CB-CG-CD1  | -12.03 | 113.78      | 121.00   |
| 35  | BB    | 2712 | C    | C6-N1-C2   | 12.03  | 125.11      | 120.30   |
| 4   | AD    | 25   | ARG  | NE-CZ-NH2  | -12.02 | 114.29      | 120.30   |
| 35  | BB    | 724  | U    | O4'-C1'-N1 | 12.02  | 117.82      | 108.20   |
| 35  | BB    | 1459 | G    | C5-C6-O6   | -12.02 | 121.39      | 128.60   |
| 35  | BB    | 1660 | G    | N1-C6-O6   | 12.02  | 127.11      | 119.90   |
| 35  | BB    | 757  | G    | C5-C6-O6   | -12.02 | 121.39      | 128.60   |
| 35  | BB    | 1381 | G    | N1-C6-O6   | 12.02  | 127.11      | 119.90   |
| 22  | AV    | 57   | A    | N1-C6-N6   | 12.01  | 125.81      | 118.60   |
| 35  | BB    | 1114 | C    | O4'-C1'-N1 | 12.01  | 117.81      | 108.20   |
| 35  | BB    | 886  | A    | N1-C6-N6   | 12.01  | 125.81      | 118.60   |
| 35  | BB    | 1804 | C    | O4'-C1'-N1 | 12.01  | 117.81      | 108.20   |
| 35  | BB    | 2015 | A    | C5-C6-N1   | -12.01 | 111.69      | 117.70   |
| 35  | BB    | 2247 | A    | N1-C6-N6   | 12.01  | 125.81      | 118.60   |
| 35  | BB    | 2706 | A    | C2-N3-C4   | -12.01 | 104.60      | 110.60   |
| 1   | AA    | 1338 | G    | O4'-C1'-N9 | 12.00  | 117.80      | 108.20   |
| 1   | AA    | 539  | A    | O4'-C1'-N9 | 12.00  | 117.80      | 108.20   |
| 35  | BB    | 2239 | G    | N3-C2-N2   | 12.00  | 128.30      | 119.90   |
| 46  | BM    | 44   | ARG  | NE-CZ-NH1  | -12.00 | 114.30      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1676 | A    | C4-C5-C6   | 12.00  | 123.00      | 117.00   |
| 35  | BB    | 1746 | A    | C4-C5-C6   | 12.00  | 123.00      | 117.00   |
| 1   | AA    | 908  | A    | N1-C6-N6   | 12.00  | 125.80      | 118.60   |
| 35  | BB    | 1873 | G    | C8-N9-C4   | -12.00 | 101.60      | 106.40   |
| 39  | BF    | 29   | ARG  | NE-CZ-NH1  | -12.00 | 114.30      | 120.30   |
| 1   | AA    | 665  | A    | N1-C6-N6   | 12.00  | 125.80      | 118.60   |
| 1   | AA    | 1362 | A    | O4'-C1'-N9 | 12.00  | 117.80      | 108.20   |
| 35  | BB    | 711  | G    | N1-C2-N3   | -12.00 | 116.70      | 123.90   |
| 35  | BB    | 2689 | U    | O4'-C1'-N1 | 12.00  | 117.80      | 108.20   |
| 38  | BE    | 40   | ARG  | NE-CZ-NH1  | 12.00  | 126.30      | 120.30   |
| 1   | AA    | 907  | A    | C5-C6-N6   | -11.99 | 114.10      | 123.70   |
| 1   | AA    | 578  | C    | C5-C6-N1   | 11.99  | 127.00      | 121.00   |
| 1   | AA    | 1499 | A    | C4-C5-C6   | 11.99  | 123.00      | 117.00   |
| 1   | AA    | 1521 | C    | N3-C4-C5   | -11.99 | 117.10      | 121.90   |
| 35  | BB    | 648  | G    | C8-N9-C4   | -11.99 | 101.60      | 106.40   |
| 35  | BB    | 1241 | A    | C5-C6-N6   | -11.99 | 114.11      | 123.70   |
| 35  | BB    | 2335 | A    | C5-C6-N1   | -11.99 | 111.71      | 117.70   |
| 34  | BA    | 59   | A    | C8-N9-C4   | -11.98 | 101.01      | 105.80   |
| 1   | AA    | 153  | C    | O4'-C1'-N1 | 11.98  | 117.78      | 108.20   |
| 1   | AA    | 262  | A    | C5-C6-N6   | -11.98 | 114.11      | 123.70   |
| 1   | AA    | 532  | A    | C5-C6-N1   | -11.98 | 111.71      | 117.70   |
| 22  | AV    | 7    | G    | N3-C2-N2   | 11.98  | 128.29      | 119.90   |
| 1   | AA    | 250  | A    | N1-C2-N3   | -11.98 | 123.31      | 129.30   |
| 1   | AA    | 1483 | A    | N1-C6-N6   | 11.98  | 125.78      | 118.60   |
| 34  | BA    | 104  | A    | C4-C5-C6   | 11.98  | 122.99      | 117.00   |
| 35  | BB    | 2402 | U    | C5-C4-O4   | -11.98 | 118.71      | 125.90   |
| 35  | BB    | 2762 | C    | N3-C4-C5   | -11.98 | 117.11      | 121.90   |
| 1   | AA    | 718  | A    | C5-C6-N1   | -11.97 | 111.71      | 117.70   |
| 35  | BB    | 514  | A    | O4'-C1'-N9 | 11.97  | 117.78      | 108.20   |
| 35  | BB    | 1353 | A    | N1-C6-N6   | 11.97  | 125.78      | 118.60   |
| 35  | BB    | 2826 | A    | N1-C2-N3   | 11.97  | 135.29      | 129.30   |
| 35  | BB    | 1857 | G    | C5-C6-O6   | -11.97 | 121.42      | 128.60   |
| 35  | BB    | 2823 | A    | N1-C2-N3   | -11.97 | 123.31      | 129.30   |
| 1   | AA    | 38   | G    | O4'-C1'-N9 | 11.97  | 117.77      | 108.20   |
| 35  | BB    | 122  | G    | C5-C6-O6   | -11.97 | 121.42      | 128.60   |
| 35  | BB    | 1136 | G    | N3-C4-C5   | -11.97 | 122.62      | 128.60   |
| 35  | BB    | 1632 | A    | C8-N9-C4   | -11.97 | 101.01      | 105.80   |
| 35  | BB    | 2228 | G    | C5-C6-O6   | -11.96 | 121.42      | 128.60   |
| 1   | AA    | 521  | G    | N7-C8-N9   | 11.96  | 119.08      | 113.10   |
| 35  | BB    | 1399 | C    | N3-C4-C5   | -11.96 | 117.12      | 121.90   |
| 35  | BB    | 2509 | G    | N7-C8-N9   | 11.96  | 119.08      | 113.10   |
| 1   | AA    | 670  | G    | N1-C6-O6   | 11.96  | 127.08      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 684  | U    | O4'-C1'-N1 | 11.96  | 117.77      | 108.20   |
| 35  | BB    | 185  | G    | N1-C6-O6   | 11.96  | 127.08      | 119.90   |
| 35  | BB    | 2150 | C    | N3-C4-C5   | -11.96 | 117.12      | 121.90   |
| 34  | BA    | 59   | A    | N1-C6-N6   | 11.95  | 125.77      | 118.60   |
| 35  | BB    | 603  | A    | N1-C6-N6   | 11.96  | 125.77      | 118.60   |
| 35  | BB    | 927  | A    | C5-C6-N1   | -11.96 | 111.72      | 117.70   |
| 35  | BB    | 1469 | A    | C4-C5-C6   | 11.96  | 122.98      | 117.00   |
| 1   | AA    | 926  | G    | N3-C4-C5   | 11.95  | 134.58      | 128.60   |
| 1   | AA    | 1190 | G    | N1-C6-O6   | 11.95  | 127.07      | 119.90   |
| 35  | BB    | 922  | C    | O4'-C1'-N1 | 11.95  | 117.76      | 108.20   |
| 35  | BB    | 637  | A    | C5-C6-N6   | -11.95 | 114.14      | 123.70   |
| 35  | BB    | 936  | A    | N1-C6-N6   | 11.95  | 125.77      | 118.60   |
| 1   | AA    | 1408 | A    | C5-C6-N6   | -11.95 | 114.14      | 123.70   |
| 35  | BB    | 2123 | G    | C6-N1-C2   | -11.95 | 117.93      | 125.10   |
| 35  | BB    | 1378 | A    | C4-C5-N7   | -11.95 | 104.73      | 110.70   |
| 35  | BB    | 2770 | G    | O4'-C1'-N9 | 11.95  | 117.76      | 108.20   |
| 35  | BB    | 727  | A    | C2-N3-C4   | -11.94 | 104.63      | 110.60   |
| 1   | AA    | 145  | G    | C5-C6-O6   | -11.94 | 121.44      | 128.60   |
| 52  | BS    | 68   | ASP  | CB-CG-OD2  | -11.94 | 107.55      | 118.30   |
| 1   | AA    | 246  | A    | N1-C6-N6   | 11.94  | 125.76      | 118.60   |
| 35  | BB    | 1891 | G    | N3-C2-N2   | 11.94  | 128.25      | 119.90   |
| 1   | AA    | 691  | G    | N1-C6-O6   | 11.93  | 127.06      | 119.90   |
| 1   | AA    | 950  | U    | O4'-C1'-N1 | 11.93  | 117.74      | 108.20   |
| 35  | BB    | 1158 | C    | O4'-C1'-N1 | 11.93  | 117.74      | 108.20   |
| 35  | BB    | 1816 | C    | N3-C4-C5   | -11.93 | 117.13      | 121.90   |
| 35  | BB    | 2274 | A    | N1-C6-N6   | 11.93  | 125.76      | 118.60   |
| 35  | BB    | 2317 | A    | C4-C5-C6   | 11.93  | 122.96      | 117.00   |
| 43  | BJ    | 44   | TYR  | CB-CG-CD1  | 11.93  | 128.16      | 121.00   |
| 1   | AA    | 1041 | G    | N1-C6-O6   | 11.93  | 127.06      | 119.90   |
| 35  | BB    | 2294 | G    | N3-C2-N2   | 11.93  | 128.25      | 119.90   |
| 35  | BB    | 2386 | A    | O4'-C1'-N9 | 11.93  | 117.74      | 108.20   |
| 1   | AA    | 799  | G    | N1-C6-O6   | 11.92  | 127.05      | 119.90   |
| 35  | BB    | 1024 | G    | C8-N9-C4   | -11.92 | 101.63      | 106.40   |
| 35  | BB    | 612  | G    | N1-C6-O6   | 11.92  | 127.05      | 119.90   |
| 1   | AA    | 1094 | G    | N1-C2-N3   | -11.92 | 116.75      | 123.90   |
| 35  | BB    | 2331 | G    | C5-C6-N1   | -11.92 | 105.54      | 111.50   |
| 1   | AA    | 98   | A    | C5-C6-N1   | -11.91 | 111.74      | 117.70   |
| 1   | AA    | 592  | G    | N1-C2-N3   | -11.91 | 116.75      | 123.90   |
| 1   | AA    | 816  | A    | C8-N9-C4   | -11.91 | 101.03      | 105.80   |
| 1   | AA    | 1332 | A    | C8-N9-C4   | -11.91 | 101.03      | 105.80   |
| 4   | AD    | 2    | ARG  | NE-CZ-NH2  | -11.91 | 114.34      | 120.30   |
| 35  | BB    | 2399 | G    | C5-C6-N1   | -11.91 | 105.55      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2412 | A    | N1-C6-N6   | 11.91  | 125.75      | 118.60   |
| 35  | BB    | 2821 | A    | C5-C6-N6   | -11.91 | 114.17      | 123.70   |
| 1   | AA    | 225  | C    | N1-C2-O2   | 11.91  | 126.04      | 118.90   |
| 35  | BB    | 2310 | C    | O4'-C1'-N1 | 11.91  | 117.73      | 108.20   |
| 3   | AC    | 163  | ARG  | NE-CZ-NH2  | -11.91 | 114.35      | 120.30   |
| 35  | BB    | 9    | G    | C5-C6-O6   | -11.91 | 121.46      | 128.60   |
| 35  | BB    | 743  | A    | N1-C6-N6   | 11.91  | 125.74      | 118.60   |
| 35  | BB    | 2452 | C    | O4'-C1'-N1 | 11.91  | 117.73      | 108.20   |
| 35  | BB    | 2529 | G    | C2-N3-C4   | 11.91  | 117.85      | 111.90   |
| 35  | BB    | 2360 | G    | N1-C6-O6   | 11.90  | 127.04      | 119.90   |
| 35  | BB    | 763  | G    | N1-C6-O6   | 11.90  | 127.04      | 119.90   |
| 1   | AA    | 487  | A    | C5-C6-N1   | -11.90 | 111.75      | 117.70   |
| 1   | AA    | 1206 | G    | C5-C6-O6   | -11.90 | 121.46      | 128.60   |
| 1   | AA    | 1239 | A    | N1-C6-N6   | 11.90  | 125.74      | 118.60   |
| 22  | AV    | 58   | A    | N1-C6-N6   | 11.90  | 125.74      | 118.60   |
| 35  | BB    | 454  | A    | C5-C6-N6   | -11.89 | 114.18      | 123.70   |
| 1   | AA    | 1071 | C    | O4'-C1'-N1 | 11.89  | 117.71      | 108.20   |
| 35  | BB    | 1797 | G    | N1-C6-O6   | 11.89  | 127.03      | 119.90   |
| 35  | BB    | 2616 | C    | N3-C4-C5   | -11.89 | 117.14      | 121.90   |
| 1   | AA    | 29   | U    | O4'-C1'-N1 | 11.89  | 117.71      | 108.20   |
| 1   | AA    | 253  | A    | N1-C6-N6   | 11.89  | 125.73      | 118.60   |
| 35  | BB    | 264  | C    | C5-C6-N1   | 11.89  | 126.94      | 121.00   |
| 35  | BB    | 1115 | G    | C6-C5-N7   | -11.89 | 123.27      | 130.40   |
| 35  | BB    | 1359 | A    | O4'-C1'-N9 | 11.89  | 117.71      | 108.20   |
| 1   | AA    | 794  | A    | C2-N3-C4   | -11.89 | 104.66      | 110.60   |
| 34  | BA    | 21   | G    | C5-C6-O6   | -11.88 | 121.47      | 128.60   |
| 35  | BB    | 165  | A    | C5-C6-N6   | -11.88 | 114.19      | 123.70   |
| 35  | BB    | 1093 | G    | N7-C8-N9   | 11.88  | 119.04      | 113.10   |
| 1   | AA    | 992  | U    | O4'-C1'-N1 | 11.88  | 117.70      | 108.20   |
| 35  | BB    | 188  | G    | N1-C6-O6   | 11.88  | 127.03      | 119.90   |
| 35  | BB    | 457  | A    | N1-C6-N6   | 11.88  | 125.73      | 118.60   |
| 35  | BB    | 1745 | A    | C8-N9-C4   | -11.88 | 101.05      | 105.80   |
| 35  | BB    | 548  | G    | N1-C6-O6   | 11.88  | 127.03      | 119.90   |
| 35  | BB    | 1334 | G    | N3-C2-N2   | 11.88  | 128.22      | 119.90   |
| 1   | AA    | 933  | G    | C5-C6-O6   | -11.88 | 121.47      | 128.60   |
| 35  | BB    | 947  | A    | C4-C5-C6   | 11.88  | 122.94      | 117.00   |
| 35  | BB    | 2426 | A    | C5-C6-N6   | -11.88 | 114.20      | 123.70   |
| 35  | BB    | 904  | G    | N1-C6-O6   | 11.88  | 127.03      | 119.90   |
| 1   | AA    | 821  | G    | C5-C6-O6   | -11.87 | 121.48      | 128.60   |
| 1   | AA    | 929  | G    | N1-C6-O6   | 11.87  | 127.02      | 119.90   |
| 35  | BB    | 1650 | A    | N7-C8-N9   | -11.87 | 107.86      | 113.80   |
| 1   | AA    | 502  | A    | N1-C6-N6   | 11.87  | 125.72      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 204  | G    | C5-C6-O6   | -11.86 | 121.48      | 128.60   |
| 1   | AA    | 913  | A    | C4-C5-N7   | -11.86 | 104.77      | 110.70   |
| 35  | BB    | 2378 | A    | N1-C6-N6   | 11.87  | 125.72      | 118.60   |
| 34  | BA    | 59   | A    | C4-C5-C6   | 11.86  | 122.93      | 117.00   |
| 35  | BB    | 77   | G    | N3-C4-N9   | 11.86  | 133.12      | 126.00   |
| 1   | AA    | 1444 | U    | N3-C4-O4   | 11.86  | 127.70      | 119.40   |
| 35  | BB    | 121  | G    | N1-C6-O6   | 11.86  | 127.02      | 119.90   |
| 1   | AA    | 15   | G    | N1-C6-O6   | 11.86  | 127.02      | 119.90   |
| 1   | AA    | 1117 | A    | N1-C6-N6   | 11.86  | 125.72      | 118.60   |
| 35  | BB    | 312  | G    | C5-C6-O6   | -11.86 | 121.48      | 128.60   |
| 1   | AA    | 288  | A    | N1-C6-N6   | 11.86  | 125.71      | 118.60   |
| 1   | AA    | 484  | G    | P-O3'-C3'  | 11.86  | 133.93      | 119.70   |
| 35  | BB    | 197  | A    | N1-C6-N6   | 11.86  | 125.71      | 118.60   |
| 35  | BB    | 861  | A    | N7-C8-N9   | -11.86 | 107.87      | 113.80   |
| 35  | BB    | 2310 | C    | N3-C4-C5   | -11.86 | 117.16      | 121.90   |
| 35  | BB    | 2470 | G    | C5-N7-C8   | 11.86  | 110.23      | 104.30   |
| 35  | BB    | 408  | G    | O4'-C1'-N9 | 11.85  | 117.68      | 108.20   |
| 1   | AA    | 545  | C    | O4'-C1'-N1 | 11.85  | 117.68      | 108.20   |
| 1   | AA    | 1070 | U    | O4'-C1'-N1 | 11.85  | 117.68      | 108.20   |
| 1   | AA    | 1520 | C    | N3-C4-C5   | -11.85 | 117.16      | 121.90   |
| 35  | BB    | 759  | G    | N1-C6-O6   | 11.85  | 127.01      | 119.90   |
| 35  | BB    | 1360 | G    | C5-C6-O6   | -11.85 | 121.49      | 128.60   |
| 35  | BB    | 1565 | C    | C6-N1-C2   | -11.85 | 115.56      | 120.30   |
| 1   | AA    | 1027 | C    | N3-C4-N4   | 11.84  | 126.29      | 118.00   |
| 1   | AA    | 996  | A    | N1-C6-N6   | 11.84  | 125.70      | 118.60   |
| 35  | BB    | 628  | G    | O4'-C1'-N9 | 11.84  | 117.67      | 108.20   |
| 35  | BB    | 2761 | A    | N1-C6-N6   | 11.84  | 125.70      | 118.60   |
| 35  | BB    | 2869 | G    | C5-C6-N1   | 11.84  | 117.42      | 111.50   |
| 35  | BB    | 1071 | G    | N1-C6-O6   | 11.83  | 127.00      | 119.90   |
| 35  | BB    | 678  | C    | N3-C4-C5   | -11.83 | 117.17      | 121.90   |
| 35  | BB    | 797  | G    | N1-C6-O6   | 11.83  | 127.00      | 119.90   |
| 34  | BA    | 45   | A    | C5-N7-C8   | 11.83  | 109.81      | 103.90   |
| 1   | AA    | 266  | G    | C5-C6-O6   | -11.83 | 121.50      | 128.60   |
| 1   | AA    | 949  | A    | N1-C6-N6   | 11.83  | 125.70      | 118.60   |
| 35  | BB    | 735  | A    | N1-C6-N6   | 11.83  | 125.70      | 118.60   |
| 35  | BB    | 2001 | C    | N3-C4-N4   | 11.83  | 126.28      | 118.00   |
| 35  | BB    | 2505 | G    | C5-C6-O6   | -11.83 | 121.50      | 128.60   |
| 35  | BB    | 57   | C    | N3-C4-N4   | 11.83  | 126.28      | 118.00   |
| 35  | BB    | 109  | C    | O4'-C1'-N1 | 11.83  | 117.66      | 108.20   |
| 35  | BB    | 2268 | A    | C4-C5-C6   | 11.83  | 122.91      | 117.00   |
| 35  | BB    | 1626 | A    | C5-C6-N1   | -11.82 | 111.79      | 117.70   |
| 35  | BB    | 2234 | G    | N1-C6-O6   | 11.82  | 127.00      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1179 | G    | N3-C2-N2   | 11.82  | 128.18      | 119.90   |
| 1   | AA    | 1018 | G    | N1-C2-N3   | -11.82 | 116.81      | 123.90   |
| 35  | BB    | 1122 | G    | N3-C2-N2   | 11.82  | 128.18      | 119.90   |
| 35  | BB    | 1452 | G    | P-O3'-C3'  | 11.82  | 133.89      | 119.70   |
| 1   | AA    | 304  | U    | C2-N3-C4   | 11.82  | 134.09      | 127.00   |
| 1   | AA    | 1433 | A    | C2-N3-C4   | -11.82 | 104.69      | 110.60   |
| 35  | BB    | 927  | A    | N1-C6-N6   | 11.82  | 125.69      | 118.60   |
| 35  | BB    | 2076 | U    | P-O3'-C3'  | 11.82  | 133.88      | 119.70   |
| 1   | AA    | 1353 | G    | N3-C2-N2   | 11.81  | 128.17      | 119.90   |
| 35  | BB    | 2777 | G    | N3-C2-N2   | 11.81  | 128.17      | 119.90   |
| 1   | AA    | 879  | C    | O4'-C1'-N1 | 11.81  | 117.65      | 108.20   |
| 1   | AA    | 911  | U    | N1-C2-O2   | 11.81  | 131.07      | 122.80   |
| 35  | BB    | 494  | G    | O4'-C1'-N9 | 11.81  | 117.65      | 108.20   |
| 35  | BB    | 1047 | G    | N1-C6-O6   | 11.81  | 126.98      | 119.90   |
| 1   | AA    | 1243 | C    | O4'-C1'-N1 | 11.81  | 117.64      | 108.20   |
| 35  | BB    | 1275 | A    | P-O3'-C3'  | 11.81  | 133.87      | 119.70   |
| 35  | BB    | 2087 | G    | N1-C6-O6   | 11.81  | 126.98      | 119.90   |
| 35  | BB    | 515  | A    | C5-C6-N6   | -11.80 | 114.26      | 123.70   |
| 35  | BB    | 1435 | G    | C5-C6-O6   | -11.80 | 121.52      | 128.60   |
| 35  | BB    | 1813 | G    | N1-C6-O6   | 11.80  | 126.98      | 119.90   |
| 35  | BB    | 2076 | U    | O4'-C1'-N1 | 11.80  | 117.64      | 108.20   |
| 1   | AA    | 1433 | A    | O4'-C1'-N9 | 11.79  | 117.63      | 108.20   |
| 35  | BB    | 2412 | A    | C8-N9-C4   | -11.79 | 101.08      | 105.80   |
| 1   | AA    | 583  | A    | N1-C6-N6   | 11.79  | 125.67      | 118.60   |
| 1   | AA    | 728  | A    | N1-C6-N6   | 11.79  | 125.67      | 118.60   |
| 35  | BB    | 535  | G    | N1-C6-O6   | 11.79  | 126.97      | 119.90   |
| 1   | AA    | 1236 | A    | N1-C6-N6   | 11.79  | 125.67      | 118.60   |
| 35  | BB    | 525  | U    | O4'-C1'-N1 | 11.78  | 117.63      | 108.20   |
| 35  | BB    | 2877 | G    | N1-C6-O6   | 11.78  | 126.97      | 119.90   |
| 1   | AA    | 860  | A    | N1-C6-N6   | 11.78  | 125.67      | 118.60   |
| 1   | AA    | 658  | C    | O4'-C1'-N1 | 11.77  | 117.62      | 108.20   |
| 35  | BB    | 1054 | A    | C8-N9-C4   | -11.77 | 101.09      | 105.80   |
| 35  | BB    | 2098 | U    | O4'-C1'-N1 | 11.77  | 117.62      | 108.20   |
| 35  | BB    | 2715 | C    | N3-C4-C5   | -11.77 | 117.19      | 121.90   |
| 35  | BB    | 861  | A    | N9-C4-C5   | -11.77 | 101.09      | 105.80   |
| 35  | BB    | 1096 | A    | C4-C5-C6   | 11.77  | 122.88      | 117.00   |
| 35  | BB    | 2466 | C    | O4'-C1'-N1 | 11.77  | 117.61      | 108.20   |
| 1   | AA    | 435  | A    | C5-C6-N6   | -11.77 | 114.29      | 123.70   |
| 35  | BB    | 322  | A    | P-O3'-C3'  | 11.77  | 133.82      | 119.70   |
| 35  | BB    | 440  | C    | O4'-C1'-N1 | 11.77  | 117.61      | 108.20   |
| 35  | BB    | 508  | A    | N1-C6-N6   | 11.77  | 125.66      | 118.60   |
| 1   | AA    | 1347 | G    | C5-C6-O6   | -11.76 | 121.54      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 749  | A    | C8-N9-C4   | -11.76 | 101.09      | 105.80   |
| 35  | BB    | 2077 | A    | N1-C6-N6   | 11.76  | 125.66      | 118.60   |
| 1   | AA    | 1239 | A    | P-O3'-C3'  | 11.76  | 133.81      | 119.70   |
| 35  | BB    | 281  | C    | N3-C4-N4   | 11.76  | 126.23      | 118.00   |
| 35  | BB    | 345  | A    | C4-C5-C6   | 11.76  | 122.88      | 117.00   |
| 1   | AA    | 417  | G    | N1-C6-O6   | 11.75  | 126.95      | 119.90   |
| 35  | BB    | 2597 | G    | N1-C6-O6   | 11.75  | 126.95      | 119.90   |
| 1   | AA    | 63   | C    | N3-C4-N4   | 11.75  | 126.22      | 118.00   |
| 35  | BB    | 1972 | G    | N1-C6-O6   | 11.75  | 126.95      | 119.90   |
| 35  | BB    | 1565 | C    | N3-C4-N4   | 11.74  | 126.22      | 118.00   |
| 35  | BB    | 1615 | C    | O4'-C1'-N1 | 11.74  | 117.60      | 108.20   |
| 1   | AA    | 186  | C    | C6-N1-C2   | -11.74 | 115.61      | 120.30   |
| 1   | AA    | 691  | G    | C5-C6-O6   | -11.74 | 121.56      | 128.60   |
| 35  | BB    | 1664 | A    | N1-C6-N6   | 11.74  | 125.64      | 118.60   |
| 35  | BB    | 2063 | C    | N3-C4-N4   | 11.73  | 126.21      | 118.00   |
| 35  | BB    | 2313 | C    | O4'-C1'-N1 | 11.73  | 117.59      | 108.20   |
| 35  | BB    | 844  | A    | C4-C5-C6   | 11.73  | 122.86      | 117.00   |
| 35  | BB    | 2495 | G    | N1-C6-O6   | 11.73  | 126.94      | 119.90   |
| 35  | BB    | 2725 | A    | C4-C5-C6   | 11.73  | 122.87      | 117.00   |
| 1   | AA    | 846  | G    | O4'-C1'-N9 | 11.73  | 117.58      | 108.20   |
| 35  | BB    | 1403 | A    | N9-C4-C5   | -11.73 | 101.11      | 105.80   |
| 35  | BB    | 1570 | A    | O4'-C1'-N9 | 11.73  | 117.58      | 108.20   |
| 35  | BB    | 1619 | G    | N1-C6-O6   | 11.73  | 126.94      | 119.90   |
| 35  | BB    | 395  | U    | O4'-C1'-N1 | 11.72  | 117.58      | 108.20   |
| 35  | BB    | 1010 | A    | N1-C6-N6   | 11.72  | 125.64      | 118.60   |
| 1   | AA    | 1164 | G    | C2-N3-C4   | 11.72  | 117.76      | 111.90   |
| 35  | BB    | 1464 | G    | C5-C6-O6   | -11.72 | 121.57      | 128.60   |
| 35  | BB    | 2873 | A    | O4'-C1'-N9 | 11.72  | 117.58      | 108.20   |
| 35  | BB    | 2013 | A    | C5-C6-N6   | -11.72 | 114.33      | 123.70   |
| 1   | AA    | 675  | A    | C5-C6-N6   | -11.72 | 114.33      | 123.70   |
| 1   | AA    | 786  | G    | N1-C6-O6   | 11.72  | 126.93      | 119.90   |
| 35  | BB    | 1928 | A    | N9-C4-C5   | 11.72  | 110.49      | 105.80   |
| 32  | B7    | 13   | PHE  | CB-CG-CD2  | 11.72  | 129.00      | 120.80   |
| 34  | BA    | 24   | G    | C8-N9-C4   | -11.71 | 101.71      | 106.40   |
| 1   | AA    | 1060 | U    | N3-C4-O4   | 11.71  | 127.60      | 119.40   |
| 35  | BB    | 1469 | A    | C6-N1-C2   | 11.71  | 125.63      | 118.60   |
| 35  | BB    | 2340 | A    | C5-C6-N6   | -11.71 | 114.33      | 123.70   |
| 35  | BB    | 2711 | A    | C8-N9-C4   | -11.71 | 101.11      | 105.80   |
| 35  | BB    | 102  | U    | O4'-C1'-N1 | 11.71  | 117.57      | 108.20   |
| 35  | BB    | 1188 | U    | C5-C6-N1   | 11.71  | 128.55      | 122.70   |
| 35  | BB    | 1480 | C    | N3-C4-C5   | -11.71 | 117.22      | 121.90   |
| 35  | BB    | 2108 | A    | C4-C5-C6   | 11.71  | 122.85      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 101  | A    | N1-C6-N6   | 11.71  | 125.62      | 118.60   |
| 35  | BB    | 402  | A    | C8-N9-C4   | -11.70 | 101.12      | 105.80   |
| 1   | AA    | 136  | C    | C5-C6-N1   | 11.70  | 126.85      | 121.00   |
| 35  | BB    | 739  | A    | C4-C5-C6   | 11.70  | 122.85      | 117.00   |
| 35  | BB    | 1552 | A    | N1-C6-N6   | 11.70  | 125.62      | 118.60   |
| 35  | BB    | 2127 | G    | O4'-C1'-N9 | 11.70  | 117.56      | 108.20   |
| 35  | BB    | 625  | G    | N3-C2-N2   | 11.70  | 128.09      | 119.90   |
| 35  | BB    | 2113 | U    | O4'-C1'-N1 | 11.70  | 117.56      | 108.20   |
| 35  | BB    | 2530 | A    | C5-C6-N6   | -11.69 | 114.34      | 123.70   |
| 35  | BB    | 1230 | A    | N1-C6-N6   | 11.69  | 125.61      | 118.60   |
| 35  | BB    | 1957 | C    | N3-C4-C5   | -11.69 | 117.22      | 121.90   |
| 35  | BB    | 2024 | G    | N1-C2-N3   | -11.69 | 116.89      | 123.90   |
| 35  | BB    | 2173 | A    | N1-C6-N6   | 11.69  | 125.61      | 118.60   |
| 35  | BB    | 1416 | G    | N1-C6-O6   | 11.69  | 126.91      | 119.90   |
| 1   | AA    | 425  | G    | N1-C6-O6   | 11.68  | 126.91      | 119.90   |
| 1   | AA    | 1329 | A    | O4'-C1'-N9 | 11.68  | 117.55      | 108.20   |
| 35  | BB    | 774  | G    | C8-N9-C4   | -11.68 | 101.73      | 106.40   |
| 1   | AA    | 541  | G    | C5-C6-O6   | -11.68 | 121.59      | 128.60   |
| 1   | AA    | 987  | G    | C6-C5-N7   | -11.68 | 123.39      | 130.40   |
| 35  | BB    | 262  | A    | N1-C6-N6   | 11.68  | 125.61      | 118.60   |
| 1   | AA    | 353  | A    | C5-C6-N6   | -11.68 | 114.36      | 123.70   |
| 1   | AA    | 609  | A    | N1-C6-N6   | 11.68  | 125.61      | 118.60   |
| 35  | BB    | 805  | G    | C5-C6-N1   | -11.68 | 105.66      | 111.50   |
| 1   | AA    | 1238 | A    | N9-C4-C5   | 11.67  | 110.47      | 105.80   |
| 1   | AA    | 432  | A    | N9-C4-C5   | 11.67  | 110.47      | 105.80   |
| 1   | AA    | 458  | U    | O4'-C1'-N1 | 11.67  | 117.54      | 108.20   |
| 35  | BB    | 2317 | A    | N1-C6-N6   | 11.67  | 125.60      | 118.60   |
| 35  | BB    | 187  | G    | C5-C6-O6   | -11.67 | 121.60      | 128.60   |
| 35  | BB    | 2577 | A    | N1-C6-N6   | 11.67  | 125.60      | 118.60   |
| 35  | BB    | 1594 | U    | C6-N1-C2   | -11.67 | 114.00      | 121.00   |
| 35  | BB    | 1117 | C    | O4'-C1'-N1 | 11.67  | 117.53      | 108.20   |
| 35  | BB    | 1924 | C    | O4'-C1'-N1 | 11.67  | 117.53      | 108.20   |
| 35  | BB    | 2423 | U    | O4'-C1'-N1 | 11.67  | 117.53      | 108.20   |
| 35  | BB    | 1479 | G    | N7-C8-N9   | -11.66 | 107.27      | 113.10   |
| 1   | AA    | 1491 | G    | C8-N9-C4   | -11.66 | 101.73      | 106.40   |
| 35  | BB    | 630  | G    | C5-C6-O6   | -11.66 | 121.60      | 128.60   |
| 1   | AA    | 923  | A    | C5-C6-N6   | -11.66 | 114.37      | 123.70   |
| 35  | BB    | 104  | A    | C8-N9-C4   | 11.66  | 110.46      | 105.80   |
| 1   | AA    | 268  | U    | O4'-C1'-N1 | 11.66  | 117.53      | 108.20   |
| 1   | AA    | 918  | A    | C4-C5-C6   | 11.66  | 122.83      | 117.00   |
| 35  | BB    | 654  | A    | C5-C6-N1   | -11.65 | 111.87      | 117.70   |
| 35  | BB    | 1387 | A    | C5-C6-N6   | -11.65 | 114.38      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 647  | C    | O4'-C1'-N1 | 11.65  | 117.52      | 108.20   |
| 35  | BB    | 1328 | A    | C4-C5-C6   | 11.65  | 122.83      | 117.00   |
| 35  | BB    | 655  | A    | O4'-C1'-N9 | 11.65  | 117.52      | 108.20   |
| 40  | BG    | 34   | ARG  | NE-CZ-NH2  | -11.65 | 114.47      | 120.30   |
| 1   | AA    | 842  | U    | O4'-C1'-N1 | 11.65  | 117.52      | 108.20   |
| 35  | BB    | 130  | C    | C4-C5-C6   | 11.65  | 123.22      | 117.40   |
| 1   | AA    | 850  | U    | O4'-C1'-N1 | 11.64  | 117.52      | 108.20   |
| 35  | BB    | 1076 | C    | C6-N1-C2   | 11.64  | 124.96      | 120.30   |
| 1   | AA    | 212  | G    | N1-C6-O6   | 11.64  | 126.89      | 119.90   |
| 1   | AA    | 279  | A    | C2-N3-C4   | -11.64 | 104.78      | 110.60   |
| 35  | BB    | 84   | A    | C4-C5-C6   | 11.64  | 122.82      | 117.00   |
| 35  | BB    | 423  | A    | O4'-C1'-N9 | 11.64  | 117.51      | 108.20   |
| 35  | BB    | 1580 | A    | C5-C6-N1   | -11.64 | 111.88      | 117.70   |
| 35  | BB    | 1807 | G    | N1-C6-O6   | 11.64  | 126.89      | 119.90   |
| 35  | BB    | 712  | G    | N1-C6-O6   | 11.64  | 126.88      | 119.90   |
| 35  | BB    | 880  | G    | P-O3'-C3'  | 11.64  | 133.66      | 119.70   |
| 1   | AA    | 44   | A    | C2-N3-C4   | -11.63 | 104.78      | 110.60   |
| 1   | AA    | 1471 | U    | O4'-C1'-N1 | 11.63  | 117.51      | 108.20   |
| 35  | BB    | 1434 | A    | C5-C6-N6   | -11.63 | 114.39      | 123.70   |
| 35  | BB    | 1688 | U    | O4'-C1'-N1 | 11.63  | 117.51      | 108.20   |
| 35  | BB    | 2189 | U    | C5-C6-N1   | 11.63  | 128.52      | 122.70   |
| 35  | BB    | 2773 | C    | N3-C4-N4   | 11.63  | 126.14      | 118.00   |
| 35  | BB    | 1532 | A    | C4-C5-C6   | 11.63  | 122.81      | 117.00   |
| 1   | AA    | 446  | G    | N1-C6-O6   | 11.63  | 126.88      | 119.90   |
| 35  | BB    | 1085 | A    | O4'-C1'-N9 | 11.63  | 117.50      | 108.20   |
| 35  | BB    | 2557 | G    | N9-C4-C5   | 11.63  | 110.05      | 105.40   |
| 35  | BB    | 1853 | A    | C5-C6-N6   | -11.63 | 114.40      | 123.70   |
| 35  | BB    | 15   | G    | C8-N9-C4   | -11.62 | 101.75      | 106.40   |
| 35  | BB    | 1361 | G    | C6-C5-N7   | -11.62 | 123.42      | 130.40   |
| 35  | BB    | 1591 | A    | N1-C6-N6   | 11.62  | 125.58      | 118.60   |
| 1   | AA    | 337  | G    | N1-C6-O6   | 11.62  | 126.87      | 119.90   |
| 35  | BB    | 152  | A    | N1-C6-N6   | 11.62  | 125.57      | 118.60   |
| 35  | BB    | 1028 | A    | C5-C6-N1   | -11.62 | 111.89      | 117.70   |
| 35  | BB    | 1421 | G    | N1-C6-O6   | 11.62  | 126.87      | 119.90   |
| 1   | AA    | 432  | A    | C5-C6-N1   | -11.62 | 111.89      | 117.70   |
| 35  | BB    | 2447 | G    | N1-C6-O6   | 11.62  | 126.87      | 119.90   |
| 1   | AA    | 1092 | A    | C8-N9-C4   | -11.62 | 101.15      | 105.80   |
| 35  | BB    | 444  | C    | O4'-C1'-N1 | 11.62  | 117.50      | 108.20   |
| 35  | BB    | 921  | C    | N3-C4-C5   | -11.62 | 117.25      | 121.90   |
| 35  | BB    | 368  | A    | C5-C6-N6   | -11.62 | 114.41      | 123.70   |
| 35  | BB    | 614  | A    | C4-C5-C6   | 11.62  | 122.81      | 117.00   |
| 1   | AA    | 176  | C    | N3-C4-C5   | -11.61 | 117.25      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 481  | G    | C5-C6-O6   | -11.62 | 121.63      | 128.60   |
| 35  | BB    | 2482 | A    | N1-C6-N6   | 11.61  | 125.57      | 118.60   |
| 35  | BB    | 2459 | A    | C8-N9-C4   | -11.61 | 101.16      | 105.80   |
| 35  | BB    | 2824 | C    | O4'-C1'-N1 | 11.61  | 117.49      | 108.20   |
| 1   | AA    | 1068 | G    | C5-C6-O6   | -11.61 | 121.63      | 128.60   |
| 35  | BB    | 372  | G    | N1-C6-O6   | 11.61  | 126.86      | 119.90   |
| 35  | BB    | 2430 | A    | N1-C6-N6   | 11.61  | 125.57      | 118.60   |
| 35  | BB    | 531  | C    | N3-C4-C5   | -11.61 | 117.26      | 121.90   |
| 1   | AA    | 1353 | G    | N3-C4-C5   | -11.61 | 122.80      | 128.60   |
| 35  | BB    | 526  | A    | N1-C6-N6   | 11.61  | 125.56      | 118.60   |
| 35  | BB    | 1269 | A    | C5-N7-C8   | 11.61  | 109.70      | 103.90   |
| 35  | BB    | 1746 | A    | N9-C4-C5   | 11.61  | 110.44      | 105.80   |
| 1   | AA    | 519  | C    | C4-C5-C6   | 11.60  | 123.20      | 117.40   |
| 35  | BB    | 1921 | G    | C4-C5-N7   | -11.60 | 106.16      | 110.80   |
| 1   | AA    | 958  | A    | C5-C6-N1   | -11.60 | 111.90      | 117.70   |
| 35  | BB    | 106  | C    | N3-C4-N4   | 11.60  | 126.12      | 118.00   |
| 35  | BB    | 1772 | A    | C8-N9-C4   | -11.60 | 101.16      | 105.80   |
| 35  | BB    | 2193 | G    | N1-C6-O6   | 11.60  | 126.86      | 119.90   |
| 35  | BB    | 380  | G    | N9-C4-C5   | 11.60  | 110.04      | 105.40   |
| 35  | BB    | 2070 | A    | C5-C6-N1   | -11.60 | 111.90      | 117.70   |
| 35  | BB    | 2330 | G    | N1-C6-O6   | 11.60  | 126.86      | 119.90   |
| 35  | BB    | 2735 | G    | N1-C6-O6   | 11.59  | 126.86      | 119.90   |
| 35  | BB    | 1616 | A    | N1-C6-N6   | 11.59  | 125.55      | 118.60   |
| 35  | BB    | 2134 | A    | O4'-C1'-N9 | 11.59  | 117.47      | 108.20   |
| 35  | BB    | 2859 | G    | N1-C6-O6   | 11.59  | 126.85      | 119.90   |
| 1   | AA    | 1002 | G    | C8-N9-C4   | -11.59 | 101.77      | 106.40   |
| 35  | BB    | 1658 | C    | O4'-C1'-N1 | 11.59  | 117.47      | 108.20   |
| 1   | AA    | 1086 | U    | O4'-C1'-N1 | 11.59  | 117.47      | 108.20   |
| 1   | AA    | 1473 | G    | O4'-C1'-N9 | 11.59  | 117.47      | 108.20   |
| 35  | BB    | 563  | A    | N1-C6-N6   | 11.59  | 125.55      | 118.60   |
| 35  | BB    | 1426 | G    | N1-C6-O6   | 11.59  | 126.85      | 119.90   |
| 1   | AA    | 126  | G    | C5-C6-O6   | -11.58 | 121.65      | 128.60   |
| 1   | AA    | 737  | C    | C4-C5-C6   | 11.58  | 123.19      | 117.40   |
| 35  | BB    | 269  | C    | N3-C4-C5   | -11.58 | 117.27      | 121.90   |
| 35  | BB    | 1984 | G    | C8-N9-C4   | 11.58  | 111.03      | 106.40   |
| 35  | BB    | 2215 | C    | C5-C6-N1   | -11.58 | 115.21      | 121.00   |
| 1   | AA    | 130  | A    | C5-N7-C8   | 11.58  | 109.69      | 103.90   |
| 52  | BS    | 95   | ARG  | NE-CZ-NH1  | -11.58 | 114.51      | 120.30   |
| 34  | BA    | 63   | C    | O4'-C1'-N1 | 11.58  | 117.46      | 108.20   |
| 1   | AA    | 1287 | A    | C5-C6-N6   | -11.57 | 114.44      | 123.70   |
| 35  | BB    | 439  | A    | C4-C5-C6   | 11.57  | 122.79      | 117.00   |
| 35  | BB    | 659  | G    | N3-C2-N2   | 11.57  | 128.00      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1681 | G    | N3-C4-C5   | -11.57 | 122.81      | 128.60   |
| 35  | BB    | 2234 | G    | N1-C2-N3   | -11.57 | 116.96      | 123.90   |
| 1   | AA    | 397  | A    | C5-C6-N1   | -11.57 | 111.92      | 117.70   |
| 35  | BB    | 336  | C    | O4'-C1'-N1 | 11.57  | 117.45      | 108.20   |
| 35  | BB    | 638  | G    | N1-C2-N3   | -11.57 | 116.96      | 123.90   |
| 35  | BB    | 1424 | G    | N3-C2-N2   | 11.57  | 128.00      | 119.90   |
| 35  | BB    | 2077 | A    | C4-C5-C6   | 11.57  | 122.78      | 117.00   |
| 35  | BB    | 744  | U    | O4'-C1'-N1 | 11.57  | 117.45      | 108.20   |
| 35  | BB    | 2665 | A    | C5-C6-N1   | -11.57 | 111.92      | 117.70   |
| 3   | AC    | 131  | ARG  | NE-CZ-NH1  | -11.56 | 114.52      | 120.30   |
| 35  | BB    | 996  | A    | O4'-C1'-N9 | 11.56  | 117.45      | 108.20   |
| 1   | AA    | 587  | G    | C8-N9-C4   | 11.56  | 111.03      | 106.40   |
| 35  | BB    | 217  | A    | C4-C5-C6   | 11.56  | 122.78      | 117.00   |
| 35  | BB    | 2624 | G    | P-O5'-C5'  | 11.56  | 139.40      | 120.90   |
| 1   | AA    | 1479 | C    | O4'-C1'-N1 | 11.56  | 117.45      | 108.20   |
| 35  | BB    | 1180 | U    | O4'-C1'-N1 | 11.56  | 117.45      | 108.20   |
| 35  | BB    | 41   | C    | C5-C4-N4   | -11.56 | 112.11      | 120.20   |
| 35  | BB    | 1034 | G    | C5-C6-O6   | -11.56 | 121.66      | 128.60   |
| 1   | AA    | 529  | G    | C4-C5-N7   | 11.56  | 115.42      | 110.80   |
| 35  | BB    | 1895 | C    | C6-N1-C2   | -11.56 | 115.68      | 120.30   |
| 35  | BB    | 1008 | A    | C4-C5-C6   | 11.56  | 122.78      | 117.00   |
| 1   | AA    | 1344 | C    | N3-C4-C5   | -11.55 | 117.28      | 121.90   |
| 35  | BB    | 669  | G    | C8-N9-C4   | -11.55 | 101.78      | 106.40   |
| 35  | BB    | 2466 | C    | N1-C2-O2   | -11.55 | 111.97      | 118.90   |
| 1   | AA    | 119  | A    | C8-N9-C4   | -11.55 | 101.18      | 105.80   |
| 35  | BB    | 533  | G    | C6-N1-C2   | 11.55  | 132.03      | 125.10   |
| 35  | BB    | 1150 | C    | O4'-C1'-N1 | 11.55  | 117.44      | 108.20   |
| 35  | BB    | 517  | C    | O4'-C1'-N1 | 11.55  | 117.44      | 108.20   |
| 35  | BB    | 1432 | G    | N1-C6-O6   | 11.55  | 126.83      | 119.90   |
| 35  | BB    | 1997 | C    | N3-C4-N4   | 11.55  | 126.08      | 118.00   |
| 35  | BB    | 1054 | A    | N9-C4-C5   | 11.55  | 110.42      | 105.80   |
| 1   | AA    | 509  | A    | N1-C6-N6   | 11.54  | 125.53      | 118.60   |
| 1   | AA    | 977  | A    | C4-C5-C6   | 11.54  | 122.77      | 117.00   |
| 35  | BB    | 209  | C    | O4'-C1'-N1 | 11.54  | 117.44      | 108.20   |
| 35  | BB    | 1339 | G    | C5-C6-N1   | 11.54  | 117.27      | 111.50   |
| 35  | BB    | 2766 | A    | C5-C6-N1   | -11.54 | 111.93      | 117.70   |
| 1   | AA    | 58   | C    | O4'-C1'-N1 | 11.54  | 117.43      | 108.20   |
| 1   | AA    | 165  | G    | C5-C6-O6   | -11.54 | 121.67      | 128.60   |
| 35  | BB    | 347  | A    | C4-C5-C6   | 11.54  | 122.77      | 117.00   |
| 35  | BB    | 1788 | C    | N3-C4-N4   | 11.54  | 126.08      | 118.00   |
| 35  | BB    | 1182 | G    | N1-C6-O6   | 11.54  | 126.82      | 119.90   |
| 1   | AA    | 655  | A    | C4-C5-C6   | 11.54  | 122.77      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 704  | A    | C5-N7-C8   | 11.54  | 109.67      | 103.90   |
| 35  | BB    | 1505 | A    | N1-C6-N6   | 11.54  | 125.52      | 118.60   |
| 39  | BF    | 149  | ARG  | NE-CZ-NH1  | 11.54  | 126.07      | 120.30   |
| 1   | AA    | 1418 | A    | C4-C5-C6   | 11.53  | 122.77      | 117.00   |
| 35  | BB    | 263  | G    | C5-C6-O6   | -11.54 | 121.68      | 128.60   |
| 35  | BB    | 312  | G    | N1-C6-O6   | 11.53  | 126.82      | 119.90   |
| 35  | BB    | 861  | A    | N1-C6-N6   | 11.53  | 125.52      | 118.60   |
| 35  | BB    | 1353 | A    | C4-C5-C6   | 11.54  | 122.77      | 117.00   |
| 35  | BB    | 2862 | G    | C4-C5-C6   | 11.54  | 125.72      | 118.80   |
| 1   | AA    | 50   | A    | C5-C6-N1   | -11.53 | 111.93      | 117.70   |
| 35  | BB    | 6    | A    | N9-C4-C5   | 11.53  | 110.41      | 105.80   |
| 35  | BB    | 2150 | C    | C2-N3-C4   | 11.53  | 125.67      | 119.90   |
| 35  | BB    | 800  | A    | C5-C6-N6   | -11.53 | 114.48      | 123.70   |
| 35  | BB    | 1734 | G    | C2-N3-C4   | 11.53  | 117.67      | 111.90   |
| 35  | BB    | 2852 | G    | O4'-C1'-N9 | 11.53  | 117.42      | 108.20   |
| 1   | AA    | 959  | A    | N1-C6-N6   | 11.53  | 125.52      | 118.60   |
| 1   | AA    | 913  | A    | C5-N7-C8   | 11.53  | 109.66      | 103.90   |
| 35  | BB    | 1154 | G    | C5-C6-O6   | -11.53 | 121.69      | 128.60   |
| 35  | BB    | 2529 | G    | N1-C6-O6   | 11.53  | 126.81      | 119.90   |
| 39  | BF    | 70   | ARG  | NE-CZ-NH2  | 11.53  | 126.06      | 120.30   |
| 35  | BB    | 602  | A    | C5-C6-N1   | -11.52 | 111.94      | 117.70   |
| 35  | BB    | 1495 | A    | N1-C6-N6   | 11.52  | 125.51      | 118.60   |
| 1   | AA    | 1167 | A    | N1-C6-N6   | 11.52  | 125.51      | 118.60   |
| 35  | BB    | 668  | A    | N1-C6-N6   | 11.52  | 125.51      | 118.60   |
| 35  | BB    | 1714 | U    | O4'-C1'-N1 | 11.52  | 117.42      | 108.20   |
| 1   | AA    | 817  | C    | C2-N3-C4   | 11.52  | 125.66      | 119.90   |
| 35  | BB    | 1802 | A    | C4-C5-C6   | 11.52  | 122.76      | 117.00   |
| 1   | AA    | 688  | G    | O4'-C1'-N9 | 11.52  | 117.41      | 108.20   |
| 1   | AA    | 935  | A    | C8-N9-C4   | -11.51 | 101.19      | 105.80   |
| 35  | BB    | 579  | G    | C5-C6-O6   | -11.51 | 121.69      | 128.60   |
| 35  | BB    | 1145 | C    | O4'-C1'-N1 | 11.51  | 117.41      | 108.20   |
| 35  | BB    | 2488 | G    | N1-C2-N3   | -11.51 | 116.99      | 123.90   |
| 1   | AA    | 911  | U    | N1-C2-N3   | -11.51 | 107.99      | 114.90   |
| 35  | BB    | 959  | A    | C2-N3-C4   | 11.51  | 116.36      | 110.60   |
| 35  | BB    | 509  | C    | C5-C4-N4   | -11.51 | 112.14      | 120.20   |
| 35  | BB    | 990  | A    | C4-C5-C6   | 11.51  | 122.75      | 117.00   |
| 35  | BB    | 2808 | G    | N1-C6-O6   | 11.51  | 126.81      | 119.90   |
| 34  | BA    | 29   | A    | C5-C6-N6   | -11.51 | 114.50      | 123.70   |
| 1   | AA    | 122  | G    | N1-C6-O6   | 11.50  | 126.80      | 119.90   |
| 35  | BB    | 1305 | C    | N3-C4-N4   | 11.50  | 126.05      | 118.00   |
| 35  | BB    | 1435 | G    | N1-C6-O6   | 11.50  | 126.80      | 119.90   |
| 35  | BB    | 2066 | C    | O4'-C1'-N1 | 11.50  | 117.40      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 179  | C    | C6-N1-C2   | 11.50  | 124.90      | 120.30   |
| 35  | BB    | 570  | G    | O4'-C1'-N9 | 11.50  | 117.40      | 108.20   |
| 1   | AA    | 903  | G    | N1-C6-O6   | 11.50  | 126.80      | 119.90   |
| 22  | AV    | 32   | A    | P-O3'-C3'  | 11.50  | 133.50      | 119.70   |
| 22  | AV    | 72   | G    | P-O3'-C3'  | 11.50  | 133.50      | 119.70   |
| 34  | BA    | 45   | A    | C5-C6-N6   | -11.50 | 114.50      | 123.70   |
| 35  | BB    | 298  | G    | C5-C6-N1   | -11.50 | 105.75      | 111.50   |
| 35  | BB    | 945  | A    | C4-C5-C6   | 11.50  | 122.75      | 117.00   |
| 35  | BB    | 363  | G    | O4'-C1'-N9 | 11.49  | 117.39      | 108.20   |
| 35  | BB    | 633  | A    | C5-C6-N1   | -11.49 | 111.95      | 117.70   |
| 35  | BB    | 1645 | G    | N1-C6-O6   | 11.49  | 126.80      | 119.90   |
| 35  | BB    | 1843 | C    | N3-C4-C5   | -11.49 | 117.30      | 121.90   |
| 35  | BB    | 2876 | G    | C5-C6-O6   | -11.49 | 121.70      | 128.60   |
| 35  | BB    | 612  | G    | C5-C6-O6   | -11.49 | 121.70      | 128.60   |
| 35  | BB    | 1364 | G    | C5-C6-O6   | -11.49 | 121.70      | 128.60   |
| 35  | BB    | 644  | A    | C5-C6-N6   | -11.49 | 114.51      | 123.70   |
| 1   | AA    | 62   | U    | O4'-C1'-N1 | 11.49  | 117.39      | 108.20   |
| 35  | BB    | 936  | A    | C4-C5-C6   | 11.49  | 122.74      | 117.00   |
| 52  | BS    | 8    | ARG  | NE-CZ-NH2  | -11.49 | 114.56      | 120.30   |
| 1   | AA    | 1339 | A    | C5-C6-N1   | -11.48 | 111.96      | 117.70   |
| 35  | BB    | 1254 | A    | C5-C6-N1   | -11.48 | 111.96      | 117.70   |
| 1   | AA    | 1179 | A    | N1-C6-N6   | 11.48  | 125.49      | 118.60   |
| 22  | AV    | 59   | A    | N1-C6-N6   | 11.48  | 125.49      | 118.60   |
| 35  | BB    | 285  | G    | C5-C6-O6   | -11.48 | 121.71      | 128.60   |
| 35  | BB    | 1935 | G    | N1-C6-O6   | 11.48  | 126.79      | 119.90   |
| 35  | BB    | 938  | G    | O4'-C1'-N9 | 11.48  | 117.38      | 108.20   |
| 35  | BB    | 2411 | A    | C4-C5-C6   | 11.48  | 122.74      | 117.00   |
| 1   | AA    | 1479 | C    | N3-C4-C5   | -11.48 | 117.31      | 121.90   |
| 35  | BB    | 1364 | G    | N3-C4-N9   | -11.48 | 119.11      | 126.00   |
| 35  | BB    | 1919 | A    | N1-C6-N6   | 11.48  | 125.49      | 118.60   |
| 35  | BB    | 2063 | C    | N3-C4-C5   | -11.48 | 117.31      | 121.90   |
| 35  | BB    | 2568 | U    | O4'-C1'-N1 | 11.48  | 117.38      | 108.20   |
| 35  | BB    | 235  | U    | C2-N3-C4   | -11.47 | 120.12      | 127.00   |
| 35  | BB    | 1024 | G    | N7-C8-N9   | 11.47  | 118.84      | 113.10   |
| 35  | BB    | 987  | C    | O4'-C1'-N1 | 11.47  | 117.38      | 108.20   |
| 35  | BB    | 1952 | A    | O4'-C1'-N9 | 11.47  | 117.38      | 108.20   |
| 35  | BB    | 439  | A    | C5-C6-N1   | -11.47 | 111.97      | 117.70   |
| 1   | AA    | 1109 | C    | N3-C4-N4   | 11.47  | 126.03      | 118.00   |
| 1   | AA    | 327  | A    | C5-C6-N6   | -11.46 | 114.53      | 123.70   |
| 35  | BB    | 49   | A    | O4'-C1'-N9 | 11.46  | 117.37      | 108.20   |
| 35  | BB    | 326  | G    | C4-C5-N7   | 11.46  | 115.38      | 110.80   |
| 35  | BB    | 784  | G    | N1-C2-N3   | -11.46 | 117.03      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 41   | G    | N1-C6-O6   | 11.45  | 126.77      | 119.90   |
| 1   | AA    | 1371 | G    | N1-C6-O6   | 11.45  | 126.77      | 119.90   |
| 44  | BK    | 71   | ARG  | NE-CZ-NH1  | 11.45  | 126.03      | 120.30   |
| 1   | AA    | 156  | C    | N3-C4-C5   | -11.45 | 117.32      | 121.90   |
| 1   | AA    | 1040 | U    | O4'-C1'-N1 | 11.45  | 117.36      | 108.20   |
| 1   | AA    | 1120 | C    | O4'-C1'-N1 | 11.45  | 117.36      | 108.20   |
| 1   | AA    | 706  | A    | N1-C6-N6   | 11.45  | 125.47      | 118.60   |
| 25  | B0    | 73   | ARG  | NE-CZ-NH2  | 11.44  | 126.02      | 120.30   |
| 35  | BB    | 1975 | G    | C5-C6-O6   | -11.44 | 121.74      | 128.60   |
| 1   | AA    | 174  | A    | C4-C5-C6   | 11.44  | 122.72      | 117.00   |
| 35  | BB    | 391  | A    | N1-C6-N6   | 11.44  | 125.46      | 118.60   |
| 35  | BB    | 1777 | U    | O4'-C1'-N1 | 11.44  | 117.35      | 108.20   |
| 1   | AA    | 722  | G    | N1-C6-O6   | 11.43  | 126.76      | 119.90   |
| 1   | AA    | 812  | G    | N1-C6-O6   | 11.43  | 126.76      | 119.90   |
| 1   | AA    | 948  | C    | O4'-C1'-N1 | 11.43  | 117.35      | 108.20   |
| 35  | BB    | 2127 | G    | C8-N9-C4   | -11.43 | 101.83      | 106.40   |
| 1   | AA    | 124  | C    | N3-C4-N4   | 11.43  | 126.00      | 118.00   |
| 1   | AA    | 941  | G    | C5-C6-O6   | -11.43 | 121.74      | 128.60   |
| 35  | BB    | 1143 | A    | C5-C6-N1   | -11.43 | 111.98      | 117.70   |
| 35  | BB    | 1438 | U    | O4'-C1'-N1 | 11.43  | 117.34      | 108.20   |
| 35  | BB    | 1770 | G    | N1-C6-O6   | 11.43  | 126.76      | 119.90   |
| 35  | BB    | 2378 | A    | N9-C4-C5   | 11.43  | 110.37      | 105.80   |
| 35  | BB    | 2389 | G    | C5-C6-O6   | -11.43 | 121.74      | 128.60   |
| 47  | BN    | 96   | ARG  | NE-CZ-NH2  | -11.43 | 114.58      | 120.30   |
| 1   | AA    | 164  | G    | O4'-C1'-N9 | 11.43  | 117.34      | 108.20   |
| 35  | BB    | 2769 | U    | O4'-C1'-N1 | 11.43  | 117.34      | 108.20   |
| 35  | BB    | 2795 | C    | O4'-C1'-N1 | 11.42  | 117.34      | 108.20   |
| 1   | AA    | 466  | A    | C5-C6-N6   | -11.42 | 114.56      | 123.70   |
| 35  | BB    | 1891 | G    | N1-C6-O6   | 11.42  | 126.75      | 119.90   |
| 35  | BB    | 2302 | U    | O4'-C1'-N1 | 11.42  | 117.34      | 108.20   |
| 35  | BB    | 2699 | C    | O4'-C1'-N1 | 11.42  | 117.33      | 108.20   |
| 35  | BB    | 311  | A    | O4'-C1'-N9 | 11.42  | 117.33      | 108.20   |
| 1   | AA    | 95   | C    | O4'-C1'-N1 | 11.42  | 117.33      | 108.20   |
| 35  | BB    | 2003 | A    | C4-C5-N7   | -11.42 | 104.99      | 110.70   |
| 1   | AA    | 953  | G    | C2-N3-C4   | -11.41 | 106.19      | 111.90   |
| 35  | BB    | 188  | G    | C5-C6-O6   | -11.41 | 121.75      | 128.60   |
| 35  | BB    | 1478 | G    | N3-C4-C5   | -11.41 | 122.89      | 128.60   |
| 35  | BB    | 136  | G    | C5-C6-O6   | -11.41 | 121.75      | 128.60   |
| 36  | BC    | 61   | TYR  | CB-CG-CD1  | 11.41  | 127.85      | 121.00   |
| 1   | AA    | 956  | U    | O4'-C1'-N1 | 11.41  | 117.32      | 108.20   |
| 35  | BB    | 401  | A    | O4'-C1'-N9 | 11.41  | 117.33      | 108.20   |
| 35  | BB    | 1534 | U    | N3-C2-O2   | -11.41 | 114.22      | 122.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2170 | A    | C5-C6-N1   | -11.41 | 112.00      | 117.70   |
| 1   | AA    | 517  | G    | C5-C6-O6   | -11.40 | 121.76      | 128.60   |
| 35  | BB    | 324  | A    | N9-C4-C5   | 11.40  | 110.36      | 105.80   |
| 1   | AA    | 988  | G    | C5-C6-O6   | -11.40 | 121.76      | 128.60   |
| 1   | AA    | 371  | A    | C4-C5-C6   | 11.40  | 122.70      | 117.00   |
| 35  | BB    | 862  | G    | N1-C6-O6   | 11.40  | 126.74      | 119.90   |
| 35  | BB    | 1310 | G    | C6-C5-N7   | -11.40 | 123.56      | 130.40   |
| 35  | BB    | 1853 | A    | C8-N9-C4   | 11.40  | 110.36      | 105.80   |
| 35  | BB    | 1749 | A    | N1-C6-N6   | 11.40  | 125.44      | 118.60   |
| 35  | BB    | 2508 | G    | N1-C6-O6   | 11.40  | 126.74      | 119.90   |
| 35  | BB    | 1256 | G    | N1-C6-O6   | 11.40  | 126.74      | 119.90   |
| 35  | BB    | 1645 | G    | C5-C6-O6   | -11.40 | 121.76      | 128.60   |
| 1   | AA    | 584  | G    | C5-C6-O6   | -11.39 | 121.76      | 128.60   |
| 1   | AA    | 1093 | A    | N1-C2-N3   | -11.39 | 123.60      | 129.30   |
| 20  | AT    | 59   | ARG  | NE-CZ-NH2  | -11.39 | 114.60      | 120.30   |
| 35  | BB    | 664  | G    | C5-C6-O6   | -11.39 | 121.76      | 128.60   |
| 35  | BB    | 2825 | G    | N1-C6-O6   | 11.39  | 126.74      | 119.90   |
| 35  | BB    | 862  | G    | C5-C6-O6   | -11.39 | 121.77      | 128.60   |
| 1   | AA    | 463  | U    | O4'-C1'-N1 | 11.39  | 117.31      | 108.20   |
| 35  | BB    | 159  | G    | N1-C6-O6   | 11.39  | 126.73      | 119.90   |
| 35  | BB    | 1304 | A    | O4'-C1'-N9 | 11.39  | 117.31      | 108.20   |
| 1   | AA    | 1013 | G    | N1-C6-O6   | 11.39  | 126.73      | 119.90   |
| 1   | AA    | 404  | G    | C5-C6-O6   | -11.39 | 121.77      | 128.60   |
| 35  | BB    | 636  | G    | C5-C6-O6   | -11.39 | 121.77      | 128.60   |
| 1   | AA    | 429  | U    | O4'-C1'-N1 | 11.39  | 117.31      | 108.20   |
| 35  | BB    | 1499 | C    | N3-C4-C5   | -11.38 | 117.35      | 121.90   |
| 35  | BB    | 1579 | A    | C5-N7-C8   | 11.38  | 109.59      | 103.90   |
| 1   | AA    | 721  | G    | C5-C6-O6   | -11.38 | 121.77      | 128.60   |
| 35  | BB    | 1541 | C    | N3-C4-C5   | -11.38 | 117.35      | 121.90   |
| 35  | BB    | 2664 | G    | N3-C2-N2   | 11.38  | 127.87      | 119.90   |
| 1   | AA    | 637  | C    | N3-C4-C5   | -11.38 | 117.35      | 121.90   |
| 35  | BB    | 2623 | G    | C5-C6-O6   | -11.38 | 121.77      | 128.60   |
| 1   | AA    | 549  | C    | C5-C6-N1   | 11.37  | 126.69      | 121.00   |
| 35  | BB    | 2307 | G    | O4'-C1'-N9 | 11.38  | 117.30      | 108.20   |
| 35  | BB    | 2633 | G    | C5-C6-N1   | -11.37 | 105.81      | 111.50   |
| 35  | BB    | 2738 | A    | N1-C6-N6   | 11.37  | 125.42      | 118.60   |
| 35  | BB    | 2094 | A    | C4-C5-C6   | 11.37  | 122.69      | 117.00   |
| 35  | BB    | 2214 | C    | N3-C4-C5   | -11.37 | 117.35      | 121.90   |
| 35  | BB    | 2399 | G    | O4'-C1'-N9 | 11.37  | 117.30      | 108.20   |
| 1   | AA    | 212  | G    | O4'-C1'-N9 | 11.37  | 117.29      | 108.20   |
| 1   | AA    | 976  | G    | N1-C6-O6   | 11.37  | 126.72      | 119.90   |
| 1   | AA    | 634  | C    | O4'-C1'-N1 | 11.36  | 117.29      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2644 | G    | N1-C6-O6   | 11.36  | 126.72      | 119.90   |
| 35  | BB    | 1368 | G    | C5-C6-N1   | -11.36 | 105.82      | 111.50   |
| 35  | BB    | 1985 | C    | O4'-C1'-N1 | 11.36  | 117.29      | 108.20   |
| 35  | BB    | 2641 | G    | C5-C6-O6   | -11.36 | 121.78      | 128.60   |
| 1   | AA    | 780  | A    | C4-C5-C6   | 11.36  | 122.68      | 117.00   |
| 1   | AA    | 1124 | G    | C5-C6-O6   | -11.36 | 121.79      | 128.60   |
| 35  | BB    | 1501 | G    | N1-C6-O6   | 11.36  | 126.71      | 119.90   |
| 1   | AA    | 28   | A    | C4-C5-C6   | 11.35  | 122.68      | 117.00   |
| 1   | AA    | 799  | G    | C5-C6-O6   | -11.35 | 121.79      | 128.60   |
| 35  | BB    | 424  | G    | C5-C6-O6   | -11.35 | 121.79      | 128.60   |
| 35  | BB    | 1652 | A    | N1-C6-N6   | 11.35  | 125.41      | 118.60   |
| 35  | BB    | 2838 | G    | C4-C5-N7   | 11.35  | 115.34      | 110.80   |
| 35  | BB    | 2875 | C    | C5-C6-N1   | 11.35  | 126.68      | 121.00   |
| 1   | AA    | 782  | A    | C5-N7-C8   | 11.35  | 109.57      | 103.90   |
| 1   | AA    | 1035 | A    | O4'-C1'-N9 | 11.35  | 117.28      | 108.20   |
| 35  | BB    | 1840 | G    | N3-C2-N2   | 11.35  | 127.84      | 119.90   |
| 1   | AA    | 805  | C    | C5-C6-N1   | 11.35  | 126.67      | 121.00   |
| 35  | BB    | 1908 | C    | O4'-C1'-N1 | 11.35  | 117.28      | 108.20   |
| 35  | BB    | 63   | A    | C5-C6-N1   | -11.34 | 112.03      | 117.70   |
| 35  | BB    | 482  | A    | C2-N3-C4   | -11.34 | 104.93      | 110.60   |
| 35  | BB    | 610  | C    | O4'-C1'-N1 | 11.34  | 117.27      | 108.20   |
| 35  | BB    | 960  | A    | C5-C6-N1   | -11.34 | 112.03      | 117.70   |
| 35  | BB    | 1797 | G    | C8-N9-C4   | -11.34 | 101.86      | 106.40   |
| 35  | BB    | 2426 | A    | C4-C5-C6   | 11.34  | 122.67      | 117.00   |
| 35  | BB    | 1525 | A    | C5-C6-N6   | -11.34 | 114.63      | 123.70   |
| 35  | BB    | 1832 | C    | N3-C4-N4   | 11.34  | 125.94      | 118.00   |
| 35  | BB    | 2594 | C    | N3-C4-N4   | 11.34  | 125.94      | 118.00   |
| 35  | BB    | 180  | G    | N3-C2-N2   | 11.34  | 127.84      | 119.90   |
| 35  | BB    | 613  | A    | O4'-C1'-N9 | 11.34  | 117.27      | 108.20   |
| 35  | BB    | 1109 | C    | O4'-C1'-N1 | 11.34  | 117.27      | 108.20   |
| 35  | BB    | 2729 | G    | C5-C6-O6   | -11.34 | 121.80      | 128.60   |
| 1   | AA    | 102  | G    | C5-C6-O6   | -11.34 | 121.80      | 128.60   |
| 35  | BB    | 1918 | A    | C5-C6-N1   | -11.34 | 112.03      | 117.70   |
| 35  | BB    | 2102 | G    | C5-C6-O6   | -11.34 | 121.80      | 128.60   |
| 35  | BB    | 2154 | A    | N1-C6-N6   | 11.34  | 125.40      | 118.60   |
| 35  | BB    | 991  | C    | O4'-C1'-N1 | 11.33  | 117.27      | 108.20   |
| 35  | BB    | 1951 | U    | O4'-C1'-N1 | 11.33  | 117.27      | 108.20   |
| 35  | BB    | 2191 | A    | C5-C6-N6   | -11.33 | 114.63      | 123.70   |
| 35  | BB    | 64   | A    | C5-C6-N1   | -11.33 | 112.03      | 117.70   |
| 35  | BB    | 1337 | G    | N1-C6-O6   | 11.33  | 126.70      | 119.90   |
| 1   | AA    | 1106 | G    | C4-C5-N7   | -11.33 | 106.27      | 110.80   |
| 35  | BB    | 1706 | C    | O4'-C1'-N1 | 11.33  | 117.26      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 1292 | G    | N1-C6-O6   | 11.32  | 126.69      | 119.90   |
| 35  | BB    | 305  | C    | O4'-C1'-N1 | 11.32  | 117.26      | 108.20   |
| 35  | BB    | 767  | U    | O4'-C1'-N1 | 11.32  | 117.26      | 108.20   |
| 1   | AA    | 111  | G    | N1-C6-O6   | 11.32  | 126.69      | 119.90   |
| 1   | AA    | 977  | A    | C5-C6-N1   | -11.32 | 112.04      | 117.70   |
| 1   | AA    | 1191 | A    | N9-C4-C5   | 11.32  | 110.33      | 105.80   |
| 35  | BB    | 2843 | G    | C2-N3-C4   | 11.32  | 117.56      | 111.90   |
| 35  | BB    | 310  | A    | C5-C6-N1   | -11.32 | 112.04      | 117.70   |
| 35  | BB    | 833  | A    | C8-N9-C4   | -11.32 | 101.27      | 105.80   |
| 35  | BB    | 838  | C    | N3-C4-N4   | 11.32  | 125.92      | 118.00   |
| 1   | AA    | 468  | A    | N1-C6-N6   | 11.32  | 125.39      | 118.60   |
| 1   | AA    | 1067 | A    | C5-C6-N6   | -11.32 | 114.65      | 123.70   |
| 35  | BB    | 476  | G    | C5-C6-O6   | -11.32 | 121.81      | 128.60   |
| 35  | BB    | 1928 | A    | C5-C6-N1   | -11.32 | 112.04      | 117.70   |
| 35  | BB    | 2717 | C    | O4'-C1'-N1 | 11.32  | 117.25      | 108.20   |
| 7   | AG    | 9    | ARG  | NE-CZ-NH1  | 11.31  | 125.96      | 120.30   |
| 1   | AA    | 1222 | G    | O4'-C1'-N9 | 11.31  | 117.25      | 108.20   |
| 1   | AA    | 1500 | A    | C4-C5-C6   | 11.31  | 122.66      | 117.00   |
| 1   | AA    | 116  | A    | C5-C6-N1   | -11.31 | 112.05      | 117.70   |
| 35  | BB    | 1175 | A    | C4-C5-C6   | 11.31  | 122.66      | 117.00   |
| 35  | BB    | 2467 | C    | N3-C4-N4   | 11.31  | 125.92      | 118.00   |
| 1   | AA    | 1006 | G    | N1-C6-O6   | 11.31  | 126.69      | 119.90   |
| 34  | BA    | 30   | C    | C5-C4-N4   | -11.31 | 112.28      | 120.20   |
| 35  | BB    | 760  | G    | N1-C6-O6   | 11.31  | 126.69      | 119.90   |
| 35  | BB    | 910  | A    | C5-C6-N6   | -11.31 | 114.65      | 123.70   |
| 35  | BB    | 1836 | C    | C6-N1-C2   | -11.31 | 115.78      | 120.30   |
| 35  | BB    | 2407 | A    | O4'-C1'-N9 | 11.31  | 117.25      | 108.20   |
| 1   | AA    | 1489 | G    | N1-C6-O6   | 11.31  | 126.68      | 119.90   |
| 34  | BA    | 52   | A    | C5-C6-N1   | -11.30 | 112.05      | 117.70   |
| 35  | BB    | 310  | A    | C5-N7-C8   | 11.31  | 109.55      | 103.90   |
| 35  | BB    | 1333 | G    | C5-C6-N1   | -11.30 | 105.85      | 111.50   |
| 35  | BB    | 2428 | G    | C5-C6-O6   | -11.30 | 121.82      | 128.60   |
| 9   | AI    | 94   | ARG  | NE-CZ-NH2  | -11.30 | 114.65      | 120.30   |
| 1   | AA    | 1114 | C    | O4'-C1'-N1 | 11.30  | 117.24      | 108.20   |
| 35  | BB    | 673  | C    | O4'-C1'-N1 | 11.30  | 117.24      | 108.20   |
| 35  | BB    | 1320 | C    | N3-C4-C5   | -11.30 | 117.38      | 121.90   |
| 35  | BB    | 2268 | A    | N3-C4-C5   | -11.30 | 118.89      | 126.80   |
| 35  | BB    | 2482 | A    | C5-C6-N6   | -11.29 | 114.67      | 123.70   |
| 35  | BB    | 583  | G    | O4'-C1'-N9 | 11.29  | 117.23      | 108.20   |
| 35  | BB    | 699  | A    | C5-C6-N1   | -11.29 | 112.05      | 117.70   |
| 35  | BB    | 2738 | A    | N9-C4-C5   | -11.29 | 101.28      | 105.80   |
| 1   | AA    | 62   | U    | C5-C6-N1   | -11.29 | 117.06      | 122.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1678 | A    | C5-C6-N6   | -11.29 | 114.67      | 123.70   |
| 35  | BB    | 1899 | A    | N1-C6-N6   | 11.29  | 125.37      | 118.60   |
| 1   | AA    | 598  | U    | O4'-C1'-N1 | 11.29  | 117.23      | 108.20   |
| 35  | BB    | 1960 | A    | C5-C6-N6   | -11.28 | 114.67      | 123.70   |
| 35  | BB    | 2585 | U    | C5-C4-O4   | -11.28 | 119.13      | 125.90   |
| 35  | BB    | 2211 | A    | C4-C5-C6   | 11.28  | 122.64      | 117.00   |
| 34  | BA    | 67   | G    | C8-N9-C4   | -11.28 | 101.89      | 106.40   |
| 1   | AA    | 330  | C    | N3-C4-C5   | -11.28 | 117.39      | 121.90   |
| 1   | AA    | 550  | G    | C5-C6-N1   | -11.28 | 105.86      | 111.50   |
| 35  | BB    | 2269 | G    | N1-C6-O6   | 11.28  | 126.67      | 119.90   |
| 1   | AA    | 150  | U    | C5-C4-O4   | -11.28 | 119.14      | 125.90   |
| 1   | AA    | 820  | U    | C5-C4-O4   | -11.28 | 119.13      | 125.90   |
| 35  | BB    | 2759 | G    | C6-C5-N7   | -11.28 | 123.63      | 130.40   |
| 1   | AA    | 71   | A    | N7-C8-N9   | -11.27 | 108.16      | 113.80   |
| 22  | AV    | 69   | G    | O4'-C1'-N9 | 11.27  | 117.22      | 108.20   |
| 35  | BB    | 94   | A    | C5-C6-N6   | -11.27 | 114.68      | 123.70   |
| 35  | BB    | 968  | C    | C6-N1-C2   | 11.27  | 124.81      | 120.30   |
| 35  | BB    | 2032 | G    | N1-C6-O6   | 11.27  | 126.66      | 119.90   |
| 35  | BB    | 2249 | U    | O4'-C1'-N1 | 11.27  | 117.22      | 108.20   |
| 35  | BB    | 2506 | U    | O4'-C1'-N1 | 11.27  | 117.22      | 108.20   |
| 35  | BB    | 1419 | A    | N9-C4-C5   | 11.27  | 110.31      | 105.80   |
| 35  | BB    | 2063 | C    | O4'-C1'-N1 | 11.27  | 117.21      | 108.20   |
| 35  | BB    | 2424 | C    | C6-N1-C2   | 11.27  | 124.81      | 120.30   |
| 1   | AA    | 284  | C    | O4'-C1'-N1 | 11.26  | 117.21      | 108.20   |
| 1   | AA    | 1475 | G    | O4'-C1'-N9 | 11.26  | 117.21      | 108.20   |
| 35  | BB    | 2534 | A    | N1-C6-N6   | 11.26  | 125.36      | 118.60   |
| 1   | AA    | 374  | A    | N1-C6-N6   | 11.26  | 125.36      | 118.60   |
| 35  | BB    | 1366 | A    | N1-C6-N6   | 11.26  | 125.36      | 118.60   |
| 35  | BB    | 2065 | C    | C4-C5-C6   | 11.26  | 123.03      | 117.40   |
| 1   | AA    | 623  | C    | N3-C4-C5   | -11.26 | 117.40      | 121.90   |
| 35  | BB    | 484  | C    | C4-C5-C6   | 11.26  | 123.03      | 117.40   |
| 35  | BB    | 1728 | C    | C4-C5-C6   | 11.26  | 123.03      | 117.40   |
| 1   | AA    | 778  | G    | N1-C2-N3   | -11.26 | 117.15      | 123.90   |
| 35  | BB    | 324  | A    | C4-C5-C6   | 11.26  | 122.63      | 117.00   |
| 35  | BB    | 549  | G    | N1-C6-O6   | 11.26  | 126.65      | 119.90   |
| 35  | BB    | 1718 | G    | C5-C6-O6   | -11.26 | 121.85      | 128.60   |
| 35  | BB    | 2623 | G    | N1-C2-N3   | -11.26 | 117.15      | 123.90   |
| 35  | BB    | 1621 | U    | O4'-C1'-N1 | 11.25  | 117.20      | 108.20   |
| 35  | BB    | 1900 | A    | C5-C6-N6   | -11.25 | 114.70      | 123.70   |
| 35  | BB    | 1969 | A    | C4-C5-C6   | 11.25  | 122.62      | 117.00   |
| 35  | BB    | 2012 | G    | O4'-C1'-N9 | 11.25  | 117.20      | 108.20   |
| 1   | AA    | 484  | G    | C5-C6-N1   | -11.25 | 105.88      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 564  | C    | C6-N1-C2   | -11.25 | 115.80      | 120.30   |
| 6   | AF    | 86   | ARG  | NE-CZ-NH2  | -11.25 | 114.68      | 120.30   |
| 35  | BB    | 1161 | C    | N3-C4-N4   | 11.25  | 125.87      | 118.00   |
| 1   | AA    | 1016 | A    | C5-C6-N1   | -11.24 | 112.08      | 117.70   |
| 35  | BB    | 1440 | U    | O4'-C1'-N1 | 11.24  | 117.19      | 108.20   |
| 1   | AA    | 808  | C    | C2-N3-C4   | 11.24  | 125.52      | 119.90   |
| 35  | BB    | 221  | A    | C4-C5-C6   | 11.24  | 122.62      | 117.00   |
| 1   | AA    | 979  | C    | P-O3'-C3'  | 11.24  | 133.19      | 119.70   |
| 35  | BB    | 23   | G    | C5-C6-O6   | -11.24 | 121.86      | 128.60   |
| 35  | BB    | 781  | A    | N9-C4-C5   | 11.24  | 110.30      | 105.80   |
| 35  | BB    | 2859 | G    | C5-C6-O6   | -11.24 | 121.86      | 128.60   |
| 1   | AA    | 385  | C    | C6-N1-C2   | -11.23 | 115.81      | 120.30   |
| 1   | AA    | 838  | G    | C5-C6-O6   | -11.23 | 121.86      | 128.60   |
| 35  | BB    | 2679 | A    | N1-C6-N6   | 11.23  | 125.34      | 118.60   |
| 1   | AA    | 821  | G    | N1-C6-O6   | 11.23  | 126.64      | 119.90   |
| 35  | BB    | 1743 | G    | N1-C6-O6   | 11.23  | 126.64      | 119.90   |
| 1   | AA    | 42   | G    | N1-C6-O6   | 11.23  | 126.64      | 119.90   |
| 1   | AA    | 1166 | G    | C5-C6-O6   | -11.23 | 121.86      | 128.60   |
| 35  | BB    | 682  | G    | C5-C6-O6   | -11.23 | 121.86      | 128.60   |
| 35  | BB    | 2407 | A    | C8-N9-C4   | -11.23 | 101.31      | 105.80   |
| 35  | BB    | 1834 | U    | O4'-C1'-N1 | 11.23  | 117.18      | 108.20   |
| 35  | BB    | 2331 | G    | C6-C5-N7   | -11.23 | 123.66      | 130.40   |
| 35  | BB    | 2835 | A    | C4-C5-N7   | -11.23 | 105.09      | 110.70   |
| 1   | AA    | 1360 | A    | N1-C6-N6   | 11.22  | 125.33      | 118.60   |
| 35  | BB    | 182  | A    | N1-C6-N6   | 11.22  | 125.33      | 118.60   |
| 35  | BB    | 1461 | C    | O4'-C1'-N1 | 11.22  | 117.18      | 108.20   |
| 35  | BB    | 624  | C    | N3-C4-C5   | -11.22 | 117.41      | 121.90   |
| 35  | BB    | 948  | C    | C5-C4-N4   | -11.22 | 112.34      | 120.20   |
| 35  | BB    | 1789 | A    | O4'-C1'-N9 | 11.22  | 117.18      | 108.20   |
| 35  | BB    | 68   | G    | N1-C2-N3   | -11.22 | 117.17      | 123.90   |
| 1   | AA    | 178  | C    | N3-C4-C5   | -11.22 | 117.41      | 121.90   |
| 1   | AA    | 319  | G    | O4'-C1'-N9 | 11.21  | 117.17      | 108.20   |
| 35  | BB    | 290  | U    | C5-C4-O4   | -11.21 | 119.17      | 125.90   |
| 35  | BB    | 679  | C    | O4'-C1'-N1 | 11.21  | 117.17      | 108.20   |
| 35  | BB    | 138  | U    | O4'-C1'-N1 | 11.21  | 117.17      | 108.20   |
| 35  | BB    | 1424 | G    | N1-C2-N3   | -11.21 | 117.17      | 123.90   |
| 35  | BB    | 1642 | G    | C5-C6-O6   | -11.21 | 121.87      | 128.60   |
| 35  | BB    | 2007 | U    | O4'-C1'-N1 | 11.21  | 117.17      | 108.20   |
| 35  | BB    | 2828 | G    | N1-C6-O6   | 11.21  | 126.63      | 119.90   |
| 35  | BB    | 1682 | G    | N1-C2-N3   | -11.21 | 117.17      | 123.90   |
| 35  | BB    | 43   | G    | C6-C5-N7   | -11.20 | 123.68      | 130.40   |
| 35  | BB    | 1754 | A    | C5-C6-N6   | -11.20 | 114.74      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2029 | G    | N1-C6-O6   | 11.20  | 126.62      | 119.90   |
| 35  | BB    | 2389 | G    | C8-N9-C4   | -11.20 | 101.92      | 106.40   |
| 35  | BB    | 2560 | A    | N9-C4-C5   | 11.20  | 110.28      | 105.80   |
| 49  | BP    | 92   | ARG  | NE-CZ-NH2  | -11.20 | 114.70      | 120.30   |
| 35  | BB    | 716  | A    | C6-C5-N7   | -11.20 | 124.46      | 132.30   |
| 35  | BB    | 2046 | G    | N1-C6-O6   | 11.20  | 126.62      | 119.90   |
| 1   | AA    | 568  | G    | C5-C6-O6   | -11.19 | 121.88      | 128.60   |
| 35  | BB    | 775  | G    | N3-C2-N2   | 11.19  | 127.74      | 119.90   |
| 35  | BB    | 1462 | C    | C5-C6-N1   | 11.20  | 126.60      | 121.00   |
| 1   | AA    | 1430 | A    | N1-C6-N6   | 11.19  | 125.32      | 118.60   |
| 16  | AP    | 31   | ARG  | NE-CZ-NH2  | 11.19  | 125.90      | 120.30   |
| 35  | BB    | 471  | A    | C5-C6-N1   | -11.19 | 112.10      | 117.70   |
| 35  | BB    | 1297 | C    | O4'-C1'-N1 | 11.19  | 117.15      | 108.20   |
| 35  | BB    | 2565 | A    | N1-C2-N3   | -11.19 | 123.70      | 129.30   |
| 1   | AA    | 86   | G    | C5-C6-O6   | -11.19 | 121.89      | 128.60   |
| 1   | AA    | 1215 | G    | N1-C6-O6   | 11.19  | 126.61      | 119.90   |
| 1   | AA    | 1241 | G    | O4'-C1'-N9 | 11.19  | 117.15      | 108.20   |
| 35  | BB    | 713  | G    | N1-C6-O6   | 11.19  | 126.61      | 119.90   |
| 35  | BB    | 1433 | A    | N1-C6-N6   | 11.19  | 125.31      | 118.60   |
| 35  | BB    | 38   | A    | C5-C6-N6   | -11.19 | 114.75      | 123.70   |
| 1   | AA    | 258  | G    | C5-C6-O6   | -11.18 | 121.89      | 128.60   |
| 35  | BB    | 163  | C    | O4'-C1'-N1 | 11.18  | 117.14      | 108.20   |
| 35  | BB    | 1975 | G    | C6-C5-N7   | -11.18 | 123.69      | 130.40   |
| 47  | BN    | 2    | ARG  | NE-CZ-NH1  | 11.18  | 125.89      | 120.30   |
| 35  | BB    | 1167 | C    | O4'-C1'-N1 | 11.18  | 117.14      | 108.20   |
| 1   | AA    | 1405 | G    | N3-C2-N2   | 11.18  | 127.72      | 119.90   |
| 35  | BB    | 2516 | A    | O4'-C1'-N9 | 11.18  | 117.14      | 108.20   |
| 1   | AA    | 1190 | G    | C5-C6-O6   | -11.17 | 121.90      | 128.60   |
| 35  | BB    | 126  | A    | N1-C6-N6   | 11.17  | 125.30      | 118.60   |
| 35  | BB    | 1362 | C    | C5-C4-N4   | -11.17 | 112.38      | 120.20   |
| 1   | AA    | 537  | G    | N1-C6-O6   | 11.17  | 126.60      | 119.90   |
| 1   | AA    | 888  | G    | C5-C6-N1   | -11.17 | 105.92      | 111.50   |
| 1   | AA    | 1175 | G    | C5-C6-O6   | -11.17 | 121.90      | 128.60   |
| 35  | BB    | 707  | G    | C5-N7-C8   | 11.17  | 109.88      | 104.30   |
| 35  | BB    | 2532 | G    | N1-C6-O6   | 11.17  | 126.60      | 119.90   |
| 34  | BA    | 116  | G    | N1-C6-O6   | 11.17  | 126.60      | 119.90   |
| 1   | AA    | 327  | A    | N9-C4-C5   | 11.17  | 110.27      | 105.80   |
| 1   | AA    | 128  | G    | N3-C2-N2   | 11.16  | 127.72      | 119.90   |
| 34  | BA    | 15   | A    | C5-C6-N1   | -11.16 | 112.12      | 117.70   |
| 35  | BB    | 1760 | C    | N3-C4-C5   | -11.16 | 117.44      | 121.90   |
| 35  | BB    | 2012 | G    | C4-C5-C6   | 11.16  | 125.50      | 118.80   |
| 1   | AA    | 111  | G    | O4'-C1'-N9 | 11.16  | 117.13      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 1435 | G    | N1-C6-O6   | 11.16  | 126.59      | 119.90   |
| 35  | BB    | 1746 | A    | N1-C6-N6   | 11.16  | 125.29      | 118.60   |
| 35  | BB    | 2227 | A    | C8-N9-C4   | -11.16 | 101.34      | 105.80   |
| 1   | AA    | 251  | G    | C5-C6-O6   | -11.15 | 121.91      | 128.60   |
| 35  | BB    | 104  | A    | C4-C5-C6   | 11.15  | 122.58      | 117.00   |
| 35  | BB    | 2476 | A    | C4-C5-C6   | 11.15  | 122.58      | 117.00   |
| 1   | AA    | 372  | C    | N3-C4-N4   | 11.15  | 125.80      | 118.00   |
| 39  | BF    | 114  | ARG  | NE-CZ-NH1  | -11.15 | 114.73      | 120.30   |
| 40  | BG    | 148  | ARG  | NE-CZ-NH2  | -11.15 | 114.73      | 120.30   |
| 1   | AA    | 145  | G    | N1-C6-O6   | 11.14  | 126.59      | 119.90   |
| 1   | AA    | 211  | G    | O4'-C1'-N9 | 11.14  | 117.11      | 108.20   |
| 1   | AA    | 814  | A    | C5-C6-N6   | -11.14 | 114.78      | 123.70   |
| 35  | BB    | 899  | A    | N1-C6-N6   | 11.14  | 125.28      | 118.60   |
| 1   | AA    | 144  | G    | O4'-C1'-N9 | 11.14  | 117.11      | 108.20   |
| 1   | AA    | 766  | A    | C5-C6-N1   | -11.14 | 112.13      | 117.70   |
| 34  | BA    | 39   | A    | C5-C6-N6   | -11.14 | 114.79      | 123.70   |
| 35  | BB    | 1527 | G    | C5-C6-O6   | -11.13 | 121.92      | 128.60   |
| 1   | AA    | 1409 | C    | C6-N1-C2   | -11.13 | 115.85      | 120.30   |
| 35  | BB    | 97   | C    | N3-C4-C5   | -11.13 | 117.45      | 121.90   |
| 34  | BA    | 21   | G    | O4'-C1'-N9 | 11.13  | 117.10      | 108.20   |
| 35  | BB    | 2078 | C    | N3-C4-N4   | 11.13  | 125.79      | 118.00   |
| 1   | AA    | 1426 | G    | C5-C6-O6   | -11.12 | 121.93      | 128.60   |
| 35  | BB    | 1496 | A    | C2-N3-C4   | 11.12  | 116.16      | 110.60   |
| 35  | BB    | 1968 | G    | N9-C4-C5   | -11.12 | 100.95      | 105.40   |
| 35  | BB    | 2271 | G    | N1-C6-O6   | 11.12  | 126.58      | 119.90   |
| 1   | AA    | 577  | G    | C6-C5-N7   | -11.12 | 123.73      | 130.40   |
| 35  | BB    | 2822 | G    | C5-N7-C8   | 11.12  | 109.86      | 104.30   |
| 1   | AA    | 56   | U    | O4'-C1'-N1 | 11.12  | 117.09      | 108.20   |
| 1   | AA    | 930  | C    | C6-N1-C2   | -11.12 | 115.85      | 120.30   |
| 35  | BB    | 821  | A    | N9-C4-C5   | 11.12  | 110.25      | 105.80   |
| 1   | AA    | 799  | G    | O4'-C1'-N9 | 11.12  | 117.09      | 108.20   |
| 1   | AA    | 961  | U    | O4'-C1'-N1 | 11.12  | 117.09      | 108.20   |
| 1   | AA    | 1421 | G    | N3-C2-N2   | 11.11  | 127.68      | 119.90   |
| 35  | BB    | 449  | A    | N1-C6-N6   | 11.11  | 125.27      | 118.60   |
| 35  | BB    | 476  | G    | C6-N1-C2   | -11.11 | 118.43      | 125.10   |
| 35  | BB    | 593  | U    | O4'-C1'-N1 | 11.11  | 117.09      | 108.20   |
| 1   | AA    | 1100 | C    | O4'-C1'-N1 | 11.11  | 117.09      | 108.20   |
| 1   | AA    | 1288 | A    | N7-C8-N9   | 11.11  | 119.35      | 113.80   |
| 35  | BB    | 1575 | C    | N3-C4-C5   | -11.11 | 117.46      | 121.90   |
| 35  | BB    | 2789 | C    | N3-C4-N4   | 11.11  | 125.78      | 118.00   |
| 36  | BC    | 160  | TYR  | CB-CG-CD2  | 11.11  | 127.67      | 121.00   |
| 35  | BB    | 2564 | A    | C4-C5-C6   | 11.11  | 122.55      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 34  | BA    | 41   | G    | O4'-C1'-N9 | 11.10  | 117.08      | 108.20   |
| 35  | BB    | 2805 | C    | O4'-C1'-N1 | 11.10  | 117.08      | 108.20   |
| 1   | AA    | 562  | U    | O4'-C1'-N1 | 11.10  | 117.08      | 108.20   |
| 1   | AA    | 987  | G    | N3-C4-C5   | -11.10 | 123.05      | 128.60   |
| 35  | BB    | 1413 | A    | O4'-C1'-N9 | 11.10  | 117.08      | 108.20   |
| 1   | AA    | 828  | U    | O4'-C1'-N1 | 11.10  | 117.08      | 108.20   |
| 35  | BB    | 1398 | C    | N1-C2-O2   | 11.10  | 125.56      | 118.90   |
| 3   | AC    | 183  | TYR  | CB-CG-CD2  | -11.10 | 114.34      | 121.00   |
| 35  | BB    | 547  | A    | C5-C6-N1   | -11.10 | 112.15      | 117.70   |
| 35  | BB    | 2616 | C    | O4'-C1'-N1 | 11.10  | 117.08      | 108.20   |
| 35  | BB    | 216  | A    | N1-C6-N6   | 11.10  | 125.26      | 118.60   |
| 1   | AA    | 247  | G    | O4'-C1'-N9 | 11.09  | 117.08      | 108.20   |
| 35  | BB    | 815  | C    | O4'-C1'-N1 | 11.09  | 117.07      | 108.20   |
| 35  | BB    | 2740 | A    | C5-C6-N6   | -11.09 | 114.83      | 123.70   |
| 1   | AA    | 214  | C    | C2-N3-C4   | 11.09  | 125.44      | 119.90   |
| 1   | AA    | 761  | G    | C5-C6-O6   | -11.09 | 121.95      | 128.60   |
| 1   | AA    | 1352 | C    | N3-C4-C5   | -11.09 | 117.46      | 121.90   |
| 35  | BB    | 317  | G    | C5-C6-O6   | -11.09 | 121.94      | 128.60   |
| 35  | BB    | 1049 | C    | N3-C4-N4   | 11.09  | 125.76      | 118.00   |
| 35  | BB    | 1256 | G    | C5-C6-O6   | -11.09 | 121.95      | 128.60   |
| 35  | BB    | 1279 | G    | N1-C6-O6   | 11.09  | 126.56      | 119.90   |
| 35  | BB    | 2111 | U    | N3-C4-O4   | 11.09  | 127.16      | 119.40   |
| 1   | AA    | 259  | G    | O4'-C1'-N9 | 11.09  | 117.07      | 108.20   |
| 35  | BB    | 2714 | G    | O4'-C1'-N9 | 11.09  | 117.07      | 108.20   |
| 1   | AA    | 205  | A    | C4-C5-C6   | 11.08  | 122.54      | 117.00   |
| 1   | AA    | 745  | G    | N1-C6-O6   | 11.08  | 126.55      | 119.90   |
| 35  | BB    | 1918 | A    | C4-C5-C6   | 11.08  | 122.54      | 117.00   |
| 1   | AA    | 470  | C    | N3-C4-C5   | -11.08 | 117.47      | 121.90   |
| 35  | BB    | 2063 | C    | C2-N3-C4   | 11.08  | 125.44      | 119.90   |
| 35  | BB    | 202  | U    | O4'-C1'-N1 | 11.08  | 117.06      | 108.20   |
| 35  | BB    | 696  | G    | O4'-C1'-N9 | 11.07  | 117.06      | 108.20   |
| 35  | BB    | 191  | A    | C4-C5-C6   | 11.07  | 122.54      | 117.00   |
| 35  | BB    | 766  | U    | C4-C5-C6   | 11.07  | 126.34      | 119.70   |
| 35  | BB    | 1196 | C    | N3-C4-C5   | -11.07 | 117.47      | 121.90   |
| 35  | BB    | 2454 | G    | N1-C6-O6   | 11.07  | 126.54      | 119.90   |
| 35  | BB    | 2391 | G    | O4'-C1'-N9 | 11.07  | 117.06      | 108.20   |
| 35  | BB    | 2425 | A    | N1-C6-N6   | 11.07  | 125.24      | 118.60   |
| 35  | BB    | 996  | A    | C5-C6-N6   | -11.07 | 114.85      | 123.70   |
| 35  | BB    | 1496 | A    | N9-C4-C5   | 11.07  | 110.23      | 105.80   |
| 1   | AA    | 524  | G    | C5-C6-O6   | -11.06 | 121.96      | 128.60   |
| 1   | AA    | 639  | G    | N1-C6-O6   | 11.06  | 126.54      | 119.90   |
| 7   | AG    | 77   | ARG  | NE-CZ-NH2  | -11.06 | 114.77      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 124  | G    | C4-C5-N7   | -11.06 | 106.37      | 110.80   |
| 35  | BB    | 2788 | C    | O4'-C1'-N1 | 11.06  | 117.05      | 108.20   |
| 35  | BB    | 176  | A    | N1-C6-N6   | 11.06  | 125.24      | 118.60   |
| 1   | AA    | 714  | G    | C5-C6-O6   | -11.06 | 121.96      | 128.60   |
| 12  | AL    | 53   | ARG  | NE-CZ-NH1  | 11.06  | 125.83      | 120.30   |
| 35  | BB    | 1519 | G    | N3-C2-N2   | 11.06  | 127.64      | 119.90   |
| 1   | AA    | 1169 | A    | C5-C6-N1   | -11.06 | 112.17      | 117.70   |
| 19  | AS    | 80   | ARG  | NE-CZ-NH1  | 11.06  | 125.83      | 120.30   |
| 34  | BA    | 35   | C    | C2-N1-C1'  | 11.06  | 130.96      | 118.80   |
| 34  | BA    | 34   | A    | C5-C6-N1   | -11.06 | 112.17      | 117.70   |
| 1   | AA    | 1206 | G    | C4-C5-N7   | 11.05  | 115.22      | 110.80   |
| 35  | BB    | 64   | A    | N1-C6-N6   | 11.05  | 125.23      | 118.60   |
| 35  | BB    | 1861 | G    | O4'-C1'-N9 | 11.05  | 117.04      | 108.20   |
| 35  | BB    | 2837 | A    | C5-C6-N6   | -11.05 | 114.86      | 123.70   |
| 1   | AA    | 201  | G    | N1-C2-N3   | -11.05 | 117.27      | 123.90   |
| 35  | BB    | 2839 | G    | O4'-C1'-N9 | 11.05  | 117.04      | 108.20   |
| 1   | AA    | 48   | C    | C2-N3-C4   | 11.05  | 125.42      | 119.90   |
| 1   | AA    | 774  | G    | N9-C4-C5   | 11.05  | 109.82      | 105.40   |
| 1   | AA    | 970  | C    | N3-C4-N4   | 11.05  | 125.73      | 118.00   |
| 40  | BG    | 148  | ARG  | NE-CZ-NH1  | 11.05  | 125.82      | 120.30   |
| 1   | AA    | 887  | G    | C5-C6-O6   | -11.04 | 121.97      | 128.60   |
| 35  | BB    | 95   | A    | C5-C6-N6   | -11.04 | 114.86      | 123.70   |
| 35  | BB    | 715  | A    | C5-C6-N6   | -11.04 | 114.86      | 123.70   |
| 35  | BB    | 1353 | A    | C5-C6-N1   | -11.04 | 112.18      | 117.70   |
| 40  | BG    | 34   | ARG  | NE-CZ-NH1  | 11.04  | 125.82      | 120.30   |
| 35  | BB    | 371  | A    | C5-C6-N1   | -11.04 | 112.18      | 117.70   |
| 35  | BB    | 2168 | G    | C5-C6-O6   | -11.04 | 121.97      | 128.60   |
| 1   | AA    | 594  | U    | O4'-C1'-N1 | 11.04  | 117.03      | 108.20   |
| 1   | AA    | 825  | A    | N7-C8-N9   | 11.04  | 119.32      | 113.80   |
| 1   | AA    | 1365 | G    | C4-C5-N7   | 11.04  | 115.22      | 110.80   |
| 35  | BB    | 885  | C    | O4'-C1'-N1 | 11.04  | 117.03      | 108.20   |
| 35  | BB    | 1500 | G    | N3-C4-C5   | -11.04 | 123.08      | 128.60   |
| 35  | BB    | 1901 | A    | C4-C5-C6   | 11.04  | 122.52      | 117.00   |
| 35  | BB    | 2688 | G    | C5-C6-O6   | -11.04 | 121.98      | 128.60   |
| 1   | AA    | 759  | A    | O4'-C1'-N9 | 11.04  | 117.03      | 108.20   |
| 35  | BB    | 2637 | U    | O4'-C1'-N1 | 11.04  | 117.03      | 108.20   |
| 34  | BA    | 110  | C    | N3-C4-N4   | 11.03  | 125.72      | 118.00   |
| 35  | BB    | 2864 | G    | O4'-C1'-N9 | 11.03  | 117.03      | 108.20   |
| 32  | B7    | 7    | ARG  | NE-CZ-NH2  | -11.03 | 114.78      | 120.30   |
| 35  | BB    | 1326 | U    | O4'-C1'-N1 | 11.03  | 117.03      | 108.20   |
| 35  | BB    | 2018 | G    | C5-C6-O6   | -11.03 | 121.98      | 128.60   |
| 35  | BB    | 857  | G    | N1-C2-N3   | -11.03 | 117.28      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 360  | G    | O4'-C1'-N9 | 11.03  | 117.02      | 108.20   |
| 12  | AL    | 93   | ARG  | NE-CZ-NH1  | -11.03 | 114.79      | 120.30   |
| 1   | AA    | 1150 | A    | C4-C5-C6   | 11.03  | 122.51      | 117.00   |
| 30  | B5    | 111  | PHE  | CB-CG-CD2  | -11.03 | 113.08      | 120.80   |
| 35  | BB    | 739  | A    | C8-N9-C4   | -11.03 | 101.39      | 105.80   |
| 1   | AA    | 49   | U    | C5-C4-O4   | 11.02  | 132.51      | 125.90   |
| 6   | AF    | 38   | ARG  | NE-CZ-NH1  | 11.02  | 125.81      | 120.30   |
| 35  | BB    | 2811 | G    | O4'-C1'-N9 | 11.02  | 117.02      | 108.20   |
| 35  | BB    | 794  | A    | N1-C6-N6   | 11.02  | 125.21      | 118.60   |
| 1   | AA    | 148  | G    | C4-C5-N7   | 11.02  | 115.21      | 110.80   |
| 1   | AA    | 838  | G    | O4'-C1'-N9 | 11.02  | 117.01      | 108.20   |
| 35  | BB    | 547  | A    | N1-C6-N6   | 11.02  | 125.21      | 118.60   |
| 35  | BB    | 645  | C    | C2-N3-C4   | 11.02  | 125.41      | 119.90   |
| 35  | BB    | 979  | A    | N1-C6-N6   | 11.02  | 125.21      | 118.60   |
| 35  | BB    | 1287 | A    | O4'-C1'-N9 | 11.02  | 117.02      | 108.20   |
| 35  | BB    | 1432 | G    | C5-C6-O6   | -11.02 | 121.99      | 128.60   |
| 1   | AA    | 1504 | G    | N1-C6-O6   | 11.02  | 126.51      | 119.90   |
| 35  | BB    | 787  | C    | O4'-C1'-N1 | 11.02  | 117.01      | 108.20   |
| 35  | BB    | 430  | A    | N1-C6-N6   | 11.01  | 125.21      | 118.60   |
| 1   | AA    | 505  | G    | N3-C2-N2   | 11.01  | 127.61      | 119.90   |
| 1   | AA    | 909  | A    | C6-C5-N7   | -11.01 | 124.59      | 132.30   |
| 1   | AA    | 1171 | A    | O4'-C1'-N9 | 11.01  | 117.01      | 108.20   |
| 35  | BB    | 181  | A    | C5-C6-N6   | -11.01 | 114.89      | 123.70   |
| 35  | BB    | 788  | A    | C4-C5-C6   | 11.01  | 122.50      | 117.00   |
| 1   | AA    | 1312 | G    | C5-C6-N1   | -11.01 | 106.00      | 111.50   |
| 1   | AA    | 1394 | A    | C5-C6-N6   | -11.01 | 114.89      | 123.70   |
| 35  | BB    | 582  | A    | N1-C6-N6   | 11.01  | 125.20      | 118.60   |
| 35  | BB    | 1681 | G    | C5-C6-O6   | -11.01 | 122.00      | 128.60   |
| 35  | BB    | 2031 | A    | C5-C6-N6   | -11.01 | 114.89      | 123.70   |
| 35  | BB    | 341  | C    | N3-C4-N4   | 11.01  | 125.70      | 118.00   |
| 35  | BB    | 741  | U    | N3-C4-O4   | 11.01  | 127.10      | 119.40   |
| 35  | BB    | 1292 | G    | C5-C6-O6   | -11.01 | 122.00      | 128.60   |
| 1   | AA    | 193  | C    | O4'-C1'-N1 | 11.00  | 117.00      | 108.20   |
| 35  | BB    | 884  | U    | C5-C4-O4   | -11.00 | 119.30      | 125.90   |
| 35  | BB    | 2119 | A    | C4-C5-C6   | 11.00  | 122.50      | 117.00   |
| 46  | BM    | 66   | ARG  | NE-CZ-NH1  | 11.00  | 125.80      | 120.30   |
| 1   | AA    | 741  | G    | N1-C6-O6   | 11.00  | 126.50      | 119.90   |
| 35  | BB    | 1310 | G    | N1-C6-O6   | 11.00  | 126.50      | 119.90   |
| 35  | BB    | 254  | G    | C8-N9-C4   | -11.00 | 102.00      | 106.40   |
| 1   | AA    | 221  | C    | N3-C4-C5   | -11.00 | 117.50      | 121.90   |
| 35  | BB    | 2868 | A    | O4'-C1'-N9 | 11.00  | 117.00      | 108.20   |
| 1   | AA    | 714  | G    | C4-C5-N7   | 10.99  | 115.20      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1   | AA    | 940  | C    | N3-C4-N4    | 10.99  | 125.70      | 118.00   |
| 35  | BB    | 1850 | G    | C5-C6-O6    | -10.99 | 122.00      | 128.60   |
| 35  | BB    | 263  | G    | C6-C5-N7    | -10.99 | 123.81      | 130.40   |
| 35  | BB    | 924  | G    | C6-C5-N7    | -10.99 | 123.81      | 130.40   |
| 35  | BB    | 2254 | C    | O4'-C1'-N1  | 10.99  | 117.00      | 108.20   |
| 35  | BB    | 2693 | G    | N1-C6-O6    | 10.99  | 126.50      | 119.90   |
| 35  | BB    | 2355 | G    | C5-C6-O6    | -10.99 | 122.01      | 128.60   |
| 1   | AA    | 1019 | A    | C4-C5-C6    | 10.99  | 122.50      | 117.00   |
| 1   | AA    | 1159 | U    | O4'-C1'-N1  | 10.99  | 116.99      | 108.20   |
| 35  | BB    | 1028 | A    | C4-C5-C6    | 10.99  | 122.49      | 117.00   |
| 35  | BB    | 2223 | G    | N1-C6-O6    | 10.99  | 126.49      | 119.90   |
| 1   | AA    | 40   | C    | N3-C4-C5    | -10.98 | 117.51      | 121.90   |
| 35  | BB    | 43   | G    | N1-C6-O6    | 10.98  | 126.49      | 119.90   |
| 35  | BB    | 153  | U    | O4'-C1'-N1  | 10.98  | 116.99      | 108.20   |
| 35  | BB    | 1253 | A    | N1-C6-N6    | 10.98  | 125.19      | 118.60   |
| 35  | BB    | 2570 | G    | N9-C4-C5    | 10.98  | 109.79      | 105.40   |
| 1   | AA    | 693  | G    | O4'-C1'-N9  | 10.98  | 116.98      | 108.20   |
| 1   | AA    | 442  | G    | O4'-C1'-N9  | 10.97  | 116.98      | 108.20   |
| 1   | AA    | 592  | G    | N1-C6-O6    | 10.97  | 126.48      | 119.90   |
| 1   | AA    | 1310 | G    | O4'-C1'-N9  | 10.97  | 116.98      | 108.20   |
| 35  | BB    | 1075 | C    | C5-C4-N4    | -10.97 | 112.52      | 120.20   |
| 35  | BB    | 363  | G    | C5-C6-O6    | -10.97 | 122.02      | 128.60   |
| 35  | BB    | 431  | U    | C5-C4-O4    | 10.97  | 132.48      | 125.90   |
| 35  | BB    | 1088 | A    | O4'-C1'-C2' | -10.97 | 94.83       | 105.80   |
| 35  | BB    | 1521 | G    | N1-C6-O6    | 10.97  | 126.48      | 119.90   |
| 35  | BB    | 2172 | U    | O4'-C1'-N1  | 10.97  | 116.98      | 108.20   |
| 35  | BB    | 1410 | G    | N1-C6-O6    | 10.97  | 126.48      | 119.90   |
| 35  | BB    | 1533 | C    | N3-C4-C5    | -10.97 | 117.51      | 121.90   |
| 1   | AA    | 297  | G    | C5-C6-O6    | -10.96 | 122.02      | 128.60   |
| 1   | AA    | 1499 | A    | N1-C6-N6    | 10.96  | 125.18      | 118.60   |
| 35  | BB    | 1756 | G    | N7-C8-N9    | -10.96 | 107.62      | 113.10   |
| 1   | AA    | 57   | G    | C5-C6-O6    | -10.96 | 122.02      | 128.60   |
| 1   | AA    | 1253 | G    | N3-C4-C5    | 10.96  | 134.08      | 128.60   |
| 35  | BB    | 1408 | G    | C4-C5-C6    | 10.96  | 125.38      | 118.80   |
| 35  | BB    | 472  | A    | N1-C6-N6    | 10.96  | 125.17      | 118.60   |
| 1   | AA    | 1028 | C    | N1-C2-O2    | 10.96  | 125.47      | 118.90   |
| 35  | BB    | 1512 | C    | O4'-C1'-N1  | 10.96  | 116.96      | 108.20   |
| 35  | BB    | 1870 | C    | N3-C4-C5    | -10.95 | 117.52      | 121.90   |
| 1   | AA    | 212  | G    | C5-C6-O6    | -10.95 | 122.03      | 128.60   |
| 35  | BB    | 779  | U    | O4'-C1'-N1  | 10.95  | 116.96      | 108.20   |
| 35  | BB    | 1279 | G    | O4'-C1'-N9  | 10.95  | 116.96      | 108.20   |
| 35  | BB    | 2234 | G    | C5-C6-N1    | -10.95 | 106.02      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 283  | G    | C5-C6-O6   | -10.95 | 122.03      | 128.60   |
| 35  | BB    | 792  | A    | C5-C6-N1   | -10.95 | 112.22      | 117.70   |
| 35  | BB    | 548  | G    | C5-C6-O6   | -10.95 | 122.03      | 128.60   |
| 35  | BB    | 1582 | C    | C5-C4-N4   | -10.95 | 112.54      | 120.20   |
| 1   | AA    | 6    | G    | N1-C6-O6   | 10.94  | 126.47      | 119.90   |
| 1   | AA    | 897  | C    | C2-N3-C4   | 10.94  | 125.37      | 119.90   |
| 1   | AA    | 1110 | A    | N1-C6-N6   | 10.95  | 125.17      | 118.60   |
| 1   | AA    | 1404 | C    | C2-N1-C1'  | 10.94  | 130.84      | 118.80   |
| 35  | BB    | 2036 | C    | C6-N1-C2   | -10.94 | 115.92      | 120.30   |
| 35  | BB    | 2291 | U    | O4'-C1'-N1 | 10.95  | 116.96      | 108.20   |
| 35  | BB    | 2733 | A    | C5-C6-N1   | -10.95 | 112.23      | 117.70   |
| 35  | BB    | 1116 | G    | N1-C6-O6   | 10.94  | 126.47      | 119.90   |
| 35  | BB    | 2073 | C    | C2-N3-C4   | 10.94  | 125.37      | 119.90   |
| 1   | AA    | 1432 | G    | N1-C6-O6   | 10.94  | 126.46      | 119.90   |
| 22  | AV    | 6    | C    | C5-C6-N1   | 10.94  | 126.47      | 121.00   |
| 1   | AA    | 87   | C    | N3-C4-C5   | -10.94 | 117.53      | 121.90   |
| 1   | AA    | 745  | G    | C5-C6-O6   | -10.94 | 122.04      | 128.60   |
| 35  | BB    | 540  | C    | C5-C6-N1   | 10.94  | 126.47      | 121.00   |
| 35  | BB    | 1967 | C    | C2-N3-C4   | 10.94  | 125.37      | 119.90   |
| 35  | BB    | 1002 | G    | O4'-C1'-N9 | 10.93  | 116.95      | 108.20   |
| 1   | AA    | 347  | G    | N3-C2-N2   | 10.93  | 127.55      | 119.90   |
| 1   | AA    | 1459 | G    | C6-C5-N7   | -10.93 | 123.84      | 130.40   |
| 35  | BB    | 299  | A    | C4-C5-N7   | -10.93 | 105.23      | 110.70   |
| 35  | BB    | 352  | A    | C8-N9-C4   | -10.93 | 101.43      | 105.80   |
| 1   | AA    | 1322 | C    | C2-N1-C1'  | 10.93  | 130.82      | 118.80   |
| 35  | BB    | 865  | C    | N3-C4-N4   | 10.93  | 125.65      | 118.00   |
| 35  | BB    | 1043 | C    | O4'-C1'-N1 | 10.93  | 116.94      | 108.20   |
| 35  | BB    | 2854 | G    | O4'-C1'-N9 | 10.93  | 116.94      | 108.20   |
| 1   | AA    | 496  | A    | C4-C5-C6   | 10.93  | 122.46      | 117.00   |
| 1   | AA    | 75   | G    | C5-C6-O6   | -10.93 | 122.04      | 128.60   |
| 1   | AA    | 105  | G    | C5-C6-O6   | -10.93 | 122.04      | 128.60   |
| 1   | AA    | 1306 | A    | N1-C6-N6   | 10.93  | 125.16      | 118.60   |
| 22  | AV    | 5    | A    | N1-C6-N6   | 10.92  | 125.16      | 118.60   |
| 35  | BB    | 2226 | C    | C6-N1-C2   | -10.92 | 115.93      | 120.30   |
| 1   | AA    | 168  | G    | C4-C5-N7   | -10.92 | 106.43      | 110.80   |
| 35  | BB    | 180  | G    | N1-C2-N3   | -10.92 | 117.35      | 123.90   |
| 35  | BB    | 977  | G    | C5-C6-N1   | -10.92 | 106.04      | 111.50   |
| 35  | BB    | 1361 | G    | N3-C4-C5   | -10.92 | 123.14      | 128.60   |
| 1   | AA    | 710  | G    | C5-C6-O6   | -10.92 | 122.05      | 128.60   |
| 1   | AA    | 1366 | C    | C6-N1-C2   | -10.92 | 115.93      | 120.30   |
| 35  | BB    | 1366 | A    | C5-C6-N1   | -10.92 | 112.24      | 117.70   |
| 35  | BB    | 6    | A    | N1-C6-N6   | 10.91  | 125.15      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1   | AA    | 129  | A    | N9-C4-C5    | 10.91  | 110.17      | 105.80   |
| 1   | AA    | 1041 | G    | C6-C5-N7    | -10.91 | 123.85      | 130.40   |
| 34  | BA    | 72   | G    | C2-N3-C4    | 10.91  | 117.36      | 111.90   |
| 35  | BB    | 2365 | G    | C5-C6-N1    | -10.91 | 106.04      | 111.50   |
| 35  | BB    | 2747 | G    | N3-C2-N2    | 10.91  | 127.54      | 119.90   |
| 35  | BB    | 1413 | A    | N1-C6-N6    | 10.91  | 125.15      | 118.60   |
| 35  | BB    | 2412 | A    | N9-C4-C5    | 10.91  | 110.16      | 105.80   |
| 35  | BB    | 2430 | A    | C5-C6-N1    | -10.91 | 112.25      | 117.70   |
| 33  | B8    | 12   | ARG  | NE-CZ-NH1   | 10.91  | 125.75      | 120.30   |
| 34  | BA    | 84   | G    | C5-C6-O6    | -10.91 | 122.06      | 128.60   |
| 35  | BB    | 627  | A    | C5'-C4'-O4' | 10.91  | 122.19      | 109.10   |
| 35  | BB    | 950  | G    | N1-C6-O6    | 10.91  | 126.44      | 119.90   |
| 35  | BB    | 1650 | A    | C5-N7-C8    | 10.91  | 109.35      | 103.90   |
| 35  | BB    | 2857 | G    | C5-C6-O6    | -10.91 | 122.06      | 128.60   |
| 1   | AA    | 255  | G    | N1-C6-O6    | 10.90  | 126.44      | 119.90   |
| 1   | AA    | 1191 | A    | C5-C6-N1    | -10.90 | 112.25      | 117.70   |
| 35  | BB    | 2900 | A    | C6-C5-N7    | -10.90 | 124.67      | 132.30   |
| 35  | BB    | 1    | G    | N1-C6-O6    | 10.90  | 126.44      | 119.90   |
| 35  | BB    | 776  | G    | C4-C5-N7    | -10.90 | 106.44      | 110.80   |
| 35  | BB    | 988  | A    | N1-C6-N6    | 10.90  | 125.14      | 118.60   |
| 35  | BB    | 1367 | A    | C5-C6-N1    | -10.90 | 112.25      | 117.70   |
| 35  | BB    | 2886 | A    | O4'-C1'-N9  | 10.90  | 116.92      | 108.20   |
| 1   | AA    | 695  | A    | N1-C6-N6    | 10.90  | 125.14      | 118.60   |
| 35  | BB    | 1087 | G    | C5-C6-O6    | -10.90 | 122.06      | 128.60   |
| 35  | BB    | 2302 | U    | N3-C4-O4    | 10.90  | 127.03      | 119.40   |
| 1   | AA    | 224  | U    | O4'-C1'-N1  | 10.89  | 116.92      | 108.20   |
| 22  | AV    | 67   | G    | C5-C6-O6    | -10.89 | 122.06      | 128.60   |
| 35  | BB    | 1945 | G    | C8-N9-C4    | -10.89 | 102.04      | 106.40   |
| 35  | BB    | 1561 | C    | O4'-C1'-N1  | 10.89  | 116.92      | 108.20   |
| 1   | AA    | 66   | A    | N1-C6-N6    | 10.89  | 125.14      | 118.60   |
| 35  | BB    | 2550 | G    | C4-C5-C6    | 10.89  | 125.33      | 118.80   |
| 1   | AA    | 456  | A    | N1-C6-N6    | 10.89  | 125.13      | 118.60   |
| 1   | AA    | 1504 | G    | C5-C6-O6    | -10.89 | 122.07      | 128.60   |
| 35  | BB    | 4    | U    | O4'-C1'-N1  | 10.89  | 116.91      | 108.20   |
| 35  | BB    | 1767 | G    | C5-C6-N1    | -10.89 | 106.06      | 111.50   |
| 35  | BB    | 835  | C    | N3-C4-C5    | -10.89 | 117.55      | 121.90   |
| 35  | BB    | 1292 | G    | N1-C6-O6    | 10.88  | 126.43      | 119.90   |
| 35  | BB    | 1731 | G    | N1-C6-O6    | 10.88  | 126.43      | 119.90   |
| 1   | AA    | 1248 | A    | O4'-C1'-N9  | 10.88  | 116.91      | 108.20   |
| 35  | BB    | 1247 | A    | N1-C6-N6    | 10.88  | 125.13      | 118.60   |
| 35  | BB    | 2831 | G    | O4'-C1'-N9  | 10.88  | 116.90      | 108.20   |
| 1   | AA    | 1357 | A    | C5-N7-C8    | 10.88  | 109.34      | 103.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 663  | G    | N3-C2-N2   | 10.88  | 127.51      | 119.90   |
| 35  | BB    | 938  | G    | C5-C6-O6   | -10.88 | 122.07      | 128.60   |
| 35  | BB    | 2433 | A    | C5-N7-C8   | 10.87  | 109.34      | 103.90   |
| 35  | BB    | 2508 | G    | C5-C6-O6   | -10.87 | 122.08      | 128.60   |
| 1   | AA    | 815  | A    | C5-C6-N1   | -10.87 | 112.26      | 117.70   |
| 1   | AA    | 1057 | G    | N1-C6-O6   | 10.87  | 126.42      | 119.90   |
| 35  | BB    | 2763 | G    | C8-N9-C4   | -10.87 | 102.05      | 106.40   |
| 35  | BB    | 221  | A    | N1-C6-N6   | 10.87  | 125.12      | 118.60   |
| 35  | BB    | 2728 | U    | O4'-C1'-N1 | 10.87  | 116.89      | 108.20   |
| 35  | BB    | 1938 | A    | N1-C6-N6   | 10.87  | 125.12      | 118.60   |
| 34  | BA    | 89   | U    | O4'-C1'-N1 | 10.86  | 116.89      | 108.20   |
| 35  | BB    | 2162 | G    | C2-N3-C4   | 10.87  | 117.33      | 111.90   |
| 1   | AA    | 152  | A    | O4'-C1'-N9 | 10.86  | 116.89      | 108.20   |
| 35  | BB    | 1933 | G    | N1-C6-O6   | 10.86  | 126.42      | 119.90   |
| 35  | BB    | 2888 | C    | O4'-C1'-N1 | 10.86  | 116.89      | 108.20   |
| 1   | AA    | 43   | C    | N3-C4-C5   | -10.86 | 117.56      | 121.90   |
| 1   | AA    | 303  | A    | C5-C6-N6   | -10.86 | 115.01      | 123.70   |
| 35  | BB    | 1247 | A    | C8-N9-C4   | -10.86 | 101.46      | 105.80   |
| 35  | BB    | 1160 | G    | C5-C6-O6   | -10.86 | 122.08      | 128.60   |
| 35  | BB    | 2789 | C    | C4-C5-C6   | 10.86  | 122.83      | 117.40   |
| 1   | AA    | 836  | G    | N1-C6-O6   | 10.86  | 126.41      | 119.90   |
| 1   | AA    | 1292 | G    | C5-C6-O6   | -10.86 | 122.09      | 128.60   |
| 35  | BB    | 1442 | U    | O4'-C1'-N1 | 10.86  | 116.89      | 108.20   |
| 35  | BB    | 1939 | U    | N3-C4-O4   | 10.86  | 127.00      | 119.40   |
| 35  | BB    | 1134 | A    | N1-C2-N3   | 10.85  | 134.72      | 129.30   |
| 1   | AA    | 750  | C    | O4'-C1'-N1 | 10.85  | 116.88      | 108.20   |
| 35  | BB    | 696  | G    | N1-C2-N3   | -10.85 | 117.39      | 123.90   |
| 35  | BB    | 1844 | C    | O4'-C1'-N1 | 10.85  | 116.88      | 108.20   |
| 1   | AA    | 299  | G    | C5-C6-O6   | -10.85 | 122.09      | 128.60   |
| 1   | AA    | 1074 | G    | N3-C2-N2   | 10.85  | 127.49      | 119.90   |
| 1   | AA    | 1449 | C    | N3-C4-C5   | -10.85 | 117.56      | 121.90   |
| 35  | BB    | 217  | A    | C5-C6-N6   | -10.85 | 115.02      | 123.70   |
| 35  | BB    | 2330 | G    | C6-C5-N7   | -10.85 | 123.89      | 130.40   |
| 35  | BB    | 160  | A    | C5-C6-N6   | -10.84 | 115.03      | 123.70   |
| 35  | BB    | 1468 | U    | C2-N3-C4   | -10.84 | 120.50      | 127.00   |
| 35  | BB    | 2409 | G    | C6-C5-N7   | -10.84 | 123.89      | 130.40   |
| 35  | BB    | 2444 | G    | C5-C6-N1   | -10.84 | 106.08      | 111.50   |
| 1   | AA    | 1302 | C    | N1-C2-O2   | 10.84  | 125.40      | 118.90   |
| 35  | BB    | 1594 | U    | O4'-C1'-N1 | 10.84  | 116.87      | 108.20   |
| 1   | AA    | 633  | G    | C4-C5-N7   | 10.84  | 115.14      | 110.80   |
| 1   | AA    | 716  | A    | C4-C5-C6   | 10.84  | 122.42      | 117.00   |
| 1   | AA    | 725  | G    | C2-N3-C4   | 10.84  | 117.32      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2042 | A    | C5-C6-N1   | -10.84 | 112.28      | 117.70   |
| 35  | BB    | 1928 | A    | C4-C5-N7   | -10.84 | 105.28      | 110.70   |
| 1   | AA    | 527  | G    | N1-C6-O6   | 10.84  | 126.40      | 119.90   |
| 1   | AA    | 1206 | G    | O4'-C1'-N9 | 10.84  | 116.87      | 108.20   |
| 35  | BB    | 178  | G    | N9-C4-C5   | -10.84 | 101.06      | 105.40   |
| 1   | AA    | 149  | A    | C5-N7-C8   | 10.83  | 109.32      | 103.90   |
| 1   | AA    | 226  | G    | C4-C5-N7   | -10.83 | 106.47      | 110.80   |
| 35  | BB    | 936  | A    | N7-C8-N9   | -10.83 | 108.38      | 113.80   |
| 1   | AA    | 192  | A    | C2-N3-C4   | -10.83 | 105.19      | 110.60   |
| 35  | BB    | 347  | A    | C5-C6-N6   | -10.83 | 115.04      | 123.70   |
| 35  | BB    | 788  | A    | C5-C6-N1   | -10.83 | 112.28      | 117.70   |
| 35  | BB    | 2579 | C    | N3-C4-N4   | 10.83  | 125.58      | 118.00   |
| 1   | AA    | 1220 | G    | C5-C6-O6   | -10.83 | 122.10      | 128.60   |
| 1   | AA    | 1497 | G    | C5-C6-O6   | -10.83 | 122.10      | 128.60   |
| 35  | BB    | 1418 | G    | C5-C6-O6   | -10.83 | 122.10      | 128.60   |
| 35  | BB    | 1984 | G    | O4'-C1'-N9 | 10.83  | 116.86      | 108.20   |
| 35  | BB    | 2003 | A    | C5-N7-C8   | 10.83  | 109.31      | 103.90   |
| 1   | AA    | 1277 | C    | O4'-C1'-N1 | 10.83  | 116.86      | 108.20   |
| 35  | BB    | 1026 | G    | N9-C4-C5   | -10.83 | 101.07      | 105.40   |
| 35  | BB    | 2048 | G    | N1-C2-N3   | -10.83 | 117.40      | 123.90   |
| 1   | AA    | 1192 | C    | O4'-C1'-N1 | 10.83  | 116.86      | 108.20   |
| 1   | AA    | 1487 | G    | N1-C6-O6   | 10.82  | 126.39      | 119.90   |
| 35  | BB    | 670  | A    | P-O3'-C3'  | 10.82  | 132.68      | 119.70   |
| 35  | BB    | 1079 | C    | O4'-C1'-N1 | 10.82  | 116.86      | 108.20   |
| 35  | BB    | 2686 | G    | N1-C6-O6   | 10.82  | 126.39      | 119.90   |
| 1   | AA    | 172  | A    | N9-C4-C5   | 10.82  | 110.13      | 105.80   |
| 35  | BB    | 1256 | G    | N3-C4-C5   | -10.82 | 123.19      | 128.60   |
| 1   | AA    | 769  | G    | O4'-C1'-N9 | 10.81  | 116.85      | 108.20   |
| 1   | AA    | 1496 | C    | C6-N1-C2   | -10.81 | 115.97      | 120.30   |
| 35  | BB    | 392  | U    | C5-C6-N1   | 10.81  | 128.11      | 122.70   |
| 35  | BB    | 75   | G    | C5-C6-O6   | -10.81 | 122.11      | 128.60   |
| 35  | BB    | 1733 | G    | N3-C2-N2   | 10.81  | 127.47      | 119.90   |
| 35  | BB    | 2225 | A    | C4-C5-C6   | 10.81  | 122.40      | 117.00   |
| 35  | BB    | 2075 | U    | C5-C4-O4   | 10.81  | 132.38      | 125.90   |
| 1   | AA    | 1201 | A    | N1-C6-N6   | 10.80  | 125.08      | 118.60   |
| 1   | AA    | 711  | G    | C5-C6-O6   | -10.80 | 122.12      | 128.60   |
| 1   | AA    | 994  | A    | C5-C6-N1   | -10.80 | 112.30      | 117.70   |
| 1   | AA    | 484  | G    | N3-C2-N2   | 10.80  | 127.46      | 119.90   |
| 1   | AA    | 1215 | G    | C5-C6-O6   | -10.80 | 122.12      | 128.60   |
| 1   | AA    | 1468 | A    | C4-C5-C6   | 10.80  | 122.40      | 117.00   |
| 35  | BB    | 159  | G    | C5-C6-N1   | -10.79 | 106.10      | 111.50   |
| 36  | BC    | 79   | ARG  | NE-CZ-NH1  | 10.79  | 125.70      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 34  | BA    | 66   | A    | N1-C6-N6   | 10.79  | 125.08      | 118.60   |
| 35  | BB    | 283  | G    | C4-C5-N7   | -10.79 | 106.48      | 110.80   |
| 35  | BB    | 2430 | A    | C6-C5-N7   | -10.79 | 124.75      | 132.30   |
| 39  | BF    | 29   | ARG  | NE-CZ-NH2  | 10.79  | 125.70      | 120.30   |
| 1   | AA    | 899  | C    | N3-C4-C5   | -10.79 | 117.58      | 121.90   |
| 35  | BB    | 2009 | A    | N1-C6-N6   | 10.79  | 125.07      | 118.60   |
| 34  | BA    | 101  | A    | N1-C6-N6   | 10.79  | 125.07      | 118.60   |
| 1   | AA    | 874  | G    | N1-C6-O6   | 10.78  | 126.37      | 119.90   |
| 35  | BB    | 2542 | A    | C5-C6-N1   | -10.78 | 112.31      | 117.70   |
| 35  | BB    | 1931 | U    | O4'-C1'-N1 | 10.78  | 116.83      | 108.20   |
| 35  | BB    | 52   | A    | O4'-C1'-N9 | 10.78  | 116.82      | 108.20   |
| 35  | BB    | 393  | C    | O4'-C1'-N1 | 10.78  | 116.83      | 108.20   |
| 35  | BB    | 551  | G    | N1-C6-O6   | 10.78  | 126.37      | 119.90   |
| 35  | BB    | 2560 | A    | C8-N9-C4   | -10.78 | 101.49      | 105.80   |
| 1   | AA    | 419  | C    | O4'-C1'-N1 | 10.78  | 116.82      | 108.20   |
| 1   | AA    | 1468 | A    | N1-C6-N6   | 10.78  | 125.07      | 118.60   |
| 1   | AA    | 73   | C    | N3-C4-N4   | 10.78  | 125.54      | 118.00   |
| 1   | AA    | 769  | G    | N3-C2-N2   | 10.78  | 127.44      | 119.90   |
| 35  | BB    | 2700 | A    | C4-C5-C6   | 10.78  | 122.39      | 117.00   |
| 34  | BA    | 41   | G    | N1-C6-O6   | 10.77  | 126.36      | 119.90   |
| 35  | BB    | 503  | A    | C5-C6-N1   | -10.77 | 112.31      | 117.70   |
| 35  | BB    | 597  | G    | C5-N7-C8   | 10.77  | 109.69      | 104.30   |
| 35  | BB    | 1807 | G    | C8-N9-C4   | -10.77 | 102.09      | 106.40   |
| 35  | BB    | 309  | A    | N1-C2-N3   | 10.77  | 134.69      | 129.30   |
| 35  | BB    | 2660 | A    | C4-C5-C6   | 10.77  | 122.39      | 117.00   |
| 35  | BB    | 2145 | C    | C6-N1-C1'  | -10.77 | 107.88      | 120.80   |
| 35  | BB    | 1389 | G    | N3-C2-N2   | 10.77  | 127.44      | 119.90   |
| 35  | BB    | 1428 | C    | C6-N1-C2   | 10.77  | 124.61      | 120.30   |
| 1   | AA    | 215  | C    | O4'-C1'-N1 | 10.77  | 116.81      | 108.20   |
| 35  | BB    | 285  | G    | C8-N9-C4   | -10.76 | 102.09      | 106.40   |
| 35  | BB    | 1536 | C    | O4'-C1'-N1 | 10.76  | 116.81      | 108.20   |
| 35  | BB    | 2661 | G    | N1-C6-O6   | 10.76  | 126.36      | 119.90   |
| 1   | AA    | 669  | G    | C6-C5-N7   | -10.76 | 123.94      | 130.40   |
| 1   | AA    | 874  | G    | C8-N9-C4   | -10.76 | 102.09      | 106.40   |
| 1   | AA    | 936  | C    | C6-N1-C2   | -10.76 | 116.00      | 120.30   |
| 35  | BB    | 2071 | A    | N1-C6-N6   | 10.76  | 125.06      | 118.60   |
| 35  | BB    | 470  | A    | C5-C6-N6   | -10.76 | 115.09      | 123.70   |
| 1   | AA    | 477  | C    | N3-C4-N4   | 10.76  | 125.53      | 118.00   |
| 1   | AA    | 771  | G    | N7-C8-N9   | -10.76 | 107.72      | 113.10   |
| 35  | BB    | 896  | A    | C5-C6-N6   | -10.76 | 115.09      | 123.70   |
| 35  | BB    | 2086 | U    | C5-C4-O4   | -10.76 | 119.45      | 125.90   |
| 1   | AA    | 1163 | A    | N1-C6-N6   | 10.76  | 125.05      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1   | AA    | 1255 | G    | O4'-C1'-N9  | 10.76  | 116.80      | 108.20   |
| 35  | BB    | 2602 | A    | O4'-C1'-N9  | 10.76  | 116.81      | 108.20   |
| 1   | AA    | 204  | G    | N1-C6-O6    | 10.75  | 126.35      | 119.90   |
| 35  | BB    | 1664 | A    | O4'-C1'-N9  | 10.75  | 116.80      | 108.20   |
| 35  | BB    | 1835 | G    | C5-C6-O6    | -10.75 | 122.15      | 128.60   |
| 35  | BB    | 2072 | C    | N3-C4-N4    | 10.75  | 125.53      | 118.00   |
| 1   | AA    | 1329 | A    | N1-C6-N6    | 10.75  | 125.05      | 118.60   |
| 35  | BB    | 613  | A    | C5'-C4'-O4' | 10.75  | 122.00      | 109.10   |
| 35  | BB    | 1794 | A    | C5-N7-C8    | 10.75  | 109.28      | 103.90   |
| 1   | AA    | 1170 | A    | N1-C6-N6    | 10.75  | 125.05      | 118.60   |
| 35  | BB    | 2204 | G    | C8-N9-C4    | 10.75  | 110.70      | 106.40   |
| 1   | AA    | 818  | G    | N1-C6-O6    | 10.75  | 126.35      | 119.90   |
| 35  | BB    | 451  | U    | O4'-C1'-N1  | 10.75  | 116.80      | 108.20   |
| 35  | BB    | 1027 | A    | N1-C2-N3    | 10.75  | 134.67      | 129.30   |
| 35  | BB    | 1380 | G    | C4-C5-N7    | 10.75  | 115.10      | 110.80   |
| 35  | BB    | 1497 | U    | O4'-C1'-N1  | 10.74  | 116.80      | 108.20   |
| 1   | AA    | 296  | U    | O4'-C1'-N1  | 10.74  | 116.79      | 108.20   |
| 35  | BB    | 1775 | U    | O4'-C1'-N1  | 10.74  | 116.79      | 108.20   |
| 1   | AA    | 264  | C    | N3-C4-C5    | -10.74 | 117.60      | 121.90   |
| 1   | AA    | 1441 | A    | N9-C4-C5    | 10.74  | 110.10      | 105.80   |
| 35  | BB    | 1899 | A    | N9-C4-C5    | 10.74  | 110.10      | 105.80   |
| 35  | BB    | 2304 | G    | C5-C6-O6    | -10.74 | 122.16      | 128.60   |
| 1   | AA    | 21   | G    | N1-C6-O6    | 10.74  | 126.34      | 119.90   |
| 35  | BB    | 1333 | G    | C5-N7-C8    | 10.74  | 109.67      | 104.30   |
| 35  | BB    | 703  | U    | O4'-C1'-N1  | 10.74  | 116.79      | 108.20   |
| 35  | BB    | 1835 | G    | N1-C6-O6    | 10.74  | 126.34      | 119.90   |
| 35  | BB    | 1843 | C    | O4'-C1'-N1  | 10.74  | 116.79      | 108.20   |
| 1   | AA    | 346  | G    | C5-C6-O6    | -10.73 | 122.16      | 128.60   |
| 1   | AA    | 1055 | A    | N1-C2-N3    | 10.73  | 134.67      | 129.30   |
| 35  | BB    | 1507 | C    | C5-C6-N1    | 10.73  | 126.37      | 121.00   |
| 35  | BB    | 2395 | C    | O4'-C1'-N1  | 10.73  | 116.79      | 108.20   |
| 35  | BB    | 2698 | U    | O4'-C1'-N1  | 10.73  | 116.79      | 108.20   |
| 35  | BB    | 1223 | G    | N1-C6-O6    | 10.73  | 126.34      | 119.90   |
| 1   | AA    | 829  | G    | O4'-C1'-N9  | 10.73  | 116.78      | 108.20   |
| 35  | BB    | 1345 | C    | N3-C4-N4    | 10.73  | 125.51      | 118.00   |
| 1   | AA    | 50   | A    | C8-N9-C4    | -10.73 | 101.51      | 105.80   |
| 1   | AA    | 792  | A    | C2-N3-C4    | -10.73 | 105.23      | 110.60   |
| 1   | AA    | 1144 | G    | O4'-C1'-N9  | 10.73  | 116.78      | 108.20   |
| 35  | BB    | 130  | C    | N3-C4-C5    | -10.73 | 117.61      | 121.90   |
| 35  | BB    | 699  | A    | C6-C5-N7    | -10.73 | 124.79      | 132.30   |
| 35  | BB    | 1608 | A    | C6-C5-N7    | -10.73 | 124.79      | 132.30   |
| 35  | BB    | 2215 | C    | C6-N1-C2    | 10.73  | 124.59      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2463 | C    | C5-C6-N1   | 10.73  | 126.36      | 121.00   |
| 35  | BB    | 103  | A    | N1-C6-N6   | 10.72  | 125.03      | 118.60   |
| 35  | BB    | 666  | A    | C4-C5-C6   | 10.72  | 122.36      | 117.00   |
| 35  | BB    | 1105 | U    | O4'-C1'-N1 | 10.72  | 116.78      | 108.20   |
| 35  | BB    | 2083 | G    | N9-C4-C5   | 10.72  | 109.69      | 105.40   |
| 1   | AA    | 1413 | A    | N1-C2-N3   | 10.72  | 134.66      | 129.30   |
| 35  | BB    | 1533 | C    | O4'-C1'-N1 | 10.72  | 116.78      | 108.20   |
| 1   | AA    | 1452 | C    | C2-N3-C4   | 10.72  | 125.26      | 119.90   |
| 35  | BB    | 1632 | A    | N9-C4-C5   | 10.72  | 110.09      | 105.80   |
| 1   | AA    | 425  | G    | C5-C6-O6   | -10.72 | 122.17      | 128.60   |
| 35  | BB    | 1094 | U    | C5-C4-O4   | 10.72  | 132.33      | 125.90   |
| 35  | BB    | 1855 | U    | C5-C6-N1   | 10.72  | 128.06      | 122.70   |
| 35  | BB    | 2729 | G    | C4-C5-N7   | 10.72  | 115.09      | 110.80   |
| 35  | BB    | 2872 | A    | C5-N7-C8   | 10.72  | 109.26      | 103.90   |
| 35  | BB    | 1067 | A    | C5-N7-C8   | 10.71  | 109.26      | 103.90   |
| 35  | BB    | 2862 | G    | N1-C6-O6   | 10.72  | 126.33      | 119.90   |
| 35  | BB    | 2463 | C    | N3-C4-N4   | 10.71  | 125.50      | 118.00   |
| 1   | AA    | 156  | C    | N3-C4-N4   | 10.71  | 125.50      | 118.00   |
| 1   | AA    | 915  | A    | C5-C6-N6   | -10.71 | 115.13      | 123.70   |
| 35  | BB    | 899  | A    | C2-N3-C4   | -10.71 | 105.25      | 110.60   |
| 35  | BB    | 904  | G    | C5-C6-O6   | -10.71 | 122.17      | 128.60   |
| 35  | BB    | 323  | C    | O4'-C1'-N1 | 10.71  | 116.77      | 108.20   |
| 35  | BB    | 432  | A    | C5-C6-N1   | -10.71 | 112.35      | 117.70   |
| 35  | BB    | 1549 | A    | C5-C6-N1   | -10.71 | 112.35      | 117.70   |
| 35  | BB    | 1936 | A    | N9-C4-C5   | 10.71  | 110.08      | 105.80   |
| 35  | BB    | 104  | A    | C5-N7-C8   | 10.71  | 109.25      | 103.90   |
| 35  | BB    | 116  | C    | O4'-C1'-N1 | 10.70  | 116.76      | 108.20   |
| 35  | BB    | 2030 | A    | C4-C5-C6   | 10.70  | 122.35      | 117.00   |
| 1   | AA    | 1318 | A    | C5-C6-N6   | -10.70 | 115.14      | 123.70   |
| 35  | BB    | 230  | G    | C4-C5-N7   | 10.70  | 115.08      | 110.80   |
| 35  | BB    | 1046 | A    | N1-C6-N6   | 10.70  | 125.02      | 118.60   |
| 35  | BB    | 1236 | G    | N1-C6-O6   | 10.70  | 126.32      | 119.90   |
| 35  | BB    | 2712 | C    | O4'-C1'-N1 | 10.70  | 116.76      | 108.20   |
| 35  | BB    | 1577 | C    | O4'-C1'-N1 | 10.70  | 116.76      | 108.20   |
| 35  | BB    | 2712 | C    | N1-C2-N3   | -10.70 | 111.71      | 119.20   |
| 1   | AA    | 1040 | U    | N3-C4-O4   | 10.70  | 126.89      | 119.40   |
| 34  | BA    | 112  | G    | O4'-C1'-N9 | 10.70  | 116.76      | 108.20   |
| 1   | AA    | 1280 | A    | C4-C5-C6   | 10.70  | 122.35      | 117.00   |
| 34  | BA    | 17   | C    | O4'-C1'-N1 | 10.70  | 116.76      | 108.20   |
| 34  | BA    | 32   | U    | O4'-C1'-N1 | 10.70  | 116.76      | 108.20   |
| 35  | BB    | 63   | A    | C4-C5-N7   | -10.70 | 105.35      | 110.70   |
| 35  | BB    | 504  | A    | C5-N7-C8   | 10.70  | 109.25      | 103.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2592 | G    | N1-C6-O6   | 10.70  | 126.32      | 119.90   |
| 1   | AA    | 1123 | U    | C5-C4-O4   | -10.69 | 119.48      | 125.90   |
| 35  | BB    | 186  | G    | C5-C6-O6   | -10.69 | 122.19      | 128.60   |
| 35  | BB    | 227  | A    | P-O3'-C3'  | 10.69  | 132.53      | 119.70   |
| 35  | BB    | 679  | C    | C6-N1-C2   | -10.69 | 116.03      | 120.30   |
| 35  | BB    | 733  | G    | N1-C6-O6   | 10.69  | 126.31      | 119.90   |
| 1   | AA    | 69   | G    | C6-C5-N7   | -10.69 | 123.99      | 130.40   |
| 1   | AA    | 422  | C    | C5-C6-N1   | 10.69  | 126.34      | 121.00   |
| 1   | AA    | 436  | C    | O4'-C1'-N1 | 10.69  | 116.75      | 108.20   |
| 35  | BB    | 2719 | G    | C5-C6-O6   | -10.69 | 122.19      | 128.60   |
| 35  | BB    | 2250 | G    | N1-C2-N3   | -10.68 | 117.49      | 123.90   |
| 1   | AA    | 198  | G    | N1-C6-O6   | 10.68  | 126.31      | 119.90   |
| 1   | AA    | 379  | C    | O4'-C1'-N1 | 10.68  | 116.74      | 108.20   |
| 1   | AA    | 792  | A    | N1-C2-N3   | 10.68  | 134.64      | 129.30   |
| 35  | BB    | 410  | G    | N7-C8-N9   | 10.68  | 118.44      | 113.10   |
| 35  | BB    | 2123 | G    | N1-C6-O6   | 10.68  | 126.31      | 119.90   |
| 34  | BA    | 23   | G    | C6-C5-N7   | -10.68 | 123.99      | 130.40   |
| 1   | AA    | 1178 | G    | O4'-C1'-N9 | 10.68  | 116.74      | 108.20   |
| 35  | BB    | 517  | C    | N3-C4-C5   | -10.68 | 117.63      | 121.90   |
| 35  | BB    | 2887 | A    | C8-N9-C4   | -10.68 | 101.53      | 105.80   |
| 35  | BB    | 478  | A    | C5-C6-N6   | -10.67 | 115.16      | 123.70   |
| 1   | AA    | 683  | G    | N1-C6-O6   | 10.67  | 126.30      | 119.90   |
| 35  | BB    | 1210 | G    | C5-C6-O6   | -10.67 | 122.20      | 128.60   |
| 35  | BB    | 59   | U    | C5-C6-N1   | 10.67  | 128.03      | 122.70   |
| 35  | BB    | 2811 | G    | N1-C2-N3   | -10.67 | 117.50      | 123.90   |
| 35  | BB    | 98   | G    | C4-C5-C6   | 10.67  | 125.20      | 118.80   |
| 35  | BB    | 1074 | G    | C5-C6-O6   | -10.67 | 122.20      | 128.60   |
| 1   | AA    | 414  | A    | O4'-C1'-N9 | 10.66  | 116.73      | 108.20   |
| 35  | BB    | 266  | G    | C5-C6-O6   | -10.66 | 122.20      | 128.60   |
| 35  | BB    | 473  | G    | O4'-C1'-N9 | 10.66  | 116.73      | 108.20   |
| 25  | B0    | 45   | PHE  | CB-CG-CD1  | 10.66  | 128.26      | 120.80   |
| 35  | BB    | 942  | G    | C2-N3-C4   | 10.66  | 117.23      | 111.90   |
| 35  | BB    | 1800 | C    | N3-C4-C5   | -10.66 | 117.64      | 121.90   |
| 35  | BB    | 2513 | A    | N1-C6-N6   | 10.66  | 125.00      | 118.60   |
| 1   | AA    | 1313 | U    | O4'-C1'-N1 | 10.66  | 116.73      | 108.20   |
| 35  | BB    | 2184 | A    | N1-C6-N6   | 10.66  | 125.00      | 118.60   |
| 1   | AA    | 77   | A    | C5-C6-N1   | -10.66 | 112.37      | 117.70   |
| 1   | AA    | 738  | C    | C6-N1-C2   | -10.66 | 116.04      | 120.30   |
| 1   | AA    | 1093 | A    | N1-C6-N6   | 10.66  | 125.00      | 118.60   |
| 1   | AA    | 1519 | A    | N1-C6-N6   | 10.66  | 125.00      | 118.60   |
| 35  | BB    | 1833 | C    | C5-C4-N4   | -10.66 | 112.74      | 120.20   |
| 35  | BB    | 66   | C    | O4'-C1'-N1 | 10.66  | 116.72      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1211 | C    | O4'-C1'-N1 | 10.66  | 116.73      | 108.20   |
| 35  | BB    | 1422 | G    | C6-N1-C2   | 10.66  | 131.49      | 125.10   |
| 35  | BB    | 1896 | G    | N1-C2-N3   | -10.66 | 117.51      | 123.90   |
| 35  | BB    | 2589 | A    | O4'-C1'-N9 | 10.66  | 116.73      | 108.20   |
| 35  | BB    | 1615 | C    | C5-C6-N1   | 10.65  | 126.33      | 121.00   |
| 45  | BL    | 2    | ARG  | NE-CZ-NH1  | 10.65  | 125.63      | 120.30   |
| 1   | AA    | 743  | A    | N7-C8-N9   | -10.65 | 108.47      | 113.80   |
| 2   | AB    | 29   | PHE  | CB-CG-CD2  | 10.65  | 128.26      | 120.80   |
| 34  | BA    | 105  | G    | O4'-C1'-N9 | 10.65  | 116.72      | 108.20   |
| 35  | BB    | 420  | C    | C2-N3-C4   | 10.65  | 125.23      | 119.90   |
| 1   | AA    | 780  | A    | C8-N9-C4   | -10.65 | 101.54      | 105.80   |
| 34  | BA    | 91   | C    | N3-C4-N4   | 10.65  | 125.45      | 118.00   |
| 35  | BB    | 415  | A    | C5-N7-C8   | 10.65  | 109.22      | 103.90   |
| 35  | BB    | 2549 | G    | C2-N3-C4   | 10.65  | 117.22      | 111.90   |
| 34  | BA    | 104  | A    | C5-C6-N1   | -10.65 | 112.38      | 117.70   |
| 35  | BB    | 1231 | U    | C5-C4-O4   | -10.65 | 119.51      | 125.90   |
| 1   | AA    | 337  | G    | C5-C6-O6   | -10.64 | 122.21      | 128.60   |
| 35  | BB    | 2881 | U    | C5-C6-N1   | 10.64  | 128.02      | 122.70   |
| 35  | BB    | 857  | G    | N1-C6-O6   | 10.64  | 126.28      | 119.90   |
| 36  | BC    | 42   | ARG  | NE-CZ-NH1  | 10.64  | 125.62      | 120.30   |
| 35  | BB    | 943  | A    | N9-C4-C5   | 10.64  | 110.06      | 105.80   |
| 1   | AA    | 110  | C    | N3-C4-N4   | 10.64  | 125.45      | 118.00   |
| 1   | AA    | 154  | U    | N3-C4-O4   | 10.64  | 126.85      | 119.40   |
| 35  | BB    | 2753 | A    | N1-C6-N6   | 10.64  | 124.98      | 118.60   |
| 35  | BB    | 231  | A    | N1-C6-N6   | 10.64  | 124.98      | 118.60   |
| 1   | AA    | 1207 | G    | N1-C6-O6   | 10.63  | 126.28      | 119.90   |
| 35  | BB    | 438  | G    | O4'-C1'-N9 | 10.63  | 116.71      | 108.20   |
| 35  | BB    | 1137 | G    | C8-N9-C4   | -10.63 | 102.15      | 106.40   |
| 35  | BB    | 147  | C    | O4'-C1'-N1 | 10.63  | 116.71      | 108.20   |
| 35  | BB    | 517  | C    | N3-C4-N4   | 10.63  | 125.44      | 118.00   |
| 35  | BB    | 2101 | A    | O4'-C1'-N9 | 10.63  | 116.71      | 108.20   |
| 1   | AA    | 864  | A    | C4-C5-C6   | 10.63  | 122.31      | 117.00   |
| 35  | BB    | 2089 | C    | O4'-C1'-N1 | 10.63  | 116.70      | 108.20   |
| 1   | AA    | 473  | U    | O4'-C1'-N1 | 10.63  | 116.70      | 108.20   |
| 35  | BB    | 2267 | A    | C5-C6-N6   | -10.63 | 115.20      | 123.70   |
| 1   | AA    | 1197 | A    | C5-N7-C8   | 10.63  | 109.21      | 103.90   |
| 35  | BB    | 10   | A    | C5-C6-N1   | -10.63 | 112.39      | 117.70   |
| 35  | BB    | 2336 | A    | C8-N9-C4   | -10.63 | 101.55      | 105.80   |
| 1   | AA    | 100  | G    | C5-C6-N1   | -10.63 | 106.19      | 111.50   |
| 35  | BB    | 28   | A    | O4'-C1'-N9 | 10.63  | 116.70      | 108.20   |
| 35  | BB    | 266  | G    | N7-C8-N9   | -10.63 | 107.79      | 113.10   |
| 1   | AA    | 61   | G    | C5-C6-O6   | -10.62 | 122.23      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 35  | BB    | 1163 | G    | C8-N9-C4    | 10.62  | 110.65      | 106.40   |
| 35  | BB    | 2328 | A    | C5-C6-N6    | -10.62 | 115.20      | 123.70   |
| 1   | AA    | 403  | C    | O4'-C1'-N1  | 10.62  | 116.70      | 108.20   |
| 35  | BB    | 1    | G    | C5-C6-O6    | -10.62 | 122.23      | 128.60   |
| 35  | BB    | 1128 | G    | C3'-C2'-C1' | 10.62  | 110.00      | 101.50   |
| 35  | BB    | 1977 | A    | C5-C6-N6    | -10.62 | 115.20      | 123.70   |
| 35  | BB    | 2780 | G    | N1-C6-O6    | 10.62  | 126.27      | 119.90   |
| 35  | BB    | 1235 | G    | N1-C6-O6    | 10.62  | 126.27      | 119.90   |
| 1   | AA    | 836  | G    | O4'-C1'-N9  | 10.62  | 116.69      | 108.20   |
| 35  | BB    | 81   | G    | C5-C6-O6    | -10.62 | 122.23      | 128.60   |
| 35  | BB    | 269  | C    | N3-C4-N4    | 10.62  | 125.43      | 118.00   |
| 35  | BB    | 1547 | C    | N3-C4-C5    | -10.62 | 117.65      | 121.90   |
| 35  | BB    | 2409 | G    | C4-C5-N7    | 10.62  | 115.05      | 110.80   |
| 1   | AA    | 267  | C    | O4'-C1'-N1  | 10.61  | 116.69      | 108.20   |
| 35  | BB    | 626  | A    | C5-C6-N6    | -10.61 | 115.21      | 123.70   |
| 35  | BB    | 1606 | C    | O4'-C1'-N1  | 10.61  | 116.69      | 108.20   |
| 35  | BB    | 2750 | A    | C5-N7-C8    | 10.61  | 109.20      | 103.90   |
| 1   | AA    | 77   | A    | C4-C5-C6    | 10.61  | 122.30      | 117.00   |
| 1   | AA    | 242  | G    | O4'-C1'-N9  | 10.61  | 116.69      | 108.20   |
| 35  | BB    | 783  | A    | N1-C6-N6    | 10.61  | 124.97      | 118.60   |
| 35  | BB    | 1024 | G    | N1-C6-O6    | 10.61  | 126.27      | 119.90   |
| 35  | BB    | 1918 | A    | O4'-C1'-N9  | 10.61  | 116.69      | 108.20   |
| 1   | AA    | 1080 | A    | C6-C5-N7    | -10.61 | 124.88      | 132.30   |
| 34  | BA    | 109  | A    | C5-C6-N6    | -10.61 | 115.22      | 123.70   |
| 1   | AA    | 116  | A    | C4-C5-C6    | 10.60  | 122.30      | 117.00   |
| 35  | BB    | 1685 | C    | C4-C5-C6    | 10.60  | 122.70      | 117.40   |
| 1   | AA    | 1066 | C    | C5-C6-N1    | 10.60  | 126.30      | 121.00   |
| 35  | BB    | 1964 | G    | N1-C6-O6    | 10.60  | 126.26      | 119.90   |
| 1   | AA    | 372  | C    | C6-N1-C2    | -10.60 | 116.06      | 120.30   |
| 35  | BB    | 1969 | A    | C5-C6-N1    | -10.60 | 112.40      | 117.70   |
| 35  | BB    | 2396 | G    | N1-C6-O6    | 10.60  | 126.26      | 119.90   |
| 35  | BB    | 2611 | C    | C5-C6-N1    | -10.60 | 115.70      | 121.00   |
| 35  | BB    | 2670 | A    | N1-C6-N6    | 10.60  | 124.96      | 118.60   |
| 48  | BO    | 2    | ASP  | CB-CG-OD1   | 10.60  | 127.83      | 118.30   |
| 1   | AA    | 883  | C    | N3-C4-N4    | 10.59  | 125.42      | 118.00   |
| 1   | AA    | 977  | A    | N9-C4-C5    | 10.59  | 110.04      | 105.80   |
| 35  | BB    | 2735 | G    | O4'-C1'-N9  | 10.59  | 116.67      | 108.20   |
| 1   | AA    | 1246 | A    | C8-N9-C4    | -10.59 | 101.56      | 105.80   |
| 35  | BB    | 549  | G    | O4'-C1'-N9  | 10.59  | 116.67      | 108.20   |
| 35  | BB    | 1412 | U    | N3-C2-O2    | -10.59 | 114.78      | 122.20   |
| 35  | BB    | 1858 | A    | C4-C5-C6    | 10.59  | 122.30      | 117.00   |
| 35  | BB    | 2357 | G    | C6-C5-N7    | -10.59 | 124.05      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 221  | C    | C6-N1-C2   | -10.59 | 116.06      | 120.30   |
| 35  | BB    | 1134 | A    | C5-C6-N1   | -10.59 | 112.41      | 117.70   |
| 35  | BB    | 2033 | A    | C5-N7-C8   | 10.59  | 109.19      | 103.90   |
| 1   | AA    | 286  | C    | C5-C4-N4   | -10.59 | 112.79      | 120.20   |
| 35  | BB    | 1208 | C    | O4'-C1'-N1 | 10.59  | 116.67      | 108.20   |
| 35  | BB    | 1704 | C    | N3-C4-N4   | 10.59  | 125.41      | 118.00   |
| 35  | BB    | 980  | A    | N1-C6-N6   | 10.58  | 124.95      | 118.60   |
| 50  | BQ    | 47   | ARG  | NE-CZ-NH1  | -10.58 | 115.01      | 120.30   |
| 1   | AA    | 1299 | A    | C8-N9-C4   | -10.58 | 101.57      | 105.80   |
| 34  | BA    | 38   | C    | O4'-C1'-N1 | 10.58  | 116.67      | 108.20   |
| 35  | BB    | 789  | A    | N1-C6-N6   | 10.58  | 124.95      | 118.60   |
| 35  | BB    | 1331 | G    | O4'-C1'-N9 | 10.58  | 116.67      | 108.20   |
| 35  | BB    | 1934 | C    | C5-C4-N4   | -10.58 | 112.79      | 120.20   |
| 1   | AA    | 1452 | C    | O4'-C1'-N1 | 10.58  | 116.66      | 108.20   |
| 35  | BB    | 1733 | G    | N1-C6-O6   | 10.58  | 126.25      | 119.90   |
| 35  | BB    | 2119 | A    | C5-C6-N6   | -10.58 | 115.24      | 123.70   |
| 1   | AA    | 395  | C    | C5-C4-N4   | -10.58 | 112.80      | 120.20   |
| 1   | AA    | 1006 | G    | N3-C2-N2   | 10.58  | 127.30      | 119.90   |
| 35  | BB    | 182  | A    | C5-N7-C8   | 10.58  | 109.19      | 103.90   |
| 35  | BB    | 879  | G    | N3-C2-N2   | 10.58  | 127.31      | 119.90   |
| 35  | BB    | 1096 | A    | C5-C6-N1   | -10.58 | 112.41      | 117.70   |
| 1   | AA    | 649  | A    | C5-C6-N6   | -10.57 | 115.24      | 123.70   |
| 35  | BB    | 1277 | G    | O4'-C1'-N9 | 10.57  | 116.66      | 108.20   |
| 35  | BB    | 1843 | C    | N3-C4-N4   | 10.57  | 125.40      | 118.00   |
| 35  | BB    | 481  | G    | N1-C6-O6   | 10.57  | 126.24      | 119.90   |
| 35  | BB    | 837  | C    | O4'-C1'-N1 | 10.57  | 116.66      | 108.20   |
| 35  | BB    | 50   | U    | O4'-C1'-N1 | 10.57  | 116.66      | 108.20   |
| 35  | BB    | 1142 | A    | N1-C6-N6   | 10.57  | 124.94      | 118.60   |
| 35  | BB    | 1357 | C    | O4'-C1'-N1 | 10.57  | 116.65      | 108.20   |
| 35  | BB    | 1823 | G    | N1-C6-O6   | 10.57  | 126.24      | 119.90   |
| 1   | AA    | 146  | G    | O4'-C1'-N9 | 10.56  | 116.65      | 108.20   |
| 1   | AA    | 224  | U    | N1-C2-N3   | -10.56 | 108.56      | 114.90   |
| 1   | AA    | 947  | G    | C5-C6-O6   | -10.56 | 122.26      | 128.60   |
| 35  | BB    | 177  | G    | C5-C6-O6   | -10.56 | 122.26      | 128.60   |
| 35  | BB    | 237  | C    | O4'-C1'-N1 | 10.56  | 116.65      | 108.20   |
| 35  | BB    | 960  | A    | C4-C5-C6   | 10.56  | 122.28      | 117.00   |
| 35  | BB    | 1021 | A    | N1-C2-N3   | 10.56  | 134.58      | 129.30   |
| 40  | BG    | 150  | TYR  | CB-CG-CD1  | -10.56 | 114.66      | 121.00   |
| 1   | AA    | 490  | C    | C6-N1-C2   | -10.56 | 116.08      | 120.30   |
| 34  | BA    | 44   | G    | C5-C6-O6   | -10.56 | 122.26      | 128.60   |
| 35  | BB    | 635  | C    | N3-C4-N4   | 10.56  | 125.39      | 118.00   |
| 35  | BB    | 974  | G    | C5-C6-O6   | -10.56 | 122.26      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1496 | A    | N1-C2-N3   | -10.56 | 124.02      | 129.30   |
| 35  | BB    | 2224 | G    | C4-C5-C6   | 10.56  | 125.14      | 118.80   |
| 35  | BB    | 2683 | C    | N3-C4-C5   | -10.56 | 117.68      | 121.90   |
| 1   | AA    | 1364 | U    | O4'-C1'-N1 | 10.56  | 116.65      | 108.20   |
| 35  | BB    | 486  | C    | O4'-C1'-N1 | 10.56  | 116.65      | 108.20   |
| 35  | BB    | 1701 | A    | C5-C6-N1   | -10.56 | 112.42      | 117.70   |
| 35  | BB    | 2653 | U    | O4'-C1'-N1 | 10.56  | 116.64      | 108.20   |
| 35  | BB    | 2903 | U    | O4'-C1'-N1 | 10.56  | 116.64      | 108.20   |
| 1   | AA    | 544  | G    | C6-C5-N7   | -10.55 | 124.07      | 130.40   |
| 35  | BB    | 706  | A    | N1-C6-N6   | 10.55  | 124.93      | 118.60   |
| 35  | BB    | 969  | G    | C5-C6-O6   | -10.55 | 122.27      | 128.60   |
| 35  | BB    | 2380 | C    | C6-N1-C2   | 10.55  | 124.52      | 120.30   |
| 35  | BB    | 2382 | G    | C4-C5-N7   | 10.55  | 115.02      | 110.80   |
| 35  | BB    | 2361 | G    | N1-C2-N3   | -10.55 | 117.57      | 123.90   |
| 35  | BB    | 263  | G    | N1-C6-O6   | 10.55  | 126.23      | 119.90   |
| 35  | BB    | 1103 | A    | C5-N7-C8   | 10.55  | 109.17      | 103.90   |
| 35  | BB    | 1129 | A    | C4-C5-C6   | 10.55  | 122.27      | 117.00   |
| 35  | BB    | 1358 | G    | O4'-C1'-N9 | 10.55  | 116.64      | 108.20   |
| 35  | BB    | 1824 | G    | C5-C6-O6   | -10.55 | 122.27      | 128.60   |
| 35  | BB    | 2712 | C    | C2-N3-C4   | 10.55  | 125.17      | 119.90   |
| 1   | AA    | 75   | G    | C5-C6-N1   | -10.54 | 106.23      | 111.50   |
| 1   | AA    | 1394 | A    | O4'-C1'-N9 | 10.54  | 116.64      | 108.20   |
| 1   | AA    | 1452 | C    | N3-C4-N4   | 10.54  | 125.38      | 118.00   |
| 35  | BB    | 1347 | A    | C4-C5-C6   | 10.55  | 122.27      | 117.00   |
| 35  | BB    | 1500 | G    | C5-C6-O6   | -10.54 | 122.27      | 128.60   |
| 35  | BB    | 1997 | C    | O4'-C1'-N1 | 10.54  | 116.64      | 108.20   |
| 35  | BB    | 2808 | G    | C5-C6-O6   | -10.54 | 122.27      | 128.60   |
| 1   | AA    | 493  | A    | C8-N9-C4   | -10.54 | 101.58      | 105.80   |
| 1   | AA    | 1210 | C    | O4'-C1'-N1 | 10.54  | 116.63      | 108.20   |
| 35  | BB    | 1196 | C    | C2-N3-C4   | 10.54  | 125.17      | 119.90   |
| 1   | AA    | 807  | A    | N1-C6-N6   | 10.54  | 124.92      | 118.60   |
| 35  | BB    | 664  | G    | N1-C6-O6   | 10.54  | 126.22      | 119.90   |
| 35  | BB    | 2736 | A    | N1-C6-N6   | 10.54  | 124.92      | 118.60   |
| 1   | AA    | 293  | G    | N3-C4-N9   | 10.54  | 132.32      | 126.00   |
| 35  | BB    | 198  | C    | O4'-C1'-N1 | 10.54  | 116.63      | 108.20   |
| 35  | BB    | 559  | G    | N1-C6-O6   | 10.54  | 126.22      | 119.90   |
| 35  | BB    | 1773 | A    | C5-N7-C8   | 10.54  | 109.17      | 103.90   |
| 35  | BB    | 1371 | G    | C5-C6-O6   | -10.54 | 122.28      | 128.60   |
| 35  | BB    | 1670 | C    | O4'-C1'-N1 | 10.54  | 116.63      | 108.20   |
| 35  | BB    | 918  | A    | C5-C6-N6   | -10.53 | 115.27      | 123.70   |
| 35  | BB    | 2003 | A    | O4'-C1'-N9 | 10.53  | 116.63      | 108.20   |
| 35  | BB    | 2791 | G    | N3-C2-N2   | 10.53  | 127.27      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 279  | A    | C5-C6-N1   | -10.53 | 112.44      | 117.70   |
| 35  | BB    | 1067 | A    | O4'-C1'-N9 | 10.53  | 116.62      | 108.20   |
| 1   | AA    | 577  | G    | C2-N3-C4   | 10.53  | 117.16      | 111.90   |
| 1   | AA    | 1027 | C    | C5-C4-N4   | -10.53 | 112.83      | 120.20   |
| 1   | AA    | 1374 | A    | O4'-C1'-N9 | 10.53  | 116.62      | 108.20   |
| 1   | AA    | 1473 | G    | N1-C6-O6   | 10.53  | 126.22      | 119.90   |
| 35  | BB    | 362  | A    | C5-C6-N6   | -10.53 | 115.28      | 123.70   |
| 1   | AA    | 492  | C    | O4'-C1'-N1 | 10.53  | 116.62      | 108.20   |
| 35  | BB    | 2800 | A    | N1-C6-N6   | 10.53  | 124.92      | 118.60   |
| 35  | BB    | 203  | A    | C5-C6-N6   | -10.53 | 115.28      | 123.70   |
| 35  | BB    | 294  | A    | N1-C6-N6   | 10.53  | 124.92      | 118.60   |
| 35  | BB    | 2230 | G    | N1-C6-O6   | 10.53  | 126.22      | 119.90   |
| 35  | BB    | 1508 | A    | O4'-C1'-N9 | 10.53  | 116.62      | 108.20   |
| 1   | AA    | 213  | G    | C5-C6-O6   | -10.52 | 122.29      | 128.60   |
| 19  | AS    | 31   | ARG  | NE-CZ-NH2  | -10.52 | 115.04      | 120.30   |
| 35  | BB    | 261  | G    | N9-C4-C5   | -10.52 | 101.19      | 105.40   |
| 4   | AD    | 110  | ARG  | NE-CZ-NH1  | -10.52 | 115.04      | 120.30   |
| 34  | BA    | 23   | G    | N1-C6-O6   | 10.52  | 126.21      | 119.90   |
| 35  | BB    | 1378 | A    | C5-N7-C8   | 10.52  | 109.16      | 103.90   |
| 35  | BB    | 1937 | A    | N1-C6-N6   | 10.52  | 124.91      | 118.60   |
| 1   | AA    | 28   | A    | O4'-C1'-N9 | 10.52  | 116.61      | 108.20   |
| 35  | BB    | 2471 | A    | C4-C5-C6   | 10.51  | 122.26      | 117.00   |
| 35  | BB    | 2675 | A    | C4-C5-C6   | 10.51  | 122.26      | 117.00   |
| 1   | AA    | 194  | C    | N3-C4-N4   | 10.51  | 125.36      | 118.00   |
| 35  | BB    | 908  | C    | O4'-C1'-N1 | 10.51  | 116.61      | 108.20   |
| 35  | BB    | 917  | A    | C6-C5-N7   | -10.51 | 124.94      | 132.30   |
| 35  | BB    | 1669 | A    | C5-C6-N1   | -10.51 | 112.44      | 117.70   |
| 35  | BB    | 2263 | C    | O4'-C1'-N1 | 10.51  | 116.61      | 108.20   |
| 1   | AA    | 672  | U    | O4'-C1'-N1 | 10.51  | 116.61      | 108.20   |
| 35  | BB    | 1309 | G    | C4-C5-C6   | 10.51  | 125.11      | 118.80   |
| 35  | BB    | 1571 | A    | C2-N3-C4   | -10.51 | 105.35      | 110.60   |
| 35  | BB    | 2112 | G    | N1-C6-O6   | 10.51  | 126.20      | 119.90   |
| 35  | BB    | 2392 | A    | C5-C6-N1   | -10.51 | 112.45      | 117.70   |
| 1   | AA    | 911  | U    | O4'-C1'-N1 | 10.50  | 116.60      | 108.20   |
| 35  | BB    | 92   | U    | O4'-C1'-N1 | 10.50  | 116.60      | 108.20   |
| 35  | BB    | 283  | G    | N3-C4-C5   | -10.50 | 123.35      | 128.60   |
| 1   | AA    | 1294 | G    | C8-N9-C4   | -10.50 | 102.20      | 106.40   |
| 1   | AA    | 908  | A    | C4-C5-C6   | 10.50  | 122.25      | 117.00   |
| 35  | BB    | 283  | G    | O4'-C1'-N9 | 10.50  | 116.60      | 108.20   |
| 35  | BB    | 1281 | G    | C5-C6-O6   | -10.50 | 122.30      | 128.60   |
| 35  | BB    | 2304 | G    | N1-C6-O6   | 10.50  | 126.20      | 119.90   |
| 1   | AA    | 507  | C    | N3-C4-C5   | -10.49 | 117.70      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 1196 | A    | C4-C5-C6   | 10.49  | 122.25      | 117.00   |
| 1   | AA    | 1432 | G    | O4'-C1'-N9 | 10.49  | 116.60      | 108.20   |
| 35  | BB    | 2042 | A    | C4-C5-C6   | 10.49  | 122.25      | 117.00   |
| 35  | BB    | 2063 | C    | C6-N1-C2   | 10.49  | 124.50      | 120.30   |
| 35  | BB    | 2175 | C    | C2-N3-C4   | 10.49  | 125.15      | 119.90   |
| 1   | AA    | 696  | A    | O4'-C1'-N9 | 10.49  | 116.59      | 108.20   |
| 1   | AA    | 1026 | G    | N1-C6-O6   | 10.49  | 126.20      | 119.90   |
| 35  | BB    | 184  | C    | N1-C2-O2   | 10.49  | 125.19      | 118.90   |
| 35  | BB    | 1940 | U    | O4'-C1'-N1 | 10.49  | 116.59      | 108.20   |
| 1   | AA    | 502  | A    | C5-C6-N6   | -10.49 | 115.31      | 123.70   |
| 35  | BB    | 2467 | C    | O4'-C1'-N1 | 10.49  | 116.59      | 108.20   |
| 1   | AA    | 1050 | G    | C5-C6-O6   | -10.49 | 122.31      | 128.60   |
| 1   | AA    | 1331 | G    | N3-C4-C5   | -10.49 | 123.36      | 128.60   |
| 35  | BB    | 604  | G    | O4'-C1'-N9 | 10.49  | 116.59      | 108.20   |
| 1   | AA    | 156  | C    | C6-N1-C2   | -10.49 | 116.11      | 120.30   |
| 1   | AA    | 192  | A    | C5-C6-N1   | -10.49 | 112.46      | 117.70   |
| 1   | AA    | 337  | G    | O4'-C1'-N9 | 10.49  | 116.59      | 108.20   |
| 35  | BB    | 19   | A    | C4-C5-N7   | -10.49 | 105.46      | 110.70   |
| 35  | BB    | 1381 | G    | C5-C6-O6   | -10.49 | 122.31      | 128.60   |
| 35  | BB    | 1388 | G    | N1-C6-O6   | 10.48  | 126.19      | 119.90   |
| 35  | BB    | 2381 | A    | C5-C6-N6   | -10.48 | 115.31      | 123.70   |
| 1   | AA    | 1163 | A    | C6-C5-N7   | -10.48 | 124.96      | 132.30   |
| 1   | AA    | 1416 | G    | N1-C6-O6   | 10.48  | 126.19      | 119.90   |
| 1   | AA    | 1289 | A    | N1-C6-N6   | 10.48  | 124.89      | 118.60   |
| 34  | BA    | 53   | A    | O4'-C1'-N9 | 10.48  | 116.58      | 108.20   |
| 35  | BB    | 981  | A    | N1-C6-N6   | 10.48  | 124.89      | 118.60   |
| 35  | BB    | 329  | G    | N1-C6-O6   | 10.48  | 126.19      | 119.90   |
| 35  | BB    | 1902 | C    | C5-C6-N1   | 10.48  | 126.24      | 121.00   |
| 35  | BB    | 1985 | C    | N3-C4-C5   | -10.48 | 117.71      | 121.90   |
| 35  | BB    | 2015 | A    | N1-C2-N3   | 10.48  | 134.54      | 129.30   |
| 35  | BB    | 2116 | G    | N1-C6-O6   | 10.48  | 126.19      | 119.90   |
| 35  | BB    | 2627 | G    | C4-C5-N7   | -10.48 | 106.61      | 110.80   |
| 1   | AA    | 1182 | G    | C5-C6-O6   | -10.47 | 122.32      | 128.60   |
| 35  | BB    | 1823 | G    | C5-C6-O6   | -10.47 | 122.32      | 128.60   |
| 35  | BB    | 2227 | A    | C5-C6-N1   | -10.47 | 112.46      | 117.70   |
| 1   | AA    | 1496 | C    | N3-C4-N4   | 10.47  | 125.33      | 118.00   |
| 34  | BA    | 69   | G    | O4'-C1'-N9 | 10.47  | 116.58      | 108.20   |
| 35  | BB    | 1649 | G    | O4'-C1'-N9 | 10.47  | 116.57      | 108.20   |
| 35  | BB    | 2524 | G    | O4'-C1'-N9 | 10.47  | 116.57      | 108.20   |
| 1   | AA    | 1018 | G    | N3-C2-N2   | 10.46  | 127.22      | 119.90   |
| 35  | BB    | 2239 | G    | N1-C2-N2   | -10.46 | 106.78      | 116.20   |
| 35  | BB    | 2778 | A    | N1-C6-N6   | 10.46  | 124.88      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 376  | G    | N3-C2-N2   | 10.46  | 127.22      | 119.90   |
| 35  | BB    | 2208 | C    | N3-C4-N4   | 10.46  | 125.32      | 118.00   |
| 35  | BB    | 2748 | A    | C5-C6-N1   | -10.46 | 112.47      | 117.70   |
| 1   | AA    | 260  | G    | O4'-C1'-N9 | 10.46  | 116.57      | 108.20   |
| 1   | AA    | 26   | A    | C4-C5-N7   | -10.46 | 105.47      | 110.70   |
| 1   | AA    | 654  | G    | N9-C4-C5   | -10.45 | 101.22      | 105.40   |
| 1   | AA    | 1435 | G    | C6-C5-N7   | -10.45 | 124.13      | 130.40   |
| 1   | AA    | 1457 | G    | N1-C6-O6   | 10.46  | 126.17      | 119.90   |
| 35  | BB    | 2268 | A    | N1-C6-N6   | 10.46  | 124.87      | 118.60   |
| 35  | BB    | 245  | G    | C5-C6-O6   | -10.45 | 122.33      | 128.60   |
| 35  | BB    | 825  | A    | C4-C5-C6   | 10.45  | 122.23      | 117.00   |
| 1   | AA    | 166  | U    | O4'-C1'-N1 | 10.45  | 116.56      | 108.20   |
| 1   | AA    | 657  | U    | N3-C4-O4   | 10.45  | 126.72      | 119.40   |
| 1   | AA    | 708  | C    | O4'-C1'-N1 | 10.45  | 116.56      | 108.20   |
| 1   | AA    | 1201 | A    | C4-C5-C6   | 10.45  | 122.23      | 117.00   |
| 1   | AA    | 1215 | G    | N9-C4-C5   | 10.45  | 109.58      | 105.40   |
| 34  | BA    | 29   | A    | O4'-C1'-N9 | 10.45  | 116.56      | 108.20   |
| 35  | BB    | 2604 | U    | O4'-C1'-N1 | 10.45  | 116.56      | 108.20   |
| 35  | BB    | 2755 | C    | C6-N1-C2   | -10.45 | 116.12      | 120.30   |
| 1   | AA    | 1375 | A    | C4-C5-C6   | 10.45  | 122.22      | 117.00   |
| 1   | AA    | 64   | G    | C8-N9-C4   | -10.45 | 102.22      | 106.40   |
| 1   | AA    | 160  | A    | N1-C2-N3   | 10.45  | 134.52      | 129.30   |
| 35  | BB    | 750  | A    | N1-C6-N6   | 10.45  | 124.87      | 118.60   |
| 35  | BB    | 1743 | G    | C6-N1-C2   | 10.45  | 131.37      | 125.10   |
| 35  | BB    | 1749 | A    | C4-C5-C6   | 10.45  | 122.22      | 117.00   |
| 35  | BB    | 2862 | G    | C5-C6-N1   | -10.45 | 106.28      | 111.50   |
| 1   | AA    | 279  | A    | P-O3'-C3'  | 10.45  | 132.23      | 119.70   |
| 35  | BB    | 1847 | A    | N1-C6-N6   | 10.44  | 124.87      | 118.60   |
| 35  | BB    | 2329 | U    | C2-N3-C4   | -10.44 | 120.73      | 127.00   |
| 35  | BB    | 2659 | G    | N1-C6-O6   | 10.45  | 126.17      | 119.90   |
| 1   | AA    | 282  | A    | C6-N1-C2   | -10.44 | 112.33      | 118.60   |
| 1   | AA    | 1078 | U    | O4'-C1'-N1 | 10.44  | 116.56      | 108.20   |
| 35  | BB    | 1401 | G    | C5-C6-O6   | -10.44 | 122.33      | 128.60   |
| 35  | BB    | 99   | U    | P-O3'-C3'  | 10.44  | 132.23      | 119.70   |
| 35  | BB    | 2748 | A    | C8-N9-C4   | 10.44  | 109.98      | 105.80   |
| 35  | BB    | 2184 | A    | C5-C6-N1   | -10.44 | 112.48      | 117.70   |
| 35  | BB    | 2169 | A    | C8-N9-C4   | -10.44 | 101.62      | 105.80   |
| 35  | BB    | 2727 | A    | C8-N9-C4   | -10.44 | 101.62      | 105.80   |
| 1   | AA    | 751  | U    | O4'-C1'-N1 | 10.44  | 116.55      | 108.20   |
| 1   | AA    | 1456 | A    | C5-C6-N6   | -10.44 | 115.35      | 123.70   |
| 35  | BB    | 2086 | U    | N3-C4-O4   | 10.44  | 126.71      | 119.40   |
| 35  | BB    | 217  | A    | C5-C6-N1   | -10.43 | 112.48      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 301  | G    | N1-C6-O6   | 10.43  | 126.16      | 119.90   |
| 35  | BB    | 504  | A    | N1-C2-N3   | 10.43  | 134.52      | 129.30   |
| 35  | BB    | 2574 | G    | N1-C6-O6   | 10.43  | 126.16      | 119.90   |
| 35  | BB    | 182  | A    | N9-C4-C5   | 10.43  | 109.97      | 105.80   |
| 1   | AA    | 925  | G    | N1-C6-O6   | 10.43  | 126.16      | 119.90   |
| 1   | AA    | 1324 | A    | N1-C6-N6   | 10.43  | 124.86      | 118.60   |
| 35  | BB    | 1319 | C    | O4'-C1'-N1 | 10.43  | 116.54      | 108.20   |
| 35  | BB    | 2850 | A    | N1-C6-N6   | 10.43  | 124.86      | 118.60   |
| 1   | AA    | 8    | A    | O4'-C1'-N9 | 10.42  | 116.54      | 108.20   |
| 1   | AA    | 88   | U    | O4'-C1'-N1 | 10.42  | 116.54      | 108.20   |
| 35  | BB    | 565  | C    | O4'-C1'-N1 | 10.42  | 116.54      | 108.20   |
| 1   | AA    | 607  | A    | N1-C6-N6   | 10.42  | 124.85      | 118.60   |
| 35  | BB    | 1210 | G    | N3-C2-N2   | 10.42  | 127.20      | 119.90   |
| 1   | AA    | 1203 | C    | O4'-C1'-N1 | 10.42  | 116.53      | 108.20   |
| 35  | BB    | 972  | A    | C5-C6-N1   | -10.42 | 112.49      | 117.70   |
| 35  | BB    | 1048 | A    | C5-C6-N6   | -10.42 | 115.37      | 123.70   |
| 35  | BB    | 1586 | A    | C8-N9-C4   | -10.42 | 101.63      | 105.80   |
| 35  | BB    | 1825 | U    | O4'-C1'-N1 | 10.42  | 116.53      | 108.20   |
| 1   | AA    | 984  | C    | C5-C4-N4   | -10.41 | 112.91      | 120.20   |
| 35  | BB    | 121  | G    | N1-C2-N3   | -10.41 | 117.65      | 123.90   |
| 35  | BB    | 458  | G    | N1-C2-N3   | -10.41 | 117.65      | 123.90   |
| 35  | BB    | 2407 | A    | C5-N7-C8   | 10.41  | 109.11      | 103.90   |
| 1   | AA    | 741  | G    | C5-C6-O6   | -10.41 | 122.36      | 128.60   |
| 1   | AA    | 372  | C    | N3-C4-C5   | -10.41 | 117.74      | 121.90   |
| 35  | BB    | 873  | C    | C5-C6-N1   | -10.41 | 115.80      | 121.00   |
| 1   | AA    | 274  | A    | C5-C6-N1   | -10.40 | 112.50      | 117.70   |
| 1   | AA    | 1262 | C    | O4'-C1'-N1 | 10.40  | 116.52      | 108.20   |
| 1   | AA    | 1285 | A    | C5-C6-N6   | -10.40 | 115.38      | 123.70   |
| 1   | AA    | 1510 | C    | O4'-C1'-N1 | 10.40  | 116.52      | 108.20   |
| 35  | BB    | 291  | G    | C6-C5-N7   | -10.40 | 124.16      | 130.40   |
| 35  | BB    | 604  | G    | N1-C6-O6   | 10.40  | 126.14      | 119.90   |
| 1   | AA    | 973  | G    | C2-N3-C4   | 10.40  | 117.10      | 111.90   |
| 35  | BB    | 1070 | A    | C4-C5-C6   | 10.40  | 122.20      | 117.00   |
| 35  | BB    | 1785 | A    | N1-C6-N6   | 10.40  | 124.84      | 118.60   |
| 35  | BB    | 2078 | C    | O4'-C1'-N1 | 10.40  | 116.52      | 108.20   |
| 1   | AA    | 655  | A    | C5-C6-N1   | -10.40 | 112.50      | 117.70   |
| 35  | BB    | 240  | C    | C5-C6-N1   | 10.40  | 126.20      | 121.00   |
| 35  | BB    | 1437 | C    | O4'-C1'-N1 | 10.40  | 116.52      | 108.20   |
| 35  | BB    | 1940 | U    | C5-C6-N1   | 10.40  | 127.90      | 122.70   |
| 35  | BB    | 2468 | A    | C5-C6-N1   | -10.39 | 112.50      | 117.70   |
| 35  | BB    | 2777 | G    | N1-C2-N3   | -10.39 | 117.66      | 123.90   |
| 35  | BB    | 250  | G    | N9-C4-C5   | -10.39 | 101.24      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2300 | C    | O4'-C1'-N1 | 10.39  | 116.51      | 108.20   |
| 35  | BB    | 22   | C    | N3-C4-C5   | -10.39 | 117.74      | 121.90   |
| 35  | BB    | 1989 | G    | N7-C8-N9   | 10.39  | 118.29      | 113.10   |
| 35  | BB    | 2771 | C    | C6-N1-C2   | -10.39 | 116.14      | 120.30   |
| 35  | BB    | 2825 | G    | C5-C6-O6   | -10.39 | 122.37      | 128.60   |
| 1   | AA    | 541  | G    | N1-C6-O6   | 10.38  | 126.13      | 119.90   |
| 35  | BB    | 1787 | A    | N1-C6-N6   | 10.39  | 124.83      | 118.60   |
| 35  | BB    | 784  | G    | C5-C6-O6   | -10.38 | 122.37      | 128.60   |
| 34  | BA    | 102  | G    | N1-C2-N2   | -10.38 | 106.86      | 116.20   |
| 35  | BB    | 2370 | G    | O4'-C1'-N9 | 10.38  | 116.51      | 108.20   |
| 1   | AA    | 747  | A    | C5-C6-N6   | -10.38 | 115.40      | 123.70   |
| 35  | BB    | 880  | G    | C5-C6-N1   | -10.38 | 106.31      | 111.50   |
| 35  | BB    | 2448 | A    | C4-C5-C6   | 10.38  | 122.19      | 117.00   |
| 35  | BB    | 2531 | A    | C5-N7-C8   | 10.38  | 109.09      | 103.90   |
| 1   | AA    | 642  | A    | C6-C5-N7   | -10.38 | 125.04      | 132.30   |
| 1   | AA    | 364  | A    | C4-C5-C6   | 10.38  | 122.19      | 117.00   |
| 1   | AA    | 1534 | A    | N1-C2-N3   | 10.38  | 134.49      | 129.30   |
| 20  | AT    | 28   | ARG  | NE-CZ-NH2  | -10.38 | 115.11      | 120.30   |
| 35  | BB    | 857  | G    | O4'-C1'-N9 | 10.38  | 116.50      | 108.20   |
| 35  | BB    | 999  | U    | O4'-C1'-N1 | 10.38  | 116.50      | 108.20   |
| 1   | AA    | 937  | A    | C8-N9-C4   | -10.37 | 101.65      | 105.80   |
| 35  | BB    | 1090 | A    | C4-C5-C6   | 10.37  | 122.19      | 117.00   |
| 35  | BB    | 1573 | G    | N1-C6-O6   | 10.37  | 126.12      | 119.90   |
| 1   | AA    | 74   | A    | C4-C5-C6   | 10.37  | 122.19      | 117.00   |
| 35  | BB    | 1364 | G    | N1-C6-O6   | 10.37  | 126.12      | 119.90   |
| 35  | BB    | 2650 | U    | O4'-C1'-N1 | 10.37  | 116.50      | 108.20   |
| 1   | AA    | 417  | G    | C5-C6-O6   | -10.37 | 122.38      | 128.60   |
| 1   | AA    | 781  | A    | C5-C6-N6   | -10.37 | 115.41      | 123.70   |
| 1   | AA    | 1107 | C    | O4'-C1'-N1 | 10.37  | 116.49      | 108.20   |
| 35  | BB    | 1184 | U    | O4'-C1'-N1 | 10.37  | 116.49      | 108.20   |
| 1   | AA    | 432  | A    | C8-N9-C4   | -10.36 | 101.66      | 105.80   |
| 1   | AA    | 1003 | G    | N1-C6-O6   | 10.36  | 126.12      | 119.90   |
| 1   | AA    | 1290 | G    | C5-C6-O6   | -10.36 | 122.38      | 128.60   |
| 1   | AA    | 1322 | C    | C6-N1-C2   | -10.36 | 116.16      | 120.30   |
| 35  | BB    | 145  | C    | N3-C4-N4   | 10.36  | 125.25      | 118.00   |
| 35  | BB    | 432  | A    | N1-C6-N6   | 10.36  | 124.82      | 118.60   |
| 1   | AA    | 459  | A    | N1-C6-N6   | 10.36  | 124.81      | 118.60   |
| 1   | AA    | 1473 | G    | C5-C6-O6   | -10.36 | 122.39      | 128.60   |
| 35  | BB    | 1345 | C    | N3-C4-C5   | -10.36 | 117.76      | 121.90   |
| 35  | BB    | 1681 | G    | N1-C6-O6   | 10.36  | 126.11      | 119.90   |
| 35  | BB    | 2747 | G    | N1-C6-O6   | 10.36  | 126.12      | 119.90   |
| 36  | BC    | 82   | TYR  | CB-CG-CD2  | 10.36  | 127.22      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1367 | A    | C4-C5-C6   | 10.36  | 122.18      | 117.00   |
| 35  | BB    | 1413 | A    | C4-C5-C6   | 10.36  | 122.18      | 117.00   |
| 35  | BB    | 2183 | A    | C6-C5-N7   | -10.36 | 125.05      | 132.30   |
| 35  | BB    | 2725 | A    | C5-C6-N1   | -10.36 | 112.52      | 117.70   |
| 1   | AA    | 605  | U    | O4'-C1'-N1 | 10.35  | 116.48      | 108.20   |
| 1   | AA    | 631  | C    | C5-C4-N4   | -10.35 | 112.95      | 120.20   |
| 35  | BB    | 1737 | G    | C6-C5-N7   | -10.35 | 124.19      | 130.40   |
| 35  | BB    | 351  | C    | C4-C5-C6   | 10.35  | 122.58      | 117.40   |
| 1   | AA    | 193  | C    | C5-C4-N4   | -10.35 | 112.95      | 120.20   |
| 35  | BB    | 86   | G    | N3-C2-N2   | 10.35  | 127.14      | 119.90   |
| 35  | BB    | 2359 | C    | N3-C4-C5   | -10.35 | 117.76      | 121.90   |
| 35  | BB    | 2792 | A    | C5-C6-N6   | -10.35 | 115.42      | 123.70   |
| 1   | AA    | 928  | G    | O4'-C1'-N9 | 10.34  | 116.47      | 108.20   |
| 35  | BB    | 2042 | A    | C5-C6-N6   | -10.34 | 115.42      | 123.70   |
| 35  | BB    | 2455 | G    | O4'-C1'-N9 | 10.34  | 116.47      | 108.20   |
| 55  | BW    | 19   | ARG  | NE-CZ-NH2  | -10.34 | 115.13      | 120.30   |
| 1   | AA    | 432  | A    | C4-C5-N7   | -10.34 | 105.53      | 110.70   |
| 35  | BB    | 2116 | G    | N9-C4-C5   | 10.34  | 109.54      | 105.40   |
| 1   | AA    | 794  | A    | N1-C6-N6   | 10.34  | 124.80      | 118.60   |
| 35  | BB    | 1237 | A    | N1-C2-N3   | -10.34 | 124.13      | 129.30   |
| 35  | BB    | 1614 | A    | N1-C6-N6   | 10.34  | 124.80      | 118.60   |
| 35  | BB    | 1444 | G    | C6-N1-C2   | -10.34 | 118.90      | 125.10   |
| 1   | AA    | 174  | A    | N1-C6-N6   | 10.34  | 124.80      | 118.60   |
| 4   | AD    | 127  | ARG  | NE-CZ-NH2  | -10.34 | 115.13      | 120.30   |
| 35  | BB    | 728  | G    | C5-C6-O6   | -10.33 | 122.40      | 128.60   |
| 35  | BB    | 2520 | C    | N3-C4-N4   | 10.33  | 125.23      | 118.00   |
| 1   | AA    | 28   | A    | C5-C6-N1   | -10.33 | 112.53      | 117.70   |
| 35  | BB    | 2281 | A    | C2-N3-C4   | -10.33 | 105.44      | 110.60   |
| 35  | BB    | 2520 | C    | C2-N3-C4   | 10.33  | 125.06      | 119.90   |
| 35  | BB    | 144  | A    | N1-C6-N6   | 10.33  | 124.80      | 118.60   |
| 35  | BB    | 716  | A    | O4'-C1'-N9 | 10.33  | 116.46      | 108.20   |
| 35  | BB    | 1949 | G    | C4-C5-C6   | 10.32  | 125.00      | 118.80   |
| 1   | AA    | 443  | C    | C6-N1-C2   | -10.32 | 116.17      | 120.30   |
| 1   | AA    | 1271 | A    | N1-C6-N6   | 10.32  | 124.79      | 118.60   |
| 35  | BB    | 2247 | A    | C8-N9-C4   | 10.32  | 109.93      | 105.80   |
| 35  | BB    | 2632 | A    | C5-N7-C8   | 10.32  | 109.06      | 103.90   |
| 1   | AA    | 26   | A    | C5-N7-C8   | 10.32  | 109.06      | 103.90   |
| 1   | AA    | 676  | A    | C5-N7-C8   | 10.32  | 109.06      | 103.90   |
| 35  | BB    | 176  | A    | O4'-C1'-N9 | 10.32  | 116.46      | 108.20   |
| 35  | BB    | 1796 | U    | N3-C4-C5   | -10.32 | 108.41      | 114.60   |
| 35  | BB    | 2741 | A    | N1-C2-N3   | 10.32  | 134.46      | 129.30   |
| 1   | AA    | 22   | G    | C5-C6-N1   | -10.32 | 106.34      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1   | AA    | 786  | G    | C5-C6-O6    | -10.32 | 122.41      | 128.60   |
| 35  | BB    | 924  | G    | N3-C4-N9    | 10.32  | 132.19      | 126.00   |
| 35  | BB    | 1852 | U    | N1-C2-O2    | -10.32 | 115.58      | 122.80   |
| 35  | BB    | 2121 | G    | N3-C4-C5    | 10.32  | 133.76      | 128.60   |
| 36  | BC    | 79   | ARG  | NE-CZ-NH2   | -10.32 | 115.14      | 120.30   |
| 43  | BJ    | 95   | ARG  | NE-CZ-NH2   | -10.32 | 115.14      | 120.30   |
| 1   | AA    | 507  | C    | C2-N3-C4    | 10.31  | 125.06      | 119.90   |
| 1   | AA    | 919  | A    | N9-C4-C5    | -10.31 | 101.67      | 105.80   |
| 1   | AA    | 1365 | G    | N1-C6-O6    | 10.31  | 126.09      | 119.90   |
| 35  | BB    | 698  | C    | C6-N1-C2    | -10.31 | 116.17      | 120.30   |
| 35  | BB    | 2019 | A    | N1-C2-N3    | 10.31  | 134.46      | 129.30   |
| 35  | BB    | 759  | G    | C6-C5-N7    | -10.31 | 124.21      | 130.40   |
| 35  | BB    | 2694 | G    | C5-C6-O6    | -10.31 | 122.41      | 128.60   |
| 35  | BB    | 2826 | A    | C4-C5-C6    | 10.31  | 122.16      | 117.00   |
| 1   | AA    | 500  | G    | C8-N9-C4    | -10.31 | 102.28      | 106.40   |
| 35  | BB    | 2349 | G    | O4'-C1'-N9  | 10.31  | 116.45      | 108.20   |
| 35  | BB    | 2692 | G    | N1-C6-O6    | 10.31  | 126.09      | 119.90   |
| 1   | AA    | 413  | G    | N3-C2-N2    | 10.31  | 127.12      | 119.90   |
| 1   | AA    | 264  | C    | N1-C2-O2    | 10.31  | 125.08      | 118.90   |
| 35  | BB    | 713  | G    | N9-C4-C5    | -10.31 | 101.28      | 105.40   |
| 35  | BB    | 1450 | G    | C5-C6-O6    | -10.31 | 122.42      | 128.60   |
| 1   | AA    | 1001 | C    | N3-C4-N4    | 10.31  | 125.21      | 118.00   |
| 35  | BB    | 1077 | A    | C4-C5-C6    | 10.30  | 122.15      | 117.00   |
| 1   | AA    | 235  | C    | O4'-C1'-N1  | 10.30  | 116.44      | 108.20   |
| 1   | AA    | 575  | G    | C5'-C4'-O4' | 10.30  | 121.46      | 109.10   |
| 1   | AA    | 1246 | A    | N9-C4-C5    | 10.30  | 109.92      | 105.80   |
| 1   | AA    | 354  | G    | C2-N3-C4    | 10.30  | 117.05      | 111.90   |
| 1   | AA    | 1048 | G    | C5-C6-O6    | -10.30 | 122.42      | 128.60   |
| 35  | BB    | 1414 | C    | N3-C4-C5    | -10.30 | 117.78      | 121.90   |
| 1   | AA    | 474  | G    | O4'-C1'-N9  | 10.30  | 116.44      | 108.20   |
| 35  | BB    | 1845 | G    | O4'-C1'-N9  | 10.30  | 116.44      | 108.20   |
| 35  | BB    | 2142 | A    | N7-C8-N9    | 10.29  | 118.95      | 113.80   |
| 35  | BB    | 2417 | C    | O4'-C1'-N1  | 10.30  | 116.44      | 108.20   |
| 35  | BB    | 2550 | G    | N3-C4-C5    | -10.29 | 123.45      | 128.60   |
| 35  | BB    | 2766 | A    | N3-C4-C5    | -10.29 | 119.59      | 126.80   |
| 1   | AA    | 679  | C    | N3-C4-C5    | -10.29 | 117.78      | 121.90   |
| 1   | AA    | 1247 | U    | O4'-C1'-N1  | 10.29  | 116.43      | 108.20   |
| 35  | BB    | 1935 | G    | C8-N9-C4    | -10.29 | 102.28      | 106.40   |
| 35  | BB    | 2377 | A    | C5-C6-N1    | -10.29 | 112.55      | 117.70   |
| 35  | BB    | 2316 | G    | O4'-C1'-N9  | 10.29  | 116.43      | 108.20   |
| 35  | BB    | 2734 | A    | C5-C6-N6    | -10.29 | 115.47      | 123.70   |
| 1   | AA    | 752  | G    | N3-C2-N2    | 10.29  | 127.10      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 1104 | G    | C5-C6-O6   | -10.29 | 122.43      | 128.60   |
| 35  | BB    | 134  | G    | O4'-C1'-N9 | 10.29  | 116.43      | 108.20   |
| 35  | BB    | 722  | A    | C4-C5-N7   | -10.29 | 105.56      | 110.70   |
| 35  | BB    | 1049 | C    | C5-C6-N1   | 10.29  | 126.14      | 121.00   |
| 35  | BB    | 1274 | A    | C8-N9-C4   | 10.29  | 109.92      | 105.80   |
| 35  | BB    | 1738 | G    | C8-N9-C4   | 10.29  | 110.52      | 106.40   |
| 35  | BB    | 2053 | G    | N7-C8-N9   | -10.29 | 107.96      | 113.10   |
| 1   | AA    | 633  | G    | C6-C5-N7   | -10.29 | 124.23      | 130.40   |
| 34  | BA    | 13   | G    | C5-C6-O6   | -10.29 | 122.43      | 128.60   |
| 35  | BB    | 1154 | G    | N1-C6-O6   | 10.29  | 126.07      | 119.90   |
| 35  | BB    | 1640 | A    | N7-C8-N9   | -10.29 | 108.66      | 113.80   |
| 35  | BB    | 2069 | G    | C5-C6-O6   | -10.29 | 122.43      | 128.60   |
| 35  | BB    | 2570 | G    | N3-C4-N9   | -10.29 | 119.83      | 126.00   |
| 1   | AA    | 124  | C    | N3-C4-C5   | -10.28 | 117.79      | 121.90   |
| 35  | BB    | 1248 | G    | N9-C4-C5   | -10.29 | 101.29      | 105.40   |
| 35  | BB    | 768  | G    | N1-C6-O6   | 10.28  | 126.07      | 119.90   |
| 35  | BB    | 2270 | A    | C5-C6-N6   | -10.28 | 115.47      | 123.70   |
| 1   | AA    | 189  | A    | C5-C6-N6   | -10.28 | 115.48      | 123.70   |
| 1   | AA    | 1141 | C    | N3-C4-C5   | -10.28 | 117.79      | 121.90   |
| 35  | BB    | 1730 | C    | C2-N3-C4   | 10.28  | 125.04      | 119.90   |
| 35  | BB    | 2463 | C    | O4'-C1'-N1 | 10.28  | 116.42      | 108.20   |
| 1   | AA    | 883  | C    | C5-C4-N4   | -10.28 | 113.01      | 120.20   |
| 1   | AA    | 1531 | A    | O4'-C1'-N9 | 10.28  | 116.42      | 108.20   |
| 34  | BA    | 76   | G    | N1-C2-N3   | -10.28 | 117.73      | 123.90   |
| 1   | AA    | 1418 | A    | C6-C5-N7   | -10.28 | 125.11      | 132.30   |
| 35  | BB    | 867  | C    | C2-N3-C4   | 10.28  | 125.04      | 119.90   |
| 1   | AA    | 371  | A    | N1-C6-N6   | 10.27  | 124.76      | 118.60   |
| 1   | AA    | 1345 | U    | N1-C2-O2   | -10.27 | 115.61      | 122.80   |
| 35  | BB    | 2057 | G    | C5-C6-O6   | -10.27 | 122.44      | 128.60   |
| 35  | BB    | 2438 | U    | O4'-C1'-N1 | 10.27  | 116.42      | 108.20   |
| 1   | AA    | 233  | C    | O4'-C1'-N1 | 10.27  | 116.41      | 108.20   |
| 1   | AA    | 244  | U    | N1-C2-O2   | -10.27 | 115.61      | 122.80   |
| 35  | BB    | 2450 | A    | C2-N3-C4   | -10.27 | 105.47      | 110.60   |
| 1   | AA    | 327  | A    | C4-C5-N7   | -10.27 | 105.57      | 110.70   |
| 1   | AA    | 836  | G    | C5-C6-O6   | -10.27 | 122.44      | 128.60   |
| 35  | BB    | 1069 | A    | C4-C5-N7   | 10.27  | 115.83      | 110.70   |
| 1   | AA    | 1357 | A    | O4'-C1'-N9 | 10.27  | 116.41      | 108.20   |
| 1   | AA    | 456  | A    | C8-N9-C4   | -10.26 | 101.69      | 105.80   |
| 1   | AA    | 1104 | G    | N9-C4-C5   | -10.26 | 101.29      | 105.40   |
| 35  | BB    | 75   | G    | C5-C6-N1   | -10.26 | 106.37      | 111.50   |
| 35  | BB    | 1681 | G    | N3-C4-N9   | 10.26  | 132.16      | 126.00   |
| 35  | BB    | 411  | G    | N1-C6-O6   | 10.26  | 126.06      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2582 | G    | O4'-C1'-N9 | 10.26  | 116.41      | 108.20   |
| 35  | BB    | 1654 | A    | C5-C6-N6   | -10.26 | 115.49      | 123.70   |
| 35  | BB    | 2706 | A    | N1-C2-N3   | 10.26  | 134.43      | 129.30   |
| 35  | BB    | 1642 | G    | C5-C6-N1   | -10.26 | 106.37      | 111.50   |
| 35  | BB    | 2778 | A    | C2-N3-C4   | -10.26 | 105.47      | 110.60   |
| 1   | AA    | 293  | G    | N3-C4-C5   | -10.26 | 123.47      | 128.60   |
| 35  | BB    | 81   | G    | C2-N3-C4   | -10.26 | 106.77      | 111.90   |
| 35  | BB    | 155  | A    | C8-N9-C4   | -10.26 | 101.70      | 105.80   |
| 35  | BB    | 877  | A    | C4-C5-C6   | 10.26  | 122.13      | 117.00   |
| 1   | AA    | 154  | U    | C5-C4-O4   | -10.25 | 119.75      | 125.90   |
| 35  | BB    | 935  | C    | C6-N1-C2   | -10.25 | 116.20      | 120.30   |
| 35  | BB    | 1529 | G    | C5-N7-C8   | -10.25 | 99.17       | 104.30   |
| 35  | BB    | 2186 | G    | N1-C6-O6   | 10.25  | 126.05      | 119.90   |
| 35  | BB    | 2241 | A    | C5-C6-N1   | -10.25 | 112.57      | 117.70   |
| 35  | BB    | 2573 | C    | N1-C2-O2   | 10.25  | 125.05      | 118.90   |
| 1   | AA    | 161  | A    | C4-C5-C6   | 10.25  | 122.12      | 117.00   |
| 1   | AA    | 1032 | G    | C5-C6-N1   | -10.25 | 106.37      | 111.50   |
| 1   | AA    | 669  | G    | C4-C5-C6   | 10.25  | 124.95      | 118.80   |
| 1   | AA    | 1005 | A    | C5-N7-C8   | 10.25  | 109.02      | 103.90   |
| 35  | BB    | 46   | G    | N3-C4-C5   | -10.25 | 123.48      | 128.60   |
| 35  | BB    | 133  | U    | O4'-C1'-N1 | 10.25  | 116.40      | 108.20   |
| 35  | BB    | 1661 | G    | C5-C6-O6   | -10.25 | 122.45      | 128.60   |
| 1   | AA    | 623  | C    | O4'-C1'-N1 | 10.24  | 116.39      | 108.20   |
| 35  | BB    | 284  | U    | O4'-C1'-N1 | 10.24  | 116.40      | 108.20   |
| 35  | BB    | 1638 | C    | N1-C2-O2   | -10.24 | 112.75      | 118.90   |
| 1   | AA    | 1109 | C    | C6-N1-C2   | -10.24 | 116.20      | 120.30   |
| 35  | BB    | 1748 | C    | C6-N1-C2   | -10.24 | 116.20      | 120.30   |
| 1   | AA    | 753  | A    | C6-N1-C2   | 10.24  | 124.75      | 118.60   |
| 30  | B5    | 163  | TYR  | CB-CG-CD1  | -10.24 | 114.86      | 121.00   |
| 35  | BB    | 1189 | A    | N1-C6-N6   | 10.24  | 124.75      | 118.60   |
| 35  | BB    | 1637 | A    | C5-N7-C8   | 10.24  | 109.02      | 103.90   |
| 35  | BB    | 1787 | A    | N9-C4-C5   | -10.24 | 101.70      | 105.80   |
| 35  | BB    | 2828 | G    | C5-C6-O6   | -10.24 | 122.45      | 128.60   |
| 1   | AA    | 1417 | G    | N1-C6-O6   | 10.24  | 126.04      | 119.90   |
| 35  | BB    | 58   | G    | C4-C5-C6   | 10.24  | 124.94      | 118.80   |
| 35  | BB    | 454  | A    | C2-N3-C4   | 10.24  | 115.72      | 110.60   |
| 35  | BB    | 1205 | A    | P-O3'-C3'  | 10.24  | 131.99      | 119.70   |
| 1   | AA    | 796  | C    | O4'-C1'-N1 | 10.24  | 116.39      | 108.20   |
| 35  | BB    | 2411 | A    | N1-C2-N3   | 10.24  | 134.42      | 129.30   |
| 1   | AA    | 958  | A    | C2-N3-C4   | -10.23 | 105.48      | 110.60   |
| 34  | BA    | 65   | U    | O4'-C1'-N1 | 10.23  | 116.39      | 108.20   |
| 35  | BB    | 1380 | G    | C6-C5-N7   | -10.23 | 124.26      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1604 | C    | N3-C4-N4   | 10.23  | 125.17      | 118.00   |
| 35  | BB    | 1811 | G    | C8-N9-C4   | -10.23 | 102.31      | 106.40   |
| 35  | BB    | 1710 | G    | C4-C5-N7   | -10.23 | 106.71      | 110.80   |
| 1   | AA    | 586  | C    | N3-C4-N4   | 10.23  | 125.16      | 118.00   |
| 1   | AA    | 908  | A    | C5-N7-C8   | 10.23  | 109.02      | 103.90   |
| 1   | AA    | 1051 | C    | O4'-C1'-N1 | 10.23  | 116.39      | 108.20   |
| 1   | AA    | 1477 | U    | N1-C2-O2   | -10.23 | 115.64      | 122.80   |
| 35  | BB    | 324  | A    | C5-C6-N1   | -10.23 | 112.58      | 117.70   |
| 1   | AA    | 80   | A    | C4-C5-C6   | 10.23  | 122.11      | 117.00   |
| 35  | BB    | 560  | C    | C6-N1-C2   | -10.23 | 116.21      | 120.30   |
| 1   | AA    | 556  | C    | C6-N1-C2   | -10.23 | 116.21      | 120.30   |
| 1   | AA    | 953  | G    | N3-C4-C5   | 10.23  | 133.71      | 128.60   |
| 35  | BB    | 37   | C    | O4'-C1'-N1 | 10.23  | 116.38      | 108.20   |
| 35  | BB    | 496  | G    | O4'-C1'-N9 | 10.23  | 116.38      | 108.20   |
| 35  | BB    | 901  | C    | N3-C4-N4   | 10.23  | 125.16      | 118.00   |
| 35  | BB    | 1067 | A    | C4-C5-C6   | 10.23  | 122.11      | 117.00   |
| 35  | BB    | 2339 | C    | O4'-C1'-N1 | 10.23  | 116.38      | 108.20   |
| 1   | AA    | 203  | G    | N1-C6-O6   | 10.22  | 126.03      | 119.90   |
| 1   | AA    | 890  | G    | C4-C5-C6   | 10.22  | 124.94      | 118.80   |
| 35  | BB    | 1828 | G    | N3-C2-N2   | 10.22  | 127.06      | 119.90   |
| 35  | BB    | 855  | G    | O4'-C1'-N9 | 10.22  | 116.38      | 108.20   |
| 35  | BB    | 1797 | G    | N7-C8-N9   | 10.22  | 118.21      | 113.10   |
| 1   | AA    | 893  | C    | N3-C4-C5   | -10.22 | 117.81      | 121.90   |
| 35  | BB    | 1850 | G    | N1-C6-O6   | 10.22  | 126.03      | 119.90   |
| 35  | BB    | 2885 | G    | N1-C2-N3   | -10.22 | 117.77      | 123.90   |
| 1   | AA    | 1460 | C    | O4'-C1'-N1 | 10.22  | 116.38      | 108.20   |
| 35  | BB    | 1577 | C    | N3-C4-N4   | 10.22  | 125.15      | 118.00   |
| 1   | AA    | 1033 | G    | C5-C6-O6   | -10.22 | 122.47      | 128.60   |
| 1   | AA    | 229  | U    | N3-C2-O2   | 10.22  | 129.35      | 122.20   |
| 35  | BB    | 254  | G    | N7-C8-N9   | 10.22  | 118.21      | 113.10   |
| 35  | BB    | 1179 | G    | N1-C6-O6   | 10.22  | 126.03      | 119.90   |
| 35  | BB    | 1348 | C    | O4'-C1'-N1 | 10.22  | 116.38      | 108.20   |
| 35  | BB    | 954  | G    | C5-C6-O6   | -10.22 | 122.47      | 128.60   |
| 35  | BB    | 969  | G    | C5-C6-N1   | -10.22 | 106.39      | 111.50   |
| 35  | BB    | 1620 | G    | N1-C6-O6   | 10.22  | 126.03      | 119.90   |
| 35  | BB    | 48   | G    | N1-C6-O6   | 10.21  | 126.03      | 119.90   |
| 1   | AA    | 259  | G    | C5-C6-O6   | -10.21 | 122.47      | 128.60   |
| 35  | BB    | 1901 | A    | N7-C8-N9   | 10.21  | 118.91      | 113.80   |
| 35  | BB    | 1952 | A    | C5-C6-N1   | -10.21 | 112.59      | 117.70   |
| 35  | BB    | 2121 | G    | N1-C2-N3   | -10.21 | 117.77      | 123.90   |
| 1   | AA    | 202  | G    | O4'-C1'-N9 | 10.21  | 116.37      | 108.20   |
| 4   | AD    | 164  | ARG  | NE-CZ-NH1  | 10.21  | 125.40      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | AA    | 363  | A    | C4-C5-C6   | 10.21  | 122.10      | 117.00   |
| 35  | BB    | 1743 | G    | C5-C6-O6   | -10.21 | 122.47      | 128.60   |
| 35  | BB    | 1938 | A    | O4'-C1'-N9 | 10.21  | 116.37      | 108.20   |
| 35  | BB    | 2006 | C    | C4-C5-C6   | 10.21  | 122.50      | 117.40   |
| 35  | BB    | 2581 | G    | C5-C6-O6   | -10.21 | 122.47      | 128.60   |
| 35  | BB    | 2893 | A    | N1-C6-N6   | 10.21  | 124.72      | 118.60   |
| 35  | BB    | 833  | A    | C4-C5-C6   | 10.21  | 122.10      | 117.00   |
| 35  | BB    | 1079 | C    | N3-C4-N4   | 10.21  | 125.14      | 118.00   |
| 35  | BB    | 1169 | A    | N1-C6-N6   | 10.21  | 124.72      | 118.60   |
| 1   | AA    | 1350 | A    | C6-C5-N7   | -10.20 | 125.16      | 132.30   |
| 35  | BB    | 2461 | A    | N9-C4-C5   | -10.20 | 101.72      | 105.80   |
| 35  | BB    | 1468 | U    | O4'-C1'-N1 | 10.20  | 116.36      | 108.20   |
| 35  | BB    | 2124 | G    | N9-C4-C5   | 10.20  | 109.48      | 105.40   |
| 35  | BB    | 2201 | G    | N7-C8-N9   | -10.20 | 108.00      | 113.10   |
| 35  | BB    | 283  | G    | C5-N7-C8   | 10.20  | 109.40      | 104.30   |
| 35  | BB    | 103  | A    | C4-C5-C6   | 10.20  | 122.10      | 117.00   |
| 35  | BB    | 933  | A    | N1-C2-N3   | 10.20  | 134.40      | 129.30   |
| 35  | BB    | 993  | G    | O4'-C1'-N9 | 10.20  | 116.36      | 108.20   |
| 35  | BB    | 1585 | C    | N3-C4-C5   | -10.20 | 117.82      | 121.90   |
| 1   | AA    | 78   | A    | N1-C6-N6   | 10.20  | 124.72      | 118.60   |
| 1   | AA    | 280  | C    | C5-C4-N4   | -10.20 | 113.06      | 120.20   |
| 1   | AA    | 498  | A    | C5-N7-C8   | 10.20  | 109.00      | 103.90   |
| 35  | BB    | 648  | G    | O4'-C1'-N9 | 10.20  | 116.36      | 108.20   |
| 1   | AA    | 1220 | G    | N7-C8-N9   | -10.19 | 108.00      | 113.10   |
| 35  | BB    | 400  | G    | C8-N9-C4   | -10.19 | 102.32      | 106.40   |
| 35  | BB    | 1558 | C    | C5-C4-N4   | -10.19 | 113.06      | 120.20   |
| 35  | BB    | 18   | U    | O4'-C1'-N1 | 10.19  | 116.35      | 108.20   |
| 1   | AA    | 16   | A    | C6-N1-C2   | 10.19  | 124.71      | 118.60   |
| 1   | AA    | 382  | A    | O4'-C1'-N9 | 10.19  | 116.35      | 108.20   |
| 35  | BB    | 2213 | U    | O4'-C1'-N1 | 10.19  | 116.35      | 108.20   |
| 35  | BB    | 2675 | A    | N9-C4-C5   | 10.19  | 109.88      | 105.80   |
| 1   | AA    | 684  | U    | C5-C4-O4   | -10.19 | 119.79      | 125.90   |
| 35  | BB    | 1906 | G    | C6-C5-N7   | -10.19 | 124.29      | 130.40   |
| 35  | BB    | 2588 | G    | C5-N7-C8   | 10.19  | 109.39      | 104.30   |
| 35  | BB    | 2762 | C    | N3-C4-N4   | 10.19  | 125.13      | 118.00   |
| 1   | AA    | 221  | C    | C5-C6-N1   | 10.18  | 126.09      | 121.00   |
| 1   | AA    | 1130 | A    | N1-C6-N6   | 10.18  | 124.71      | 118.60   |
| 1   | AA    | 21   | G    | N3-C2-N2   | 10.18  | 127.03      | 119.90   |
| 1   | AA    | 450  | G    | N1-C6-O6   | 10.18  | 126.01      | 119.90   |
| 1   | AA    | 1374 | A    | N1-C6-N6   | 10.18  | 124.71      | 118.60   |
| 35  | BB    | 2034 | U    | N3-C2-O2   | -10.18 | 115.07      | 122.20   |
| 1   | AA    | 175  | C    | N3-C4-N4   | 10.18  | 125.13      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2485 | G    | N3-C2-N2   | 10.18  | 127.03      | 119.90   |
| 1   | AA    | 432  | A    | C5-N7-C8   | 10.18  | 108.99      | 103.90   |
| 1   | AA    | 459  | A    | C4-C5-C6   | 10.18  | 122.09      | 117.00   |
| 35  | BB    | 1232 | G    | N1-C6-O6   | 10.18  | 126.01      | 119.90   |
| 1   | AA    | 817  | C    | C5-C6-N1   | 10.18  | 126.09      | 121.00   |
| 35  | BB    | 1473 | G    | C5-C6-O6   | -10.18 | 122.49      | 128.60   |
| 35  | BB    | 1692 | U    | C2-N3-C4   | -10.18 | 120.89      | 127.00   |
| 35  | BB    | 2285 | C    | O4'-C1'-N1 | 10.18  | 116.34      | 108.20   |
| 35  | BB    | 2499 | C    | O4'-C1'-N1 | 10.18  | 116.34      | 108.20   |
| 35  | BB    | 2808 | G    | C6-N1-C2   | 10.18  | 131.21      | 125.10   |
| 1   | AA    | 657  | U    | O4'-C1'-N1 | 10.17  | 116.34      | 108.20   |
| 1   | AA    | 1092 | A    | C5-C6-N6   | -10.17 | 115.56      | 123.70   |
| 35  | BB    | 412  | A    | C5-C6-N1   | -10.17 | 112.61      | 117.70   |
| 35  | BB    | 942  | G    | N3-C2-N2   | 10.17  | 127.02      | 119.90   |
| 35  | BB    | 977  | G    | C4-C5-C6   | 10.17  | 124.90      | 118.80   |
| 35  | BB    | 2146 | C    | C2-N3-C4   | 10.17  | 124.99      | 119.90   |
| 35  | BB    | 2878 | U    | O4'-C1'-N1 | 10.17  | 116.34      | 108.20   |
| 34  | BA    | 9    | G    | N1-C6-O6   | 10.17  | 126.00      | 119.90   |
| 35  | BB    | 408  | G    | C5-C6-O6   | -10.17 | 122.50      | 128.60   |
| 35  | BB    | 506  | G    | N1-C6-O6   | 10.17  | 126.00      | 119.90   |
| 35  | BB    | 1515 | A    | O4'-C1'-N9 | 10.17  | 116.34      | 108.20   |
| 35  | BB    | 697  | G    | N1-C6-O6   | 10.17  | 126.00      | 119.90   |
| 35  | BB    | 1488 | C    | O4'-C1'-N1 | 10.17  | 116.33      | 108.20   |
| 35  | BB    | 2082 | A    | C4-C5-C6   | 10.17  | 122.08      | 117.00   |
| 35  | BB    | 2159 | G    | O4'-C1'-N9 | 10.17  | 116.33      | 108.20   |
| 35  | BB    | 2663 | G    | C4-C5-N7   | 10.17  | 114.87      | 110.80   |
| 1   | AA    | 849  | G    | N1-C6-O6   | 10.16  | 126.00      | 119.90   |
| 1   | AA    | 987  | G    | C5-C6-N1   | -10.16 | 106.42      | 111.50   |
| 35  | BB    | 1296 | G    | C8-N9-C4   | -10.16 | 102.33      | 106.40   |
| 35  | BB    | 2737 | G    | C5-C6-O6   | -10.16 | 122.50      | 128.60   |
| 35  | BB    | 572  | A    | N1-C6-N6   | 10.16  | 124.70      | 118.60   |
| 1   | AA    | 710  | G    | C5-C6-N1   | -10.16 | 106.42      | 111.50   |
| 35  | BB    | 2271 | G    | C8-N9-C4   | -10.16 | 102.34      | 106.40   |
| 35  | BB    | 2620 | C    | O4'-C1'-N1 | 10.16  | 116.33      | 108.20   |
| 35  | BB    | 2884 | U    | N3-C4-O4   | 10.16  | 126.51      | 119.40   |
| 1   | AA    | 1307 | U    | C5-C4-O4   | -10.16 | 119.81      | 125.90   |
| 35  | BB    | 2412 | A    | C4-C5-C6   | 10.16  | 122.08      | 117.00   |
| 1   | AA    | 1198 | G    | O4'-C1'-N9 | 10.15  | 116.32      | 108.20   |
| 35  | BB    | 927  | A    | C4-C5-C6   | 10.15  | 122.08      | 117.00   |
| 35  | BB    | 1871 | A    | C5-C6-N1   | -10.15 | 112.62      | 117.70   |
| 1   | AA    | 940  | C    | O4'-C1'-N1 | 10.15  | 116.32      | 108.20   |
| 1   | AA    | 1102 | A    | C5-C6-N6   | -10.15 | 115.58      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 947  | A    | O4'-C1'-N9 | 10.15  | 116.32      | 108.20   |
| 35  | BB    | 1140 | C    | O4'-C1'-N1 | 10.15  | 116.32      | 108.20   |
| 35  | BB    | 2570 | G    | C8-N9-C4   | -10.15 | 102.34      | 106.40   |
| 35  | BB    | 2890 | G    | N1-C2-N3   | -10.15 | 117.81      | 123.90   |
| 35  | BB    | 1534 | U    | O4'-C1'-N1 | 10.15  | 116.32      | 108.20   |
| 1   | AA    | 443  | C    | C5-C4-N4   | -10.15 | 113.09      | 120.20   |
| 35  | BB    | 1631 | G    | C5-C6-N1   | -10.15 | 106.42      | 111.50   |
| 35  | BB    | 1822 | C    | O4'-C1'-N1 | 10.15  | 116.32      | 108.20   |
| 35  | BB    | 2394 | C    | N3-C4-N4   | 10.15  | 125.11      | 118.00   |
| 1   | AA    | 126  | G    | N1-C6-O6   | 10.15  | 125.99      | 119.90   |
| 1   | AA    | 1347 | G    | C4-C5-N7   | -10.15 | 106.74      | 110.80   |
| 35  | BB    | 657  | U    | O4'-C1'-N1 | 10.15  | 116.32      | 108.20   |
| 35  | BB    | 2071 | A    | C8-N9-C4   | -10.15 | 101.74      | 105.80   |
| 35  | BB    | 2163 | A    | C4-C5-C6   | 10.15  | 122.07      | 117.00   |
| 1   | AA    | 33   | A    | C5-C6-N6   | -10.15 | 115.58      | 123.70   |
| 1   | AA    | 654  | G    | N1-C6-O6   | 10.15  | 125.99      | 119.90   |
| 1   | AA    | 1225 | A    | N1-C6-N6   | 10.15  | 124.69      | 118.60   |
| 1   | AA    | 1419 | G    | C8-N9-C4   | 10.15  | 110.46      | 106.40   |
| 35  | BB    | 1293 | C    | N3-C4-N4   | 10.15  | 125.10      | 118.00   |
| 35  | BB    | 1490 | A    | C8-N9-C4   | -10.15 | 101.74      | 105.80   |
| 35  | BB    | 2726 | A    | C5-N7-C8   | 10.15  | 108.97      | 103.90   |
| 35  | BB    | 11   | C    | N3-C4-N4   | 10.14  | 125.10      | 118.00   |
| 35  | BB    | 453  | A    | O4'-C1'-N9 | 10.14  | 116.32      | 108.20   |
| 1   | AA    | 190  | A    | C4-C5-C6   | 10.14  | 122.07      | 117.00   |
| 35  | BB    | 1585 | C    | O4'-C1'-N1 | 10.14  | 116.31      | 108.20   |
| 1   | AA    | 1426 | G    | N1-C6-O6   | 10.14  | 125.98      | 119.90   |
| 34  | BA    | 70   | C    | C5-C4-N4   | -10.14 | 113.10      | 120.20   |
| 34  | BA    | 100  | G    | N1-C6-O6   | 10.14  | 125.98      | 119.90   |
| 35  | BB    | 2165 | C    | P-O3'-C3'  | 10.14  | 131.87      | 119.70   |
| 35  | BB    | 787  | C    | C6-N1-C2   | 10.14  | 124.36      | 120.30   |
| 35  | BB    | 1640 | A    | C5-N7-C8   | 10.14  | 108.97      | 103.90   |
| 35  | BB    | 141  | G    | N1-C6-O6   | 10.14  | 125.98      | 119.90   |
| 35  | BB    | 1362 | C    | N3-C4-N4   | 10.14  | 125.09      | 118.00   |
| 35  | BB    | 1416 | G    | C5-N7-C8   | 10.14  | 109.37      | 104.30   |
| 1   | AA    | 1289 | A    | C8-N9-C4   | -10.13 | 101.75      | 105.80   |
| 35  | BB    | 2369 | A    | C8-N9-C4   | -10.13 | 101.75      | 105.80   |
| 1   | AA    | 1437 | A    | N1-C6-N6   | 10.13  | 124.68      | 118.60   |
| 35  | BB    | 1281 | G    | C4-C5-N7   | -10.13 | 106.75      | 110.80   |
| 35  | BB    | 1398 | C    | O4'-C1'-N1 | 10.13  | 116.31      | 108.20   |
| 35  | BB    | 2028 | U    | O4'-C1'-N1 | 10.13  | 116.31      | 108.20   |
| 35  | BB    | 2364 | C    | N3-C4-C5   | -10.13 | 117.85      | 121.90   |
| 35  | BB    | 2298 | A    | N1-C6-N6   | 10.13  | 124.68      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2649 | C    | O4'-C1'-N1 | 10.13  | 116.30      | 108.20   |
| 1   | AA    | 588  | G    | N1-C6-O6   | 10.12  | 125.97      | 119.90   |
| 35  | BB    | 416  | U    | O4'-C1'-N1 | 10.12  | 116.30      | 108.20   |
| 35  | BB    | 2880 | C    | C4-C5-C6   | 10.12  | 122.46      | 117.40   |
| 1   | AA    | 681  | A    | C5-C6-N1   | -10.12 | 112.64      | 117.70   |
| 35  | BB    | 340  | A    | C5-N7-C8   | 10.12  | 108.96      | 103.90   |
| 34  | BA    | 25   | U    | O4'-C1'-N1 | 10.12  | 116.30      | 108.20   |
| 1   | AA    | 186  | C    | C5-C4-N4   | -10.12 | 113.12      | 120.20   |
| 34  | BA    | 27   | C    | P-O5'-C5'  | 10.12  | 137.09      | 120.90   |
| 35  | BB    | 2338 | C    | N1-C2-O2   | -10.12 | 112.83      | 118.90   |
| 35  | BB    | 2702 | G    | C5-C6-O6   | -10.12 | 122.53      | 128.60   |
| 1   | AA    | 1048 | G    | O4'-C1'-N9 | 10.12  | 116.30      | 108.20   |
| 35  | BB    | 463  | G    | N3-C2-N2   | 10.12  | 126.98      | 119.90   |
| 35  | BB    | 1852 | U    | O4'-C1'-N1 | 10.12  | 116.29      | 108.20   |
| 35  | BB    | 2333 | A    | N1-C2-N3   | 10.12  | 134.36      | 129.30   |
| 1   | AA    | 498  | A    | N1-C6-N6   | 10.12  | 124.67      | 118.60   |
| 1   | AA    | 743  | A    | N1-C6-N6   | 10.12  | 124.67      | 118.60   |
| 35  | BB    | 707  | G    | N3-C2-N2   | 10.12  | 126.98      | 119.90   |
| 35  | BB    | 2383 | G    | C5-C6-O6   | -10.12 | 122.53      | 128.60   |
| 35  | BB    | 1877 | A    | C2-N3-C4   | -10.11 | 105.54      | 110.60   |
| 35  | BB    | 2447 | G    | P-O3'-C3'  | 10.12  | 131.84      | 119.70   |
| 35  | BB    | 2561 | U    | C5-C6-N1   | 10.12  | 127.76      | 122.70   |
| 1   | AA    | 363  | A    | C5-C6-N1   | -10.11 | 112.64      | 117.70   |
| 1   | AA    | 1346 | A    | N1-C2-N3   | 10.11  | 134.36      | 129.30   |
| 35  | BB    | 1338 | G    | N1-C2-N3   | -10.11 | 117.83      | 123.90   |
| 35  | BB    | 1759 | A    | C5-C6-N6   | -10.11 | 115.61      | 123.70   |
| 35  | BB    | 1879 | C    | C5-C4-N4   | -10.11 | 113.12      | 120.20   |
| 38  | BE    | 40   | ARG  | NE-CZ-NH2  | -10.11 | 115.25      | 120.30   |
| 35  | BB    | 915  | C    | C6-N1-C2   | -10.11 | 116.26      | 120.30   |
| 1   | AA    | 273  | U    | C5-C6-N1   | 10.11  | 127.75      | 122.70   |
| 1   | AA    | 522  | C    | C2-N3-C4   | 10.11  | 124.95      | 119.90   |
| 1   | AA    | 689  | C    | O4'-C1'-N1 | 10.11  | 116.29      | 108.20   |
| 1   | AA    | 1151 | A    | N3-C4-C5   | -10.11 | 119.72      | 126.80   |
| 35  | BB    | 97   | C    | C6-N1-C2   | -10.11 | 116.26      | 120.30   |
| 35  | BB    | 417  | C    | C6-N1-C2   | -10.11 | 116.26      | 120.30   |
| 35  | BB    | 1113 | U    | O4'-C1'-N1 | 10.11  | 116.29      | 108.20   |
| 35  | BB    | 1450 | G    | O4'-C1'-N9 | 10.11  | 116.29      | 108.20   |
| 35  | BB    | 1786 | A    | C5-C6-N1   | -10.11 | 112.64      | 117.70   |
| 35  | BB    | 2234 | G    | C6-C5-N7   | -10.11 | 124.33      | 130.40   |
| 35  | BB    | 2294 | G    | O4'-C1'-N9 | 10.11  | 116.29      | 108.20   |
| 35  | BB    | 2838 | G    | N9-C4-C5   | -10.11 | 101.36      | 105.40   |
| 35  | BB    | 785  | G    | N1-C6-O6   | 10.11  | 125.96      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1535 | A    | O4'-C1'-N9 | 10.11  | 116.29      | 108.20   |
| 35  | BB    | 2474 | U    | C5-C6-N1   | 10.11  | 127.75      | 122.70   |
| 1   | AA    | 1445 | U    | O4'-C1'-N1 | 10.10  | 116.28      | 108.20   |
| 35  | BB    | 177  | G    | N1-C6-O6   | 10.10  | 125.96      | 119.90   |
| 1   | AA    | 627  | G    | C5-C6-N1   | -10.10 | 106.45      | 111.50   |
| 1   | AA    | 816  | A    | C5-C6-N1   | -10.10 | 112.65      | 117.70   |
| 1   | AA    | 949  | A    | C4-C5-C6   | 10.10  | 122.05      | 117.00   |
| 35  | BB    | 140  | C    | C5-C6-N1   | 10.10  | 126.05      | 121.00   |
| 35  | BB    | 801  | G    | C4-C5-C6   | 10.10  | 124.86      | 118.80   |
| 35  | BB    | 2015 | A    | C4-C5-C6   | 10.10  | 122.05      | 117.00   |
| 22  | AV    | 37   | G    | N3-C4-C5   | -10.10 | 123.55      | 128.60   |
| 35  | BB    | 302  | C    | N3-C4-C5   | -10.10 | 117.86      | 121.90   |
| 35  | BB    | 1444 | G    | O4'-C1'-N9 | 10.10  | 116.28      | 108.20   |
| 21  | AU    | 17   | ARG  | NE-CZ-NH1  | 10.10  | 125.35      | 120.30   |
| 35  | BB    | 197  | A    | O4'-C1'-N9 | 10.10  | 116.28      | 108.20   |
| 35  | BB    | 301  | G    | C8-N9-C4   | -10.10 | 102.36      | 106.40   |
| 35  | BB    | 835  | C    | N3-C4-N4   | 10.10  | 125.07      | 118.00   |
| 35  | BB    | 958  | U    | N3-C4-C5   | -10.10 | 108.54      | 114.60   |
| 1   | AA    | 485  | U    | N1-C2-N3   | -10.10 | 108.84      | 114.90   |
| 35  | BB    | 222  | A    | N1-C6-N6   | 10.10  | 124.66      | 118.60   |
| 35  | BB    | 635  | C    | N3-C4-C5   | -10.10 | 117.86      | 121.90   |
| 1   | AA    | 660  | C    | O4'-C1'-N1 | 10.09  | 116.27      | 108.20   |
| 35  | BB    | 1591 | A    | C4-C5-C6   | 10.09  | 122.05      | 117.00   |
| 35  | BB    | 1837 | C    | O4'-C1'-N1 | 10.09  | 116.28      | 108.20   |
| 1   | AA    | 691  | G    | N9-C4-C5   | -10.09 | 101.36      | 105.40   |
| 1   | AA    | 1127 | G    | C4-C5-C6   | 10.09  | 124.86      | 118.80   |
| 35  | BB    | 187  | G    | P-O5'-C5'  | 10.09  | 137.05      | 120.90   |
| 35  | BB    | 1106 | G    | N1-C6-O6   | 10.09  | 125.96      | 119.90   |
| 35  | BB    | 2413 | G    | C5-C6-O6   | -10.09 | 122.54      | 128.60   |
| 35  | BB    | 2877 | G    | C5-N7-C8   | 10.09  | 109.35      | 104.30   |
| 1   | AA    | 136  | C    | O4'-C1'-N1 | 10.09  | 116.27      | 108.20   |
| 35  | BB    | 1400 | U    | O4'-C1'-N1 | 10.09  | 116.27      | 108.20   |
| 1   | AA    | 1039 | G    | N1-C6-O6   | 10.09  | 125.95      | 119.90   |
| 35  | BB    | 921  | C    | O4'-C1'-N1 | 10.09  | 116.27      | 108.20   |
| 35  | BB    | 2206 | C    | C6-N1-C2   | -10.09 | 116.27      | 120.30   |
| 35  | BB    | 2758 | A    | C5-C6-N6   | -10.09 | 115.63      | 123.70   |
| 35  | BB    | 1464 | G    | O4'-C1'-N9 | 10.09  | 116.27      | 108.20   |
| 1   | AA    | 114  | U    | O4'-C1'-N1 | 10.08  | 116.27      | 108.20   |
| 1   | AA    | 496  | A    | C8-N9-C4   | -10.08 | 101.77      | 105.80   |
| 1   | AA    | 973  | G    | O4'-C1'-N9 | 10.08  | 116.27      | 108.20   |
| 35  | BB    | 1822 | C    | N3-C4-N4   | 10.08  | 125.06      | 118.00   |
| 35  | BB    | 1588 | G    | N1-C6-O6   | 10.08  | 125.95      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 2331 | G    | C4-C5-C6   | 10.08  | 124.85      | 118.80   |
| 1   | AA    | 65   | A    | C5-C6-N1   | -10.08 | 112.66      | 117.70   |
| 1   | AA    | 716  | A    | C6-C5-N7   | -10.08 | 125.25      | 132.30   |
| 34  | BA    | 56   | G    | N7-C8-N9   | 10.08  | 118.14      | 113.10   |
| 35  | BB    | 432  | A    | C4-C5-C6   | 10.08  | 122.04      | 117.00   |
| 35  | BB    | 2597 | G    | N1-C2-N3   | -10.08 | 117.85      | 123.90   |
| 35  | BB    | 2846 | G    | C5-C6-O6   | -10.08 | 122.55      | 128.60   |
| 18  | AR    | 50   | TYR  | CB-CG-CD2  | 10.08  | 127.05      | 121.00   |
| 35  | BB    | 197  | A    | C5-C6-N1   | -10.08 | 112.66      | 117.70   |
| 35  | BB    | 839  | U    | O4'-C1'-N1 | 10.08  | 116.26      | 108.20   |
| 35  | BB    | 1837 | C    | N3-C4-C5   | -10.08 | 117.87      | 121.90   |
| 35  | BB    | 1416 | G    | O4'-C1'-N9 | 10.07  | 116.26      | 108.20   |
| 35  | BB    | 1570 | A    | C5-C6-N6   | -10.07 | 115.64      | 123.70   |
| 1   | AA    | 301  | G    | C5-C6-O6   | -10.07 | 122.56      | 128.60   |
| 1   | AA    | 1404 | C    | N1-C2-O2   | -10.07 | 112.86      | 118.90   |
| 35  | BB    | 246  | C    | O4'-C1'-N1 | 10.07  | 116.26      | 108.20   |
| 1   | AA    | 361  | G    | C8-N9-C4   | -10.07 | 102.37      | 106.40   |
| 1   | AA    | 649  | A    | N7-C8-N9   | -10.07 | 108.76      | 113.80   |
| 35  | BB    | 1962 | C    | N3-C4-N4   | 10.07  | 125.05      | 118.00   |
| 53  | BT    | 12   | ARG  | NE-CZ-NH2  | -10.07 | 115.26      | 120.30   |
| 1   | AA    | 11   | G    | C4-C5-N7   | 10.07  | 114.83      | 110.80   |
| 1   | AA    | 570  | G    | C5-C6-O6   | -10.07 | 122.56      | 128.60   |
| 1   | AA    | 778  | G    | C4-C5-N7   | 10.07  | 114.83      | 110.80   |
| 1   | AA    | 890  | G    | C6-C5-N7   | -10.07 | 124.36      | 130.40   |
| 1   | AA    | 1163 | A    | C4-C5-C6   | 10.07  | 122.03      | 117.00   |
| 35  | BB    | 952  | G    | C5-C6-O6   | -10.07 | 122.56      | 128.60   |
| 35  | BB    | 2636 | C    | O4'-C1'-N1 | 10.07  | 116.26      | 108.20   |
| 35  | BB    | 417  | C    | N3-C4-N4   | 10.07  | 125.05      | 118.00   |
| 35  | BB    | 1100 | C    | N3-C4-N4   | 10.07  | 125.05      | 118.00   |
| 35  | BB    | 1336 | A    | N1-C6-N6   | 10.07  | 124.64      | 118.60   |
| 1   | AA    | 201  | G    | C4-C5-C6   | 10.07  | 124.84      | 118.80   |
| 1   | AA    | 937  | A    | N1-C2-N3   | -10.07 | 124.27      | 129.30   |
| 1   | AA    | 60   | A    | C5-C6-N6   | -10.07 | 115.65      | 123.70   |
| 35  | BB    | 1289 | C    | C5-C4-N4   | -10.07 | 113.15      | 120.20   |
| 35  | BB    | 1405 | U    | O4'-C1'-N1 | 10.07  | 116.25      | 108.20   |
| 1   | AA    | 182  | A    | O4'-C1'-N9 | 10.06  | 116.25      | 108.20   |
| 35  | BB    | 1549 | A    | N1-C6-N6   | 10.06  | 124.64      | 118.60   |
| 35  | BB    | 509  | C    | N3-C4-N4   | 10.06  | 125.04      | 118.00   |
| 35  | BB    | 759  | G    | C4-C5-C6   | 10.06  | 124.84      | 118.80   |
| 35  | BB    | 2741 | A    | N1-C6-N6   | 10.06  | 124.64      | 118.60   |
| 1   | AA    | 51   | A    | C5-C6-N6   | -10.06 | 115.65      | 123.70   |
| 35  | BB    | 354  | A    | C5-C6-N1   | -10.06 | 112.67      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 1699 | G    | N1-C6-O6   | 10.06  | 125.94      | 119.90   |
| 35  | BB    | 2853 | C    | N3-C4-N4   | 10.06  | 125.04      | 118.00   |
| 1   | AA    | 1114 | C    | C6-N1-C2   | -10.06 | 116.28      | 120.30   |
| 35  | BB    | 620  | G    | N1-C2-N3   | -10.06 | 117.87      | 123.90   |
| 35  | BB    | 1385 | A    | C5-C6-N6   | -10.06 | 115.65      | 123.70   |
| 1   | AA    | 1074 | G    | N7-C8-N9   | 10.05  | 118.13      | 113.10   |
| 1   | AA    | 1256 | A    | C5-C6-N6   | -10.06 | 115.66      | 123.70   |
| 22  | AV    | 53   | G    | N1-C6-O6   | 10.06  | 125.93      | 119.90   |
| 34  | BA    | 57   | A    | O4'-C1'-N9 | 10.06  | 116.25      | 108.20   |
| 35  | BB    | 1010 | A    | C5-C6-N1   | -10.06 | 112.67      | 117.70   |
| 1   | AA    | 1206 | G    | C6-C5-N7   | -10.05 | 124.37      | 130.40   |
| 35  | BB    | 560  | C    | C5-C4-N4   | -10.05 | 113.16      | 120.20   |
| 35  | BB    | 798  | G    | N1-C6-O6   | 10.05  | 125.93      | 119.90   |
| 1   | AA    | 10   | A    | C5-C6-N6   | -10.05 | 115.66      | 123.70   |
| 1   | AA    | 151  | A    | N9-C4-C5   | 10.05  | 109.82      | 105.80   |
| 35  | BB    | 76   | C    | N3-C4-N4   | 10.05  | 125.04      | 118.00   |
| 35  | BB    | 1545 | A    | C8-N9-C4   | -10.05 | 101.78      | 105.80   |
| 1   | AA    | 1137 | C    | N3-C4-N4   | 10.05  | 125.03      | 118.00   |
| 35  | BB    | 122  | G    | C4-C5-C6   | 10.05  | 124.83      | 118.80   |
| 35  | BB    | 371  | A    | P-O3'-C3'  | 10.05  | 131.76      | 119.70   |
| 35  | BB    | 595  | C    | O4'-C1'-N1 | 10.05  | 116.24      | 108.20   |
| 35  | BB    | 856  | G    | N1-C6-O6   | 10.05  | 125.93      | 119.90   |
| 35  | BB    | 1482 | G    | C4-C5-N7   | -10.05 | 106.78      | 110.80   |
| 35  | BB    | 1598 | A    | C5-C6-N1   | -10.05 | 112.67      | 117.70   |
| 35  | BB    | 1858 | A    | N1-C6-N6   | 10.05  | 124.63      | 118.60   |
| 35  | BB    | 2019 | A    | C2-N3-C4   | -10.05 | 105.58      | 110.60   |
| 35  | BB    | 2551 | C    | O4'-C1'-N1 | 10.05  | 116.24      | 108.20   |
| 1   | AA    | 105  | G    | C6-N1-C2   | 10.05  | 131.13      | 125.10   |
| 35  | BB    | 492  | A    | N1-C6-N6   | 10.05  | 124.63      | 118.60   |
| 35  | BB    | 1026 | G    | N3-C4-N9   | 10.05  | 132.03      | 126.00   |
| 35  | BB    | 1331 | G    | N1-C6-O6   | 10.05  | 125.93      | 119.90   |
| 1   | AA    | 1299 | A    | C6-C5-N7   | -10.04 | 125.27      | 132.30   |
| 35  | BB    | 1318 | U    | C5-C6-N1   | 10.04  | 127.72      | 122.70   |
| 35  | BB    | 1853 | A    | O4'-C1'-N9 | 10.04  | 116.23      | 108.20   |
| 35  | BB    | 2556 | C    | N3-C4-N4   | 10.04  | 125.03      | 118.00   |
| 1   | AA    | 876  | C    | N3-C4-C5   | -10.04 | 117.88      | 121.90   |
| 35  | BB    | 621  | A    | C5-C6-N6   | -10.04 | 115.67      | 123.70   |
| 35  | BB    | 727  | A    | C5-C6-N6   | -10.04 | 115.67      | 123.70   |
| 35  | BB    | 2224 | G    | N1-C6-O6   | 10.04  | 125.92      | 119.90   |
| 1   | AA    | 1420 | U    | O4'-C1'-N1 | 10.04  | 116.23      | 108.20   |
| 35  | BB    | 314  | C    | O4'-C1'-N1 | 10.04  | 116.23      | 108.20   |
| 35  | BB    | 515  | A    | O4'-C1'-N9 | 10.04  | 116.23      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 35  | BB    | 1783 | A    | C8-N9-C4    | 10.04  | 109.82      | 105.80   |
| 35  | BB    | 1979 | U    | N1-C2-O2    | -10.04 | 115.77      | 122.80   |
| 35  | BB    | 1781 | U    | O4'-C1'-N1  | 10.04  | 116.23      | 108.20   |
| 35  | BB    | 1456 | G    | O4'-C1'-N9  | 10.04  | 116.23      | 108.20   |
| 35  | BB    | 1752 | C    | O4'-C1'-N1  | 10.03  | 116.23      | 108.20   |
| 1   | AA    | 558  | G    | N1-C6-O6    | 10.03  | 125.92      | 119.90   |
| 35  | BB    | 1284 | A    | C5-C6-N6    | -10.03 | 115.67      | 123.70   |
| 35  | BB    | 2602 | A    | C5-C6-N1    | -10.03 | 112.68      | 117.70   |
| 35  | BB    | 1970 | A    | C2-N3-C4    | 10.03  | 115.61      | 110.60   |
| 35  | BB    | 2189 | U    | C6-N1-C2    | -10.03 | 114.98      | 121.00   |
| 35  | BB    | 2648 | G    | N1-C6-O6    | 10.03  | 125.92      | 119.90   |
| 1   | AA    | 949  | A    | N1-C2-N3    | -10.03 | 124.28      | 129.30   |
| 35  | BB    | 1630 | A    | N1-C6-N6    | 10.03  | 124.62      | 118.60   |
| 9   | AI    | 79   | ARG  | NE-CZ-NH2   | -10.03 | 115.29      | 120.30   |
| 35  | BB    | 145  | C    | C5-C4-N4    | -10.03 | 113.18      | 120.20   |
| 35  | BB    | 611  | C    | N3-C4-C5    | -10.03 | 117.89      | 121.90   |
| 35  | BB    | 1000 | A    | C5-C6-N6    | -10.03 | 115.68      | 123.70   |
| 35  | BB    | 1434 | A    | N9-C4-C5    | -10.03 | 101.79      | 105.80   |
| 1   | AA    | 1023 | U    | C5-C4-O4    | 10.03  | 131.91      | 125.90   |
| 1   | AA    | 1324 | A    | O4'-C1'-N9  | 10.03  | 116.22      | 108.20   |
| 35  | BB    | 1938 | A    | N7-C8-N9    | -10.03 | 108.79      | 113.80   |
| 35  | BB    | 2053 | G    | O4'-C1'-N9  | 10.02  | 116.22      | 108.20   |
| 53  | BT    | 73   | ARG  | NE-CZ-NH1   | 10.02  | 125.31      | 120.30   |
| 1   | AA    | 264  | C    | C2-N3-C4    | 10.02  | 124.91      | 119.90   |
| 35  | BB    | 855  | G    | C8-N9-C4    | 10.02  | 110.41      | 106.40   |
| 35  | BB    | 2361 | G    | N1-C6-O6    | 10.02  | 125.91      | 119.90   |
| 1   | AA    | 790  | A    | N1-C6-N6    | 10.02  | 124.61      | 118.60   |
| 1   | AA    | 1225 | A    | C3'-C2'-C1' | 10.02  | 109.51      | 101.50   |
| 1   | AA    | 861  | G    | N1-C6-O6    | 10.02  | 125.91      | 119.90   |
| 35  | BB    | 26   | G    | C5-C6-O6    | -10.02 | 122.59      | 128.60   |
| 35  | BB    | 898  | C    | O4'-C1'-N1  | 10.01  | 116.21      | 108.20   |
| 1   | AA    | 1431 | A    | C5-C6-N6    | -10.01 | 115.69      | 123.70   |
| 34  | BA    | 98   | G    | P-O3'-C3'   | 10.01  | 131.71      | 119.70   |
| 35  | BB    | 104  | A    | C5-C6-N1    | -10.01 | 112.69      | 117.70   |
| 1   | AA    | 42   | G    | C5-C6-O6    | -10.01 | 122.59      | 128.60   |
| 1   | AA    | 665  | A    | C5-N7-C8    | 10.01  | 108.91      | 103.90   |
| 35  | BB    | 243  | U    | N1-C2-N3    | -10.01 | 108.89      | 114.90   |
| 35  | BB    | 690  | G    | N9-C4-C5    | 10.01  | 109.40      | 105.40   |
| 35  | BB    | 2160 | C    | C5-C6-N1    | 10.01  | 126.00      | 121.00   |
| 35  | BB    | 2881 | U    | O4'-C1'-N1  | 10.01  | 116.21      | 108.20   |
| 47  | BN    | 30   | ARG  | NE-CZ-NH1   | 10.01  | 125.31      | 120.30   |
| 55  | BW    | 57   | TYR  | CB-CG-CD2   | -10.01 | 114.99      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 35  | BB    | 597  | G    | C2-N3-C4   | 10.01  | 116.90      | 111.90   |
| 35  | BB    | 2793 | C    | N3-C4-C5   | -10.01 | 117.90      | 121.90   |
| 1   | AA    | 488  | C    | O4'-C1'-N1 | 10.01  | 116.20      | 108.20   |
| 35  | BB    | 156  | A    | N1-C6-N6   | 10.01  | 124.60      | 118.60   |
| 35  | BB    | 157  | C    | O4'-C1'-N1 | 10.01  | 116.20      | 108.20   |
| 35  | BB    | 199  | A    | N1-C6-N6   | 10.01  | 124.60      | 118.60   |
| 35  | BB    | 540  | C    | C6-N1-C2   | -10.01 | 116.30      | 120.30   |
| 35  | BB    | 1006 | C    | N3-C4-N4   | 10.01  | 125.00      | 118.00   |
| 1   | AA    | 1246 | A    | O4'-C1'-N9 | 10.00  | 116.20      | 108.20   |
| 35  | BB    | 833  | A    | C5-C6-N6   | -10.00 | 115.70      | 123.70   |
| 1   | AA    | 115  | G    | N1-C2-N3   | -10.00 | 117.90      | 123.90   |
| 1   | AA    | 806  | C    | O4'-C1'-N1 | 10.00  | 116.20      | 108.20   |
| 34  | BA    | 102  | G    | C2-N3-C4   | -10.00 | 106.90      | 111.90   |
| 35  | BB    | 2892 | G    | C5-C6-O6   | -10.00 | 122.60      | 128.60   |
| 1   | AA    | 699  | C    | O4'-C1'-N1 | 10.00  | 116.20      | 108.20   |
| 35  | BB    | 1589 | U    | C2-N3-C4   | -10.00 | 121.00      | 127.00   |
| 35  | BB    | 2287 | A    | C5-C6-N6   | -10.00 | 115.70      | 123.70   |
| 1   | AA    | 544  | G    | N3-C2-N2   | 10.00  | 126.90      | 119.90   |
| 1   | AA    | 563  | A    | C4-C5-C6   | 10.00  | 122.00      | 117.00   |
| 1   | AA    | 625  | U    | N3-C2-O2   | 10.00  | 129.20      | 122.20   |
| 35  | BB    | 1579 | A    | O4'-C1'-N9 | 10.00  | 116.20      | 108.20   |
| 35  | BB    | 2623 | G    | N7-C8-N9   | 10.00  | 118.10      | 113.10   |
| 35  | BB    | 2017 | U    | C5-C4-O4   | -9.99  | 119.90      | 125.90   |
| 1   | AA    | 993  | G    | O4'-C1'-N9 | 9.99   | 116.19      | 108.20   |
| 1   | AA    | 1161 | C    | C6-N1-C2   | -9.99  | 116.30      | 120.30   |
| 35  | BB    | 2801 | G    | C6-C5-N7   | -9.99  | 124.40      | 130.40   |
| 40  | BG    | 54   | ARG  | NE-CZ-NH1  | 9.99   | 125.30      | 120.30   |
| 1   | AA    | 29   | U    | C5-C4-O4   | -9.99  | 119.91      | 125.90   |
| 1   | AA    | 447  | G    | C8-N9-C4   | -9.99  | 102.40      | 106.40   |
| 1   | AA    | 536  | C    | N3-C4-N4   | 9.99   | 124.99      | 118.00   |
| 1   | AA    | 953  | G    | C4-C5-N7   | 9.99   | 114.80      | 110.80   |
| 35  | BB    | 2649 | C    | N3-C4-N4   | 9.99   | 124.99      | 118.00   |
| 1   | AA    | 403  | C    | N3-C4-N4   | 9.99   | 124.99      | 118.00   |
| 35  | BB    | 928  | A    | N1-C6-N6   | 9.99   | 124.59      | 118.60   |
| 35  | BB    | 2354 | C    | N1-C2-O2   | -9.99  | 112.91      | 118.90   |
| 1   | AA    | 68   | G    | N1-C6-O6   | 9.98   | 125.89      | 119.90   |
| 1   | AA    | 1343 | G    | C2-N3-C4   | 9.98   | 116.89      | 111.90   |
| 1   | AA    | 1419 | G    | N3-C4-C5   | 9.98   | 133.59      | 128.60   |
| 35  | BB    | 1118 | C    | N3-C4-N4   | 9.98   | 124.99      | 118.00   |
| 1   | AA    | 774  | G    | N1-C2-N3   | -9.98  | 117.91      | 123.90   |
| 1   | AA    | 1374 | A    | C5-C6-N6   | -9.98  | 115.72      | 123.70   |
| 35  | BB    | 1331 | G    | C5-C6-O6   | -9.98  | 122.61      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 400  | C    | O4'-C1'-N1  | 9.98  | 116.18      | 108.20   |
| 1   | AA    | 416  | G    | C4-C5-C6    | 9.98  | 124.79      | 118.80   |
| 1   | AA    | 916  | U    | C5-C6-N1    | 9.98  | 127.69      | 122.70   |
| 1   | AA    | 1316 | G    | N1-C6-O6    | 9.98  | 125.89      | 119.90   |
| 1   | AA    | 1339 | A    | O4'-C1'-N9  | 9.98  | 116.18      | 108.20   |
| 2   | AB    | 21   | TYR  | CB-CG-CD2   | 9.98  | 126.99      | 121.00   |
| 1   | AA    | 929  | G    | C5-C6-O6    | -9.97 | 122.62      | 128.60   |
| 35  | BB    | 146  | A    | C5-C6-N1    | -9.97 | 112.71      | 117.70   |
| 35  | BB    | 1008 | A    | N1-C6-N6    | 9.97  | 124.58      | 118.60   |
| 1   | AA    | 567  | G    | N1-C6-O6    | 9.97  | 125.88      | 119.90   |
| 1   | AA    | 1005 | A    | N1-C6-N6    | 9.97  | 124.58      | 118.60   |
| 34  | BA    | 106  | G    | C5-C6-O6    | -9.97 | 122.62      | 128.60   |
| 35  | BB    | 492  | A    | C4-C5-C6    | 9.97  | 121.98      | 117.00   |
| 35  | BB    | 555  | G    | C3'-C2'-C1' | 9.97  | 109.47      | 101.50   |
| 13  | AM    | 78   | ARG  | NE-CZ-NH1   | 9.97  | 125.28      | 120.30   |
| 35  | BB    | 1778 | U    | O4'-C1'-N1  | 9.97  | 116.17      | 108.20   |
| 35  | BB    | 2059 | A    | C2-N3-C4    | -9.97 | 105.62      | 110.60   |
| 1   | AA    | 944  | G    | N1-C2-N3    | -9.97 | 117.92      | 123.90   |
| 1   | AA    | 1310 | G    | N1-C6-O6    | 9.96  | 125.88      | 119.90   |
| 1   | AA    | 1386 | G    | C4-C5-N7    | -9.96 | 106.81      | 110.80   |
| 1   | AA    | 1405 | G    | C5-C6-O6    | -9.96 | 122.62      | 128.60   |
| 35  | BB    | 708  | G    | N1-C6-O6    | 9.96  | 125.88      | 119.90   |
| 1   | AA    | 87   | C    | N3-C4-N4    | 9.96  | 124.97      | 118.00   |
| 35  | BB    | 1755 | A    | C2-N3-C4    | -9.96 | 105.62      | 110.60   |
| 35  | BB    | 1901 | A    | N1-C2-N3    | -9.96 | 124.32      | 129.30   |
| 35  | BB    | 2255 | G    | N1-C6-O6    | 9.96  | 125.88      | 119.90   |
| 1   | AA    | 276  | G    | O4'-C1'-N9  | 9.96  | 116.17      | 108.20   |
| 1   | AA    | 550  | G    | C6-C5-N7    | -9.96 | 124.43      | 130.40   |
| 1   | AA    | 670  | G    | C5-C6-O6    | -9.96 | 122.62      | 128.60   |
| 1   | AA    | 873  | A    | N1-C6-N6    | 9.96  | 124.58      | 118.60   |
| 1   | AA    | 1352 | C    | N1-C2-O2    | -9.96 | 112.92      | 118.90   |
| 1   | AA    | 753  | A    | C4-C5-C6    | 9.96  | 121.98      | 117.00   |
| 35  | BB    | 1002 | G    | C6-C5-N7    | -9.96 | 124.43      | 130.40   |
| 35  | BB    | 1150 | C    | C6-N1-C2    | -9.96 | 116.32      | 120.30   |
| 35  | BB    | 1937 | A    | C5-C6-N1    | -9.96 | 112.72      | 117.70   |
| 35  | BB    | 2341 | G    | C2-N3-C4    | 9.96  | 116.88      | 111.90   |
| 1   | AA    | 681  | A    | C6-C5-N7    | -9.96 | 125.33      | 132.30   |
| 35  | BB    | 2465 | C    | C6-N1-C2    | -9.96 | 116.32      | 120.30   |
| 1   | AA    | 1462 | C    | N3-C4-N4    | 9.95  | 124.97      | 118.00   |
| 1   | AA    | 1506 | U    | O4'-C1'-N1  | 9.95  | 116.16      | 108.20   |
| 35  | BB    | 2875 | C    | N3-C4-C5    | -9.95 | 117.92      | 121.90   |
| 1   | AA    | 535  | A    | N1-C2-N3    | 9.95  | 134.28      | 129.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 705  | G    | C6-C5-N7   | -9.95 | 124.43      | 130.40   |
| 35  | BB    | 2158 | A    | C4-C5-C6   | 9.95  | 121.97      | 117.00   |
| 1   | AA    | 1097 | C    | O4'-C1'-N1 | 9.95  | 116.16      | 108.20   |
| 1   | AA    | 739  | C    | N3-C4-N4   | 9.95  | 124.96      | 118.00   |
| 1   | AA    | 848  | C    | N3-C4-N4   | 9.95  | 124.96      | 118.00   |
| 35  | BB    | 933  | A    | N1-C6-N6   | 9.95  | 124.57      | 118.60   |
| 35  | BB    | 2126 | A    | C8-N9-C4   | -9.95 | 101.82      | 105.80   |
| 35  | BB    | 2677 | G    | O4'-C1'-N9 | 9.95  | 116.16      | 108.20   |
| 35  | BB    | 81   | G    | N1-C6-O6   | 9.94  | 125.87      | 119.90   |
| 35  | BB    | 2357 | G    | C4-C5-C6   | 9.94  | 124.77      | 118.80   |
| 1   | AA    | 651  | C    | O4'-C1'-N1 | 9.94  | 116.15      | 108.20   |
| 35  | BB    | 854  | C    | C5-C4-N4   | -9.94 | 113.24      | 120.20   |
| 1   | AA    | 1438 | G    | N3-C2-N2   | 9.94  | 126.86      | 119.90   |
| 1   | AA    | 1441 | A    | C4-C5-C6   | 9.94  | 121.97      | 117.00   |
| 35  | BB    | 1024 | G    | C5-C6-O6   | -9.94 | 122.64      | 128.60   |
| 35  | BB    | 2505 | G    | N7-C8-N9   | -9.94 | 108.13      | 113.10   |
| 1   | AA    | 848  | C    | N3-C4-C5   | -9.94 | 117.92      | 121.90   |
| 35  | BB    | 1582 | C    | N3-C4-N4   | 9.94  | 124.96      | 118.00   |
| 1   | AA    | 48   | C    | O4'-C1'-N1 | 9.93  | 116.15      | 108.20   |
| 1   | AA    | 153  | C    | C5-C6-N1   | 9.93  | 125.97      | 121.00   |
| 22  | AV    | 33   | U    | P-O3'-C3'  | 9.93  | 131.62      | 119.70   |
| 35  | BB    | 446  | G    | N1-C6-O6   | 9.93  | 125.86      | 119.90   |
| 35  | BB    | 1749 | A    | C4-C5-N7   | -9.93 | 105.73      | 110.70   |
| 35  | BB    | 2585 | U    | O4'-C1'-N1 | 9.93  | 116.15      | 108.20   |
| 1   | AA    | 6    | G    | N7-C8-N9   | 9.93  | 118.06      | 113.10   |
| 1   | AA    | 280  | C    | N3-C4-N4   | 9.93  | 124.95      | 118.00   |
| 1   | AA    | 1458 | G    | N1-C6-O6   | 9.93  | 125.86      | 119.90   |
| 35  | BB    | 574  | A    | C5-C6-N1   | -9.93 | 112.74      | 117.70   |
| 35  | BB    | 1237 | A    | C5-N7-C8   | 9.93  | 108.86      | 103.90   |
| 35  | BB    | 1994 | C    | C2-N3-C4   | 9.93  | 124.86      | 119.90   |
| 1   | AA    | 452  | A    | O4'-C1'-N9 | 9.92  | 116.14      | 108.20   |
| 1   | AA    | 151  | A    | C8-N9-C4   | -9.92 | 101.83      | 105.80   |
| 35  | BB    | 943  | A    | C8-N9-C4   | -9.92 | 101.83      | 105.80   |
| 35  | BB    | 1133 | A    | P-O3'-C3'  | 9.92  | 131.61      | 119.70   |
| 35  | BB    | 1750 | G    | C8-N9-C4   | -9.92 | 102.43      | 106.40   |
| 1   | AA    | 142  | G    | N7-C8-N9   | 9.92  | 118.06      | 113.10   |
| 1   | AA    | 165  | G    | N1-C6-O6   | 9.92  | 125.85      | 119.90   |
| 35  | BB    | 1901 | A    | C5-C6-N1   | -9.92 | 112.74      | 117.70   |
| 35  | BB    | 2611 | C    | C4-C5-C6   | 9.92  | 122.36      | 117.40   |
| 1   | AA    | 1251 | A    | O4'-C1'-N9 | 9.92  | 116.14      | 108.20   |
| 35  | BB    | 1691 | C    | C5-C6-N1   | 9.92  | 125.96      | 121.00   |
| 35  | BB    | 1692 | U    | N1-C2-N3   | 9.92  | 120.85      | 114.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2732 | G    | O4'-C1'-N9  | 9.92  | 116.14      | 108.20   |
| 35  | BB    | 64   | A    | C6-C5-N7    | -9.92 | 125.36      | 132.30   |
| 35  | BB    | 2589 | A    | N1-C6-N6    | 9.92  | 124.55      | 118.60   |
| 35  | BB    | 1592 | C    | C5-C6-N1    | 9.91  | 125.96      | 121.00   |
| 1   | AA    | 13   | U    | N3-C2-O2    | 9.91  | 129.14      | 122.20   |
| 1   | AA    | 1515 | G    | N1-C6-O6    | 9.91  | 125.85      | 119.90   |
| 35  | BB    | 1337 | G    | C5-C6-O6    | -9.91 | 122.65      | 128.60   |
| 35  | BB    | 2327 | A    | C8-N9-C4    | -9.91 | 101.83      | 105.80   |
| 35  | BB    | 2437 | G    | C5-C6-O6    | -9.91 | 122.65      | 128.60   |
| 1   | AA    | 995  | C    | O4'-C1'-N1  | 9.91  | 116.13      | 108.20   |
| 35  | BB    | 199  | A    | O4'-C1'-N9  | 9.91  | 116.13      | 108.20   |
| 1   | AA    | 280  | C    | C5-C6-N1    | -9.91 | 116.05      | 121.00   |
| 1   | AA    | 683  | G    | C5-C6-O6    | -9.91 | 122.65      | 128.60   |
| 35  | BB    | 1537 | G    | C5-C6-N1    | -9.91 | 106.55      | 111.50   |
| 35  | BB    | 2167 | U    | O4'-C1'-N1  | 9.91  | 116.13      | 108.20   |
| 35  | BB    | 1669 | A    | C4-C5-C6    | 9.91  | 121.95      | 117.00   |
| 35  | BB    | 2191 | A    | C4-C5-N7    | -9.91 | 105.75      | 110.70   |
| 35  | BB    | 2739 | U    | O4'-C1'-N1  | 9.91  | 116.13      | 108.20   |
| 1   | AA    | 318  | G    | N1-C6-O6    | 9.91  | 125.84      | 119.90   |
| 1   | AA    | 728  | A    | C6-C5-N7    | -9.91 | 125.37      | 132.30   |
| 1   | AA    | 1128 | C    | O4'-C1'-N1  | 9.91  | 116.12      | 108.20   |
| 35  | BB    | 120  | U    | O4'-C1'-N1  | 9.91  | 116.12      | 108.20   |
| 35  | BB    | 233  | A    | C5-C6-N6    | -9.91 | 115.77      | 123.70   |
| 35  | BB    | 675  | A    | N1-C2-N3    | 9.91  | 134.25      | 129.30   |
| 35  | BB    | 1041 | G    | O4'-C1'-N9  | 9.91  | 116.12      | 108.20   |
| 35  | BB    | 2059 | A    | N7-C8-N9    | -9.91 | 108.85      | 113.80   |
| 1   | AA    | 741  | G    | O4'-C1'-N9  | 9.90  | 116.12      | 108.20   |
| 1   | AA    | 1215 | G    | N1-C2-N3    | -9.90 | 117.96      | 123.90   |
| 1   | AA    | 1498 | U    | O4'-C1'-N1  | 9.90  | 116.12      | 108.20   |
| 5   | AE    | 137  | ARG  | NE-CZ-NH1   | 9.90  | 125.25      | 120.30   |
| 35  | BB    | 36   | G    | C5-N7-C8    | 9.90  | 109.25      | 104.30   |
| 35  | BB    | 992  | C    | C5-C6-N1    | 9.90  | 125.95      | 121.00   |
| 1   | AA    | 1372 | U    | C5-C4-O4    | -9.90 | 119.96      | 125.90   |
| 35  | BB    | 1733 | G    | C5-C6-O6    | -9.90 | 122.66      | 128.60   |
| 35  | BB    | 2885 | G    | N1-C6-O6    | 9.90  | 125.84      | 119.90   |
| 1   | AA    | 1199 | U    | O4'-C1'-N1  | 9.90  | 116.12      | 108.20   |
| 1   | AA    | 1524 | C    | N3-C4-N4    | 9.90  | 124.93      | 118.00   |
| 35  | BB    | 310  | A    | N1-C6-N6    | 9.90  | 124.54      | 118.60   |
| 35  | BB    | 876  | C    | C6-N1-C2    | -9.90 | 116.34      | 120.30   |
| 35  | BB    | 922  | C    | O4'-C4'-C3' | -9.90 | 94.10       | 104.00   |
| 35  | BB    | 1881 | C    | O4'-C1'-N1  | 9.90  | 116.12      | 108.20   |
| 35  | BB    | 2858 | C    | N3-C4-C5    | -9.90 | 117.94      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 737  | C    | C5-C6-N1   | -9.90 | 116.05      | 121.00   |
| 1   | AA    | 960  | U    | P-O3'-C3'  | 9.90  | 131.58      | 119.70   |
| 35  | BB    | 1470 | A    | N1-C2-N3   | 9.90  | 134.25      | 129.30   |
| 1   | AA    | 172  | A    | C4-C5-N7   | -9.90 | 105.75      | 110.70   |
| 34  | BA    | 114  | C    | O4'-C1'-N1 | 9.90  | 116.12      | 108.20   |
| 35  | BB    | 2864 | G    | C5-C6-N1   | -9.90 | 106.55      | 111.50   |
| 35  | BB    | 513  | A    | C2-N3-C4   | -9.89 | 105.65      | 110.60   |
| 35  | BB    | 264  | C    | N3-C4-N4   | 9.89  | 124.92      | 118.00   |
| 35  | BB    | 1480 | C    | C4-C5-C6   | 9.89  | 122.35      | 117.40   |
| 35  | BB    | 2672 | U    | O4'-C1'-N1 | 9.89  | 116.11      | 108.20   |
| 1   | AA    | 1136 | C    | N3-C4-N4   | 9.89  | 124.92      | 118.00   |
| 35  | BB    | 15   | G    | N3-C2-N2   | 9.89  | 126.82      | 119.90   |
| 35  | BB    | 580  | U    | O4'-C1'-N1 | 9.89  | 116.11      | 108.20   |
| 35  | BB    | 995  | C    | O4'-C1'-N1 | 9.89  | 116.11      | 108.20   |
| 1   | AA    | 1254 | A    | C5-C6-N6   | -9.89 | 115.79      | 123.70   |
| 35  | BB    | 1037 | G    | C5-C6-O6   | -9.89 | 122.67      | 128.60   |
| 35  | BB    | 1129 | A    | N1-C6-N6   | 9.89  | 124.53      | 118.60   |
| 35  | BB    | 2130 | U    | O4'-C1'-N1 | 9.89  | 116.11      | 108.20   |
| 35  | BB    | 2717 | C    | N1-C2-O2   | -9.89 | 112.97      | 118.90   |
| 1   | AA    | 1014 | A    | C5-C6-N1   | -9.88 | 112.76      | 117.70   |
| 35  | BB    | 391  | A    | C4-C5-C6   | 9.88  | 121.94      | 117.00   |
| 56  | BY    | 19   | ARG  | NE-CZ-NH1  | 9.89  | 125.24      | 120.30   |
| 35  | BB    | 887  | U    | P-O3'-C3'  | 9.88  | 131.56      | 119.70   |
| 35  | BB    | 1221 | C    | O4'-C1'-N1 | 9.88  | 116.11      | 108.20   |
| 35  | BB    | 1101 | U    | O4'-C1'-N1 | 9.88  | 116.10      | 108.20   |
| 35  | BB    | 1786 | A    | N1-C6-N6   | 9.88  | 124.53      | 118.60   |
| 35  | BB    | 2433 | A    | O4'-C1'-N9 | 9.88  | 116.10      | 108.20   |
| 35  | BB    | 2900 | A    | N1-C6-N6   | 9.88  | 124.53      | 118.60   |
| 1   | AA    | 1097 | C    | N3-C4-N4   | 9.88  | 124.91      | 118.00   |
| 35  | BB    | 1062 | G    | C4-C5-C6   | 9.88  | 124.73      | 118.80   |
| 35  | BB    | 1158 | C    | N3-C4-C5   | -9.88 | 117.95      | 121.90   |
| 35  | BB    | 1557 | C    | N3-C4-N4   | 9.88  | 124.92      | 118.00   |
| 35  | BB    | 1827 | U    | O4'-C1'-N1 | 9.88  | 116.10      | 108.20   |
| 35  | BB    | 2410 | G    | N1-C6-O6   | 9.88  | 125.83      | 119.90   |
| 35  | BB    | 1485 | U    | C5-C4-O4   | -9.88 | 119.97      | 125.90   |
| 1   | AA    | 28   | A    | N1-C6-N6   | 9.87  | 124.52      | 118.60   |
| 1   | AA    | 1457 | G    | C6-C5-N7   | -9.88 | 124.47      | 130.40   |
| 35  | BB    | 1853 | A    | N9-C4-C5   | -9.88 | 101.85      | 105.80   |
| 35  | BB    | 1961 | C    | O4'-C1'-N1 | 9.88  | 116.10      | 108.20   |
| 35  | BB    | 2338 | C    | N3-C4-C5   | -9.88 | 117.95      | 121.90   |
| 35  | BB    | 936  | A    | N3-C4-C5   | -9.87 | 119.89      | 126.80   |
| 35  | BB    | 2802 | G    | N1-C6-O6   | 9.87  | 125.82      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 98   | G    | C5-C6-N1   | -9.87 | 106.57      | 111.50   |
| 35  | BB    | 924  | G    | C8-N9-C4   | 9.87  | 110.35      | 106.40   |
| 35  | BB    | 298  | G    | N9-C4-C5   | -9.87 | 101.45      | 105.40   |
| 35  | BB    | 891  | G    | N7-C8-N9   | 9.87  | 118.03      | 113.10   |
| 35  | BB    | 2421 | G    | O4'-C1'-N9 | 9.87  | 116.09      | 108.20   |
| 35  | BB    | 2720 | U    | O4'-C1'-N1 | 9.87  | 116.10      | 108.20   |
| 35  | BB    | 1558 | C    | O4'-C1'-N1 | 9.87  | 116.09      | 108.20   |
| 35  | BB    | 2886 | A    | C5-C6-N1   | -9.87 | 112.77      | 117.70   |
| 1   | AA    | 1252 | A    | C5-C6-N6   | -9.86 | 115.81      | 123.70   |
| 35  | BB    | 771  | G    | O4'-C1'-N9 | 9.87  | 116.09      | 108.20   |
| 35  | BB    | 2621 | G    | C5-C6-N1   | -9.87 | 106.57      | 111.50   |
| 1   | AA    | 743  | A    | C5-N7-C8   | 9.86  | 108.83      | 103.90   |
| 34  | BA    | 83   | G    | O4'-C1'-N9 | 9.86  | 116.09      | 108.20   |
| 48  | BO    | 102  | ARG  | NE-CZ-NH2  | -9.86 | 115.37      | 120.30   |
| 1   | AA    | 925  | G    | C4-C5-N7   | 9.86  | 114.74      | 110.80   |
| 1   | AA    | 1004 | A    | O4'-C1'-N9 | 9.86  | 116.09      | 108.20   |
| 1   | AA    | 1387 | G    | O4'-C1'-N9 | 9.86  | 116.09      | 108.20   |
| 35  | BB    | 1155 | A    | N1-C6-N6   | 9.86  | 124.52      | 118.60   |
| 35  | BB    | 1909 | C    | C5-C6-N1   | 9.86  | 125.93      | 121.00   |
| 35  | BB    | 464  | U    | O4'-C1'-N1 | 9.86  | 116.08      | 108.20   |
| 35  | BB    | 2468 | A    | C6-C5-N7   | -9.86 | 125.40      | 132.30   |
| 35  | BB    | 1087 | G    | N7-C8-N9   | 9.86  | 118.03      | 113.10   |
| 35  | BB    | 1380 | G    | O4'-C1'-N9 | 9.86  | 116.08      | 108.20   |
| 35  | BB    | 1407 | G    | O4'-C1'-N9 | 9.86  | 116.08      | 108.20   |
| 35  | BB    | 2185 | U    | O4'-C1'-N1 | 9.86  | 116.08      | 108.20   |
| 1   | AA    | 942  | G    | N1-C6-O6   | 9.85  | 125.81      | 119.90   |
| 35  | BB    | 251  | A    | N1-C6-N6   | 9.85  | 124.51      | 118.60   |
| 35  | BB    | 324  | A    | C4-C5-N7   | -9.85 | 105.77      | 110.70   |
| 35  | BB    | 1226 | A    | C5-C6-N6   | -9.85 | 115.82      | 123.70   |
| 35  | BB    | 1537 | G    | C4-C5-N7   | -9.85 | 106.86      | 110.80   |
| 35  | BB    | 1977 | A    | O4'-C1'-N9 | 9.85  | 116.08      | 108.20   |
| 1   | AA    | 270  | A    | C5-N7-C8   | 9.85  | 108.83      | 103.90   |
| 1   | AA    | 1306 | A    | C5-C6-N6   | -9.85 | 115.82      | 123.70   |
| 1   | AA    | 1525 | G    | N1-C2-N3   | -9.85 | 117.99      | 123.90   |
| 35  | BB    | 29   | U    | P-O3'-C3'  | -9.85 | 107.88      | 119.70   |
| 35  | BB    | 182  | A    | C5-C6-N1   | -9.85 | 112.78      | 117.70   |
| 35  | BB    | 723  | C    | N3-C4-N4   | 9.85  | 124.89      | 118.00   |
| 35  | BB    | 1840 | G    | O4'-C1'-N9 | 9.85  | 116.08      | 108.20   |
| 35  | BB    | 1972 | G    | C5-C6-N1   | -9.85 | 106.58      | 111.50   |
| 35  | BB    | 2010 | G    | O4'-C1'-N9 | 9.85  | 116.08      | 108.20   |
| 1   | AA    | 271  | C    | N3-C4-C5   | -9.85 | 117.96      | 121.90   |
| 1   | AA    | 938  | A    | N1-C6-N6   | 9.85  | 124.51      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1008 | U    | C5-C6-N1    | 9.85  | 127.62      | 122.70   |
| 35  | BB    | 1237 | A    | C3'-C2'-C1' | 9.85  | 109.38      | 101.50   |
| 17  | AQ    | 76   | ARG  | NE-CZ-NH1   | 9.85  | 125.22      | 120.30   |
| 35  | BB    | 2811 | G    | N7-C8-N9    | 9.85  | 118.02      | 113.10   |
| 1   | AA    | 238  | A    | C5-C6-N6    | -9.84 | 115.83      | 123.70   |
| 35  | BB    | 722  | A    | N9-C4-C5    | 9.84  | 109.74      | 105.80   |
| 1   | AA    | 1516 | G    | C5-N7-C8    | 9.84  | 109.22      | 104.30   |
| 35  | BB    | 142  | A    | C5-C6-N6    | -9.84 | 115.83      | 123.70   |
| 35  | BB    | 705  | A    | N1-C6-N6    | 9.84  | 124.51      | 118.60   |
| 35  | BB    | 807  | U    | O4'-C1'-N1  | 9.84  | 116.08      | 108.20   |
| 35  | BB    | 2003 | A    | C4-C5-C6    | 9.84  | 121.92      | 117.00   |
| 35  | BB    | 1046 | A    | C5'-C4'-O4' | 9.84  | 120.91      | 109.10   |
| 1   | AA    | 1108 | G    | O4'-C1'-N9  | 9.84  | 116.07      | 108.20   |
| 1   | AA    | 1164 | G    | N3-C2-N2    | 9.84  | 126.79      | 119.90   |
| 35  | BB    | 1731 | G    | P-O3'-C3'   | 9.84  | 131.51      | 119.70   |
| 35  | BB    | 1057 | A    | O4'-C1'-N9  | 9.84  | 116.07      | 108.20   |
| 1   | AA    | 536  | C    | N3-C4-C5    | -9.84 | 117.97      | 121.90   |
| 1   | AA    | 1480 | A    | N9-C4-C5    | 9.84  | 109.73      | 105.80   |
| 35  | BB    | 750  | A    | C8-N9-C4    | -9.84 | 101.86      | 105.80   |
| 35  | BB    | 928  | A    | C5-C6-N6    | -9.84 | 115.83      | 123.70   |
| 35  | BB    | 1462 | C    | N3-C4-C5    | -9.84 | 117.97      | 121.90   |
| 35  | BB    | 1973 | G    | C6-N1-C2    | 9.84  | 131.00      | 125.10   |
| 8   | AH    | 65   | PHE  | CB-CG-CD2   | 9.84  | 127.69      | 120.80   |
| 35  | BB    | 263  | G    | C4-C5-N7    | 9.84  | 114.73      | 110.80   |
| 35  | BB    | 283  | G    | N9-C4-C5    | 9.84  | 109.33      | 105.40   |
| 35  | BB    | 1430 | G    | N3-C2-N2    | 9.84  | 126.79      | 119.90   |
| 35  | BB    | 1462 | C    | C6-N1-C2    | -9.84 | 116.37      | 120.30   |
| 35  | BB    | 2800 | A    | C4-C5-C6    | 9.84  | 121.92      | 117.00   |
| 1   | AA    | 460  | A    | O4'-C1'-N9  | 9.83  | 116.07      | 108.20   |
| 35  | BB    | 523  | C    | O4'-C1'-N1  | 9.83  | 116.07      | 108.20   |
| 35  | BB    | 627  | A    | N9-C4-C5    | 9.83  | 109.73      | 105.80   |
| 35  | BB    | 850  | U    | C5-C6-N1    | 9.83  | 127.62      | 122.70   |
| 1   | AA    | 1105 | A    | N1-C6-N6    | 9.83  | 124.50      | 118.60   |
| 35  | BB    | 2082 | A    | N1-C6-N6    | 9.83  | 124.50      | 118.60   |
| 35  | BB    | 722  | A    | C5-C6-N6    | -9.83 | 115.84      | 123.70   |
| 35  | BB    | 1647 | U    | O4'-C1'-N1  | 9.83  | 116.06      | 108.20   |
| 35  | BB    | 2437 | G    | N1-C6-O6    | 9.83  | 125.80      | 119.90   |
| 49  | BP    | 112  | ARG  | NE-CZ-NH1   | 9.83  | 125.21      | 120.30   |
| 22  | AV    | 34   | G    | P-O5'-C5'   | 9.83  | 136.62      | 120.90   |
| 35  | BB    | 895  | U    | C5-C6-N1    | 9.83  | 127.61      | 122.70   |
| 35  | BB    | 1535 | A    | C5'-C4'-O4' | 9.83  | 120.89      | 109.10   |
| 35  | BB    | 2860 | A    | C5-C6-N1    | -9.83 | 112.79      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 128  | G    | O4'-C1'-N9 | 9.82  | 116.06      | 108.20   |
| 35  | BB    | 13   | A    | N7-C8-N9   | -9.82 | 108.89      | 113.80   |
| 35  | BB    | 2012 | G    | C6-C5-N7   | -9.82 | 124.50      | 130.40   |
| 35  | BB    | 969  | G    | C6-C5-N7   | -9.82 | 124.51      | 130.40   |
| 1   | AA    | 239  | U    | P-O5'-C5'  | 9.82  | 136.61      | 120.90   |
| 34  | BA    | 116  | G    | C5-C6-O6   | -9.82 | 122.71      | 128.60   |
| 35  | BB    | 934  | U    | O4'-C1'-N1 | 9.82  | 116.06      | 108.20   |
| 35  | BB    | 1998 | A    | C5-C6-N6   | -9.82 | 115.84      | 123.70   |
| 1   | AA    | 302  | G    | C6-C5-N7   | -9.82 | 124.51      | 130.40   |
| 1   | AA    | 1349 | A    | N1-C2-N3   | 9.82  | 134.21      | 129.30   |
| 35  | BB    | 900  | A    | C5-C6-N6   | -9.82 | 115.85      | 123.70   |
| 35  | BB    | 1069 | A    | N9-C4-C5   | -9.82 | 101.87      | 105.80   |
| 35  | BB    | 1339 | G    | C5-C6-O6   | -9.82 | 122.71      | 128.60   |
| 35  | BB    | 2141 | G    | N1-C6-O6   | 9.82  | 125.79      | 119.90   |
| 35  | BB    | 2764 | A    | C4-C5-C6   | 9.82  | 121.91      | 117.00   |
| 1   | AA    | 161  | A    | C5-C6-N1   | -9.81 | 112.79      | 117.70   |
| 1   | AA    | 441  | A    | C8-N9-C4   | -9.81 | 101.87      | 105.80   |
| 1   | AA    | 1177 | G    | C5-C6-O6   | -9.81 | 122.71      | 128.60   |
| 1   | AA    | 819  | A    | N7-C8-N9   | 9.81  | 118.71      | 113.80   |
| 1   | AA    | 175  | C    | O4'-C1'-N1 | 9.81  | 116.05      | 108.20   |
| 1   | AA    | 251  | G    | N1-C6-O6   | 9.81  | 125.79      | 119.90   |
| 35  | BB    | 342  | A    | C4-C5-C6   | 9.81  | 121.91      | 117.00   |
| 35  | BB    | 2410 | G    | C6-N1-C2   | 9.81  | 130.99      | 125.10   |
| 1   | AA    | 580  | C    | N3-C4-C5   | 9.81  | 125.82      | 121.90   |
| 1   | AA    | 912  | C    | C6-N1-C2   | -9.81 | 116.38      | 120.30   |
| 35  | BB    | 699  | A    | N1-C2-N3   | 9.81  | 134.21      | 129.30   |
| 35  | BB    | 2422 | C    | O4'-C1'-N1 | 9.81  | 116.05      | 108.20   |
| 1   | AA    | 448  | A    | N1-C2-N3   | 9.81  | 134.20      | 129.30   |
| 1   | AA    | 1041 | G    | C4-C5-N7   | 9.80  | 114.72      | 110.80   |
| 1   | AA    | 1465 | A    | C5-C6-N6   | -9.80 | 115.86      | 123.70   |
| 35  | BB    | 1233 | C    | C5-C4-N4   | -9.80 | 113.34      | 120.20   |
| 35  | BB    | 1591 | A    | C5-C6-N1   | -9.81 | 112.80      | 117.70   |
| 34  | BA    | 18   | G    | O4'-C1'-N9 | 9.80  | 116.04      | 108.20   |
| 35  | BB    | 279  | A    | N7-C8-N9   | 9.80  | 118.70      | 113.80   |
| 35  | BB    | 1162 | G    | O4'-C1'-N9 | 9.80  | 116.04      | 108.20   |
| 1   | AA    | 419  | C    | C5-C4-N4   | -9.80 | 113.34      | 120.20   |
| 35  | BB    | 1179 | G    | N1-C2-N3   | -9.80 | 118.02      | 123.90   |
| 35  | BB    | 253  | C    | N3-C4-C5   | -9.80 | 117.98      | 121.90   |
| 35  | BB    | 1005 | C    | N3-C4-C5   | -9.80 | 117.98      | 121.90   |
| 35  | BB    | 1776 | G    | C5-C6-O6   | -9.80 | 122.72      | 128.60   |
| 35  | BB    | 1986 | C    | N3-C4-C5   | -9.80 | 117.98      | 121.90   |
| 35  | BB    | 98   | G    | N3-C4-C5   | -9.80 | 123.70      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 925  | A    | N1-C6-N6   | 9.80  | 124.48      | 118.60   |
| 35  | BB    | 1290 | C    | O4'-C1'-N1 | 9.80  | 116.04      | 108.20   |
| 1   | AA    | 360  | G    | C8-N9-C4   | -9.79 | 102.48      | 106.40   |
| 1   | AA    | 497  | G    | N1-C6-O6   | 9.79  | 125.78      | 119.90   |
| 35  | BB    | 1330 | C    | O4'-C1'-N1 | 9.79  | 116.03      | 108.20   |
| 35  | BB    | 2458 | G    | N1-C6-O6   | 9.79  | 125.78      | 119.90   |
| 35  | BB    | 1026 | G    | O4'-C1'-N9 | 9.79  | 116.03      | 108.20   |
| 35  | BB    | 1085 | A    | C5-C6-N1   | -9.79 | 112.80      | 117.70   |
| 35  | BB    | 1880 | U    | O4'-C1'-N1 | 9.79  | 116.03      | 108.20   |
| 35  | BB    | 2001 | C    | O4'-C1'-N1 | 9.79  | 116.03      | 108.20   |
| 35  | BB    | 2116 | G    | C4-C5-C6   | 9.79  | 124.67      | 118.80   |
| 35  | BB    | 2382 | G    | N1-C6-O6   | 9.79  | 125.78      | 119.90   |
| 1   | AA    | 108  | G    | C4-C5-N7   | 9.79  | 114.72      | 110.80   |
| 1   | AA    | 462  | G    | N3-C2-N2   | 9.79  | 126.75      | 119.90   |
| 1   | AA    | 728  | A    | C6-N1-C2   | 9.79  | 124.47      | 118.60   |
| 35  | BB    | 2013 | A    | N9-C4-C5   | -9.79 | 101.88      | 105.80   |
| 1   | AA    | 339  | C    | O4'-C1'-N1 | 9.79  | 116.03      | 108.20   |
| 1   | AA    | 684  | U    | C6-N1-C2   | -9.79 | 115.13      | 121.00   |
| 1   | AA    | 877  | G    | O4'-C1'-N9 | 9.79  | 116.03      | 108.20   |
| 35  | BB    | 211  | C    | N3-C2-O2   | -9.79 | 115.05      | 121.90   |
| 35  | BB    | 368  | A    | C5-N7-C8   | 9.79  | 108.79      | 103.90   |
| 35  | BB    | 686  | U    | N1-C2-N3   | -9.79 | 109.03      | 114.90   |
| 35  | BB    | 1383 | A    | O4'-C1'-N9 | 9.79  | 116.03      | 108.20   |
| 35  | BB    | 1730 | C    | N3-C4-C5   | -9.79 | 117.98      | 121.90   |
| 1   | AA    | 1483 | A    | C4-C5-C6   | 9.79  | 121.89      | 117.00   |
| 34  | BA    | 84   | G    | C4-C5-N7   | 9.79  | 114.72      | 110.80   |
| 35  | BB    | 1970 | A    | C4-C5-C6   | 9.79  | 121.89      | 117.00   |
| 35  | BB    | 1361 | G    | N1-C6-O6   | 9.78  | 125.77      | 119.90   |
| 35  | BB    | 2424 | C    | C5-C6-N1   | -9.79 | 116.11      | 121.00   |
| 43  | BJ    | 16   | TYR  | CB-CG-CD2  | -9.79 | 115.13      | 121.00   |
| 1   | AA    | 444  | G    | O4'-C1'-N9 | 9.78  | 116.03      | 108.20   |
| 1   | AA    | 676  | A    | N7-C8-N9   | -9.78 | 108.91      | 113.80   |
| 35  | BB    | 1544 | A    | C5-C6-N6   | -9.78 | 115.87      | 123.70   |
| 1   | AA    | 714  | G    | N1-C6-O6   | 9.78  | 125.77      | 119.90   |
| 35  | BB    | 240  | C    | C4-C5-C6   | -9.78 | 112.51      | 117.40   |
| 35  | BB    | 247  | G    | C5-C6-N1   | -9.78 | 106.61      | 111.50   |
| 35  | BB    | 1189 | A    | C5-N7-C8   | 9.78  | 108.79      | 103.90   |
| 35  | BB    | 1948 | G    | C5-C6-O6   | 9.78  | 134.47      | 128.60   |
| 35  | BB    | 1738 | G    | N9-C4-C5   | -9.78 | 101.49      | 105.40   |
| 48  | BO    | 102  | ARG  | NE-CZ-NH1  | 9.78  | 125.19      | 120.30   |
| 1   | AA    | 786  | G    | O4'-C1'-N9 | 9.78  | 116.02      | 108.20   |
| 35  | BB    | 394  | C    | O4'-C1'-N1 | 9.78  | 116.02      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 2882 | A    | C5-C6-N6   | -9.78 | 115.88      | 123.70   |
| 1   | AA    | 1442 | G    | O4'-C1'-N9 | 9.77  | 116.02      | 108.20   |
| 35  | BB    | 10   | A    | C4-C5-C6   | 9.77  | 121.89      | 117.00   |
| 35  | BB    | 469  | G    | N1-C6-O6   | 9.77  | 125.77      | 119.90   |
| 1   | AA    | 1147 | C    | N3-C4-C5   | -9.77 | 117.99      | 121.90   |
| 22  | AV    | 4    | C    | O4'-C1'-N1 | 9.77  | 116.02      | 108.20   |
| 35  | BB    | 924  | G    | N7-C8-N9   | -9.77 | 108.22      | 113.10   |
| 35  | BB    | 1752 | C    | N3-C4-C5   | -9.77 | 117.99      | 121.90   |
| 35  | BB    | 2345 | G    | C6-C5-N7   | -9.77 | 124.54      | 130.40   |
| 35  | BB    | 2723 | C    | O4'-C1'-N1 | 9.77  | 116.02      | 108.20   |
| 1   | AA    | 817  | C    | N3-C4-N4   | 9.77  | 124.84      | 118.00   |
| 12  | AL    | 13   | ARG  | NE-CZ-NH1  | 9.77  | 125.19      | 120.30   |
| 35  | BB    | 1510 | G    | N1-C6-O6   | 9.77  | 125.76      | 119.90   |
| 35  | BB    | 2204 | G    | O4'-C1'-N9 | 9.77  | 116.02      | 108.20   |
| 1   | AA    | 115  | G    | N3-C2-N2   | 9.77  | 126.74      | 119.90   |
| 35  | BB    | 159  | G    | C6-N1-C2   | 9.77  | 130.96      | 125.10   |
| 34  | BA    | 60   | C    | O4'-C1'-N1 | 9.77  | 116.01      | 108.20   |
| 1   | AA    | 217  | C    | O4'-C1'-N1 | 9.76  | 116.01      | 108.20   |
| 35  | BB    | 977  | G    | C5-C6-O6   | -9.76 | 122.74      | 128.60   |
| 35  | BB    | 581  | C    | O4'-C1'-N1 | 9.76  | 116.01      | 108.20   |
| 35  | BB    | 2508 | G    | O4'-C1'-N9 | 9.76  | 116.01      | 108.20   |
| 1   | AA    | 306  | A    | C4-C5-C6   | 9.76  | 121.88      | 117.00   |
| 1   | AA    | 969  | A    | C4-C5-C6   | 9.76  | 121.88      | 117.00   |
| 3   | AC    | 171  | ARG  | NE-CZ-NH1  | 9.76  | 125.18      | 120.30   |
| 35  | BB    | 2171 | A    | N1-C6-N6   | 9.76  | 124.46      | 118.60   |
| 35  | BB    | 2839 | G    | N1-C6-O6   | 9.76  | 125.76      | 119.90   |
| 1   | AA    | 756  | C    | N3-C4-N4   | 9.76  | 124.83      | 118.00   |
| 1   | AA    | 1215 | G    | C2-N3-C4   | 9.76  | 116.78      | 111.90   |
| 34  | BA    | 2    | G    | C5-C6-O6   | -9.76 | 122.75      | 128.60   |
| 35  | BB    | 276  | U    | C5-C4-O4   | -9.76 | 120.05      | 125.90   |
| 35  | BB    | 654  | A    | O4'-C1'-N9 | 9.76  | 116.00      | 108.20   |
| 1   | AA    | 527  | G    | C5-C6-O6   | -9.75 | 122.75      | 128.60   |
| 35  | BB    | 401  | A    | N1-C6-N6   | 9.75  | 124.45      | 118.60   |
| 35  | BB    | 624  | C    | C6-N1-C2   | -9.75 | 116.40      | 120.30   |
| 35  | BB    | 814  | C    | O4'-C1'-N1 | 9.75  | 116.00      | 108.20   |
| 1   | AA    | 744  | C    | C6-N1-C2   | 9.75  | 124.20      | 120.30   |
| 1   | AA    | 874  | G    | N3-C4-C5   | -9.75 | 123.73      | 128.60   |
| 22  | AV    | 7    | G    | P-O3'-C3'  | 9.75  | 131.40      | 119.70   |
| 35  | BB    | 668  | A    | C5-C6-N6   | -9.75 | 115.90      | 123.70   |
| 35  | BB    | 916  | G    | C8-N9-C4   | -9.75 | 102.50      | 106.40   |
| 35  | BB    | 2448 | A    | C6-C5-N7   | -9.75 | 125.47      | 132.30   |
| 35  | BB    | 2635 | A    | C5-C6-N6   | -9.75 | 115.90      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 2681 | C    | N3-C4-N4   | 9.75  | 124.83      | 118.00   |
| 35  | BB    | 240  | C    | C2-N3-C4   | 9.75  | 124.77      | 119.90   |
| 35  | BB    | 383  | C    | O4'-C1'-N1 | 9.75  | 116.00      | 108.20   |
| 35  | BB    | 1099 | G    | C2-N3-C4   | 9.75  | 116.77      | 111.90   |
| 1   | AA    | 59   | A    | N3-C4-C5   | -9.75 | 119.98      | 126.80   |
| 1   | AA    | 254  | G    | C5-C6-N1   | -9.75 | 106.63      | 111.50   |
| 35  | BB    | 2375 | G    | O4'-C1'-N9 | 9.75  | 116.00      | 108.20   |
| 1   | AA    | 577  | G    | C4-C5-C6   | 9.74  | 124.65      | 118.80   |
| 1   | AA    | 1015 | G    | C5-C6-O6   | -9.74 | 122.75      | 128.60   |
| 35  | BB    | 411  | G    | C8-N9-C4   | -9.74 | 102.50      | 106.40   |
| 35  | BB    | 1556 | C    | N3-C4-C5   | -9.74 | 118.00      | 121.90   |
| 1   | AA    | 445  | G    | N1-C6-O6   | 9.74  | 125.75      | 119.90   |
| 35  | BB    | 54   | G    | N3-C4-C5   | -9.74 | 123.73      | 128.60   |
| 35  | BB    | 610  | C    | C6-N1-C2   | -9.74 | 116.40      | 120.30   |
| 35  | BB    | 2627 | G    | N9-C4-C5   | 9.74  | 109.30      | 105.40   |
| 35  | BB    | 2893 | A    | C5-C6-N1   | -9.74 | 112.83      | 117.70   |
| 45  | BL    | 2    | ARG  | NE-CZ-NH2  | -9.74 | 115.43      | 120.30   |
| 35  | BB    | 849  | A    | N1-C6-N6   | 9.74  | 124.44      | 118.60   |
| 35  | BB    | 885  | C    | C5-C6-N1   | 9.74  | 125.87      | 121.00   |
| 35  | BB    | 1136 | G    | C5-C6-O6   | -9.74 | 122.76      | 128.60   |
| 35  | BB    | 2178 | C    | C6-N1-C1'  | -9.74 | 109.11      | 120.80   |
| 35  | BB    | 2590 | A    | N1-C6-N6   | 9.74  | 124.44      | 118.60   |
| 35  | BB    | 2791 | G    | C5-C6-O6   | -9.74 | 122.76      | 128.60   |
| 35  | BB    | 2447 | G    | N3-C2-N2   | 9.74  | 126.72      | 119.90   |
| 35  | BB    | 2809 | A    | C5-C6-N1   | -9.74 | 112.83      | 117.70   |
| 1   | AA    | 307  | C    | C4-C5-C6   | 9.74  | 122.27      | 117.40   |
| 1   | AA    | 621  | A    | O4'-C1'-N9 | 9.74  | 115.99      | 108.20   |
| 35  | BB    | 1895 | C    | C4-C5-C6   | 9.74  | 122.27      | 117.40   |
| 35  | BB    | 921  | C    | C6-N1-C2   | -9.73 | 116.41      | 120.30   |
| 35  | BB    | 245  | G    | N1-C6-O6   | 9.73  | 125.74      | 119.90   |
| 35  | BB    | 1802 | A    | C5-C6-N1   | -9.73 | 112.83      | 117.70   |
| 35  | BB    | 920  | A    | N1-C6-N6   | 9.73  | 124.44      | 118.60   |
| 35  | BB    | 1750 | G    | N1-C6-O6   | 9.73  | 125.74      | 119.90   |
| 35  | BB    | 2309 | A    | N1-C6-N6   | 9.73  | 124.44      | 118.60   |
| 35  | BB    | 2324 | U    | O4'-C1'-N1 | 9.73  | 115.98      | 108.20   |
| 1   | AA    | 357  | G    | N1-C6-O6   | 9.73  | 125.74      | 119.90   |
| 1   | AA    | 580  | C    | O4'-C1'-N1 | 9.73  | 115.98      | 108.20   |
| 1   | AA    | 1350 | A    | N9-C4-C5   | -9.73 | 101.91      | 105.80   |
| 1   | AA    | 1413 | A    | C2-N3-C4   | -9.73 | 105.74      | 110.60   |
| 35  | BB    | 1932 | A    | N1-C6-N6   | 9.73  | 124.44      | 118.60   |
| 35  | BB    | 2333 | A    | C6-N1-C2   | -9.73 | 112.76      | 118.60   |
| 35  | BB    | 2606 | C    | N3-C4-N4   | 9.73  | 124.81      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 2767 | C    | C4-C5-C6   | 9.73  | 122.26      | 117.40   |
| 35  | BB    | 1017 | G    | O4'-C1'-N9 | 9.73  | 115.98      | 108.20   |
| 1   | AA    | 710  | G    | C4-C5-N7   | -9.72 | 106.91      | 110.80   |
| 1   | AA    | 1032 | G    | N1-C6-O6   | 9.72  | 125.73      | 119.90   |
| 1   | AA    | 1348 | U    | O4'-C1'-N1 | 9.72  | 115.98      | 108.20   |
| 35  | BB    | 1317 | G    | N1-C6-O6   | 9.72  | 125.73      | 119.90   |
| 23  | AX    | 19   | A    | C4-C5-C6   | 9.72  | 121.86      | 117.00   |
| 35  | BB    | 2089 | C    | N3-C4-N4   | 9.72  | 124.81      | 118.00   |
| 35  | BB    | 2234 | G    | C4-C5-C6   | 9.72  | 124.63      | 118.80   |
| 35  | BB    | 943  | A    | N1-C6-N6   | 9.72  | 124.43      | 118.60   |
| 35  | BB    | 1589 | U    | C5-C4-O4   | -9.72 | 120.07      | 125.90   |
| 35  | BB    | 2635 | A    | N7-C8-N9   | 9.72  | 118.66      | 113.80   |
| 1   | AA    | 505  | G    | C5-N7-C8   | -9.72 | 99.44       | 104.30   |
| 1   | AA    | 783  | C    | O4'-C1'-N1 | 9.72  | 115.97      | 108.20   |
| 35  | BB    | 1071 | G    | N3-C2-N2   | 9.72  | 126.70      | 119.90   |
| 1   | AA    | 1481 | U    | O4'-C1'-N1 | 9.72  | 115.97      | 108.20   |
| 35  | BB    | 2421 | G    | N1-C6-O6   | 9.72  | 125.73      | 119.90   |
| 1   | AA    | 813  | U    | N3-C4-C5   | -9.71 | 108.77      | 114.60   |
| 35  | BB    | 206  | U    | O4'-C1'-N1 | 9.71  | 115.97      | 108.20   |
| 35  | BB    | 1735 | A    | C5-C6-N1   | -9.71 | 112.84      | 117.70   |
| 35  | BB    | 2586 | U    | O4'-C1'-N1 | 9.71  | 115.97      | 108.20   |
| 1   | AA    | 1353 | G    | C2-N3-C4   | 9.71  | 116.76      | 111.90   |
| 1   | AA    | 1520 | C    | N3-C4-N4   | 9.71  | 124.80      | 118.00   |
| 35  | BB    | 881  | G    | N7-C8-N9   | 9.71  | 117.96      | 113.10   |
| 35  | BB    | 1660 | G    | N1-C2-N3   | -9.71 | 118.07      | 123.90   |
| 1   | AA    | 501  | C    | O4'-C1'-N1 | 9.71  | 115.97      | 108.20   |
| 35  | BB    | 1341 | G    | O4'-C1'-N9 | 9.71  | 115.97      | 108.20   |
| 35  | BB    | 1709 | U    | O4'-C1'-N1 | 9.71  | 115.97      | 108.20   |
| 35  | BB    | 1888 | G    | N1-C6-O6   | 9.71  | 125.73      | 119.90   |
| 35  | BB    | 2283 | C    | C6-N1-C2   | -9.71 | 116.42      | 120.30   |
| 1   | AA    | 295  | C    | N3-C4-N4   | 9.71  | 124.80      | 118.00   |
| 1   | AA    | 1082 | A    | C8-N9-C4   | -9.71 | 101.92      | 105.80   |
| 35  | BB    | 419  | U    | O4'-C1'-N1 | 9.71  | 115.97      | 108.20   |
| 35  | BB    | 2129 | C    | N3-C4-C5   | -9.71 | 118.02      | 121.90   |
| 1   | AA    | 749  | A    | C5-C6-N1   | -9.70 | 112.85      | 117.70   |
| 35  | BB    | 293  | U    | C4-C5-C6   | -9.71 | 113.88      | 119.70   |
| 35  | BB    | 330  | A    | C2-N3-C4   | -9.71 | 105.75      | 110.60   |
| 35  | BB    | 354  | A    | C5-C6-N6   | -9.71 | 115.94      | 123.70   |
| 35  | BB    | 445  | C    | N3-C4-C5   | -9.71 | 118.02      | 121.90   |
| 35  | BB    | 507  | A    | C2-N3-C4   | 9.70  | 115.45      | 110.60   |
| 35  | BB    | 1937 | A    | C6-N1-C2   | 9.71  | 124.42      | 118.60   |
| 39  | BF    | 174  | PHE  | CB-CG-CD2  | 9.71  | 127.59      | 120.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 181  | A    | O4'-C1'-N9 | 9.70  | 115.96      | 108.20   |
| 1   | AA    | 263  | A    | C4-C5-C6   | 9.70  | 121.85      | 117.00   |
| 1   | AA    | 612  | C    | N3-C4-N4   | 9.70  | 124.79      | 118.00   |
| 1   | AA    | 702  | A    | C5-C6-N6   | -9.70 | 115.94      | 123.70   |
| 35  | BB    | 152  | A    | C4-C5-C6   | 9.70  | 121.85      | 117.00   |
| 35  | BB    | 498  | G    | N3-C2-N2   | 9.70  | 126.69      | 119.90   |
| 35  | BB    | 1493 | C    | C2-N3-C4   | 9.70  | 124.75      | 119.90   |
| 35  | BB    | 2262 | U    | O4'-C1'-N1 | 9.70  | 115.96      | 108.20   |
| 35  | BB    | 2546 | U    | O4'-C1'-N1 | 9.70  | 115.96      | 108.20   |
| 35  | BB    | 1514 | G    | C5-C6-O6   | -9.70 | 122.78      | 128.60   |
| 35  | BB    | 2785 | C    | O4'-C1'-N1 | 9.70  | 115.96      | 108.20   |
| 1   | AA    | 603  | U    | O4'-C1'-N1 | 9.70  | 115.96      | 108.20   |
| 1   | AA    | 849  | G    | P-O5'-C5'  | 9.70  | 136.42      | 120.90   |
| 34  | BA    | 52   | A    | C4-C5-C6   | 9.70  | 121.85      | 117.00   |
| 35  | BB    | 808  | G    | C6-C5-N7   | -9.70 | 124.58      | 130.40   |
| 35  | BB    | 816  | C    | N3-C4-N4   | 9.70  | 124.79      | 118.00   |
| 35  | BB    | 1368 | G    | O4'-C1'-N9 | 9.70  | 115.96      | 108.20   |
| 35  | BB    | 1913 | A    | C5-N7-C8   | 9.70  | 108.75      | 103.90   |
| 35  | BB    | 2358 | A    | C5-C6-N6   | -9.70 | 115.94      | 123.70   |
| 35  | BB    | 2808 | G    | N3-C2-N2   | 9.70  | 126.69      | 119.90   |
| 35  | BB    | 2853 | C    | O4'-C1'-N1 | 9.70  | 115.96      | 108.20   |
| 1   | AA    | 890  | G    | N1-C2-N3   | -9.70 | 118.08      | 123.90   |
| 36  | BC    | 257  | ARG  | NE-CZ-NH2  | -9.70 | 115.45      | 120.30   |
| 35  | BB    | 2284 | A    | C4-C5-C6   | 9.69  | 121.85      | 117.00   |
| 1   | AA    | 1269 | A    | N1-C2-N3   | -9.69 | 124.45      | 129.30   |
| 35  | BB    | 1390 | U    | N3-C4-C5   | -9.69 | 108.78      | 114.60   |
| 1   | AA    | 975  | A    | C5-C6-N1   | -9.69 | 112.86      | 117.70   |
| 35  | BB    | 600  | G    | C5-C6-O6   | -9.69 | 122.79      | 128.60   |
| 35  | BB    | 1303 | G    | O4'-C1'-N9 | 9.69  | 115.95      | 108.20   |
| 1   | AA    | 1371 | G    | C5-C6-O6   | -9.69 | 122.79      | 128.60   |
| 35  | BB    | 696  | G    | C5-C6-N1   | -9.69 | 106.66      | 111.50   |
| 34  | BA    | 93   | C    | O4'-C1'-N1 | 9.69  | 115.95      | 108.20   |
| 35  | BB    | 1147 | A    | C5-C6-N1   | -9.69 | 112.86      | 117.70   |
| 35  | BB    | 1482 | G    | C5-C6-N1   | -9.69 | 106.66      | 111.50   |
| 35  | BB    | 2060 | A    | N1-C6-N6   | 9.69  | 124.41      | 118.60   |
| 35  | BB    | 2839 | G    | C5-C6-O6   | -9.69 | 122.79      | 128.60   |
| 1   | AA    | 1276 | G    | O4'-C1'-N9 | 9.68  | 115.95      | 108.20   |
| 35  | BB    | 209  | C    | N3-C4-C5   | -9.68 | 118.03      | 121.90   |
| 35  | BB    | 2144 | G    | N1-C6-O6   | 9.68  | 125.71      | 119.90   |
| 35  | BB    | 2351 | G    | C5-C6-O6   | -9.68 | 122.79      | 128.60   |
| 35  | BB    | 1852 | U    | N1-C2-N3   | 9.68  | 120.71      | 114.90   |
| 35  | BB    | 1879 | C    | O4'-C1'-N1 | 9.68  | 115.95      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 329  | G    | C5-C6-N1   | -9.68 | 106.66      | 111.50   |
| 35  | BB    | 1457 | U    | O4'-C1'-N1 | 9.68  | 115.94      | 108.20   |
| 35  | BB    | 2171 | A    | C4-C5-C6   | 9.68  | 121.84      | 117.00   |
| 1   | AA    | 1318 | A    | O4'-C1'-N9 | 9.68  | 115.94      | 108.20   |
| 35  | BB    | 1191 | G    | N1-C6-O6   | 9.68  | 125.71      | 119.90   |
| 1   | AA    | 144  | G    | N1-C6-O6   | 9.68  | 125.70      | 119.90   |
| 1   | AA    | 1104 | G    | C4-C5-N7   | 9.68  | 114.67      | 110.80   |
| 35  | BB    | 686  | U    | O4'-C1'-N1 | 9.68  | 115.94      | 108.20   |
| 35  | BB    | 1509 | A    | O4'-C1'-N9 | 9.68  | 115.94      | 108.20   |
| 35  | BB    | 2676 | C    | C5-C6-N1   | 9.68  | 125.84      | 121.00   |
| 1   | AA    | 69   | G    | N1-C6-O6   | 9.67  | 125.70      | 119.90   |
| 1   | AA    | 299  | G    | N9-C4-C5   | -9.67 | 101.53      | 105.40   |
| 1   | AA    | 520  | A    | C5-C6-N6   | -9.67 | 115.96      | 123.70   |
| 35  | BB    | 1714 | U    | C5-C6-N1   | -9.67 | 117.86      | 122.70   |
| 35  | BB    | 20   | C    | O4'-C1'-N1 | 9.67  | 115.94      | 108.20   |
| 35  | BB    | 409  | G    | O4'-C1'-N9 | 9.67  | 115.94      | 108.20   |
| 35  | BB    | 2564 | A    | C8-N9-C4   | -9.67 | 101.93      | 105.80   |
| 1   | AA    | 771  | G    | C6-N1-C2   | -9.67 | 119.30      | 125.10   |
| 1   | AA    | 940  | C    | N3-C4-C5   | -9.67 | 118.03      | 121.90   |
| 35  | BB    | 1355 | G    | N1-C6-O6   | 9.67  | 125.70      | 119.90   |
| 35  | BB    | 1635 | A    | N9-C4-C5   | 9.67  | 109.67      | 105.80   |
| 1   | AA    | 192  | A    | C5-C6-N6   | -9.67 | 115.97      | 123.70   |
| 35  | BB    | 184  | C    | N3-C4-N4   | 9.67  | 124.77      | 118.00   |
| 35  | BB    | 1253 | A    | N7-C8-N9   | -9.67 | 108.97      | 113.80   |
| 35  | BB    | 1686 | C    | N3-C4-C5   | -9.67 | 118.03      | 121.90   |
| 35  | BB    | 2627 | G    | O4'-C1'-N9 | 9.67  | 115.93      | 108.20   |
| 1   | AA    | 863  | U    | C5-C6-N1   | 9.66  | 127.53      | 122.70   |
| 16  | AP    | 56   | ARG  | NE-CZ-NH1  | 9.66  | 125.13      | 120.30   |
| 35  | BB    | 2050 | C    | N3-C4-C5   | -9.66 | 118.03      | 121.90   |
| 35  | BB    | 2753 | A    | C4-C5-C6   | 9.66  | 121.83      | 117.00   |
| 35  | BB    | 2835 | A    | C5-N7-C8   | 9.66  | 108.73      | 103.90   |
| 35  | BB    | 758  | C    | O4'-C1'-N1 | 9.66  | 115.93      | 108.20   |
| 35  | BB    | 1115 | G    | C5-C6-N1   | -9.66 | 106.67      | 111.50   |
| 35  | BB    | 1503 | A    | C5-N7-C8   | 9.66  | 108.73      | 103.90   |
| 35  | BB    | 1516 | G    | C6-C5-N7   | -9.66 | 124.60      | 130.40   |
| 35  | BB    | 2459 | A    | C5-C6-N6   | -9.66 | 115.97      | 123.70   |
| 35  | BB    | 2682 | A    | C5-C6-N6   | -9.66 | 115.97      | 123.70   |
| 1   | AA    | 1289 | A    | C4-C5-C6   | 9.66  | 121.83      | 117.00   |
| 34  | BA    | 26   | C    | N3-C4-N4   | 9.66  | 124.76      | 118.00   |
| 1   | AA    | 366  | A    | C4-C5-C6   | 9.66  | 121.83      | 117.00   |
| 35  | BB    | 255  | A    | N1-C6-N6   | 9.66  | 124.39      | 118.60   |
| 34  | BA    | 109  | A    | N9-C4-C5   | -9.66 | 101.94      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 105  | G    | N3-C2-N2   | 9.65  | 126.66      | 119.90   |
| 1   | AA    | 1251 | A    | C6-C5-N7   | -9.65 | 125.54      | 132.30   |
| 1   | AA    | 1373 | G    | N3-C2-N2   | 9.65  | 126.66      | 119.90   |
| 35  | BB    | 217  | A    | N1-C2-N3   | -9.65 | 124.47      | 129.30   |
| 35  | BB    | 1059 | G    | O4'-C1'-N9 | 9.65  | 115.92      | 108.20   |
| 35  | BB    | 2856 | A    | N9-C4-C5   | -9.65 | 101.94      | 105.80   |
| 35  | BB    | 2120 | G    | N3-C2-N2   | 9.65  | 126.66      | 119.90   |
| 1   | AA    | 805  | C    | O4'-C1'-N1 | 9.65  | 115.92      | 108.20   |
| 1   | AA    | 1153 | G    | N1-C6-O6   | 9.65  | 125.69      | 119.90   |
| 35  | BB    | 392  | U    | C6-N1-C2   | -9.65 | 115.21      | 121.00   |
| 1   | AA    | 484  | G    | C5-C6-O6   | -9.65 | 122.81      | 128.60   |
| 35  | BB    | 1598 | A    | C8-N9-C4   | -9.65 | 101.94      | 105.80   |
| 34  | BA    | 30   | C    | N3-C4-C5   | -9.65 | 118.04      | 121.90   |
| 35  | BB    | 1693 | U    | N3-C4-O4   | 9.65  | 126.15      | 119.40   |
| 1   | AA    | 51   | A    | C2-N3-C4   | 9.65  | 115.42      | 110.60   |
| 1   | AA    | 1516 | G    | N7-C8-N9   | -9.65 | 108.28      | 113.10   |
| 35  | BB    | 951  | C    | C5-C4-N4   | -9.65 | 113.45      | 120.20   |
| 35  | BB    | 1000 | A    | O4'-C1'-N9 | 9.65  | 115.92      | 108.20   |
| 35  | BB    | 1088 | A    | C5-C6-N6   | -9.65 | 115.98      | 123.70   |
| 1   | AA    | 1454 | G    | C2-N3-C4   | 9.64  | 116.72      | 111.90   |
| 34  | BA    | 107  | G    | C4-C5-N7   | 9.64  | 114.66      | 110.80   |
| 35  | BB    | 1683 | U    | O4'-C1'-N1 | 9.64  | 115.92      | 108.20   |
| 1   | AA    | 896  | C    | N3-C4-N4   | 9.64  | 124.75      | 118.00   |
| 1   | AA    | 1169 | A    | O4'-C1'-N9 | 9.64  | 115.91      | 108.20   |
| 35  | BB    | 533  | G    | N1-C2-N3   | -9.64 | 118.12      | 123.90   |
| 35  | BB    | 1329 | U    | N3-C4-O4   | 9.64  | 126.15      | 119.40   |
| 35  | BB    | 1333 | G    | C6-C5-N7   | -9.64 | 124.61      | 130.40   |
| 35  | BB    | 2053 | G    | C8-N9-C4   | 9.64  | 110.26      | 106.40   |
| 35  | BB    | 2424 | C    | C4-C5-C6   | 9.64  | 122.22      | 117.40   |
| 1   | AA    | 102  | G    | N1-C6-O6   | 9.64  | 125.68      | 119.90   |
| 1   | AA    | 505  | G    | C6-C5-N7   | -9.64 | 124.62      | 130.40   |
| 1   | AA    | 784  | A    | O4'-C1'-N9 | 9.64  | 115.91      | 108.20   |
| 35  | BB    | 993  | G    | C8-N9-C4   | -9.64 | 102.55      | 106.40   |
| 1   | AA    | 657  | U    | N3-C2-O2   | 9.64  | 128.95      | 122.20   |
| 1   | AA    | 924  | C    | N3-C4-C5   | -9.64 | 118.05      | 121.90   |
| 1   | AA    | 1012 | A    | N1-C2-N3   | 9.64  | 134.12      | 129.30   |
| 34  | BA    | 19   | C    | C4-C5-C6   | 9.64  | 122.22      | 117.40   |
| 34  | BA    | 53   | A    | C4-C5-C6   | 9.64  | 121.82      | 117.00   |
| 34  | BA    | 76   | G    | C5-C6-O6   | -9.64 | 122.82      | 128.60   |
| 1   | AA    | 1191 | A    | C8-N9-C4   | -9.64 | 101.94      | 105.80   |
| 1   | AA    | 1520 | C    | C4-C5-C6   | 9.64  | 122.22      | 117.40   |
| 35  | BB    | 1376 | C    | N3-C4-C5   | -9.63 | 118.05      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2465 | C    | O4'-C1'-N1  | 9.63  | 115.91      | 108.20   |
| 1   | AA    | 647  | C    | C6-N1-C2    | 9.63  | 124.15      | 120.30   |
| 1   | AA    | 684  | U    | C5-C6-N1    | 9.63  | 127.52      | 122.70   |
| 35  | BB    | 692  | C    | O4'-C1'-N1  | 9.63  | 115.90      | 108.20   |
| 35  | BB    | 1566 | A    | C5-C6-N6    | -9.63 | 116.00      | 123.70   |
| 1   | AA    | 1147 | C    | O4'-C1'-N1  | 9.63  | 115.90      | 108.20   |
| 1   | AA    | 300  | A    | N1-C6-N6    | 9.63  | 124.38      | 118.60   |
| 1   | AA    | 1257 | A    | C5-C6-N6    | -9.63 | 116.00      | 123.70   |
| 34  | BA    | 75   | G    | N7-C8-N9    | -9.63 | 108.29      | 113.10   |
| 35  | BB    | 260  | G    | O4'-C1'-N9  | 9.63  | 115.90      | 108.20   |
| 35  | BB    | 945  | A    | N7-C8-N9    | -9.63 | 108.99      | 113.80   |
| 35  | BB    | 1054 | A    | C4-C5-N7    | -9.63 | 105.89      | 110.70   |
| 35  | BB    | 57   | C    | C3'-C2'-C1' | 9.62  | 109.20      | 101.50   |
| 35  | BB    | 256  | A    | O4'-C1'-N9  | 9.62  | 115.90      | 108.20   |
| 35  | BB    | 717  | C    | C6-N1-C2    | 9.62  | 124.15      | 120.30   |
| 35  | BB    | 1558 | C    | N3-C4-N4    | 9.62  | 124.74      | 118.00   |
| 1   | AA    | 81   | A    | C5-C6-N6    | -9.62 | 116.00      | 123.70   |
| 35  | BB    | 326  | G    | C5-C6-N1    | -9.62 | 106.69      | 111.50   |
| 35  | BB    | 1071 | G    | C6-C5-N7    | -9.62 | 124.63      | 130.40   |
| 35  | BB    | 2337 | G    | C8-N9-C4    | -9.62 | 102.55      | 106.40   |
| 35  | BB    | 2524 | G    | N7-C8-N9    | 9.62  | 117.91      | 113.10   |
| 1   | AA    | 999  | C    | O4'-C1'-N1  | 9.62  | 115.89      | 108.20   |
| 30  | B5    | 51   | ASP  | CB-CG-OD1   | 9.62  | 126.96      | 118.30   |
| 35  | BB    | 1396 | U    | O4'-C1'-N1  | 9.62  | 115.90      | 108.20   |
| 35  | BB    | 2436 | G    | N1-C6-O6    | 9.62  | 125.67      | 119.90   |
| 35  | BB    | 297  | G    | N1-C6-O6    | 9.62  | 125.67      | 119.90   |
| 35  | BB    | 2570 | G    | C4-C5-N7    | -9.62 | 106.95      | 110.80   |
| 35  | BB    | 1439 | A    | N7-C8-N9    | -9.62 | 108.99      | 113.80   |
| 35  | BB    | 2360 | G    | C5-N7-C8    | 9.62  | 109.11      | 104.30   |
| 35  | BB    | 2843 | G    | N1-C2-N3    | -9.62 | 118.13      | 123.90   |
| 1   | AA    | 24   | U    | C2-N3-C4    | -9.62 | 121.23      | 127.00   |
| 35  | BB    | 1734 | G    | N1-C2-N3    | -9.61 | 118.13      | 123.90   |
| 35  | BB    | 2327 | A    | O4'-C1'-N9  | 9.62  | 115.89      | 108.20   |
| 35  | BB    | 494  | G    | C8-N9-C4    | -9.61 | 102.56      | 106.40   |
| 35  | BB    | 2289 | G    | C2-N3-C4    | -9.61 | 107.09      | 111.90   |
| 46  | BM    | 18   | ARG  | NE-CZ-NH1   | -9.61 | 115.50      | 120.30   |
| 1   | AA    | 1055 | A    | C5-C6-N1    | -9.61 | 112.90      | 117.70   |
| 35  | BB    | 2148 | G    | N1-C2-N3    | -9.61 | 118.14      | 123.90   |
| 1   | AA    | 341  | C    | O4'-C1'-N1  | 9.61  | 115.89      | 108.20   |
| 1   | AA    | 1360 | A    | C5-C6-N1    | -9.61 | 112.90      | 117.70   |
| 35  | BB    | 678  | C    | C4-C5-C6    | 9.61  | 122.20      | 117.40   |
| 1   | AA    | 402  | G    | N3-C4-C5    | -9.60 | 123.80      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1475 | G    | C5-C6-O6    | -9.60 | 122.84      | 128.60   |
| 35  | BB    | 1359 | A    | N1-C6-N6    | 9.60  | 124.36      | 118.60   |
| 35  | BB    | 1840 | G    | N1-C2-N3    | -9.60 | 118.14      | 123.90   |
| 1   | AA    | 29   | U    | C3'-C2'-C1' | 9.60  | 109.18      | 101.50   |
| 1   | AA    | 625  | U    | N1-C2-O2    | -9.60 | 116.08      | 122.80   |
| 35  | BB    | 218  | A    | C5-C6-N6    | -9.60 | 116.02      | 123.70   |
| 35  | BB    | 590  | A    | N1-C6-N6    | 9.60  | 124.36      | 118.60   |
| 35  | BB    | 680  | C    | C6-N1-C2    | -9.60 | 116.46      | 120.30   |
| 35  | BB    | 2180 | U    | C5-C4-O4    | -9.60 | 120.14      | 125.90   |
| 1   | AA    | 1028 | C    | C5-C6-N1    | 9.60  | 125.80      | 121.00   |
| 1   | AA    | 1534 | A    | C5-C6-N1    | -9.60 | 112.90      | 117.70   |
| 35  | BB    | 252  | G    | O4'-C1'-N9  | 9.60  | 115.88      | 108.20   |
| 1   | AA    | 760  | G    | O4'-C1'-N9  | 9.60  | 115.88      | 108.20   |
| 1   | AA    | 922  | G    | N1-C6-O6    | 9.60  | 125.66      | 119.90   |
| 35  | BB    | 638  | G    | C6-C5-N7    | -9.60 | 124.64      | 130.40   |
| 35  | BB    | 2550 | G    | N3-C4-N9    | 9.60  | 131.76      | 126.00   |
| 35  | BB    | 458  | G    | C4-C5-C6    | 9.59  | 124.56      | 118.80   |
| 35  | BB    | 2639 | A    | C5-C6-N6    | -9.59 | 116.02      | 123.70   |
| 1   | AA    | 231  | U    | O4'-C1'-N1  | 9.59  | 115.87      | 108.20   |
| 1   | AA    | 334  | C    | O4'-C1'-N1  | 9.59  | 115.87      | 108.20   |
| 1   | AA    | 759  | A    | C8-N9-C4    | -9.59 | 101.96      | 105.80   |
| 1   | AA    | 947  | G    | N3-C2-N2    | 9.59  | 126.61      | 119.90   |
| 35  | BB    | 116  | C    | N3-C4-N4    | 9.59  | 124.71      | 118.00   |
| 1   | AA    | 1034 | G    | O4'-C1'-N9  | 9.59  | 115.87      | 108.20   |
| 1   | AA    | 1299 | A    | C5-C6-N1    | -9.59 | 112.91      | 117.70   |
| 35  | BB    | 75   | G    | C4-C5-N7    | -9.59 | 106.97      | 110.80   |
| 35  | BB    | 643  | A    | C4-C5-C6    | 9.59  | 121.80      | 117.00   |
| 35  | BB    | 656  | G    | N9-C4-C5    | 9.59  | 109.24      | 105.40   |
| 35  | BB    | 2679 | A    | O4'-C1'-N9  | 9.59  | 115.87      | 108.20   |
| 1   | AA    | 217  | C    | N3-C4-N4    | 9.59  | 124.71      | 118.00   |
| 1   | AA    | 592  | G    | N9-C4-C5    | 9.59  | 109.23      | 105.40   |
| 35  | BB    | 1047 | G    | N1-C2-N3    | -9.59 | 118.15      | 123.90   |
| 35  | BB    | 273  | G    | C8-N9-C4    | -9.59 | 102.57      | 106.40   |
| 35  | BB    | 1772 | A    | C5-C6-N6    | -9.59 | 116.03      | 123.70   |
| 35  | BB    | 2020 | A    | C5-C6-N6    | -9.59 | 116.03      | 123.70   |
| 35  | BB    | 1888 | G    | C5-N7-C8    | 9.59  | 109.09      | 104.30   |
| 35  | BB    | 2712 | C    | N1-C2-O2    | 9.59  | 124.65      | 118.90   |
| 1   | AA    | 1225 | A    | C1'-O4'-C4' | 9.58  | 117.57      | 109.90   |
| 35  | BB    | 48   | G    | N1-C2-N3    | -9.58 | 118.15      | 123.90   |
| 35  | BB    | 763  | G    | C4-C5-N7    | -9.58 | 106.97      | 110.80   |
| 35  | BB    | 1194 | A    | N1-C6-N6    | 9.58  | 124.35      | 118.60   |
| 35  | BB    | 1420 | A    | C6-C5-N7    | -9.58 | 125.59      | 132.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1823 | G    | C6-N1-C2   | 9.58  | 130.85      | 125.10   |
| 35  | BB    | 1978 | A    | C5-C6-N6   | -9.58 | 116.03      | 123.70   |
| 35  | BB    | 1982 | U    | C5-C4-O4   | -9.58 | 120.15      | 125.90   |
| 27  | B2    | 44   | ARG  | NE-CZ-NH1  | -9.58 | 115.51      | 120.30   |
| 35  | BB    | 1823 | G    | O4'-C1'-N9 | 9.58  | 115.86      | 108.20   |
| 35  | BB    | 2638 | G    | N1-C6-O6   | 9.58  | 125.65      | 119.90   |
| 1   | AA    | 459  | A    | C5-C6-N1   | -9.58 | 112.91      | 117.70   |
| 1   | AA    | 1480 | A    | C5-C6-N6   | -9.58 | 116.04      | 123.70   |
| 35  | BB    | 827  | U    | O4'-C1'-N1 | 9.58  | 115.86      | 108.20   |
| 35  | BB    | 989  | G    | C8-N9-C4   | -9.58 | 102.57      | 106.40   |
| 35  | BB    | 1365 | A    | N1-C6-N6   | 9.58  | 124.35      | 118.60   |
| 35  | BB    | 1822 | C    | P-O3'-C3'  | -9.58 | 108.21      | 119.70   |
| 35  | BB    | 2135 | A    | O4'-C1'-N9 | 9.58  | 115.86      | 108.20   |
| 35  | BB    | 2749 | A    | O4'-C1'-N9 | 9.58  | 115.86      | 108.20   |
| 1   | AA    | 31   | G    | C6-C5-N7   | -9.58 | 124.65      | 130.40   |
| 35  | BB    | 699  | A    | N1-C6-N6   | 9.58  | 124.35      | 118.60   |
| 1   | AA    | 1032 | G    | N3-C2-N2   | 9.58  | 126.60      | 119.90   |
| 1   | AA    | 1036 | A    | C5-C6-N6   | -9.58 | 116.04      | 123.70   |
| 35  | BB    | 91   | A    | C2-N3-C4   | 9.58  | 115.39      | 110.60   |
| 35  | BB    | 411  | G    | N9-C4-C5   | 9.58  | 109.23      | 105.40   |
| 35  | BB    | 674  | G    | N1-C6-O6   | 9.58  | 125.65      | 119.90   |
| 35  | BB    | 770  | G    | O4'-C1'-N9 | 9.58  | 115.86      | 108.20   |
| 35  | BB    | 1912 | A    | C5-C6-N1   | -9.58 | 112.91      | 117.70   |
| 35  | BB    | 2014 | A    | C4-C5-C6   | 9.58  | 121.79      | 117.00   |
| 1   | AA    | 124  | C    | O4'-C1'-N1 | 9.57  | 115.86      | 108.20   |
| 1   | AA    | 1478 | U    | O4'-C1'-N1 | 9.57  | 115.86      | 108.20   |
| 35  | BB    | 79   | C    | N3-C4-C5   | -9.57 | 118.07      | 121.90   |
| 35  | BB    | 1634 | A    | C5-C6-N6   | -9.57 | 116.04      | 123.70   |
| 35  | BB    | 1507 | C    | C6-N1-C2   | -9.57 | 116.47      | 120.30   |
| 35  | BB    | 1984 | G    | N9-C4-C5   | -9.57 | 101.57      | 105.40   |
| 35  | BB    | 2476 | A    | C6-C5-N7   | -9.57 | 125.60      | 132.30   |
| 35  | BB    | 2565 | A    | N1-C6-N6   | 9.57  | 124.34      | 118.60   |
| 1   | AA    | 602  | A    | C8-N9-C4   | -9.57 | 101.97      | 105.80   |
| 1   | AA    | 946  | A    | C5-C6-N6   | -9.57 | 116.04      | 123.70   |
| 35  | BB    | 475  | C    | C2-N3-C4   | 9.57  | 124.69      | 119.90   |
| 35  | BB    | 911  | A    | C4-C5-C6   | 9.57  | 121.78      | 117.00   |
| 35  | BB    | 943  | A    | C6-C5-N7   | -9.57 | 125.60      | 132.30   |
| 1   | AA    | 752  | G    | C2-N3-C4   | 9.57  | 116.68      | 111.90   |
| 1   | AA    | 1503 | A    | N1-C6-N6   | 9.57  | 124.34      | 118.60   |
| 35  | BB    | 1913 | A    | C4-C5-C6   | 9.57  | 121.78      | 117.00   |
| 1   | AA    | 243  | A    | C4-C5-C6   | 9.57  | 121.78      | 117.00   |
| 1   | AA    | 362  | G    | N1-C6-O6   | 9.57  | 125.64      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 116  | C    | N3-C4-C5    | -9.57 | 118.07      | 121.90   |
| 35  | BB    | 1240 | U    | N1-C2-N3    | -9.57 | 109.16      | 114.90   |
| 35  | BB    | 2830 | C    | C6-N1-C2    | -9.57 | 116.47      | 120.30   |
| 35  | BB    | 2076 | U    | O4'-C4'-C3' | -9.57 | 94.43       | 104.00   |
| 35  | BB    | 2332 | C    | C6-N1-C2    | -9.57 | 116.47      | 120.30   |
| 35  | BB    | 2737 | G    | N1-C6-O6    | 9.57  | 125.64      | 119.90   |
| 1   | AA    | 429  | U    | N3-C4-O4    | 9.56  | 126.09      | 119.40   |
| 35  | BB    | 1755 | A    | N1-C6-N6    | 9.56  | 124.34      | 118.60   |
| 1   | AA    | 447  | G    | N1-C6-O6    | 9.56  | 125.64      | 119.90   |
| 1   | AA    | 796  | C    | N3-C4-N4    | 9.56  | 124.69      | 118.00   |
| 1   | AA    | 1329 | A    | C2-N3-C4    | 9.56  | 115.38      | 110.60   |
| 34  | BA    | 44   | G    | N1-C6-O6    | 9.56  | 125.64      | 119.90   |
| 35  | BB    | 543  | G    | N1-C6-O6    | 9.56  | 125.64      | 119.90   |
| 35  | BB    | 2777 | G    | C8-N9-C4    | 9.56  | 110.23      | 106.40   |
| 1   | AA    | 335  | C    | C5-C6-N1    | 9.56  | 125.78      | 121.00   |
| 35  | BB    | 1087 | G    | N1-C6-O6    | 9.56  | 125.64      | 119.90   |
| 35  | BB    | 2470 | G    | N1-C6-O6    | 9.56  | 125.64      | 119.90   |
| 35  | BB    | 2773 | C    | N3-C4-C5    | -9.56 | 118.08      | 121.90   |
| 35  | BB    | 161  | A    | N9-C4-C5    | 9.56  | 109.62      | 105.80   |
| 35  | BB    | 802  | A    | C8-N9-C4    | -9.56 | 101.98      | 105.80   |
| 35  | BB    | 2463 | C    | C5-C4-N4    | -9.56 | 113.51      | 120.20   |
| 1   | AA    | 57   | G    | C2-N3-C4    | 9.56  | 116.68      | 111.90   |
| 1   | AA    | 315  | A    | P-O3'-C3'   | 9.56  | 131.17      | 119.70   |
| 1   | AA    | 1261 | A    | C5-C6-N6    | -9.56 | 116.05      | 123.70   |
| 1   | AA    | 1365 | G    | N1-C2-N3    | -9.56 | 118.16      | 123.90   |
| 35  | BB    | 110  | G    | O4'-C1'-N9  | 9.56  | 115.85      | 108.20   |
| 35  | BB    | 656  | G    | C6-C5-N7    | -9.56 | 124.66      | 130.40   |
| 1   | AA    | 331  | G    | N1-C6-O6    | 9.56  | 125.63      | 119.90   |
| 35  | BB    | 245  | G    | N9-C4-C5    | 9.56  | 109.22      | 105.40   |
| 35  | BB    | 901  | C    | O4'-C1'-N1  | 9.56  | 115.85      | 108.20   |
| 35  | BB    | 1432 | G    | N9-C4-C5    | -9.56 | 101.58      | 105.40   |
| 1   | AA    | 1236 | A    | C5-C6-N1    | -9.55 | 112.92      | 117.70   |
| 35  | BB    | 1271 | G    | N1-C6-O6    | 9.56  | 125.63      | 119.90   |
| 35  | BB    | 1532 | A    | N3-C4-C5    | -9.56 | 120.11      | 126.80   |
| 35  | BB    | 173  | A    | N7-C8-N9    | -9.55 | 109.02      | 113.80   |
| 35  | BB    | 1694 | C    | N3-C4-N4    | 9.55  | 124.69      | 118.00   |
| 35  | BB    | 2261 | C    | C6-N1-C2    | -9.55 | 116.48      | 120.30   |
| 35  | BB    | 2481 | G    | N3-C2-N2    | 9.55  | 126.59      | 119.90   |
| 35  | BB    | 2729 | G    | C6-C5-N7    | -9.55 | 124.67      | 130.40   |
| 1   | AA    | 151  | A    | N1-C6-N6    | 9.55  | 124.33      | 118.60   |
| 1   | AA    | 356  | A    | O4'-C1'-N9  | 9.55  | 115.84      | 108.20   |
| 1   | AA    | 758  | C    | C5-C4-N4    | -9.55 | 113.51      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 809  | G    | C4-C5-C6   | 9.55  | 124.53      | 118.80   |
| 1   | AA    | 1385 | G    | O4'-C1'-N9 | 9.55  | 115.84      | 108.20   |
| 35  | BB    | 1364 | G    | N3-C4-C5   | 9.55  | 133.37      | 128.60   |
| 35  | BB    | 1899 | A    | C6-N1-C2   | -9.55 | 112.87      | 118.60   |
| 35  | BB    | 1930 | G    | N1-C2-N3   | -9.55 | 118.17      | 123.90   |
| 35  | BB    | 2199 | A    | C5-C6-N1   | -9.55 | 112.93      | 117.70   |
| 35  | BB    | 2706 | A    | C4-C5-C6   | 9.55  | 121.77      | 117.00   |
| 1   | AA    | 449  | G    | N1-C6-O6   | 9.54  | 125.63      | 119.90   |
| 35  | BB    | 417  | C    | C2-N3-C4   | 9.54  | 124.67      | 119.90   |
| 35  | BB    | 2341 | G    | N1-C2-N3   | -9.54 | 118.17      | 123.90   |
| 35  | BB    | 2573 | C    | N3-C4-C5   | -9.55 | 118.08      | 121.90   |
| 1   | AA    | 158  | G    | N9-C4-C5   | 9.54  | 109.22      | 105.40   |
| 3   | AC    | 35   | ASP  | CB-CG-OD1  | 9.54  | 126.89      | 118.30   |
| 34  | BA    | 31   | C    | O4'-C1'-N1 | 9.54  | 115.83      | 108.20   |
| 40  | BG    | 169  | ARG  | NE-CZ-NH1  | -9.54 | 115.53      | 120.30   |
| 35  | BB    | 252  | G    | N1-C6-O6   | 9.54  | 125.62      | 119.90   |
| 35  | BB    | 733  | G    | C5-N7-C8   | 9.54  | 109.07      | 104.30   |
| 35  | BB    | 2535 | G    | N9-C4-C5   | -9.54 | 101.58      | 105.40   |
| 56  | BY    | 10   | ARG  | NE-CZ-NH1  | 9.54  | 125.07      | 120.30   |
| 35  | BB    | 184  | C    | C5-C4-N4   | -9.54 | 113.52      | 120.20   |
| 1   | AA    | 219  | U    | O4'-C1'-N1 | 9.54  | 115.83      | 108.20   |
| 1   | AA    | 553  | A    | N1-C2-N3   | 9.54  | 134.07      | 129.30   |
| 1   | AA    | 1139 | G    | C5-C6-O6   | -9.54 | 122.88      | 128.60   |
| 35  | BB    | 901  | C    | P-O5'-C5'  | 9.54  | 136.16      | 120.90   |
| 1   | AA    | 1488 | G    | C4-C5-N7   | -9.54 | 106.98      | 110.80   |
| 35  | BB    | 371  | A    | C2-N3-C4   | -9.54 | 105.83      | 110.60   |
| 35  | BB    | 1576 | U    | O4'-C1'-N1 | 9.54  | 115.83      | 108.20   |
| 1   | AA    | 115  | G    | C6-C5-N7   | -9.53 | 124.68      | 130.40   |
| 1   | AA    | 682  | G    | C6-C5-N7   | -9.54 | 124.68      | 130.40   |
| 1   | AA    | 700  | G    | N1-C6-O6   | 9.53  | 125.62      | 119.90   |
| 1   | AA    | 1304 | G    | N7-C8-N9   | 9.53  | 117.87      | 113.10   |
| 2   | AB    | 21   | TYR  | CB-CG-CD1  | -9.53 | 115.28      | 121.00   |
| 19  | AS    | 35   | ARG  | NE-CZ-NH1  | 9.54  | 125.07      | 120.30   |
| 34  | BA    | 110  | C    | N3-C4-C5   | -9.54 | 118.09      | 121.90   |
| 35  | BB    | 649  | G    | O4'-C1'-N9 | 9.53  | 115.83      | 108.20   |
| 35  | BB    | 739  | A    | C5-C6-N1   | -9.53 | 112.93      | 117.70   |
| 1   | AA    | 23   | C    | O4'-C1'-N1 | 9.53  | 115.83      | 108.20   |
| 1   | AA    | 179  | A    | C5-C6-N6   | -9.53 | 116.08      | 123.70   |
| 1   | AA    | 1357 | A    | C5-C6-N6   | -9.53 | 116.07      | 123.70   |
| 35  | BB    | 870  | U    | N1-C2-N3   | -9.53 | 109.18      | 114.90   |
| 35  | BB    | 1951 | U    | C5-C6-N1   | -9.53 | 117.93      | 122.70   |
| 35  | BB    | 2736 | A    | C5-C6-N1   | -9.53 | 112.93      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 491  | G    | O4'-C1'-N9  | 9.53  | 115.82      | 108.20   |
| 35  | BB    | 2710 | C    | O4'-C1'-N1  | 9.53  | 115.82      | 108.20   |
| 1   | AA    | 1014 | A    | N1-C6-N6    | 9.53  | 124.32      | 118.60   |
| 1   | AA    | 1217 | C    | O4'-C1'-N1  | 9.53  | 115.82      | 108.20   |
| 35  | BB    | 1672 | A    | C8-N9-C4    | -9.53 | 101.99      | 105.80   |
| 35  | BB    | 1802 | A    | N1-C6-N6    | 9.53  | 124.32      | 118.60   |
| 1   | AA    | 1327 | C    | C5-C6-N1    | 9.53  | 125.76      | 121.00   |
| 35  | BB    | 275  | C    | N3-C4-C5    | -9.53 | 118.09      | 121.90   |
| 35  | BB    | 805  | G    | C4-C5-C6    | 9.53  | 124.52      | 118.80   |
| 35  | BB    | 2142 | A    | N1-C6-N6    | 9.53  | 124.32      | 118.60   |
| 35  | BB    | 2069 | G    | C8-N9-C4    | 9.53  | 110.21      | 106.40   |
| 35  | BB    | 2674 | G    | N1-C6-O6    | 9.53  | 125.61      | 119.90   |
| 35  | BB    | 2719 | G    | C6-C5-N7    | -9.53 | 124.68      | 130.40   |
| 34  | BA    | 41   | G    | C5-C6-O6    | -9.52 | 122.89      | 128.60   |
| 35  | BB    | 1126 | A    | C5-N7-C8    | 9.52  | 108.66      | 103.90   |
| 37  | BD    | 82   | PHE  | CB-CG-CD1   | 9.52  | 127.47      | 120.80   |
| 1   | AA    | 668  | G    | N1-C6-O6    | 9.52  | 125.61      | 119.90   |
| 35  | BB    | 842  | U    | O4'-C1'-N1  | 9.52  | 115.82      | 108.20   |
| 35  | BB    | 964  | C    | N3-C4-N4    | 9.52  | 124.67      | 118.00   |
| 35  | BB    | 2072 | C    | N3-C4-C5    | -9.52 | 118.09      | 121.90   |
| 35  | BB    | 1867 | G    | N1-C2-N3    | -9.52 | 118.19      | 123.90   |
| 1   | AA    | 159  | G    | C5-C6-O6    | -9.52 | 122.89      | 128.60   |
| 1   | AA    | 356  | A    | C5-C6-N6    | -9.52 | 116.08      | 123.70   |
| 1   | AA    | 1323 | G    | C2-N3-C4    | -9.52 | 107.14      | 111.90   |
| 35  | BB    | 13   | A    | C1'-O4'-C4' | 9.52  | 117.51      | 109.90   |
| 1   | AA    | 299  | G    | O4'-C1'-N9  | 9.51  | 115.81      | 108.20   |
| 35  | BB    | 230  | G    | C6-C5-N7    | -9.51 | 124.69      | 130.40   |
| 35  | BB    | 1776 | G    | N1-C6-O6    | 9.51  | 125.61      | 119.90   |
| 35  | BB    | 2592 | G    | C5-C6-O6    | -9.51 | 122.89      | 128.60   |
| 35  | BB    | 2759 | G    | N9-C4-C5    | -9.51 | 101.59      | 105.40   |
| 35  | BB    | 2843 | G    | C5-C6-O6    | -9.51 | 122.89      | 128.60   |
| 1   | AA    | 1333 | A    | C5-C6-N6    | -9.51 | 116.09      | 123.70   |
| 34  | BA    | 97   | C    | C5-C4-N4    | -9.51 | 113.54      | 120.20   |
| 35  | BB    | 3    | U    | C5-C4-O4    | -9.51 | 120.19      | 125.90   |
| 35  | BB    | 487  | C    | N3-C4-N4    | 9.51  | 124.66      | 118.00   |
| 35  | BB    | 528  | A    | O4'-C1'-N9  | 9.51  | 115.81      | 108.20   |
| 35  | BB    | 547  | A    | C4-C5-C6    | 9.51  | 121.75      | 117.00   |
| 35  | BB    | 663  | G    | C8-N9-C4    | -9.51 | 102.60      | 106.40   |
| 35  | BB    | 932  | U    | O4'-C1'-N1  | 9.51  | 115.81      | 108.20   |
| 35  | BB    | 945  | A    | C5-N7-C8    | 9.51  | 108.65      | 103.90   |
| 35  | BB    | 2712 | C    | N3-C4-C5    | -9.51 | 118.10      | 121.90   |
| 35  | BB    | 2801 | G    | C2-N3-C4    | 9.51  | 116.65      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 546  | A    | N1-C6-N6   | 9.51  | 124.31      | 118.60   |
| 34  | BA    | 15   | A    | C6-C5-N7   | -9.51 | 125.64      | 132.30   |
| 35  | BB    | 683  | U    | N1-C2-O2   | -9.51 | 116.14      | 122.80   |
| 35  | BB    | 2468 | A    | N9-C4-C5   | 9.51  | 109.60      | 105.80   |
| 35  | BB    | 458  | G    | N1-C6-O6   | 9.51  | 125.60      | 119.90   |
| 35  | BB    | 1774 | C    | O4'-C1'-N1 | 9.51  | 115.81      | 108.20   |
| 35  | BB    | 1939 | U    | C5-C4-O4   | -9.51 | 120.20      | 125.90   |
| 1   | AA    | 187  | G    | C5-C6-O6   | -9.50 | 122.90      | 128.60   |
| 1   | AA    | 847  | G    | C5-C6-O6   | -9.50 | 122.90      | 128.60   |
| 1   | AA    | 50   | A    | N1-C2-N3   | -9.50 | 124.55      | 129.30   |
| 1   | AA    | 676  | A    | C4-C5-C6   | 9.50  | 121.75      | 117.00   |
| 1   | AA    | 799  | G    | N3-C2-N2   | 9.50  | 126.55      | 119.90   |
| 35  | BB    | 1426 | G    | C6-C5-N7   | -9.50 | 124.70      | 130.40   |
| 35  | BB    | 1713 | A    | C5-C6-N6   | -9.50 | 116.10      | 123.70   |
| 35  | BB    | 2445 | G    | C5-C6-O6   | -9.50 | 122.90      | 128.60   |
| 1   | AA    | 1250 | A    | O4'-C1'-N9 | 9.50  | 115.80      | 108.20   |
| 1   | AA    | 1516 | G    | O4'-C1'-N9 | 9.50  | 115.80      | 108.20   |
| 35  | BB    | 1230 | A    | C5-C6-N1   | -9.50 | 112.95      | 117.70   |
| 35  | BB    | 2273 | A    | N1-C6-N6   | 9.50  | 124.30      | 118.60   |
| 34  | BA    | 8    | C    | O4'-C1'-N1 | 9.50  | 115.80      | 108.20   |
| 53  | BT    | 79   | ASP  | CB-CG-OD1  | 9.50  | 126.85      | 118.30   |
| 35  | BB    | 862  | G    | C8-N9-C4   | -9.50 | 102.60      | 106.40   |
| 35  | BB    | 1779 | U    | C5-C6-N1   | 9.50  | 127.45      | 122.70   |
| 35  | BB    | 2458 | G    | C5-C6-O6   | -9.50 | 122.90      | 128.60   |
| 35  | BB    | 2614 | A    | C6-C5-N7   | -9.50 | 125.65      | 132.30   |
| 35  | BB    | 2222 | C    | N3-C4-N4   | 9.49  | 124.65      | 118.00   |
| 1   | AA    | 668  | G    | C8-N9-C4   | 9.49  | 110.20      | 106.40   |
| 1   | AA    | 893  | C    | N3-C4-N4   | 9.49  | 124.64      | 118.00   |
| 30  | B5    | 43   | ASP  | CB-CG-OD1  | 9.49  | 126.84      | 118.30   |
| 35  | BB    | 156  | A    | C5-C6-N6   | -9.49 | 116.11      | 123.70   |
| 1   | AA    | 724  | G    | N1-C6-O6   | 9.49  | 125.59      | 119.90   |
| 35  | BB    | 19   | A    | N9-C4-C5   | 9.49  | 109.60      | 105.80   |
| 35  | BB    | 1322 | A    | C6-N1-C2   | 9.49  | 124.29      | 118.60   |
| 35  | BB    | 1395 | A    | N1-C6-N6   | 9.49  | 124.29      | 118.60   |
| 35  | BB    | 2655 | G    | N1-C6-O6   | 9.49  | 125.59      | 119.90   |
| 34  | BA    | 99   | A    | C4-C5-C6   | 9.49  | 121.74      | 117.00   |
| 35  | BB    | 413  | C    | N3-C4-N4   | 9.49  | 124.64      | 118.00   |
| 35  | BB    | 1628 | G    | C4-C5-N7   | 9.49  | 114.59      | 110.80   |
| 35  | BB    | 2666 | C    | C2-N1-C1'  | 9.49  | 129.24      | 118.80   |
| 1   | AA    | 975  | A    | C5-C6-N6   | -9.48 | 116.11      | 123.70   |
| 1   | AA    | 927  | G    | C5-C6-N1   | -9.48 | 106.76      | 111.50   |
| 35  | BB    | 877  | A    | C5-C6-N1   | -9.48 | 112.96      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1586 | A    | N1-C6-N6   | 9.48  | 124.29      | 118.60   |
| 35  | BB    | 2894 | G    | C5-C6-O6   | -9.48 | 122.91      | 128.60   |
| 35  | BB    | 72   | U    | N1-C2-O2   | 9.48  | 129.44      | 122.80   |
| 35  | BB    | 1770 | G    | C5-C6-O6   | -9.48 | 122.91      | 128.60   |
| 35  | BB    | 1716 | U    | O4'-C1'-N1 | 9.48  | 115.78      | 108.20   |
| 35  | BB    | 1729 | U    | O4'-C1'-N1 | 9.48  | 115.78      | 108.20   |
| 35  | BB    | 2294 | G    | C5-N7-C8   | 9.48  | 109.04      | 104.30   |
| 1   | AA    | 491  | G    | N7-C8-N9   | 9.48  | 117.84      | 113.10   |
| 1   | AA    | 516  | U    | C5-C4-O4   | 9.48  | 131.59      | 125.90   |
| 1   | AA    | 1253 | G    | N1-C6-O6   | 9.48  | 125.59      | 119.90   |
| 35  | BB    | 67   | U    | O4'-C1'-N1 | 9.48  | 115.78      | 108.20   |
| 35  | BB    | 1529 | G    | N3-C4-C5   | 9.48  | 133.34      | 128.60   |
| 43  | BJ    | 96   | ARG  | NE-CZ-NH2  | 9.48  | 125.04      | 120.30   |
| 23  | AX    | 19   | A    | C5-C6-N1   | -9.48 | 112.96      | 117.70   |
| 34  | BA    | 67   | G    | N7-C8-N9   | 9.48  | 117.84      | 113.10   |
| 35  | BB    | 1059 | G    | C5-C6-O6   | -9.48 | 122.91      | 128.60   |
| 35  | BB    | 1891 | G    | C5-C6-O6   | -9.48 | 122.91      | 128.60   |
| 35  | BB    | 2447 | G    | N3-C4-C5   | 9.48  | 133.34      | 128.60   |
| 35  | BB    | 2475 | C    | P-O3'-C3'  | 9.48  | 131.07      | 119.70   |
| 1   | AA    | 127  | G    | N1-C6-O6   | 9.47  | 125.58      | 119.90   |
| 35  | BB    | 722  | A    | C8-N9-C4   | -9.47 | 102.01      | 105.80   |
| 34  | BA    | 83   | G    | C5-C6-O6   | -9.47 | 122.92      | 128.60   |
| 35  | BB    | 493  | G    | N7-C8-N9   | 9.47  | 117.84      | 113.10   |
| 35  | BB    | 1954 | G    | N3-C2-N2   | 9.47  | 126.53      | 119.90   |
| 35  | BB    | 2176 | A    | N1-C6-N6   | 9.47  | 124.28      | 118.60   |
| 35  | BB    | 1830 | C    | O4'-C1'-N1 | 9.47  | 115.78      | 108.20   |
| 35  | BB    | 2177 | C    | O4'-C1'-N1 | 9.47  | 115.78      | 108.20   |
| 35  | BB    | 2421 | G    | C5-N7-C8   | 9.47  | 109.04      | 104.30   |
| 35  | BB    | 2543 | G    | O4'-C1'-N9 | 9.47  | 115.78      | 108.20   |
| 1   | AA    | 925  | G    | N3-C2-N2   | 9.47  | 126.53      | 119.90   |
| 1   | AA    | 1042 | A    | C2-N3-C4   | -9.47 | 105.86      | 110.60   |
| 35  | BB    | 1287 | A    | C4-C5-N7   | -9.47 | 105.96      | 110.70   |
| 35  | BB    | 878  | A    | C5-C6-N6   | -9.47 | 116.12      | 123.70   |
| 35  | BB    | 2114 | A    | C5-C6-N6   | -9.47 | 116.12      | 123.70   |
| 35  | BB    | 2627 | G    | N3-C4-C5   | -9.47 | 123.86      | 128.60   |
| 1   | AA    | 512  | U    | N3-C4-O4   | 9.47  | 126.03      | 119.40   |
| 22  | AV    | 46   | G    | N1-C6-O6   | 9.47  | 125.58      | 119.90   |
| 35  | BB    | 792  | A    | C4-C5-C6   | 9.47  | 121.73      | 117.00   |
| 35  | BB    | 1877 | A    | N1-C6-N6   | 9.47  | 124.28      | 118.60   |
| 1   | AA    | 1253 | G    | N9-C4-C5   | -9.47 | 101.61      | 105.40   |
| 35  | BB    | 274  | C    | N3-C4-N4   | 9.46  | 124.62      | 118.00   |
| 35  | BB    | 788  | A    | C5-C6-N6   | -9.46 | 116.13      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1459 | G    | P-O3'-C3'  | 9.46  | 131.06      | 119.70   |
| 35  | BB    | 1890 | A    | C5-C6-N1   | -9.46 | 112.97      | 117.70   |
| 1   | AA    | 378  | G    | N1-C2-N3   | -9.46 | 118.22      | 123.90   |
| 35  | BB    | 1257 | C    | C5-C4-N4   | -9.46 | 113.58      | 120.20   |
| 1   | AA    | 417  | G    | O4'-C1'-N9 | 9.46  | 115.77      | 108.20   |
| 1   | AA    | 1280 | A    | C5-C6-N6   | -9.46 | 116.13      | 123.70   |
| 35  | BB    | 1163 | G    | C5-C6-O6   | -9.46 | 122.92      | 128.60   |
| 35  | BB    | 1550 | C    | O4'-C1'-N1 | 9.46  | 115.77      | 108.20   |
| 35  | BB    | 2527 | C    | N3-C4-N4   | 9.46  | 124.62      | 118.00   |
| 35  | BB    | 731  | C    | O4'-C1'-N1 | 9.46  | 115.77      | 108.20   |
| 35  | BB    | 1907 | G    | C8-N9-C4   | -9.46 | 102.62      | 106.40   |
| 35  | BB    | 2335 | A    | C6-N1-C2   | 9.46  | 124.28      | 118.60   |
| 1   | AA    | 780  | A    | C5-C6-N1   | -9.46 | 112.97      | 117.70   |
| 35  | BB    | 475  | C    | N3-C4-C5   | -9.46 | 118.12      | 121.90   |
| 35  | BB    | 733  | G    | N1-C2-N3   | -9.46 | 118.23      | 123.90   |
| 35  | BB    | 1429 | G    | N3-C2-N2   | 9.46  | 126.52      | 119.90   |
| 1   | AA    | 47   | C    | C5-C6-N1   | 9.46  | 125.73      | 121.00   |
| 1   | AA    | 1243 | C    | C6-N1-C2   | 9.46  | 124.08      | 120.30   |
| 1   | AA    | 755  | G    | C8-N9-C4   | -9.45 | 102.62      | 106.40   |
| 1   | AA    | 1055 | A    | C4-C5-C6   | 9.46  | 121.73      | 117.00   |
| 1   | AA    | 1079 | G    | N1-C6-O6   | 9.45  | 125.57      | 119.90   |
| 35  | BB    | 1509 | A    | C5-C6-N6   | -9.45 | 116.14      | 123.70   |
| 35  | BB    | 1757 | A    | C5-C6-N6   | -9.46 | 116.14      | 123.70   |
| 35  | BB    | 2061 | G    | C8-N9-C4   | -9.45 | 102.62      | 106.40   |
| 35  | BB    | 2462 | C    | O4'-C1'-N1 | 9.46  | 115.76      | 108.20   |
| 1   | AA    | 125  | U    | O4'-C1'-N1 | 9.45  | 115.76      | 108.20   |
| 1   | AA    | 1041 | G    | N9-C4-C5   | -9.45 | 101.62      | 105.40   |
| 1   | AA    | 1189 | U    | N3-C2-O2   | 9.45  | 128.82      | 122.20   |
| 1   | AA    | 1307 | U    | C2-N3-C4   | -9.45 | 121.33      | 127.00   |
| 35  | BB    | 1653 | G    | N1-C2-N3   | -9.45 | 118.23      | 123.90   |
| 35  | BB    | 2138 | G    | N1-C6-O6   | 9.45  | 125.57      | 119.90   |
| 1   | AA    | 89   | U    | O4'-C1'-N1 | 9.45  | 115.76      | 108.20   |
| 35  | BB    | 247  | G    | N7-C8-N9   | -9.45 | 108.38      | 113.10   |
| 35  | BB    | 1197 | G    | O4'-C1'-N9 | 9.45  | 115.76      | 108.20   |
| 35  | BB    | 1784 | A    | N9-C4-C5   | -9.45 | 102.02      | 105.80   |
| 35  | BB    | 2399 | G    | N3-C2-N2   | 9.45  | 126.52      | 119.90   |
| 35  | BB    | 2861 | U    | C4-C5-C6   | 9.45  | 125.37      | 119.70   |
| 1   | AA    | 518  | C    | O4'-C1'-N1 | 9.45  | 115.76      | 108.20   |
| 1   | AA    | 577  | G    | N3-C4-N9   | 9.45  | 131.67      | 126.00   |
| 35  | BB    | 16   | C    | O4'-C1'-N1 | 9.45  | 115.76      | 108.20   |
| 35  | BB    | 1575 | C    | N3-C4-N4   | 9.45  | 124.61      | 118.00   |
| 35  | BB    | 88   | G    | C2-N3-C4   | 9.45  | 116.62      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1794 | A    | N7-C8-N9    | -9.45 | 109.08      | 113.80   |
| 35  | BB    | 1722 | A    | C2-N3-C4    | -9.44 | 105.88      | 110.60   |
| 1   | AA    | 487  | A    | C4-C5-C6    | 9.44  | 121.72      | 117.00   |
| 35  | BB    | 1383 | A    | C4-C5-C6    | 9.44  | 121.72      | 117.00   |
| 35  | BB    | 2439 | A    | C6-C5-N7    | -9.44 | 125.69      | 132.30   |
| 48  | BO    | 2    | ASP  | CB-CG-OD2   | -9.44 | 109.80      | 118.30   |
| 35  | BB    | 88   | G    | N3-C2-N2    | 9.44  | 126.51      | 119.90   |
| 1   | AA    | 169  | C    | C5-C4-N4    | -9.44 | 113.59      | 120.20   |
| 1   | AA    | 1497 | G    | N1-C2-N3    | -9.44 | 118.24      | 123.90   |
| 35  | BB    | 807  | U    | C4'-C3'-C2' | -9.44 | 93.16       | 102.60   |
| 35  | BB    | 998  | C    | C2-N3-C4    | -9.44 | 115.18      | 119.90   |
| 35  | BB    | 1375 | U    | C4-C5-C6    | -9.44 | 114.04      | 119.70   |
| 35  | BB    | 1516 | G    | C5-N7-C8    | -9.44 | 99.58       | 104.30   |
| 1   | AA    | 67   | C    | C4-C5-C6    | 9.44  | 122.12      | 117.40   |
| 1   | AA    | 847  | G    | N3-C4-N9    | 9.44  | 131.66      | 126.00   |
| 22  | AV    | 32   | A    | N7-C8-N9    | -9.44 | 109.08      | 113.80   |
| 35  | BB    | 622  | G    | O4'-C1'-N9  | 9.44  | 115.75      | 108.20   |
| 35  | BB    | 1874 | C    | C6-N1-C2    | -9.44 | 116.53      | 120.30   |
| 35  | BB    | 1893 | C    | N3-C4-N4    | 9.44  | 124.61      | 118.00   |
| 35  | BB    | 2850 | A    | N1-C2-N3    | -9.44 | 124.58      | 129.30   |
| 35  | BB    | 2446 | G    | N3-C2-N2    | 9.44  | 126.50      | 119.90   |
| 35  | BB    | 2531 | A    | C4-C5-C6    | 9.44  | 121.72      | 117.00   |
| 1   | AA    | 207  | C    | C2-N3-C4    | -9.43 | 115.18      | 119.90   |
| 35  | BB    | 335  | C    | N3-C4-C5    | -9.43 | 118.13      | 121.90   |
| 35  | BB    | 1023 | U    | C5-C4-O4    | -9.43 | 120.24      | 125.90   |
| 1   | AA    | 477  | C    | N3-C4-C5    | -9.43 | 118.13      | 121.90   |
| 1   | AA    | 674  | G    | C5-C6-O6    | -9.43 | 122.94      | 128.60   |
| 1   | AA    | 682  | G    | C5-C6-O6    | -9.43 | 122.94      | 128.60   |
| 1   | AA    | 1109 | C    | O4'-C1'-N1  | 9.43  | 115.75      | 108.20   |
| 22  | AV    | 10   | G    | N1-C6-O6    | 9.43  | 125.56      | 119.90   |
| 34  | BA    | 118  | C    | C6-N1-C2    | -9.43 | 116.53      | 120.30   |
| 34  | BA    | 118  | C    | C2-N3-C4    | 9.43  | 124.61      | 119.90   |
| 35  | BB    | 973  | A    | N1-C6-N6    | 9.43  | 124.26      | 118.60   |
| 1   | AA    | 29   | U    | C6-N1-C2    | 9.43  | 126.66      | 121.00   |
| 1   | AA    | 1152 | A    | C4-C5-C6    | 9.43  | 121.71      | 117.00   |
| 1   | AA    | 1170 | A    | C4-C5-C6    | 9.43  | 121.71      | 117.00   |
| 1   | AA    | 1439 | G    | N1-C6-O6    | 9.43  | 125.56      | 119.90   |
| 1   | AA    | 1455 | G    | C5-C6-O6    | -9.43 | 122.94      | 128.60   |
| 22  | AV    | 65   | U    | P-O3'-C3'   | 9.43  | 131.01      | 119.70   |
| 35  | BB    | 854  | C    | N3-C4-N4    | 9.43  | 124.60      | 118.00   |
| 35  | BB    | 1279 | G    | C5-C6-O6    | -9.43 | 122.94      | 128.60   |
| 35  | BB    | 2415 | G    | N3-C2-N2    | 9.43  | 126.50      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 2503 | A    | C4-C5-C6   | 9.43  | 121.71      | 117.00   |
| 35  | BB    | 1611 | C    | C2-N3-C4   | 9.43  | 124.61      | 119.90   |
| 1   | AA    | 758  | C    | O4'-C1'-N1 | 9.42  | 115.74      | 108.20   |
| 1   | AA    | 808  | C    | O4'-C1'-N1 | 9.42  | 115.74      | 108.20   |
| 35  | BB    | 636  | G    | N1-C6-O6   | 9.42  | 125.56      | 119.90   |
| 35  | BB    | 700  | G    | C5-C6-O6   | -9.42 | 122.95      | 128.60   |
| 35  | BB    | 1851 | U    | O4'-C1'-N1 | 9.42  | 115.74      | 108.20   |
| 1   | AA    | 295  | C    | C5-C6-N1   | 9.42  | 125.71      | 121.00   |
| 1   | AA    | 606  | G    | C5-C6-O6   | -9.42 | 122.95      | 128.60   |
| 1   | AA    | 890  | G    | C5-C6-N1   | -9.42 | 106.79      | 111.50   |
| 35  | BB    | 80   | G    | N3-C2-N2   | 9.42  | 126.49      | 119.90   |
| 35  | BB    | 584  | C    | O4'-C1'-N1 | 9.42  | 115.74      | 108.20   |
| 35  | BB    | 1118 | C    | O4'-C1'-N1 | 9.42  | 115.74      | 108.20   |
| 35  | BB    | 2378 | A    | C4-C5-N7   | -9.42 | 105.99      | 110.70   |
| 35  | BB    | 350  | G    | C4-C5-C6   | 9.42  | 124.45      | 118.80   |
| 35  | BB    | 1588 | G    | C6-C5-N7   | -9.42 | 124.75      | 130.40   |
| 35  | BB    | 2335 | A    | C4-C5-C6   | 9.42  | 121.71      | 117.00   |
| 1   | AA    | 1314 | C    | O4'-C1'-N1 | 9.42  | 115.73      | 108.20   |
| 1   | AA    | 1322 | C    | C4-C5-C6   | -9.42 | 112.69      | 117.40   |
| 35  | BB    | 458  | G    | O4'-C1'-N9 | 9.42  | 115.73      | 108.20   |
| 35  | BB    | 961  | C    | N3-C4-N4   | 9.42  | 124.59      | 118.00   |
| 35  | BB    | 2455 | G    | N3-C2-N2   | 9.42  | 126.49      | 119.90   |
| 35  | BB    | 1888 | G    | N3-C2-N2   | 9.42  | 126.49      | 119.90   |
| 35  | BB    | 701  | G    | N3-C4-C5   | 9.41  | 133.31      | 128.60   |
| 35  | BB    | 876  | C    | O4'-C1'-N1 | 9.41  | 115.73      | 108.20   |
| 35  | BB    | 1606 | C    | N3-C4-C5   | -9.41 | 118.13      | 121.90   |
| 35  | BB    | 2345 | G    | O4'-C1'-N9 | 9.41  | 115.73      | 108.20   |
| 1   | AA    | 539  | A    | C5-C6-N6   | -9.41 | 116.17      | 123.70   |
| 1   | AA    | 683  | G    | O4'-C1'-N9 | 9.41  | 115.73      | 108.20   |
| 35  | BB    | 435  | C    | N3-C4-N4   | 9.41  | 124.59      | 118.00   |
| 35  | BB    | 1891 | G    | O4'-C1'-N9 | 9.41  | 115.73      | 108.20   |
| 35  | BB    | 2184 | A    | N1-C2-N3   | -9.41 | 124.59      | 129.30   |
| 1   | AA    | 1434 | A    | C2-N3-C4   | -9.41 | 105.89      | 110.60   |
| 34  | BA    | 80   | U    | O4'-C1'-N1 | 9.41  | 115.73      | 108.20   |
| 35  | BB    | 739  | A    | O4'-C1'-N9 | 9.41  | 115.73      | 108.20   |
| 35  | BB    | 1672 | A    | C5-C6-N1   | -9.41 | 113.00      | 117.70   |
| 35  | BB    | 216  | A    | C4-C5-C6   | 9.41  | 121.70      | 117.00   |
| 35  | BB    | 742  | A    | C5-C6-N6   | -9.41 | 116.17      | 123.70   |
| 35  | BB    | 1425 | G    | C6-C5-N7   | -9.41 | 124.75      | 130.40   |
| 35  | BB    | 2447 | G    | N1-C2-N3   | -9.41 | 118.25      | 123.90   |
| 35  | BB    | 2617 | U    | N1-C2-O2   | -9.41 | 116.21      | 122.80   |
| 1   | AA    | 71   | A    | C5-N7-C8   | 9.41  | 108.60      | 103.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | BA    | 91   | C    | O4'-C1'-N1  | 9.41  | 115.72      | 108.20   |
| 35  | BB    | 459  | U    | N3-C4-C5    | -9.41 | 108.96      | 114.60   |
| 35  | BB    | 1810 | A    | C5-C6-N6    | -9.41 | 116.17      | 123.70   |
| 35  | BB    | 2718 | G    | N1-C6-O6    | 9.41  | 125.54      | 119.90   |
| 35  | BB    | 2726 | A    | C4-C5-C6    | 9.41  | 121.70      | 117.00   |
| 1   | AA    | 293  | G    | C5-C6-N1    | -9.40 | 106.80      | 111.50   |
| 1   | AA    | 766  | A    | C6-N1-C2    | 9.40  | 124.24      | 118.60   |
| 35  | BB    | 401  | A    | N9-C4-C5    | 9.40  | 109.56      | 105.80   |
| 1   | AA    | 329  | A    | P-O3'-C3'   | 9.40  | 130.98      | 119.70   |
| 1   | AA    | 1250 | A    | N1-C6-N6    | 9.40  | 124.24      | 118.60   |
| 35  | BB    | 1788 | C    | C6-N1-C2    | -9.40 | 116.54      | 120.30   |
| 35  | BB    | 2512 | C    | C5-C4-N4    | -9.40 | 113.62      | 120.20   |
| 1   | AA    | 80   | A    | C8-N9-C4    | -9.40 | 102.04      | 105.80   |
| 1   | AA    | 818  | G    | N3-C2-N2    | 9.40  | 126.48      | 119.90   |
| 35  | BB    | 774  | G    | C5-C6-O6    | -9.40 | 122.96      | 128.60   |
| 35  | BB    | 1583 | A    | C8-N9-C4    | -9.40 | 102.04      | 105.80   |
| 35  | BB    | 2313 | C    | N1-C2-N3    | 9.40  | 125.78      | 119.20   |
| 1   | AA    | 352  | C    | N1-C2-O2    | 9.40  | 124.54      | 118.90   |
| 1   | AA    | 1065 | U    | O4'-C1'-N1  | 9.40  | 115.72      | 108.20   |
| 1   | AA    | 1294 | G    | O4'-C1'-N9  | 9.40  | 115.72      | 108.20   |
| 22  | AV    | 37   | G    | C2-N3-C4    | 9.40  | 116.60      | 111.90   |
| 34  | BA    | 72   | G    | O4'-C1'-N9  | 9.40  | 115.72      | 108.20   |
| 35  | BB    | 2123 | G    | P-O3'-C3'   | 9.40  | 130.98      | 119.70   |
| 35  | BB    | 1749 | A    | C5-N7-C8    | 9.40  | 108.60      | 103.90   |
| 35  | BB    | 2435 | A    | C5-C6-N1    | -9.40 | 113.00      | 117.70   |
| 1   | AA    | 438  | U    | C5-C4-O4    | -9.39 | 120.26      | 125.90   |
| 35  | BB    | 1135 | C    | C5-C4-N4    | -9.39 | 113.62      | 120.20   |
| 35  | BB    | 1301 | A    | N1-C6-N6    | 9.39  | 124.24      | 118.60   |
| 35  | BB    | 1351 | C    | O4'-C1'-N1  | 9.39  | 115.72      | 108.20   |
| 35  | BB    | 2666 | C    | C2-N3-C4    | 9.39  | 124.60      | 119.90   |
| 35  | BB    | 867  | C    | O4'-C1'-N1  | 9.39  | 115.72      | 108.20   |
| 35  | BB    | 1057 | A    | C5'-C4'-O4' | 9.39  | 120.37      | 109.10   |
| 35  | BB    | 2145 | C    | C5-C4-N4    | -9.39 | 113.62      | 120.20   |
| 35  | BB    | 2583 | G    | C2-N3-C4    | -9.39 | 107.20      | 111.90   |
| 35  | BB    | 1466 | U    | N1-C2-O2    | -9.39 | 116.23      | 122.80   |
| 35  | BB    | 1566 | A    | N7-C8-N9    | -9.39 | 109.10      | 113.80   |
| 1   | AA    | 549  | C    | O4'-C1'-N1  | 9.39  | 115.71      | 108.20   |
| 35  | BB    | 1360 | G    | C6-N1-C2    | -9.39 | 119.47      | 125.10   |
| 35  | BB    | 1553 | A    | O4'-C1'-N9  | 9.39  | 115.71      | 108.20   |
| 34  | BA    | 108  | A    | C4-C5-C6    | 9.39  | 121.69      | 117.00   |
| 35  | BB    | 209  | C    | N3-C4-N4    | 9.39  | 124.57      | 118.00   |
| 35  | BB    | 858  | G    | C5-C6-O6    | -9.39 | 122.97      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1377 | G    | N3-C2-N2    | 9.39  | 126.47      | 119.90   |
| 1   | AA    | 667  | G    | C5-C6-O6    | -9.39 | 122.97      | 128.60   |
| 34  | BA    | 85   | G    | C2-N3-C4    | -9.38 | 107.21      | 111.90   |
| 35  | BB    | 405  | U    | O4'-C1'-N1  | 9.39  | 115.71      | 108.20   |
| 35  | BB    | 885  | C    | N3-C4-N4    | 9.38  | 124.57      | 118.00   |
| 35  | BB    | 2244 | U    | O4'-C1'-N1  | 9.39  | 115.71      | 108.20   |
| 35  | BB    | 2212 | A    | O4'-C1'-N9  | 9.38  | 115.71      | 108.20   |
| 35  | BB    | 2271 | G    | N7-C8-N9    | 9.38  | 117.79      | 113.10   |
| 35  | BB    | 2578 | G    | C5-C6-O6    | -9.38 | 122.97      | 128.60   |
| 35  | BB    | 17   | G    | C5-C6-O6    | -9.38 | 122.97      | 128.60   |
| 1   | AA    | 1174 | G    | O4'-C1'-N9  | 9.38  | 115.70      | 108.20   |
| 35  | BB    | 865  | C    | N3-C4-C5    | -9.38 | 118.15      | 121.90   |
| 35  | BB    | 2648 | G    | C4-C5-N7    | 9.38  | 114.55      | 110.80   |
| 1   | AA    | 815  | A    | C1'-O4'-C4' | -9.38 | 102.40      | 109.90   |
| 34  | BA    | 5    | U    | O4'-C1'-N1  | 9.38  | 115.70      | 108.20   |
| 34  | BA    | 20   | G    | O4'-C1'-N9  | 9.38  | 115.70      | 108.20   |
| 52  | BS    | 89   | ALA  | N-CA-CB     | 9.38  | 123.23      | 110.10   |
| 1   | AA    | 1384 | C    | C5-C4-N4    | -9.37 | 113.64      | 120.20   |
| 35  | BB    | 404  | A    | C5-C6-N6    | -9.38 | 116.20      | 123.70   |
| 35  | BB    | 631  | A    | N1-C6-N6    | 9.38  | 124.22      | 118.60   |
| 35  | BB    | 2503 | A    | C5-C6-N1    | -9.38 | 113.01      | 117.70   |
| 35  | BB    | 2783 | U    | C2-N3-C4    | -9.38 | 121.38      | 127.00   |
| 35  | BB    | 579  | G    | C8-N9-C4    | -9.37 | 102.65      | 106.40   |
| 35  | BB    | 1039 | A    | C5-C6-N1    | -9.37 | 113.02      | 117.70   |
| 35  | BB    | 1432 | G    | O4'-C1'-N9  | 9.37  | 115.70      | 108.20   |
| 35  | BB    | 1907 | G    | N1-C2-N3    | -9.37 | 118.28      | 123.90   |
| 35  | BB    | 2748 | A    | C4-C5-C6    | 9.37  | 121.69      | 117.00   |
| 1   | AA    | 1403 | C    | O4'-C1'-N1  | 9.37  | 115.70      | 108.20   |
| 4   | AD    | 13   | ARG  | NE-CZ-NH1   | 9.37  | 124.98      | 120.30   |
| 35  | BB    | 1016 | G    | C6-C5-N7    | -9.37 | 124.78      | 130.40   |
| 35  | BB    | 2159 | G    | C8-N9-C4    | -9.37 | 102.65      | 106.40   |
| 35  | BB    | 2425 | A    | C8-N9-C4    | -9.37 | 102.05      | 105.80   |
| 1   | AA    | 149  | A    | C4-C5-N7    | -9.37 | 106.02      | 110.70   |
| 1   | AA    | 337  | G    | N3-C4-C5    | -9.37 | 123.92      | 128.60   |
| 35  | BB    | 2298 | A    | O4'-C1'-N9  | 9.37  | 115.69      | 108.20   |
| 35  | BB    | 2702 | G    | C4-C5-N7    | -9.37 | 107.05      | 110.80   |
| 1   | AA    | 1376 | U    | O4'-C1'-N1  | 9.37  | 115.69      | 108.20   |
| 35  | BB    | 54   | G    | O4'-C1'-N9  | 9.37  | 115.69      | 108.20   |
| 35  | BB    | 112  | U    | N1-C2-N3    | 9.37  | 120.52      | 114.90   |
| 35  | BB    | 1612 | C    | N3-C4-N4    | 9.37  | 124.56      | 118.00   |
| 35  | BB    | 2371 | G    | C6-C5-N7    | -9.37 | 124.78      | 130.40   |
| 1   | AA    | 357  | G    | C5-C6-O6    | -9.37 | 122.98      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1357 | A    | C4-C5-N7   | -9.37 | 106.02      | 110.70   |
| 35  | BB    | 300  | A    | C6-C5-N7   | -9.36 | 125.75      | 132.30   |
| 52  | BS    | 68   | ASP  | CB-CG-OD1  | 9.37  | 126.73      | 118.30   |
| 35  | BB    | 2158 | A    | C5-C6-N6   | -9.36 | 116.21      | 123.70   |
| 25  | B0    | 26   | ARG  | NE-CZ-NH1  | 9.36  | 124.98      | 120.30   |
| 35  | BB    | 1320 | C    | N3-C4-N4   | 9.36  | 124.55      | 118.00   |
| 35  | BB    | 1708 | C    | C6-N1-C2   | -9.36 | 116.56      | 120.30   |
| 35  | BB    | 1813 | G    | C6-C5-N7   | -9.36 | 124.78      | 130.40   |
| 35  | BB    | 1999 | C    | N3-C4-C5   | -9.36 | 118.16      | 121.90   |
| 35  | BB    | 2107 | G    | O4'-C1'-N9 | 9.36  | 115.69      | 108.20   |
| 35  | BB    | 2279 | G    | C5-N7-C8   | -9.36 | 99.62       | 104.30   |
| 35  | BB    | 2357 | G    | C2-N3-C4   | 9.36  | 116.58      | 111.90   |
| 1   | AA    | 35   | G    | N1-C2-N3   | -9.36 | 118.28      | 123.90   |
| 1   | AA    | 154  | U    | C5-C6-N1   | 9.36  | 127.38      | 122.70   |
| 1   | AA    | 1356 | G    | N9-C4-C5   | -9.36 | 101.66      | 105.40   |
| 1   | AA    | 1423 | G    | N7-C8-N9   | 9.36  | 117.78      | 113.10   |
| 35  | BB    | 69   | C    | O4'-C1'-N1 | 9.36  | 115.69      | 108.20   |
| 35  | BB    | 361  | G    | N1-C6-O6   | 9.36  | 125.52      | 119.90   |
| 34  | BA    | 71   | C    | N3-C4-C5   | -9.36 | 118.16      | 121.90   |
| 35  | BB    | 645  | C    | N3-C4-N4   | 9.36  | 124.55      | 118.00   |
| 35  | BB    | 2320 | U    | C5-C6-N1   | 9.36  | 127.38      | 122.70   |
| 1   | AA    | 362  | G    | C4-C5-N7   | 9.36  | 114.54      | 110.80   |
| 1   | AA    | 1452 | C    | C6-N1-C2   | -9.36 | 116.56      | 120.30   |
| 34  | BA    | 7    | G    | O4'-C1'-N9 | 9.36  | 115.69      | 108.20   |
| 35  | BB    | 2543 | G    | C8-N9-C4   | -9.36 | 102.66      | 106.40   |
| 35  | BB    | 2168 | G    | C6-C5-N7   | -9.36 | 124.79      | 130.40   |
| 35  | BB    | 2673 | G    | O4'-C1'-N9 | 9.36  | 115.68      | 108.20   |
| 1   | AA    | 601  | G    | N1-C6-O6   | 9.35  | 125.51      | 119.90   |
| 1   | AA    | 714  | G    | C6-C5-N7   | -9.35 | 124.79      | 130.40   |
| 1   | AA    | 749  | A    | C4-C5-C6   | 9.35  | 121.68      | 117.00   |
| 1   | AA    | 768  | A    | C5-C6-N6   | -9.35 | 116.22      | 123.70   |
| 35  | BB    | 2604 | U    | N3-C4-O4   | 9.35  | 125.95      | 119.40   |
| 35  | BB    | 2876 | G    | N1-C6-O6   | 9.35  | 125.51      | 119.90   |
| 35  | BB    | 2255 | G    | C5-C6-O6   | -9.35 | 122.99      | 128.60   |
| 1   | AA    | 721  | G    | N1-C6-O6   | 9.35  | 125.51      | 119.90   |
| 35  | BB    | 1030 | C    | N3-C4-C5   | -9.35 | 118.16      | 121.90   |
| 35  | BB    | 1635 | A    | C8-N9-C4   | -9.35 | 102.06      | 105.80   |
| 35  | BB    | 1800 | C    | N3-C4-N4   | 9.35  | 124.54      | 118.00   |
| 35  | BB    | 2044 | C    | C2-N3-C4   | 9.35  | 124.57      | 119.90   |
| 35  | BB    | 2263 | C    | N3-C4-C5   | -9.35 | 118.16      | 121.90   |
| 1   | AA    | 896  | C    | C6-N1-C2   | -9.35 | 116.56      | 120.30   |
| 1   | AA    | 983  | A    | C5-C6-N1   | -9.35 | 113.03      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 409  | G    | C5-C6-O6    | -9.35 | 122.99      | 128.60   |
| 35  | BB    | 485  | C    | C6-N1-C2    | -9.35 | 116.56      | 120.30   |
| 35  | BB    | 2681 | C    | C4-C5-C6    | 9.35  | 122.07      | 117.40   |
| 1   | AA    | 1042 | A    | C5-C6-N6    | -9.34 | 116.23      | 123.70   |
| 1   | AA    | 1409 | C    | C2-N3-C4    | 9.34  | 124.57      | 119.90   |
| 1   | AA    | 1472 | U    | O4'-C1'-N1  | 9.34  | 115.68      | 108.20   |
| 35  | BB    | 2208 | C    | N3-C4-C5    | -9.34 | 118.16      | 121.90   |
| 1   | AA    | 1423 | G    | C5-N7-C8    | -9.34 | 99.63       | 104.30   |
| 35  | BB    | 37   | C    | N3-C4-N4    | 9.34  | 124.54      | 118.00   |
| 35  | BB    | 427  | U    | O4'-C1'-N1  | 9.34  | 115.67      | 108.20   |
| 35  | BB    | 1079 | C    | N3-C4-C5    | -9.34 | 118.16      | 121.90   |
| 35  | BB    | 1839 | G    | C6-C5-N7    | -9.34 | 124.79      | 130.40   |
| 1   | AA    | 386  | C    | C5-C4-N4    | -9.34 | 113.66      | 120.20   |
| 35  | BB    | 277  | G    | O4'-C1'-N9  | 9.34  | 115.67      | 108.20   |
| 35  | BB    | 1213 | A    | O4'-C1'-N9  | 9.34  | 115.67      | 108.20   |
| 50  | BQ    | 2    | ARG  | NE-CZ-NH1   | -9.34 | 115.63      | 120.30   |
| 1   | AA    | 969  | A    | C4-C5-N7    | -9.34 | 106.03      | 110.70   |
| 35  | BB    | 813  | U    | O4'-C1'-N1  | 9.34  | 115.67      | 108.20   |
| 35  | BB    | 1952 | A    | C5-N7-C8    | 9.34  | 108.57      | 103.90   |
| 1   | AA    | 1138 | G    | N3-C2-N2    | 9.34  | 126.44      | 119.90   |
| 35  | BB    | 345  | A    | N9-C4-C5    | 9.34  | 109.53      | 105.80   |
| 1   | AA    | 663  | A    | O4'-C1'-N9  | 9.34  | 115.67      | 108.20   |
| 34  | BA    | 42   | C    | N3-C4-N4    | 9.34  | 124.54      | 118.00   |
| 35  | BB    | 368  | A    | C4'-C3'-C2' | -9.34 | 93.26       | 102.60   |
| 35  | BB    | 1699 | G    | C8-N9-C4    | -9.34 | 102.67      | 106.40   |
| 35  | BB    | 2047 | C    | C2-N3-C4    | -9.34 | 115.23      | 119.90   |
| 35  | BB    | 1304 | A    | N1-C6-N6    | 9.34  | 124.20      | 118.60   |
| 35  | BB    | 2364 | C    | N3-C4-N4    | 9.34  | 124.53      | 118.00   |
| 1   | AA    | 420  | U    | O4'-C1'-N1  | 9.33  | 115.67      | 108.20   |
| 1   | AA    | 977  | A    | C8-N9-C4    | -9.33 | 102.07      | 105.80   |
| 1   | AA    | 1061 | G    | C8-N9-C4    | -9.33 | 102.67      | 106.40   |
| 16  | AP    | 14   | ARG  | NE-CZ-NH2   | -9.33 | 115.63      | 120.30   |
| 34  | BA    | 14   | U    | O4'-C1'-N1  | 9.33  | 115.67      | 108.20   |
| 35  | BB    | 428  | A    | C5-C6-N1    | -9.33 | 113.03      | 117.70   |
| 35  | BB    | 1478 | G    | C4-C5-C6    | 9.33  | 124.40      | 118.80   |
| 35  | BB    | 1899 | A    | C5-N7-C8    | 9.33  | 108.57      | 103.90   |
| 35  | BB    | 2470 | G    | C5-C6-O6    | -9.33 | 123.00      | 128.60   |
| 35  | BB    | 2763 | G    | N1-C2-N2    | -9.33 | 107.80      | 116.20   |
| 1   | AA    | 1136 | C    | C5-C4-N4    | -9.33 | 113.67      | 120.20   |
| 35  | BB    | 1110 | G    | C8-N9-C4    | -9.33 | 102.67      | 106.40   |
| 1   | AA    | 1517 | G    | O4'-C1'-N9  | 9.33  | 115.66      | 108.20   |
| 34  | BA    | 116  | G    | N1-C2-N3    | -9.33 | 118.30      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 55   | G    | N7-C8-N9   | -9.33 | 108.44      | 113.10   |
| 40  | BG    | 93   | TYR  | CB-CG-CD1  | -9.33 | 115.40      | 121.00   |
| 1   | AA    | 352  | C    | N3-C4-C5   | -9.33 | 118.17      | 121.90   |
| 35  | BB    | 2119 | A    | O4'-C1'-N9 | 9.33  | 115.66      | 108.20   |
| 1   | AA    | 485  | U    | O4'-C1'-N1 | 9.33  | 115.66      | 108.20   |
| 1   | AA    | 1173 | U    | O4'-C1'-N1 | 9.33  | 115.66      | 108.20   |
| 35  | BB    | 1719 | G    | N1-C6-O6   | 9.33  | 125.50      | 119.90   |
| 35  | BB    | 2749 | A    | C4-C5-C6   | 9.33  | 121.66      | 117.00   |
| 1   | AA    | 310  | G    | C5-C6-O6   | -9.32 | 123.01      | 128.60   |
| 1   | AA    | 688  | G    | N1-C6-O6   | 9.32  | 125.49      | 119.90   |
| 8   | AH    | 96   | ALA  | N-CA-CB    | 9.32  | 123.15      | 110.10   |
| 35  | BB    | 2489 | U    | N1-C2-O2   | 9.32  | 129.33      | 122.80   |
| 35  | BB    | 1500 | G    | C8-N9-C4   | -9.32 | 102.67      | 106.40   |
| 1   | AA    | 1427 | C    | N3-C4-N4   | 9.32  | 124.53      | 118.00   |
| 1   | AA    | 1220 | G    | O4'-C1'-N9 | 9.32  | 115.66      | 108.20   |
| 1   | AA    | 1275 | A    | N1-C2-N3   | 9.32  | 133.96      | 129.30   |
| 35  | BB    | 298  | G    | C6-N1-C2   | 9.32  | 130.69      | 125.10   |
| 35  | BB    | 1284 | A    | C8-N9-C4   | -9.32 | 102.07      | 105.80   |
| 35  | BB    | 1436 | G    | N9-C4-C5   | -9.32 | 101.67      | 105.40   |
| 35  | BB    | 1542 | U    | N3-C4-O4   | -9.32 | 112.88      | 119.40   |
| 1   | AA    | 632  | U    | O4'-C1'-N1 | 9.32  | 115.65      | 108.20   |
| 34  | BA    | 71   | C    | N1-C2-N3   | 9.32  | 125.72      | 119.20   |
| 35  | BB    | 272  | A    | C6-C5-N7   | -9.32 | 125.78      | 132.30   |
| 35  | BB    | 541  | A    | C2-N3-C4   | -9.31 | 105.94      | 110.60   |
| 35  | BB    | 1957 | C    | O4'-C1'-N1 | 9.31  | 115.65      | 108.20   |
| 35  | BB    | 1910 | G    | N1-C6-O6   | 9.31  | 125.49      | 119.90   |
| 35  | BB    | 2351 | G    | N1-C6-O6   | 9.31  | 125.49      | 119.90   |
| 35  | BB    | 2581 | G    | N3-C2-N2   | 9.31  | 126.42      | 119.90   |
| 1   | AA    | 627  | G    | C5-C6-O6   | -9.31 | 123.01      | 128.60   |
| 1   | AA    | 1263 | C    | N3-C4-C5   | -9.31 | 118.17      | 121.90   |
| 35  | BB    | 1244 | A    | N1-C6-N6   | 9.31  | 124.19      | 118.60   |
| 35  | BB    | 2141 | G    | C5-C6-N1   | -9.31 | 106.84      | 111.50   |
| 35  | BB    | 2448 | A    | C5-C6-N1   | -9.31 | 113.04      | 117.70   |
| 35  | BB    | 96   | C    | O4'-C1'-N1 | 9.31  | 115.65      | 108.20   |
| 35  | BB    | 750  | A    | N1-C2-N3   | -9.31 | 124.64      | 129.30   |
| 35  | BB    | 1678 | A    | O4'-C1'-N9 | 9.31  | 115.65      | 108.20   |
| 1   | AA    | 1151 | A    | C4-C5-C6   | 9.31  | 121.65      | 117.00   |
| 35  | BB    | 1486 | U    | O4'-C1'-N1 | 9.31  | 115.65      | 108.20   |
| 34  | BA    | 72   | G    | N3-C4-C5   | -9.31 | 123.95      | 128.60   |
| 35  | BB    | 1293 | C    | C5-C4-N4   | -9.31 | 113.69      | 120.20   |
| 35  | BB    | 1603 | A    | C5-N7-C8   | 9.31  | 108.55      | 103.90   |
| 35  | BB    | 2574 | G    | O4'-C1'-N9 | 9.31  | 115.64      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 330  | C    | N3-C4-N4    | 9.30  | 124.51      | 118.00   |
| 1   | AA    | 785  | G    | N9-C4-C5    | -9.30 | 101.68      | 105.40   |
| 1   | AA    | 1155 | A    | C5-C6-N6    | -9.30 | 116.26      | 123.70   |
| 35  | BB    | 1295 | C    | C6-N1-C2    | -9.30 | 116.58      | 120.30   |
| 35  | BB    | 2198 | A    | C5-N7-C8    | 9.30  | 108.55      | 103.90   |
| 35  | BB    | 2810 | A    | N9-C4-C5    | 9.31  | 109.52      | 105.80   |
| 1   | AA    | 1305 | G    | C4-C5-N7    | -9.30 | 107.08      | 110.80   |
| 35  | BB    | 1127 | A    | N1-C6-N6    | 9.30  | 124.18      | 118.60   |
| 35  | BB    | 2509 | G    | N1-C6-O6    | 9.30  | 125.48      | 119.90   |
| 1   | AA    | 530  | G    | N1-C6-O6    | 9.30  | 125.48      | 119.90   |
| 35  | BB    | 2497 | A    | C5-C6-N1    | -9.30 | 113.05      | 117.70   |
| 1   | AA    | 570  | G    | N1-C6-O6    | 9.30  | 125.48      | 119.90   |
| 1   | AA    | 931  | C    | C4-C5-C6    | -9.30 | 112.75      | 117.40   |
| 34  | BA    | 43   | C    | O4'-C1'-N1  | 9.30  | 115.64      | 108.20   |
| 35  | BB    | 75   | G    | N7-C8-N9    | -9.30 | 108.45      | 113.10   |
| 1   | AA    | 309  | A    | O4'-C1'-N9  | 9.30  | 115.64      | 108.20   |
| 35  | BB    | 942  | G    | C8-N9-C4    | -9.30 | 102.68      | 106.40   |
| 35  | BB    | 77   | G    | N3-C4-C5    | -9.30 | 123.95      | 128.60   |
| 35  | BB    | 780  | G    | N1-C6-O6    | 9.30  | 125.48      | 119.90   |
| 35  | BB    | 977  | G    | C4-C5-N7    | -9.30 | 107.08      | 110.80   |
| 35  | BB    | 2681 | C    | N3-C4-C5    | -9.30 | 118.18      | 121.90   |
| 1   | AA    | 9    | G    | C5-C6-O6    | -9.30 | 123.02      | 128.60   |
| 1   | AA    | 11   | G    | C6-C5-N7    | -9.29 | 124.82      | 130.40   |
| 1   | AA    | 958  | A    | C4-C5-C6    | 9.30  | 121.65      | 117.00   |
| 1   | AA    | 1201 | A    | N9-C4-C5    | 9.30  | 109.52      | 105.80   |
| 1   | AA    | 1457 | G    | C8-N9-C4    | -9.29 | 102.68      | 106.40   |
| 35  | BB    | 995  | C    | C6-N1-C2    | -9.29 | 116.58      | 120.30   |
| 1   | AA    | 255  | G    | C5-C6-N1    | -9.29 | 106.85      | 111.50   |
| 1   | AA    | 405  | U    | C5-C6-N1    | 9.29  | 127.35      | 122.70   |
| 35  | BB    | 121  | G    | N3-C2-N2    | 9.29  | 126.41      | 119.90   |
| 35  | BB    | 1735 | A    | C4-C5-C6    | 9.29  | 121.64      | 117.00   |
| 35  | BB    | 2412 | A    | N1-C2-N3    | 9.29  | 133.94      | 129.30   |
| 1   | AA    | 514  | C    | N3-C4-N4    | 9.29  | 124.50      | 118.00   |
| 35  | BB    | 406  | G    | C5-C6-O6    | -9.29 | 123.03      | 128.60   |
| 35  | BB    | 504  | A    | C6-N1-C2    | -9.29 | 113.03      | 118.60   |
| 35  | BB    | 814  | C    | C4'-C3'-C2' | -9.29 | 93.31       | 102.60   |
| 35  | BB    | 1378 | A    | C4-C5-C6    | 9.29  | 121.64      | 117.00   |
| 34  | BA    | 57   | A    | N1-C6-N6    | 9.29  | 124.17      | 118.60   |
| 35  | BB    | 2278 | A    | C5-C6-N6    | -9.29 | 116.27      | 123.70   |
| 55  | BW    | 50   | MET  | CG-SD-CE    | -9.29 | 85.34       | 100.20   |
| 1   | AA    | 942  | G    | C5-C6-O6    | -9.28 | 123.03      | 128.60   |
| 35  | BB    | 1859 | U    | O4'-C1'-N1  | 9.28  | 115.63      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 265  | G    | O4'-C1'-N9  | 9.28  | 115.62      | 108.20   |
| 1   | AA    | 1242 | G    | N7-C8-N9    | -9.28 | 108.46      | 113.10   |
| 35  | BB    | 1529 | G    | C6-C5-N7    | -9.28 | 124.83      | 130.40   |
| 35  | BB    | 2371 | G    | C5-C6-O6    | -9.28 | 123.03      | 128.60   |
| 35  | BB    | 2516 | A    | C4-C5-C6    | 9.28  | 121.64      | 117.00   |
| 35  | BB    | 2639 | A    | C2-N3-C4    | -9.28 | 105.96      | 110.60   |
| 35  | BB    | 2794 | C    | N3-C4-N4    | 9.28  | 124.50      | 118.00   |
| 1   | AA    | 141  | G    | C8-N9-C4    | -9.28 | 102.69      | 106.40   |
| 1   | AA    | 371  | A    | C4-C5-N7    | -9.28 | 106.06      | 110.70   |
| 35  | BB    | 1376 | C    | C2-N3-C4    | 9.28  | 124.54      | 119.90   |
| 35  | BB    | 1689 | A    | O4'-C1'-N9  | 9.28  | 115.62      | 108.20   |
| 1   | AA    | 162  | A    | C5-N7-C8    | 9.28  | 108.54      | 103.90   |
| 1   | AA    | 779  | C    | C6-N1-C2    | -9.28 | 116.59      | 120.30   |
| 1   | AA    | 831  | A    | C4-C5-N7    | -9.28 | 106.06      | 110.70   |
| 1   | AA    | 1090 | U    | N3-C2-O2    | 9.28  | 128.69      | 122.20   |
| 35  | BB    | 103  | A    | N9-C4-C5    | 9.28  | 109.51      | 105.80   |
| 2   | AB    | 193  | ASP  | CB-CG-OD1   | 9.28  | 126.65      | 118.30   |
| 34  | BA    | 97   | C    | N3-C4-N4    | 9.28  | 124.49      | 118.00   |
| 35  | BB    | 1732 | C    | N3-C4-C5    | -9.28 | 118.19      | 121.90   |
| 35  | BB    | 1901 | A    | N9-C4-C5    | 9.28  | 109.51      | 105.80   |
| 1   | AA    | 92   | U    | C4-C5-C6    | -9.27 | 114.14      | 119.70   |
| 1   | AA    | 1360 | A    | C4-C5-C6    | 9.27  | 121.64      | 117.00   |
| 35  | BB    | 638  | G    | N3-C2-N2    | 9.27  | 126.39      | 119.90   |
| 35  | BB    | 1184 | U    | N1-C2-N3    | -9.27 | 109.34      | 114.90   |
| 35  | BB    | 1430 | G    | N1-C2-N3    | -9.27 | 118.34      | 123.90   |
| 35  | BB    | 2559 | C    | O4'-C1'-N1  | 9.27  | 115.62      | 108.20   |
| 35  | BB    | 2833 | U    | C1'-O4'-C4' | -9.27 | 102.48      | 109.90   |
| 1   | AA    | 546  | A    | C2-N3-C4    | -9.27 | 105.97      | 110.60   |
| 1   | AA    | 1500 | A    | N1-C6-N6    | 9.27  | 124.16      | 118.60   |
| 35  | BB    | 2663 | G    | O4'-C1'-N9  | 9.27  | 115.61      | 108.20   |
| 35  | BB    | 2668 | G    | N1-C6-O6    | 9.27  | 125.46      | 119.90   |
| 1   | AA    | 199  | A    | C4-C5-C6    | 9.27  | 121.63      | 117.00   |
| 1   | AA    | 554  | A    | C5-C6-N6    | -9.27 | 116.29      | 123.70   |
| 1   | AA    | 987  | G    | N9-C4-C5    | 9.27  | 109.11      | 105.40   |
| 35  | BB    | 1990 | C    | N3-C4-C5    | -9.27 | 118.19      | 121.90   |
| 35  | BB    | 2178 | C    | C2-N1-C1'   | 9.27  | 128.99      | 118.80   |
| 35  | BB    | 2327 | A    | C5-C6-N6    | -9.27 | 116.29      | 123.70   |
| 35  | BB    | 2855 | C    | N3-C4-N4    | 9.27  | 124.49      | 118.00   |
| 1   | AA    | 943  | U    | C6-N1-C2    | -9.26 | 115.44      | 121.00   |
| 22  | AV    | 22   | G    | N1-C6-O6    | 9.26  | 125.46      | 119.90   |
| 35  | BB    | 226  | A    | O4'-C1'-N9  | 9.26  | 115.61      | 108.20   |
| 35  | BB    | 1001 | A    | N1-C6-N6    | 9.26  | 124.16      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1301 | A    | C5-N7-C8   | 9.26  | 108.53      | 103.90   |
| 35  | BB    | 1388 | G    | C5-C6-N1   | 9.26  | 116.13      | 111.50   |
| 35  | BB    | 2198 | A    | C5-C6-N6   | -9.26 | 116.29      | 123.70   |
| 1   | AA    | 74   | A    | C5-C6-N1   | -9.26 | 113.07      | 117.70   |
| 1   | AA    | 347  | G    | N1-C6-O6   | 9.26  | 125.46      | 119.90   |
| 31  | B6    | 33   | ARG  | NE-CZ-NH2  | 9.26  | 124.93      | 120.30   |
| 35  | BB    | 1532 | A    | N1-C6-N6   | 9.26  | 124.16      | 118.60   |
| 1   | AA    | 1001 | C    | C5-C4-N4   | -9.26 | 113.72      | 120.20   |
| 1   | AA    | 1391 | U    | N1-C2-N3   | -9.26 | 109.34      | 114.90   |
| 34  | BA    | 59   | A    | C4-C5-N7   | -9.26 | 106.07      | 110.70   |
| 1   | AA    | 1151 | A    | C5-C6-N6   | -9.26 | 116.29      | 123.70   |
| 35  | BB    | 527  | C    | N3-C4-N4   | 9.26  | 124.48      | 118.00   |
| 35  | BB    | 713  | G    | N1-C2-N3   | -9.26 | 118.35      | 123.90   |
| 35  | BB    | 974  | G    | C6-C5-N7   | -9.26 | 124.85      | 130.40   |
| 35  | BB    | 1927 | A    | O4'-C1'-N9 | 9.26  | 115.61      | 108.20   |
| 35  | BB    | 2465 | C    | N3-C4-N4   | 9.26  | 124.48      | 118.00   |
| 35  | BB    | 2635 | A    | O4'-C1'-N9 | 9.26  | 115.60      | 108.20   |
| 41  | BH    | 46   | PHE  | CB-CG-CD2  | -9.26 | 114.32      | 120.80   |
| 1   | AA    | 840  | C    | C5-C4-N4   | -9.25 | 113.72      | 120.20   |
| 35  | BB    | 1990 | C    | O4'-C1'-N1 | 9.25  | 115.60      | 108.20   |
| 35  | BB    | 2579 | C    | C5-C4-N4   | -9.25 | 113.72      | 120.20   |
| 1   | AA    | 582  | C    | C5-C6-N1   | 9.25  | 125.63      | 121.00   |
| 1   | AA    | 648  | A    | C5-C6-N6   | -9.25 | 116.30      | 123.70   |
| 1   | AA    | 1366 | C    | O4'-C1'-N1 | 9.25  | 115.60      | 108.20   |
| 27  | B2    | 30   | ARG  | NE-CZ-NH2  | 9.25  | 124.92      | 120.30   |
| 35  | BB    | 290  | U    | O4'-C1'-N1 | 9.25  | 115.60      | 108.20   |
| 35  | BB    | 466  | A    | O4'-C1'-N9 | 9.25  | 115.60      | 108.20   |
| 35  | BB    | 882  | G    | O4'-C1'-N9 | 9.25  | 115.60      | 108.20   |
| 35  | BB    | 2096 | C    | C6-N1-C2   | -9.25 | 116.60      | 120.30   |
| 35  | BB    | 2260 | C    | C4-C5-C6   | 9.25  | 122.02      | 117.40   |
| 35  | BB    | 1206 | G    | C5-C6-O6   | -9.25 | 123.05      | 128.60   |
| 7   | AG    | 43   | TYR  | CG-CD2-CE2 | -9.25 | 113.90      | 121.30   |
| 35  | BB    | 816  | C    | O4'-C1'-N1 | 9.25  | 115.60      | 108.20   |
| 35  | BB    | 1748 | C    | N3-C4-N4   | 9.25  | 124.47      | 118.00   |
| 35  | BB    | 2319 | G    | O4'-C1'-N9 | 9.25  | 115.60      | 108.20   |
| 35  | BB    | 2595 | G    | C5-C6-O6   | 9.25  | 134.15      | 128.60   |
| 35  | BB    | 2758 | A    | C6-N1-C2   | -9.25 | 113.05      | 118.60   |
| 1   | AA    | 61   | G    | N1-C6-O6   | 9.24  | 125.45      | 119.90   |
| 2   | AB    | 197  | PHE  | CB-CG-CD1  | -9.24 | 114.33      | 120.80   |
| 35  | BB    | 407  | G    | N1-C6-O6   | 9.24  | 125.45      | 119.90   |
| 35  | BB    | 409  | G    | N1-C6-O6   | 9.24  | 125.45      | 119.90   |
| 35  | BB    | 1283 | G    | O4'-C1'-N9 | 9.24  | 115.60      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1656 | C    | O4'-C1'-N1 | 9.24  | 115.60      | 108.20   |
| 1   | AA    | 443  | C    | C5-C6-N1   | 9.24  | 125.62      | 121.00   |
| 1   | AA    | 513  | C    | N3-C4-N4   | 9.24  | 124.47      | 118.00   |
| 1   | AA    | 1375 | A    | C5-C6-N1   | -9.24 | 113.08      | 117.70   |
| 35  | BB    | 456  | C    | N1-C2-O2   | 9.24  | 124.44      | 118.90   |
| 35  | BB    | 545  | U    | O4'-C1'-N1 | 9.24  | 115.59      | 108.20   |
| 1   | AA    | 528  | C    | N3-C4-C5   | -9.24 | 118.20      | 121.90   |
| 1   | AA    | 941  | G    | N9-C4-C5   | -9.24 | 101.70      | 105.40   |
| 1   | AA    | 1251 | A    | C5-C6-N6   | -9.24 | 116.31      | 123.70   |
| 35  | BB    | 1792 | G    | C5-C6-O6   | -9.24 | 123.06      | 128.60   |
| 1   | AA    | 610  | U    | N3-C4-C5   | -9.24 | 109.06      | 114.60   |
| 1   | AA    | 1338 | G    | N1-C6-O6   | 9.24  | 125.44      | 119.90   |
| 35  | BB    | 500  | G    | C5-C6-O6   | -9.24 | 123.06      | 128.60   |
| 35  | BB    | 680  | C    | C5-C6-N1   | 9.24  | 125.62      | 121.00   |
| 35  | BB    | 1136 | G    | C2-N3-C4   | 9.24  | 116.52      | 111.90   |
| 35  | BB    | 2161 | C    | O4'-C1'-N1 | 9.24  | 115.59      | 108.20   |
| 35  | BB    | 2065 | C    | C5-C6-N1   | -9.24 | 116.38      | 121.00   |
| 1   | AA    | 271  | C    | C4-C5-C6   | 9.24  | 122.02      | 117.40   |
| 1   | AA    | 1507 | A    | O4'-C1'-N9 | 9.24  | 115.59      | 108.20   |
| 1   | AA    | 1306 | A    | N9-C4-C5   | -9.24 | 102.11      | 105.80   |
| 35  | BB    | 211  | C    | N3-C4-N4   | 9.24  | 124.47      | 118.00   |
| 35  | BB    | 688  | U    | O4'-C1'-N1 | 9.24  | 115.59      | 108.20   |
| 35  | BB    | 829  | A    | N1-C2-N3   | -9.24 | 124.68      | 129.30   |
| 35  | BB    | 2025 | C    | O4'-C1'-N1 | 9.24  | 115.59      | 108.20   |
| 35  | BB    | 2869 | G    | N1-C2-N3   | -9.23 | 118.36      | 123.90   |
| 1   | AA    | 399  | G    | O4'-C1'-N9 | 9.23  | 115.59      | 108.20   |
| 1   | AA    | 908  | A    | C4-C5-N7   | -9.23 | 106.08      | 110.70   |
| 1   | AA    | 1419 | G    | N1-C6-O6   | 9.23  | 125.44      | 119.90   |
| 35  | BB    | 326  | G    | C4-C5-C6   | 9.23  | 124.34      | 118.80   |
| 1   | AA    | 727  | G    | N1-C6-O6   | 9.23  | 125.44      | 119.90   |
| 35  | BB    | 960  | A    | C4-C5-N7   | -9.23 | 106.08      | 110.70   |
| 35  | BB    | 1487 | U    | O4'-C1'-N1 | 9.23  | 115.59      | 108.20   |
| 35  | BB    | 1993 | U    | O4'-C1'-N1 | 9.23  | 115.59      | 108.20   |
| 35  | BB    | 1256 | G    | C4-C5-N7   | -9.23 | 107.11      | 110.80   |
| 35  | BB    | 1993 | U    | C5-C4-O4   | -9.23 | 120.36      | 125.90   |
| 35  | BB    | 2126 | A    | C5-C6-N6   | -9.23 | 116.31      | 123.70   |
| 1   | AA    | 132  | C    | C4-C5-C6   | 9.23  | 122.01      | 117.40   |
| 1   | AA    | 1242 | G    | C5-N7-C8   | 9.23  | 108.92      | 104.30   |
| 35  | BB    | 1017 | G    | C6-C5-N7   | -9.23 | 124.86      | 130.40   |
| 1   | AA    | 1142 | G    | C5-C6-O6   | -9.23 | 123.06      | 128.60   |
| 35  | BB    | 291  | G    | C5-C6-O6   | -9.23 | 123.06      | 128.60   |
| 35  | BB    | 1387 | A    | C8-N9-C4   | -9.23 | 102.11      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1588 | G    | N3-C4-C5   | -9.23 | 123.99      | 128.60   |
| 35  | BB    | 1701 | A    | C4-C5-C6   | 9.23  | 121.61      | 117.00   |
| 35  | BB    | 2444 | G    | C6-N1-C2   | 9.23  | 130.64      | 125.10   |
| 35  | BB    | 2787 | C    | O4'-C1'-N1 | 9.23  | 115.58      | 108.20   |
| 1   | AA    | 228  | A    | C8-N9-C4   | -9.22 | 102.11      | 105.80   |
| 35  | BB    | 798  | G    | C2-N3-C4   | -9.22 | 107.29      | 111.90   |
| 1   | AA    | 1193 | G    | C5-C6-O6   | -9.22 | 123.07      | 128.60   |
| 25  | B0    | 59   | ASP  | CB-CG-OD2  | 9.22  | 126.60      | 118.30   |
| 35  | BB    | 425  | G    | N1-C6-O6   | 9.22  | 125.43      | 119.90   |
| 35  | BB    | 2659 | G    | C8-N9-C4   | -9.22 | 102.71      | 106.40   |
| 1   | AA    | 628  | G    | C5-C6-O6   | -9.22 | 123.07      | 128.60   |
| 35  | BB    | 83   | A    | C8-N9-C4   | -9.22 | 102.11      | 105.80   |
| 35  | BB    | 103  | A    | C5-C6-N1   | -9.22 | 113.09      | 117.70   |
| 35  | BB    | 468  | G    | C5-C6-O6   | -9.22 | 123.07      | 128.60   |
| 35  | BB    | 676  | A    | C5-C6-N6   | -9.22 | 116.32      | 123.70   |
| 35  | BB    | 1028 | A    | N9-C4-C5   | 9.22  | 109.49      | 105.80   |
| 35  | BB    | 1717 | A    | N1-C6-N6   | 9.22  | 124.13      | 118.60   |
| 35  | BB    | 1691 | C    | O4'-C1'-N1 | 9.22  | 115.58      | 108.20   |
| 35  | BB    | 1808 | A    | N7-C8-N9   | 9.22  | 118.41      | 113.80   |
| 35  | BB    | 2502 | G    | N1-C6-O6   | 9.22  | 125.43      | 119.90   |
| 35  | BB    | 2675 | A    | O4'-C1'-N9 | 9.22  | 115.58      | 108.20   |
| 35  | BB    | 1570 | A    | N1-C6-N6   | 9.22  | 124.13      | 118.60   |
| 35  | BB    | 2585 | U    | N3-C4-O4   | 9.22  | 125.85      | 119.40   |
| 1   | AA    | 1150 | A    | C5-C6-N1   | -9.22 | 113.09      | 117.70   |
| 35  | BB    | 2566 | A    | N1-C6-N6   | 9.22  | 124.13      | 118.60   |
| 1   | AA    | 944  | G    | O4'-C1'-N9 | 9.22  | 115.57      | 108.20   |
| 1   | AA    | 1332 | A    | O4'-C1'-N9 | 9.22  | 115.57      | 108.20   |
| 1   | AA    | 1389 | C    | O4'-C1'-N1 | 9.22  | 115.57      | 108.20   |
| 1   | AA    | 1295 | U    | O4'-C1'-N1 | 9.21  | 115.57      | 108.20   |
| 34  | BA    | 91   | C    | C5-C4-N4   | -9.21 | 113.75      | 120.20   |
| 35  | BB    | 712  | G    | C5-C6-O6   | -9.21 | 123.07      | 128.60   |
| 35  | BB    | 1470 | A    | C4-C5-C6   | 9.21  | 121.61      | 117.00   |
| 35  | BB    | 1869 | G    | C5-C6-N1   | -9.21 | 106.89      | 111.50   |
| 35  | BB    | 2661 | G    | N9-C4-C5   | -9.22 | 101.71      | 105.40   |
| 1   | AA    | 71   | A    | N1-C6-N6   | 9.21  | 124.13      | 118.60   |
| 1   | AA    | 1300 | G    | N1-C6-O6   | 9.21  | 125.43      | 119.90   |
| 35  | BB    | 1701 | A    | C5-C6-N6   | -9.21 | 116.33      | 123.70   |
| 1   | AA    | 37   | U    | O4'-C1'-N1 | 9.21  | 115.57      | 108.20   |
| 1   | AA    | 394  | G    | C5-C6-O6   | -9.21 | 123.07      | 128.60   |
| 1   | AA    | 715  | A    | C4-C5-C6   | 9.21  | 121.61      | 117.00   |
| 34  | BA    | 107  | G    | N3-C2-N2   | 9.21  | 126.35      | 119.90   |
| 35  | BB    | 594  | U    | N3-C4-O4   | 9.21  | 125.85      | 119.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 2597 | G    | N3-C2-N2   | 9.21  | 126.35      | 119.90   |
| 35  | BB    | 1873 | G    | N1-C2-N3   | -9.21 | 118.37      | 123.90   |
| 1   | AA    | 448  | A    | O4'-C1'-N9 | 9.21  | 115.57      | 108.20   |
| 1   | AA    | 480  | U    | O4'-C1'-N1 | 9.21  | 115.57      | 108.20   |
| 1   | AA    | 1079 | G    | N9-C4-C5   | 9.21  | 109.08      | 105.40   |
| 35  | BB    | 350  | G    | C5-C6-O6   | -9.21 | 123.08      | 128.60   |
| 35  | BB    | 616  | A    | C5-C6-N6   | -9.21 | 116.33      | 123.70   |
| 35  | BB    | 2644 | G    | C5-C6-O6   | -9.21 | 123.08      | 128.60   |
| 1   | AA    | 774  | G    | N3-C4-C5   | -9.20 | 124.00      | 128.60   |
| 35  | BB    | 477  | A    | C4-C5-N7   | -9.20 | 106.10      | 110.70   |
| 35  | BB    | 2236 | U    | O4'-C1'-N1 | 9.21  | 115.56      | 108.20   |
| 9   | AI    | 37   | TYR  | CB-CG-CD1  | -9.20 | 115.48      | 121.00   |
| 35  | BB    | 895  | U    | C6-N1-C2   | -9.20 | 115.48      | 121.00   |
| 35  | BB    | 1794 | A    | O4'-C1'-N9 | 9.20  | 115.56      | 108.20   |
| 35  | BB    | 1936 | A    | C5-C6-N6   | -9.20 | 116.34      | 123.70   |
| 1   | AA    | 80   | A    | C5-C6-N1   | -9.20 | 113.10      | 117.70   |
| 1   | AA    | 569  | C    | O4'-C1'-N1 | 9.20  | 115.56      | 108.20   |
| 35  | BB    | 177  | G    | N9-C4-C5   | -9.20 | 101.72      | 105.40   |
| 35  | BB    | 1721 | G    | C8-N9-C4   | -9.20 | 102.72      | 106.40   |
| 1   | AA    | 1296 | C    | C5-C6-N1   | -9.20 | 116.40      | 121.00   |
| 11  | AK    | 26   | PHE  | CB-CG-CD1  | 9.20  | 127.24      | 120.80   |
| 35  | BB    | 489  | G    | N1-C6-O6   | 9.20  | 125.42      | 119.90   |
| 35  | BB    | 707  | G    | O4'-C1'-N9 | 9.20  | 115.56      | 108.20   |
| 35  | BB    | 1122 | G    | C6-C5-N7   | -9.20 | 124.88      | 130.40   |
| 35  | BB    | 1231 | U    | C5-C6-N1   | 9.20  | 127.30      | 122.70   |
| 1   | AA    | 1076 | U    | O4'-C1'-N1 | 9.20  | 115.56      | 108.20   |
| 1   | AA    | 1386 | G    | N1-C6-O6   | 9.20  | 125.42      | 119.90   |
| 35  | BB    | 84   | A    | C5-C6-N1   | -9.20 | 113.10      | 117.70   |
| 35  | BB    | 2433 | A    | C4-C5-C6   | 9.20  | 121.60      | 117.00   |
| 1   | AA    | 40   | C    | C4-C5-C6   | 9.19  | 122.00      | 117.40   |
| 1   | AA    | 606  | G    | C6-C5-N7   | -9.19 | 124.88      | 130.40   |
| 35  | BB    | 1490 | A    | C4-C5-C6   | 9.19  | 121.60      | 117.00   |
| 35  | BB    | 2802 | G    | C5-C6-O6   | -9.20 | 123.08      | 128.60   |
| 1   | AA    | 1446 | A    | C5-C6-N1   | -9.19 | 113.10      | 117.70   |
| 35  | BB    | 375  | G    | C5-C6-O6   | -9.19 | 123.08      | 128.60   |
| 35  | BB    | 1251 | C    | C5-C4-N4   | -9.19 | 113.77      | 120.20   |
| 35  | BB    | 1359 | A    | C5-C6-N1   | -9.19 | 113.10      | 117.70   |
| 35  | BB    | 2191 | A    | O4'-C1'-N9 | 9.19  | 115.55      | 108.20   |
| 1   | AA    | 345  | C    | N3-C4-N4   | 9.19  | 124.43      | 118.00   |
| 1   | AA    | 440  | C    | N3-C4-C5   | -9.19 | 118.22      | 121.90   |
| 1   | AA    | 573  | A    | C4-C5-N7   | -9.19 | 106.11      | 110.70   |
| 35  | BB    | 735  | A    | C5-C6-N1   | -9.19 | 113.11      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 879  | C    | N3-C4-N4    | 9.19  | 124.43      | 118.00   |
| 1   | AA    | 1377 | A    | C8-N9-C4    | -9.19 | 102.12      | 105.80   |
| 35  | BB    | 1232 | G    | N1-C2-N3    | -9.19 | 118.39      | 123.90   |
| 35  | BB    | 1415 | U    | C2-N3-C4    | 9.19  | 132.51      | 127.00   |
| 35  | BB    | 1915 | U    | C4-C5-C6    | -9.19 | 114.19      | 119.70   |
| 35  | BB    | 531  | C    | C5-C4-N4    | -9.19 | 113.77      | 120.20   |
| 35  | BB    | 1998 | A    | O4'-C1'-N9  | 9.19  | 115.55      | 108.20   |
| 35  | BB    | 2040 | G    | N9-C4-C5    | -9.19 | 101.72      | 105.40   |
| 35  | BB    | 2027 | G    | O4'-C1'-N9  | 9.19  | 115.55      | 108.20   |
| 35  | BB    | 2855 | C    | O4'-C1'-N1  | 9.19  | 115.55      | 108.20   |
| 34  | BA    | 69   | G    | N1-C6-O6    | 9.19  | 125.41      | 119.90   |
| 35  | BB    | 2705 | A    | N1-C6-N6    | 9.19  | 124.11      | 118.60   |
| 1   | AA    | 792  | A    | O4'-C1'-N9  | 9.18  | 115.55      | 108.20   |
| 1   | AA    | 994  | A    | C6-N1-C2    | 9.18  | 124.11      | 118.60   |
| 1   | AA    | 1201 | A    | O4'-C1'-N9  | 9.18  | 115.55      | 108.20   |
| 35  | BB    | 1773 | A    | C5-C6-N6    | -9.18 | 116.35      | 123.70   |
| 1   | AA    | 187  | G    | N3-C2-N2    | 9.18  | 126.33      | 119.90   |
| 1   | AA    | 195  | A    | C8-N9-C4    | -9.18 | 102.13      | 105.80   |
| 35  | BB    | 1139 | G    | C5-C6-O6    | -9.18 | 123.09      | 128.60   |
| 35  | BB    | 129  | C    | C5-C4-N4    | -9.18 | 113.78      | 120.20   |
| 35  | BB    | 295  | G    | N9-C4-C5    | -9.18 | 101.73      | 105.40   |
| 35  | BB    | 485  | C    | C5-C6-N1    | 9.18  | 125.59      | 121.00   |
| 35  | BB    | 728  | G    | O4'-C1'-N9  | 9.18  | 115.54      | 108.20   |
| 35  | BB    | 2151 | U    | C5-C4-O4    | -9.18 | 120.39      | 125.90   |
| 35  | BB    | 2509 | G    | C8-N9-C4    | -9.18 | 102.73      | 106.40   |
| 35  | BB    | 2888 | C    | N3-C4-N4    | 9.18  | 124.42      | 118.00   |
| 35  | BB    | 2893 | A    | C4-C5-C6    | 9.18  | 121.59      | 117.00   |
| 1   | AA    | 564  | C    | O4'-C1'-N1  | 9.18  | 115.54      | 108.20   |
| 1   | AA    | 923  | A    | N7-C8-N9    | -9.18 | 109.21      | 113.80   |
| 1   | AA    | 977  | A    | C6-N1-C2    | 9.17  | 124.10      | 118.60   |
| 35  | BB    | 487  | C    | C2-N3-C4    | 9.17  | 124.49      | 119.90   |
| 35  | BB    | 742  | A    | O4'-C1'-N9  | 9.17  | 115.54      | 108.20   |
| 35  | BB    | 1485 | U    | O4'-C1'-N1  | 9.17  | 115.54      | 108.20   |
| 35  | BB    | 2250 | G    | N1-C6-O6    | 9.17  | 125.41      | 119.90   |
| 1   | AA    | 509  | A    | C5-C6-N6    | -9.17 | 116.36      | 123.70   |
| 1   | AA    | 1368 | A    | C4'-C3'-C2' | -9.17 | 93.43       | 102.60   |
| 9   | AI    | 79   | ARG  | NE-CZ-NH1   | 9.17  | 124.88      | 120.30   |
| 22  | AV    | 72   | G    | O4'-C1'-N9  | 9.17  | 115.54      | 108.20   |
| 1   | AA    | 223  | A    | C5-C6-N1    | -9.17 | 113.12      | 117.70   |
| 1   | AA    | 586  | C    | P-O3'-C3'   | -9.17 | 108.70      | 119.70   |
| 35  | BB    | 669  | G    | C5'-C4'-O4' | 9.17  | 120.10      | 109.10   |
| 1   | AA    | 889  | A    | C4-C5-N7    | -9.17 | 106.12      | 110.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1188 | A    | C2-N3-C4   | -9.17 | 106.02      | 110.60   |
| 35  | BB    | 675  | A    | C4-C5-C6   | 9.17  | 121.58      | 117.00   |
| 1   | AA    | 506  | G    | O4'-C1'-N9 | 9.16  | 115.53      | 108.20   |
| 1   | AA    | 519  | C    | N3-C4-N4   | 9.16  | 124.42      | 118.00   |
| 1   | AA    | 1174 | G    | N1-C6-O6   | 9.16  | 125.40      | 119.90   |
| 35  | BB    | 36   | G    | N1-C6-O6   | 9.16  | 125.40      | 119.90   |
| 35  | BB    | 929  | U    | C4-C5-C6   | -9.16 | 114.20      | 119.70   |
| 35  | BB    | 1005 | C    | N3-C4-N4   | 9.16  | 124.42      | 118.00   |
| 35  | BB    | 1085 | A    | C4-C5-C6   | 9.16  | 121.58      | 117.00   |
| 47  | BN    | 64   | ARG  | NE-CZ-NH2  | -9.16 | 115.72      | 120.30   |
| 35  | BB    | 192  | C    | C4-C5-C6   | 9.16  | 121.98      | 117.40   |
| 35  | BB    | 764  | A    | C4-C5-C6   | 9.16  | 121.58      | 117.00   |
| 35  | BB    | 1618 | A    | C5-C6-N6   | -9.16 | 116.37      | 123.70   |
| 35  | BB    | 2631 | G    | N9-C4-C5   | -9.16 | 101.73      | 105.40   |
| 4   | AD    | 43   | ARG  | NE-CZ-NH2  | -9.16 | 115.72      | 120.30   |
| 1   | AA    | 510  | A    | N1-C6-N6   | 9.16  | 124.09      | 118.60   |
| 1   | AA    | 1379 | G    | N1-C6-O6   | 9.16  | 125.39      | 119.90   |
| 35  | BB    | 150  | U    | O4'-C1'-N1 | 9.16  | 115.53      | 108.20   |
| 35  | BB    | 436  | C    | P-O3'-C3'  | -9.16 | 108.71      | 119.70   |
| 35  | BB    | 2889 | C    | O4'-C1'-N1 | 9.16  | 115.53      | 108.20   |
| 1   | AA    | 491  | G    | C5-N7-C8   | -9.16 | 99.72       | 104.30   |
| 35  | BB    | 605  | G    | N9-C4-C5   | -9.16 | 101.74      | 105.40   |
| 35  | BB    | 1758 | U    | C6-N1-C1'  | -9.16 | 108.38      | 121.20   |
| 35  | BB    | 1491 | G    | C5-C6-N1   | -9.16 | 106.92      | 111.50   |
| 35  | BB    | 1749 | A    | C5-C6-N1   | -9.15 | 113.12      | 117.70   |
| 1   | AA    | 194  | C    | N3-C4-C5   | -9.15 | 118.24      | 121.90   |
| 1   | AA    | 1163 | A    | C5-C6-N1   | -9.15 | 113.12      | 117.70   |
| 1   | AA    | 1171 | A    | N1-C6-N6   | 9.15  | 124.09      | 118.60   |
| 35  | BB    | 1968 | G    | C5-C6-O6   | -9.15 | 123.11      | 128.60   |
| 35  | BB    | 2224 | G    | C6-C5-N7   | -9.15 | 124.91      | 130.40   |
| 35  | BB    | 2600 | A    | C5-C6-N1   | -9.15 | 113.12      | 117.70   |
| 35  | BB    | 2632 | A    | C5-C6-N1   | -9.15 | 113.12      | 117.70   |
| 35  | BB    | 2864 | G    | N3-C2-N2   | 9.15  | 126.31      | 119.90   |
| 1   | AA    | 1311 | A    | N1-C6-N6   | 9.15  | 124.09      | 118.60   |
| 3   | AC    | 168  | ARG  | NE-CZ-NH2  | -9.15 | 115.72      | 120.30   |
| 35  | BB    | 314  | C    | C6-N1-C2   | -9.15 | 116.64      | 120.30   |
| 35  | BB    | 371  | A    | C6-N1-C2   | 9.15  | 124.09      | 118.60   |
| 35  | BB    | 1232 | G    | C5-C6-O6   | -9.15 | 123.11      | 128.60   |
| 1   | AA    | 1498 | U    | C6-N1-C2   | 9.15  | 126.49      | 121.00   |
| 35  | BB    | 1074 | G    | C4-C5-N7   | -9.15 | 107.14      | 110.80   |
| 35  | BB    | 2311 | A    | C4-C5-N7   | -9.15 | 106.12      | 110.70   |
| 35  | BB    | 2564 | A    | N1-C6-N6   | 9.15  | 124.09      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2688 | G    | O4'-C1'-N9  | 9.15  | 115.52      | 108.20   |
| 1   | AA    | 517  | G    | C4-C5-C6    | 9.15  | 124.29      | 118.80   |
| 35  | BB    | 653  | U    | N1-C2-O2    | 9.15  | 129.20      | 122.80   |
| 1   | AA    | 640  | A    | C5-N7-C8    | 9.15  | 108.47      | 103.90   |
| 1   | AA    | 1526 | G    | N1-C6-O6    | 9.15  | 125.39      | 119.90   |
| 35  | BB    | 49   | A    | C6-C5-N7    | -9.15 | 125.90      | 132.30   |
| 35  | BB    | 2198 | A    | P-O3'-C3'   | 9.15  | 130.68      | 119.70   |
| 35  | BB    | 2212 | A    | N1-C6-N6    | 9.15  | 124.09      | 118.60   |
| 35  | BB    | 2478 | A    | C4-C5-C6    | 9.15  | 121.58      | 117.00   |
| 35  | BB    | 679  | C    | N3-C4-C5    | -9.15 | 118.24      | 121.90   |
| 35  | BB    | 1237 | A    | C4-C5-C6    | 9.15  | 121.57      | 117.00   |
| 35  | BB    | 2201 | G    | C6-C5-N7    | -9.15 | 124.91      | 130.40   |
| 35  | BB    | 1451 | C    | C3'-C2'-C1' | 9.15  | 108.82      | 101.50   |
| 35  | BB    | 2614 | A    | N1-C6-N6    | 9.15  | 124.09      | 118.60   |
| 1   | AA    | 30   | U    | O4'-C1'-N1  | 9.14  | 115.52      | 108.20   |
| 1   | AA    | 568  | G    | N1-C6-O6    | 9.14  | 125.39      | 119.90   |
| 35  | BB    | 1270 | C    | C5-C4-N4    | -9.14 | 113.80      | 120.20   |
| 1   | AA    | 136  | C    | N3-C4-N4    | 9.14  | 124.40      | 118.00   |
| 1   | AA    | 592  | G    | C4-C5-C6    | 9.14  | 124.29      | 118.80   |
| 1   | AA    | 1024 | G    | N1-C6-O6    | 9.14  | 125.39      | 119.90   |
| 35  | BB    | 1062 | G    | C5-N7-C8    | 9.14  | 108.87      | 104.30   |
| 35  | BB    | 1083 | U    | O4'-C1'-N1  | 9.14  | 115.51      | 108.20   |
| 35  | BB    | 1634 | A    | C5-C6-N1    | -9.14 | 113.13      | 117.70   |
| 35  | BB    | 2379 | G    | C6-C5-N7    | -9.14 | 124.91      | 130.40   |
| 1   | AA    | 338  | A    | O4'-C1'-N9  | 9.14  | 115.51      | 108.20   |
| 35  | BB    | 1639 | C    | N3-C4-C5    | -9.14 | 118.24      | 121.90   |
| 35  | BB    | 238  | C    | C5-C4-N4    | -9.14 | 113.80      | 120.20   |
| 35  | BB    | 728  | G    | N1-C6-O6    | 9.14  | 125.38      | 119.90   |
| 35  | BB    | 1539 | U    | O4'-C1'-N1  | 9.14  | 115.51      | 108.20   |
| 35  | BB    | 1908 | C    | N3-C4-N4    | 9.14  | 124.40      | 118.00   |
| 35  | BB    | 2428 | G    | O4'-C1'-N9  | 9.14  | 115.51      | 108.20   |
| 1   | AA    | 667  | G    | C5-C6-N1    | -9.14 | 106.93      | 111.50   |
| 22  | AV    | 39   | G    | N3-C4-C5    | -9.14 | 124.03      | 128.60   |
| 22  | AV    | 43   | G    | N1-C6-O6    | 9.14  | 125.38      | 119.90   |
| 35  | BB    | 1020 | A    | C5-C6-N1    | -9.14 | 113.13      | 117.70   |
| 35  | BB    | 1736 | U    | O4'-C1'-N1  | 9.14  | 115.51      | 108.20   |
| 35  | BB    | 2407 | A    | C4-C5-C6    | 9.14  | 121.57      | 117.00   |
| 35  | BB    | 2754 | U    | O4'-C1'-N1  | 9.14  | 115.51      | 108.20   |
| 1   | AA    | 384  | G    | C5-N7-C8    | -9.14 | 99.73       | 104.30   |
| 1   | AA    | 471  | U    | O4'-C1'-N1  | 9.13  | 115.51      | 108.20   |
| 1   | AA    | 1080 | A    | N1-C6-N6    | 9.13  | 124.08      | 118.60   |
| 16  | AP    | 32   | PHE  | CB-CG-CD2   | 9.14  | 127.19      | 120.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1412 | U    | C2-N3-C4    | -9.13 | 121.52      | 127.00   |
| 35  | BB    | 2028 | U    | C5-C6-N1    | 9.14  | 127.27      | 122.70   |
| 35  | BB    | 1740 | G    | N3-C2-N2    | 9.13  | 126.29      | 119.90   |
| 35  | BB    | 2458 | G    | O4'-C1'-N9  | 9.13  | 115.51      | 108.20   |
| 1   | AA    | 206  | C    | N3-C4-C5    | -9.13 | 118.25      | 121.90   |
| 18  | AR    | 31   | TYR  | CB-CG-CD2   | -9.13 | 115.52      | 121.00   |
| 35  | BB    | 426  | C    | O4'-C1'-N1  | 9.13  | 115.51      | 108.20   |
| 35  | BB    | 1341 | G    | C8-N9-C4    | -9.13 | 102.75      | 106.40   |
| 35  | BB    | 1959 | G    | N3-C4-C5    | 9.13  | 133.16      | 128.60   |
| 35  | BB    | 2678 | C    | O4'-C1'-N1  | 9.13  | 115.51      | 108.20   |
| 1   | AA    | 67   | C    | O4'-C1'-N1  | 9.13  | 115.50      | 108.20   |
| 1   | AA    | 865  | A    | C5-C6-N6    | -9.13 | 116.40      | 123.70   |
| 3   | AC    | 192  | TYR  | CB-CG-CD2   | -9.13 | 115.52      | 121.00   |
| 35  | BB    | 505  | A    | C5-C6-N6    | -9.13 | 116.40      | 123.70   |
| 1   | AA    | 1485 | U    | O4'-C1'-N1  | 9.13  | 115.50      | 108.20   |
| 35  | BB    | 423  | A    | N1-C6-N6    | 9.13  | 124.08      | 118.60   |
| 35  | BB    | 1983 | G    | P-O3'-C3'   | -9.13 | 108.75      | 119.70   |
| 35  | BB    | 2669 | G    | N1-C2-N3    | -9.13 | 118.42      | 123.90   |
| 35  | BB    | 1237 | A    | O4'-C1'-N9  | 9.13  | 115.50      | 108.20   |
| 35  | BB    | 2397 | G    | C6-C5-N7    | -9.13 | 124.92      | 130.40   |
| 1   | AA    | 410  | G    | N3-C2-N2    | 9.13  | 126.29      | 119.90   |
| 1   | AA    | 1397 | C    | N3-C4-N4    | 9.12  | 124.39      | 118.00   |
| 1   | AA    | 1486 | G    | C5-C6-O6    | -9.12 | 123.12      | 128.60   |
| 35  | BB    | 342  | A    | C5-C6-N1    | -9.12 | 113.14      | 117.70   |
| 35  | BB    | 1435 | G    | C5-N7-C8    | 9.13  | 108.86      | 104.30   |
| 35  | BB    | 2229 | U    | N3-C2-O2    | -9.13 | 115.81      | 122.20   |
| 35  | BB    | 457  | A    | C5-N7-C8    | 9.12  | 108.46      | 103.90   |
| 35  | BB    | 1626 | A    | C6-N1-C2    | 9.12  | 124.08      | 118.60   |
| 35  | BB    | 1768 | C    | N3-C4-C5    | -9.12 | 118.25      | 121.90   |
| 35  | BB    | 2829 | A    | N9-C4-C5    | -9.12 | 102.15      | 105.80   |
| 1   | AA    | 556  | C    | O4'-C1'-N1  | 9.12  | 115.50      | 108.20   |
| 1   | AA    | 1316 | G    | C6-N1-C2    | 9.12  | 130.57      | 125.10   |
| 22  | AV    | 31   | C    | O4'-C1'-N1  | 9.12  | 115.50      | 108.20   |
| 35  | BB    | 299  | A    | N9-C4-C5    | 9.12  | 109.45      | 105.80   |
| 35  | BB    | 498  | G    | O4'-C4'-C3' | -9.12 | 94.88       | 104.00   |
| 35  | BB    | 634  | C    | N3-C4-N4    | 9.12  | 124.39      | 118.00   |
| 1   | AA    | 241  | G    | C5-C6-O6    | -9.12 | 123.13      | 128.60   |
| 1   | AA    | 910  | C    | C6-N1-C2    | -9.12 | 116.65      | 120.30   |
| 1   | AA    | 1222 | G    | N9-C4-C5    | 9.12  | 109.05      | 105.40   |
| 35  | BB    | 706  | A    | C6-C5-N7    | -9.12 | 125.92      | 132.30   |
| 35  | BB    | 1540 | G    | N1-C2-N3    | -9.12 | 118.43      | 123.90   |
| 35  | BB    | 2073 | C    | N3-C4-C5    | -9.12 | 118.25      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 601  | C    | O4'-C1'-N1 | 9.12  | 115.49      | 108.20   |
| 35  | BB    | 1834 | U    | C5-C6-N1   | 9.12  | 127.26      | 122.70   |
| 35  | BB    | 2292 | U    | O4'-C1'-N1 | 9.12  | 115.49      | 108.20   |
| 35  | BB    | 2895 | G    | C4-C5-N7   | -9.12 | 107.15      | 110.80   |
| 1   | AA    | 1033 | G    | N1-C6-O6   | 9.12  | 125.37      | 119.90   |
| 34  | BA    | 98   | G    | C4-C5-N7   | 9.12  | 114.45      | 110.80   |
| 35  | BB    | 191  | A    | C4-C5-N7   | -9.12 | 106.14      | 110.70   |
| 35  | BB    | 254  | G    | N1-C6-O6   | 9.12  | 125.37      | 119.90   |
| 35  | BB    | 2325 | G    | C6-C5-N7   | -9.12 | 124.93      | 130.40   |
| 35  | BB    | 350  | G    | C6-C5-N7   | -9.11 | 124.93      | 130.40   |
| 35  | BB    | 2896 | C    | N3-C4-N4   | 9.11  | 124.38      | 118.00   |
| 1   | AA    | 838  | G    | N9-C4-C5   | -9.11 | 101.75      | 105.40   |
| 35  | BB    | 408  | G    | N1-C6-O6   | 9.11  | 125.37      | 119.90   |
| 1   | AA    | 117  | G    | N1-C2-N3   | -9.11 | 118.43      | 123.90   |
| 1   | AA    | 535  | A    | N9-C4-C5   | 9.11  | 109.44      | 105.80   |
| 1   | AA    | 901  | A    | N1-C6-N6   | 9.11  | 124.07      | 118.60   |
| 1   | AA    | 1164 | G    | C6-C5-N7   | -9.11 | 124.93      | 130.40   |
| 34  | BA    | 35   | C    | C6-N1-C1'  | -9.11 | 109.87      | 120.80   |
| 35  | BB    | 1989 | G    | C5-C6-N1   | -9.11 | 106.94      | 111.50   |
| 1   | AA    | 419  | C    | N3-C4-N4   | 9.11  | 124.38      | 118.00   |
| 1   | AA    | 229  | U    | N1-C2-N3   | -9.11 | 109.44      | 114.90   |
| 1   | AA    | 1500 | A    | C6-C5-N7   | -9.11 | 125.92      | 132.30   |
| 35  | BB    | 51   | G    | C6-C5-N7   | -9.11 | 124.94      | 130.40   |
| 35  | BB    | 115  | C    | N3-C4-C5   | -9.11 | 118.26      | 121.90   |
| 35  | BB    | 1992 | G    | C8-N9-C4   | -9.11 | 102.76      | 106.40   |
| 35  | BB    | 2046 | G    | C6-C5-N7   | -9.11 | 124.94      | 130.40   |
| 35  | BB    | 2055 | C    | O4'-C1'-N1 | 9.11  | 115.49      | 108.20   |
| 35  | BB    | 2530 | A    | C4-C5-C6   | 9.11  | 121.56      | 117.00   |
| 4   | AD    | 2    | ARG  | NE-CZ-NH1  | 9.11  | 124.85      | 120.30   |
| 35  | BB    | 299  | A    | C5-C6-N1   | -9.11 | 113.15      | 117.70   |
| 1   | AA    | 1384 | C    | N3-C4-N4   | 9.10  | 124.37      | 118.00   |
| 35  | BB    | 485  | C    | O4'-C1'-N1 | 9.10  | 115.48      | 108.20   |
| 35  | BB    | 834  | G    | O4'-C1'-N9 | 9.10  | 115.48      | 108.20   |
| 35  | BB    | 1530 | G    | C5-C6-N1   | -9.10 | 106.95      | 111.50   |
| 1   | AA    | 538  | G    | O4'-C1'-N9 | 9.10  | 115.48      | 108.20   |
| 1   | AA    | 1377 | A    | N9-C4-C5   | 9.10  | 109.44      | 105.80   |
| 34  | BA    | 94   | A    | N1-C6-N6   | 9.10  | 124.06      | 118.60   |
| 35  | BB    | 1793 | C    | C5-C6-N1   | 9.10  | 125.55      | 121.00   |
| 35  | BB    | 528  | A    | C5-C6-N1   | -9.10 | 113.15      | 117.70   |
| 35  | BB    | 2750 | A    | O4'-C1'-N9 | 9.10  | 115.48      | 108.20   |
| 1   | AA    | 6    | G    | C5-N7-C8   | -9.10 | 99.75       | 104.30   |
| 1   | AA    | 773  | G    | C6-C5-N7   | -9.10 | 124.94      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1363 | A    | N1-C6-N6    | 9.10  | 124.06      | 118.60   |
| 1   | AA    | 1468 | A    | N1-C2-N3    | 9.10  | 133.85      | 129.30   |
| 35  | BB    | 250  | G    | C5-C6-N1    | -9.10 | 106.95      | 111.50   |
| 35  | BB    | 330  | A    | C5-C6-N6    | -9.10 | 116.42      | 123.70   |
| 35  | BB    | 428  | A    | N1-C6-N6    | 9.10  | 124.06      | 118.60   |
| 1   | AA    | 6    | G    | N3-C4-C5    | 9.10  | 133.15      | 128.60   |
| 1   | AA    | 89   | U    | C5-C6-N1    | 9.10  | 127.25      | 122.70   |
| 2   | AB    | 207  | ARG  | NE-CZ-NH2   | -9.10 | 115.75      | 120.30   |
| 35  | BB    | 665  | U    | O4'-C1'-N1  | 9.10  | 115.48      | 108.20   |
| 35  | BB    | 956  | G    | N1-C6-O6    | 9.10  | 125.36      | 119.90   |
| 35  | BB    | 1218 | G    | O4'-C1'-N9  | 9.10  | 115.48      | 108.20   |
| 35  | BB    | 1828 | G    | N1-C2-N3    | -9.10 | 118.44      | 123.90   |
| 35  | BB    | 1858 | A    | O4'-C1'-N9  | 9.10  | 115.48      | 108.20   |
| 1   | AA    | 1290 | G    | C6-C5-N7    | -9.09 | 124.94      | 130.40   |
| 1   | AA    | 41   | G    | N9-C4-C5    | -9.09 | 101.76      | 105.40   |
| 35  | BB    | 122  | G    | P-O3'-C3'   | -9.09 | 108.79      | 119.70   |
| 35  | BB    | 900  | A    | C5-N7-C8    | 9.09  | 108.45      | 103.90   |
| 35  | BB    | 965  | C    | O4'-C1'-N1  | 9.09  | 115.47      | 108.20   |
| 1   | AA    | 435  | A    | C8-N9-C4    | -9.09 | 102.16      | 105.80   |
| 1   | AA    | 398  | U    | O4'-C1'-N1  | 9.09  | 115.47      | 108.20   |
| 35  | BB    | 494  | G    | N7-C8-N9    | 9.09  | 117.64      | 113.10   |
| 35  | BB    | 780  | G    | C4-C5-N7    | -9.09 | 107.16      | 110.80   |
| 35  | BB    | 2751 | G    | N1-C6-O6    | 9.09  | 125.35      | 119.90   |
| 1   | AA    | 65   | A    | N1-C6-N6    | 9.09  | 124.05      | 118.60   |
| 1   | AA    | 845  | A    | C5-N7-C8    | 9.09  | 108.44      | 103.90   |
| 1   | AA    | 988  | G    | C5-C6-N1    | 9.09  | 116.04      | 111.50   |
| 13  | AM    | 82   | LEU  | CB-CG-CD2   | 9.09  | 126.45      | 111.00   |
| 35  | BB    | 1341 | G    | N3-C2-N2    | 9.09  | 126.26      | 119.90   |
| 35  | BB    | 1615 | C    | C6-N1-C2    | -9.09 | 116.67      | 120.30   |
| 1   | AA    | 1117 | A    | C5-C6-N1    | -9.09 | 113.16      | 117.70   |
| 1   | AA    | 1173 | U    | N3-C4-O4    | 9.09  | 125.76      | 119.40   |
| 35  | BB    | 361  | G    | C4-C5-C6    | 9.09  | 124.25      | 118.80   |
| 35  | BB    | 1472 | C    | C2-N3-C4    | 9.09  | 124.44      | 119.90   |
| 35  | BB    | 1787 | A    | C5-C6-N6    | -9.09 | 116.43      | 123.70   |
| 35  | BB    | 2091 | C    | O4'-C1'-N1  | 9.09  | 115.47      | 108.20   |
| 1   | AA    | 1331 | G    | N3-C4-N9    | 9.08  | 131.45      | 126.00   |
| 1   | AA    | 1499 | A    | C5-C6-N1    | -9.08 | 113.16      | 117.70   |
| 35  | BB    | 543  | G    | N1-C2-N3    | -9.08 | 118.45      | 123.90   |
| 35  | BB    | 1070 | A    | C4'-C3'-C2' | -9.08 | 93.52       | 102.60   |
| 35  | BB    | 1617 | C    | N3-C4-C5    | -9.08 | 118.27      | 121.90   |
| 35  | BB    | 2225 | A    | C5-C6-N6    | -9.08 | 116.43      | 123.70   |
| 35  | BB    | 2267 | A    | C8-N9-C4    | -9.08 | 102.17      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1480 | A    | O4'-C1'-N9 | 9.08  | 115.46      | 108.20   |
| 34  | BA    | 45   | A    | C4-C5-N7   | -9.08 | 106.16      | 110.70   |
| 35  | BB    | 2707 | U    | O4'-C1'-N1 | 9.08  | 115.47      | 108.20   |
| 35  | BB    | 159  | G    | N1-C2-N3   | -9.08 | 118.45      | 123.90   |
| 35  | BB    | 721  | A    | C5-C6-N6   | -9.08 | 116.44      | 123.70   |
| 35  | BB    | 283  | G    | N1-C2-N3   | -9.08 | 118.45      | 123.90   |
| 35  | BB    | 741  | U    | C5-C4-O4   | -9.08 | 120.45      | 125.90   |
| 35  | BB    | 1597 | A    | C5-C6-N1   | -9.08 | 113.16      | 117.70   |
| 35  | BB    | 1975 | G    | N3-C2-N2   | 9.08  | 126.25      | 119.90   |
| 35  | BB    | 2110 | G    | N1-C2-N3   | -9.08 | 118.45      | 123.90   |
| 35  | BB    | 2221 | G    | C6-C5-N7   | -9.08 | 124.95      | 130.40   |
| 35  | BB    | 2351 | G    | N3-C2-N2   | 9.08  | 126.25      | 119.90   |
| 1   | AA    | 389  | A    | N1-C2-N3   | 9.07  | 133.84      | 129.30   |
| 1   | AA    | 738  | C    | C2-N3-C4   | 9.07  | 124.44      | 119.90   |
| 35  | BB    | 578  | G    | N1-C6-O6   | 9.07  | 125.34      | 119.90   |
| 35  | BB    | 1118 | C    | C5-C4-N4   | -9.07 | 113.85      | 120.20   |
| 35  | BB    | 1347 | A    | C5-C6-N1   | -9.07 | 113.16      | 117.70   |
| 35  | BB    | 1677 | A    | C5-C6-N1   | -9.07 | 113.16      | 117.70   |
| 35  | BB    | 1802 | A    | C5-N7-C8   | 9.07  | 108.44      | 103.90   |
| 35  | BB    | 260  | G    | C2-N3-C4   | 9.07  | 116.44      | 111.90   |
| 35  | BB    | 979  | A    | N7-C8-N9   | -9.07 | 109.27      | 113.80   |
| 35  | BB    | 1426 | G    | N3-C2-N2   | 9.07  | 126.25      | 119.90   |
| 35  | BB    | 1760 | C    | N3-C4-N4   | 9.07  | 124.35      | 118.00   |
| 35  | BB    | 1823 | G    | N3-C4-C5   | 9.07  | 133.13      | 128.60   |
| 53  | BT    | 20   | ALA  | N-CA-CB    | 9.07  | 122.80      | 110.10   |
| 35  | BB    | 2440 | C    | N3-C4-N4   | 9.07  | 124.35      | 118.00   |
| 35  | BB    | 896  | A    | C5-C6-N1   | -9.07 | 113.17      | 117.70   |
| 35  | BB    | 421  | C    | C5-C6-N1   | 9.07  | 125.53      | 121.00   |
| 35  | BB    | 1439 | A    | O4'-C1'-N9 | 9.07  | 115.45      | 108.20   |
| 35  | BB    | 1745 | A    | N1-C2-N3   | 9.07  | 133.83      | 129.30   |
| 35  | BB    | 2722 | G    | C5-C6-O6   | -9.07 | 123.16      | 128.60   |
| 1   | AA    | 596  | A    | O4'-C1'-N9 | 9.06  | 115.45      | 108.20   |
| 30  | B5    | 7    | ARG  | NE-CZ-NH1  | 9.06  | 124.83      | 120.30   |
| 35  | BB    | 198  | C    | C5-C4-N4   | -9.06 | 113.86      | 120.20   |
| 35  | BB    | 476  | G    | C5-C6-N1   | 9.06  | 116.03      | 111.50   |
| 35  | BB    | 1916 | A    | C4-C5-C6   | 9.06  | 121.53      | 117.00   |
| 35  | BB    | 2428 | G    | N1-C6-O6   | 9.06  | 125.34      | 119.90   |
| 35  | BB    | 57   | C    | O4'-C1'-N1 | 9.06  | 115.45      | 108.20   |
| 35  | BB    | 1487 | U    | C5-C6-N1   | 9.06  | 127.23      | 122.70   |
| 1   | AA    | 416  | G    | N1-C6-O6   | 9.06  | 125.34      | 119.90   |
| 1   | AA    | 1134 | G    | N1-C6-O6   | 9.06  | 125.34      | 119.90   |
| 1   | AA    | 1144 | G    | N9-C4-C5   | 9.06  | 109.02      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 32  | B7    | 12   | ARG  | NE-CZ-NH1  | -9.06 | 115.77      | 120.30   |
| 35  | BB    | 161  | A    | C5-C6-N1   | -9.06 | 113.17      | 117.70   |
| 35  | BB    | 172  | A    | N1-C6-N6   | 9.06  | 124.04      | 118.60   |
| 35  | BB    | 453  | A    | N1-C6-N6   | 9.06  | 124.04      | 118.60   |
| 35  | BB    | 578  | G    | C6-C5-N7   | -9.06 | 124.96      | 130.40   |
| 35  | BB    | 697  | G    | C2-N3-C4   | 9.06  | 116.43      | 111.90   |
| 35  | BB    | 1617 | C    | C2-N1-C1'  | 9.06  | 128.77      | 118.80   |
| 35  | BB    | 1873 | G    | C5-C6-O6   | -9.06 | 123.16      | 128.60   |
| 1   | AA    | 512  | U    | C5-C4-O4   | -9.06 | 120.47      | 125.90   |
| 1   | AA    | 595  | A    | C4-C5-C6   | 9.06  | 121.53      | 117.00   |
| 35  | BB    | 189  | G    | O4'-C1'-N9 | 9.06  | 115.45      | 108.20   |
| 35  | BB    | 1085 | A    | C4-C5-N7   | -9.06 | 106.17      | 110.70   |
| 35  | BB    | 1121 | C    | O4'-C1'-N1 | 9.06  | 115.45      | 108.20   |
| 35  | BB    | 1677 | A    | C5-N7-C8   | 9.06  | 108.43      | 103.90   |
| 35  | BB    | 1888 | G    | O4'-C1'-N9 | 9.06  | 115.45      | 108.20   |
| 35  | BB    | 2275 | C    | N3-C4-N4   | 9.06  | 124.34      | 118.00   |
| 35  | BB    | 2433 | A    | C2-N3-C4   | -9.06 | 106.07      | 110.60   |
| 1   | AA    | 15   | G    | C6-C5-N7   | -9.06 | 124.97      | 130.40   |
| 1   | AA    | 959  | A    | P-O3'-C3'  | 9.06  | 130.57      | 119.70   |
| 1   | AA    | 1429 | A    | C5-C6-N6   | -9.06 | 116.45      | 123.70   |
| 35  | BB    | 338  | G    | C5-C6-O6   | -9.06 | 123.17      | 128.60   |
| 35  | BB    | 2451 | A    | N1-C6-N6   | 9.06  | 124.03      | 118.60   |
| 35  | BB    | 2561 | U    | O4'-C1'-N1 | 9.06  | 115.44      | 108.20   |
| 47  | BN    | 69   | ARG  | NE-CZ-NH1  | 9.06  | 124.83      | 120.30   |
| 1   | AA    | 138  | G    | N9-C4-C5   | -9.05 | 101.78      | 105.40   |
| 1   | AA    | 674  | G    | N1-C6-O6   | 9.05  | 125.33      | 119.90   |
| 1   | AA    | 677  | U    | O4'-C1'-N1 | 9.05  | 115.44      | 108.20   |
| 35  | BB    | 2883 | A    | C5-C6-N6   | -9.05 | 116.46      | 123.70   |
| 35  | BB    | 1266 | G    | C5-C6-O6   | -9.05 | 123.17      | 128.60   |
| 35  | BB    | 681  | G    | O4'-C1'-N9 | 9.05  | 115.44      | 108.20   |
| 35  | BB    | 808  | G    | C4-C5-N7   | 9.05  | 114.42      | 110.80   |
| 35  | BB    | 870  | U    | O4'-C1'-N1 | 9.05  | 115.44      | 108.20   |
| 35  | BB    | 1168 | G    | C5-C6-N1   | -9.05 | 106.97      | 111.50   |
| 35  | BB    | 310  | A    | N7-C8-N9   | -9.05 | 109.28      | 113.80   |
| 35  | BB    | 1407 | G    | N9-C4-C5   | 9.05  | 109.02      | 105.40   |
| 35  | BB    | 1483 | G    | C5-C6-O6   | -9.05 | 123.17      | 128.60   |
| 35  | BB    | 2114 | A    | C4-C5-C6   | 9.05  | 121.52      | 117.00   |
| 35  | BB    | 2573 | C    | N3-C4-N4   | 9.05  | 124.33      | 118.00   |
| 1   | AA    | 179  | A    | N1-C2-N3   | -9.04 | 124.78      | 129.30   |
| 1   | AA    | 220  | G    | C5-C6-O6   | -9.04 | 123.17      | 128.60   |
| 7   | AG    | 137  | ARG  | NE-CZ-NH1  | 9.04  | 124.82      | 120.30   |
| 35  | BB    | 713  | G    | C8-N9-C4   | 9.05  | 110.02      | 106.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 2686 | G    | N1-C2-N3   | -9.04 | 118.47      | 123.90   |
| 1   | AA    | 174  | A    | C8-N9-C4   | 9.04  | 109.42      | 105.80   |
| 1   | AA    | 728  | A    | N1-C2-N3   | -9.04 | 124.78      | 129.30   |
| 1   | AA    | 1079 | G    | C8-N9-C4   | -9.04 | 102.78      | 106.40   |
| 35  | BB    | 625  | G    | N1-C2-N3   | -9.04 | 118.47      | 123.90   |
| 35  | BB    | 1123 | C    | N3-C4-C5   | -9.04 | 118.28      | 121.90   |
| 1   | AA    | 860  | A    | C5-C6-N6   | -9.04 | 116.47      | 123.70   |
| 1   | AA    | 964  | A    | C5-C6-N6   | -9.04 | 116.47      | 123.70   |
| 35  | BB    | 670  | A    | C8-N9-C4   | -9.04 | 102.19      | 105.80   |
| 35  | BB    | 1984 | G    | C4-C5-N7   | 9.04  | 114.42      | 110.80   |
| 35  | BB    | 2432 | A    | C5-C6-N1   | -9.04 | 113.18      | 117.70   |
| 1   | AA    | 665  | A    | O4'-C1'-N9 | 9.04  | 115.43      | 108.20   |
| 1   | AA    | 1072 | G    | C5-C6-O6   | -9.04 | 123.18      | 128.60   |
| 1   | AA    | 1163 | A    | C8-N9-C4   | -9.04 | 102.19      | 105.80   |
| 1   | AA    | 1458 | G    | C2-N3-C4   | -9.04 | 107.38      | 111.90   |
| 34  | BA    | 92   | C    | N3-C4-C5   | -9.04 | 118.28      | 121.90   |
| 35  | BB    | 1894 | C    | C5-C6-N1   | 9.04  | 125.52      | 121.00   |
| 35  | BB    | 2645 | G    | N1-C6-O6   | 9.04  | 125.32      | 119.90   |
| 35  | BB    | 2649 | C    | C5-C4-N4   | -9.04 | 113.88      | 120.20   |
| 35  | BB    | 2844 | G    | C5-C6-O6   | -9.04 | 123.18      | 128.60   |
| 22  | AV    | 15   | G    | N1-C6-O6   | 9.03  | 125.32      | 119.90   |
| 35  | BB    | 141  | G    | O4'-C1'-N9 | 9.03  | 115.43      | 108.20   |
| 35  | BB    | 693  | A    | N1-C2-N3   | 9.03  | 133.82      | 129.30   |
| 35  | BB    | 1129 | A    | O4'-C1'-N9 | 9.03  | 115.43      | 108.20   |
| 35  | BB    | 1458 | U    | O4'-C1'-N1 | 9.03  | 115.42      | 108.20   |
| 35  | BB    | 1521 | G    | O4'-C1'-N9 | 9.03  | 115.42      | 108.20   |
| 35  | BB    | 2158 | A    | C5-C6-N1   | -9.03 | 113.18      | 117.70   |
| 35  | BB    | 1927 | A    | P-O3'-C3'  | 9.03  | 130.54      | 119.70   |
| 35  | BB    | 2842 | G    | C4-C5-N7   | -9.03 | 107.19      | 110.80   |
| 1   | AA    | 275  | G    | O4'-C1'-N9 | 9.03  | 115.42      | 108.20   |
| 1   | AA    | 373  | A    | C2-N3-C4   | 9.03  | 115.11      | 110.60   |
| 1   | AA    | 490  | C    | N3-C4-N4   | 9.03  | 124.32      | 118.00   |
| 1   | AA    | 825  | A    | C5-C6-N6   | -9.03 | 116.48      | 123.70   |
| 1   | AA    | 829  | G    | N1-C6-O6   | 9.03  | 125.32      | 119.90   |
| 1   | AA    | 1482 | G    | P-O3'-C3'  | 9.03  | 130.53      | 119.70   |
| 34  | BA    | 87   | U    | C4-C5-C6   | -9.03 | 114.28      | 119.70   |
| 35  | BB    | 254  | G    | N3-C2-N2   | 9.03  | 126.22      | 119.90   |
| 35  | BB    | 785  | G    | C5-C6-N1   | -9.03 | 106.98      | 111.50   |
| 35  | BB    | 1574 | C    | C2-N3-C4   | 9.03  | 124.41      | 119.90   |
| 35  | BB    | 1632 | A    | C2-N3-C4   | 9.03  | 115.11      | 110.60   |
| 35  | BB    | 1811 | G    | N9-C4-C5   | 9.03  | 109.01      | 105.40   |
| 35  | BB    | 1922 | G    | O4'-C1'-N9 | 9.03  | 115.42      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | AM    | 92   | ARG  | NE-CZ-NH2   | -9.03 | 115.79      | 120.30   |
| 30  | B5    | 9    | ARG  | NE-CZ-NH1   | 9.03  | 124.81      | 120.30   |
| 35  | BB    | 319  | G    | N3-C2-N2    | 9.03  | 126.22      | 119.90   |
| 35  | BB    | 1874 | C    | O4'-C1'-N1  | 9.03  | 115.42      | 108.20   |
| 1   | AA    | 626  | G    | C5-C6-O6    | -9.02 | 123.19      | 128.60   |
| 1   | AA    | 762  | U    | O4'-C1'-N1  | 9.02  | 115.42      | 108.20   |
| 1   | AA    | 873  | A    | C4-C5-C6    | 9.02  | 121.51      | 117.00   |
| 1   | AA    | 1249 | C    | N3-C4-C5    | -9.02 | 118.29      | 121.90   |
| 35  | BB    | 2124 | G    | C8-N9-C4    | -9.02 | 102.79      | 106.40   |
| 1   | AA    | 1188 | A    | N1-C2-N3    | 9.02  | 133.81      | 129.30   |
| 34  | BA    | 78   | A    | O4'-C1'-N9  | 9.02  | 115.42      | 108.20   |
| 1   | AA    | 885  | G    | C8-N9-C4    | -9.02 | 102.79      | 106.40   |
| 1   | AA    | 1486 | G    | N1-C2-N3    | -9.02 | 118.49      | 123.90   |
| 1   | AA    | 382  | A    | C4-C5-C6    | 9.02  | 121.51      | 117.00   |
| 1   | AA    | 1442 | G    | N9-C4-C5    | 9.02  | 109.01      | 105.40   |
| 35  | BB    | 1585 | C    | C2-N3-C4    | 9.02  | 124.41      | 119.90   |
| 31  | B6    | 5    | PHE  | CB-CG-CD1   | -9.02 | 114.49      | 120.80   |
| 35  | BB    | 441  | U    | N3-C4-C5    | -9.02 | 109.19      | 114.60   |
| 35  | BB    | 1419 | A    | C4-C5-N7    | -9.02 | 106.19      | 110.70   |
| 1   | AA    | 403  | C    | C5-C6-N1    | 9.02  | 125.51      | 121.00   |
| 1   | AA    | 1013 | G    | N3-C2-N2    | 9.02  | 126.21      | 119.90   |
| 35  | BB    | 649  | G    | C5-N7-C8    | -9.02 | 99.79       | 104.30   |
| 35  | BB    | 1257 | C    | N3-C4-N4    | 9.02  | 124.31      | 118.00   |
| 35  | BB    | 1705 | A    | N1-C2-N3    | 9.02  | 133.81      | 129.30   |
| 35  | BB    | 2147 | A    | C2-N3-C4    | -9.02 | 106.09      | 110.60   |
| 46  | BM    | 91   | TYR  | CB-CG-CD1   | 9.02  | 126.41      | 121.00   |
| 1   | AA    | 26   | A    | N1-C6-N6    | 9.01  | 124.01      | 118.60   |
| 1   | AA    | 785  | G    | C6-C5-N7    | -9.01 | 124.99      | 130.40   |
| 35  | BB    | 2023 | C    | C6-N1-C2    | -9.01 | 116.69      | 120.30   |
| 35  | BB    | 2369 | A    | N9-C4-C5    | 9.01  | 109.41      | 105.80   |
| 35  | BB    | 1527 | G    | N3-C2-N2    | 9.01  | 126.21      | 119.90   |
| 35  | BB    | 2760 | C    | N3-C4-N4    | 9.01  | 124.31      | 118.00   |
| 35  | BB    | 2848 | G    | N3-C2-N2    | 9.01  | 126.21      | 119.90   |
| 1   | AA    | 130  | A    | C4-C5-N7    | -9.01 | 106.19      | 110.70   |
| 1   | AA    | 305  | G    | C1'-O4'-C4' | 9.01  | 117.11      | 109.90   |
| 1   | AA    | 457  | G    | C5-C6-N1    | -9.01 | 107.00      | 111.50   |
| 1   | AA    | 633  | G    | N3-C4-N9    | 9.01  | 131.41      | 126.00   |
| 1   | AA    | 828  | U    | C5-C6-N1    | 9.01  | 127.20      | 122.70   |
| 1   | AA    | 1386 | G    | C5-C6-O6    | -9.01 | 123.19      | 128.60   |
| 35  | BB    | 313  | G    | N1-C2-N3    | -9.01 | 118.50      | 123.90   |
| 35  | BB    | 1202 | G    | N1-C6-O6    | 9.01  | 125.31      | 119.90   |
| 35  | BB    | 1248 | G    | N1-C2-N3    | -9.01 | 118.50      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1254 | A    | C2-N3-C4   | -9.01 | 106.09      | 110.60   |
| 35  | BB    | 2722 | G    | N3-C2-N2   | 9.01  | 126.21      | 119.90   |
| 1   | AA    | 138  | G    | C4-C5-N7   | 9.01  | 114.40      | 110.80   |
| 1   | AA    | 586  | C    | N3-C4-C5   | -9.01 | 118.30      | 121.90   |
| 1   | AA    | 1299 | A    | N9-C4-C5   | 9.01  | 109.40      | 105.80   |
| 35  | BB    | 1713 | A    | C5-C6-N1   | -9.01 | 113.20      | 117.70   |
| 1   | AA    | 514  | C    | C5-C6-N1   | 9.01  | 125.50      | 121.00   |
| 1   | AA    | 1488 | G    | N1-C6-O6   | 9.01  | 125.30      | 119.90   |
| 35  | BB    | 795  | C    | O4'-C1'-N1 | 9.01  | 115.41      | 108.20   |
| 35  | BB    | 2429 | G    | C5-C6-O6   | -9.01 | 123.20      | 128.60   |
| 35  | BB    | 2346 | A    | O4'-C1'-N9 | 9.01  | 115.40      | 108.20   |
| 1   | AA    | 792  | A    | C4-C5-C6   | 9.00  | 121.50      | 117.00   |
| 1   | AA    | 876  | C    | O4'-C1'-N1 | 9.00  | 115.40      | 108.20   |
| 34  | BA    | 109  | A    | C6-C5-N7   | -9.00 | 126.00      | 132.30   |
| 35  | BB    | 901  | C    | C4-C5-C6   | 9.00  | 121.90      | 117.40   |
| 35  | BB    | 2740 | A    | C6-N1-C2   | -9.00 | 113.20      | 118.60   |
| 22  | AV    | 24   | G    | N1-C6-O6   | 9.00  | 125.30      | 119.90   |
| 22  | AV    | 50   | G    | N1-C6-O6   | 9.00  | 125.30      | 119.90   |
| 35  | BB    | 2744 | G    | N1-C6-O6   | 9.00  | 125.30      | 119.90   |
| 1   | AA    | 295  | C    | O4'-C1'-N1 | 9.00  | 115.40      | 108.20   |
| 1   | AA    | 1163 | A    | C6-N1-C2   | 9.00  | 124.00      | 118.60   |
| 5   | AE    | 137  | ARG  | NE-CZ-NH2  | -9.00 | 115.80      | 120.30   |
| 34  | BA    | 53   | A    | C5-C6-N6   | -9.00 | 116.50      | 123.70   |
| 35  | BB    | 213  | A    | C5-C6-N1   | -9.00 | 113.20      | 117.70   |
| 35  | BB    | 619  | G    | O4'-C1'-N9 | 9.00  | 115.40      | 108.20   |
| 35  | BB    | 1030 | C    | O4'-C1'-N1 | 9.00  | 115.40      | 108.20   |
| 1   | AA    | 635  | A    | C5-C6-N6   | -9.00 | 116.50      | 123.70   |
| 35  | BB    | 159  | G    | O4'-C1'-N9 | 9.00  | 115.40      | 108.20   |
| 35  | BB    | 389  | G    | N1-C2-N3   | -9.00 | 118.50      | 123.90   |
| 35  | BB    | 1014 | A    | C5-C6-N1   | -9.00 | 113.20      | 117.70   |
| 35  | BB    | 2765 | A    | C5-C6-N6   | -9.00 | 116.50      | 123.70   |
| 35  | BB    | 2823 | A    | N1-C6-N6   | 9.00  | 124.00      | 118.60   |
| 1   | AA    | 1366 | C    | C5-C4-N4   | -8.99 | 113.91      | 120.20   |
| 1   | AA    | 1521 | C    | N3-C4-N4   | 8.99  | 124.30      | 118.00   |
| 35  | BB    | 2201 | G    | C5-C6-N1   | -8.99 | 107.00      | 111.50   |
| 35  | BB    | 2777 | G    | N7-C8-N9   | -8.99 | 108.60      | 113.10   |
| 35  | BB    | 1010 | A    | C5-N7-C8   | 8.99  | 108.40      | 103.90   |
| 1   | AA    | 238  | A    | N1-C6-N6   | 8.99  | 124.00      | 118.60   |
| 35  | BB    | 603  | A    | C5-C6-N6   | -8.99 | 116.51      | 123.70   |
| 35  | BB    | 942  | G    | C5-C6-O6   | -8.99 | 123.21      | 128.60   |
| 35  | BB    | 2304 | G    | N1-C2-N3   | -8.99 | 118.50      | 123.90   |
| 35  | BB    | 1480 | C    | O4'-C1'-N1 | 8.99  | 115.39      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 2241 | A    | N9-C4-C5   | 8.99  | 109.39      | 105.80   |
| 1   | AA    | 175  | C    | N3-C4-C5   | -8.99 | 118.31      | 121.90   |
| 1   | AA    | 744  | C    | O4'-C1'-N1 | 8.99  | 115.39      | 108.20   |
| 35  | BB    | 172  | A    | C5-N7-C8   | 8.99  | 108.39      | 103.90   |
| 35  | BB    | 1349 | C    | O4'-C1'-N1 | 8.99  | 115.39      | 108.20   |
| 35  | BB    | 2345 | G    | N1-C6-O6   | 8.99  | 125.29      | 119.90   |
| 35  | BB    | 2715 | C    | N3-C4-N4   | 8.99  | 124.29      | 118.00   |
| 1   | AA    | 419  | C    | C6-N1-C2   | -8.98 | 116.71      | 120.30   |
| 35  | BB    | 193  | U    | C5-C4-O4   | -8.98 | 120.51      | 125.90   |
| 35  | BB    | 482  | A    | N1-C2-N3   | 8.98  | 133.79      | 129.30   |
| 35  | BB    | 1191 | G    | C5-C6-O6   | -8.98 | 123.21      | 128.60   |
| 35  | BB    | 1383 | A    | N9-C4-C5   | 8.98  | 109.39      | 105.80   |
| 35  | BB    | 1550 | C    | N3-C2-O2   | -8.98 | 115.61      | 121.90   |
| 35  | BB    | 2241 | A    | C4-C5-N7   | -8.98 | 106.21      | 110.70   |
| 35  | BB    | 2712 | C    | P-O3'-C3'  | 8.98  | 130.48      | 119.70   |
| 35  | BB    | 2611 | C    | C6-N1-C2   | 8.98  | 123.89      | 120.30   |
| 35  | BB    | 2759 | G    | C4-C5-N7   | 8.98  | 114.39      | 110.80   |
| 1   | AA    | 1002 | G    | N3-C4-C5   | -8.98 | 124.11      | 128.60   |
| 35  | BB    | 2889 | C    | N3-C4-N4   | 8.98  | 124.29      | 118.00   |
| 35  | BB    | 667  | U    | O4'-C1'-N1 | 8.98  | 115.38      | 108.20   |
| 1   | AA    | 125  | U    | C5-C4-O4   | -8.98 | 120.51      | 125.90   |
| 1   | AA    | 475  | C    | N3-C4-C5   | -8.98 | 118.31      | 121.90   |
| 1   | AA    | 864  | A    | C5-C6-N1   | -8.98 | 113.21      | 117.70   |
| 35  | BB    | 261  | G    | C6-C5-N7   | -8.98 | 125.01      | 130.40   |
| 35  | BB    | 1767 | G    | N1-C6-O6   | 8.98  | 125.29      | 119.90   |
| 35  | BB    | 432  | A    | O4'-C1'-N9 | 8.98  | 115.38      | 108.20   |
| 35  | BB    | 1272 | A    | C4-C5-C6   | 8.98  | 121.49      | 117.00   |
| 1   | AA    | 874  | G    | C5-C6-O6   | -8.97 | 123.22      | 128.60   |
| 1   | AA    | 1337 | G    | N1-C6-O6   | 8.97  | 125.28      | 119.90   |
| 35  | BB    | 425  | G    | N3-C4-N9   | -8.97 | 120.62      | 126.00   |
| 1   | AA    | 371  | A    | N3-C4-C5   | -8.97 | 120.52      | 126.80   |
| 1   | AA    | 1024 | G    | C5-C6-N1   | -8.97 | 107.01      | 111.50   |
| 1   | AA    | 1134 | G    | O4'-C1'-N9 | 8.97  | 115.38      | 108.20   |
| 1   | AA    | 918  | A    | C5-C6-N1   | -8.97 | 113.22      | 117.70   |
| 35  | BB    | 377  | G    | O4'-C1'-N9 | 8.97  | 115.38      | 108.20   |
| 35  | BB    | 689  | A    | N1-C6-N6   | 8.97  | 123.98      | 118.60   |
| 35  | BB    | 939  | G    | N3-C2-N2   | 8.97  | 126.18      | 119.90   |
| 35  | BB    | 1560 | G    | C5-C6-O6   | -8.97 | 123.22      | 128.60   |
| 1   | AA    | 300  | A    | O4'-C1'-N9 | 8.97  | 115.38      | 108.20   |
| 1   | AA    | 1446 | A    | O4'-C1'-N9 | 8.97  | 115.38      | 108.20   |
| 35  | BB    | 44   | A    | C5-C6-N6   | -8.97 | 116.53      | 123.70   |
| 35  | BB    | 901  | C    | C2-N3-C4   | 8.97  | 124.38      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1049 | C    | N3-C4-C5   | -8.97 | 118.31      | 121.90   |
| 35  | BB    | 1763 | G    | N1-C6-O6   | 8.97  | 125.28      | 119.90   |
| 35  | BB    | 2657 | A    | O4'-C1'-N9 | 8.97  | 115.37      | 108.20   |
| 35  | BB    | 2801 | G    | O4'-C1'-N9 | 8.97  | 115.37      | 108.20   |
| 35  | BB    | 239  | C    | O4'-C1'-N1 | 8.97  | 115.37      | 108.20   |
| 35  | BB    | 2370 | G    | N1-C6-O6   | 8.97  | 125.28      | 119.90   |
| 1   | AA    | 21   | G    | C8-N9-C4   | -8.96 | 102.81      | 106.40   |
| 1   | AA    | 666  | G    | N3-C2-N2   | 8.96  | 126.17      | 119.90   |
| 1   | AA    | 1073 | U    | P-O3'-C3'  | -8.96 | 108.94      | 119.70   |
| 1   | AA    | 153  | C    | N3-C4-C5   | -8.96 | 118.31      | 121.90   |
| 1   | AA    | 327  | A    | C5-N7-C8   | 8.96  | 108.38      | 103.90   |
| 1   | AA    | 546  | A    | C5-C6-N1   | -8.96 | 113.22      | 117.70   |
| 1   | AA    | 413  | G    | N7-C8-N9   | -8.96 | 108.62      | 113.10   |
| 1   | AA    | 610  | U    | N3-C4-O4   | 8.96  | 125.67      | 119.40   |
| 1   | AA    | 1267 | C    | O4'-C1'-N1 | 8.96  | 115.37      | 108.20   |
| 4   | AD    | 145  | ARG  | NE-CZ-NH2  | 8.96  | 124.78      | 120.30   |
| 35  | BB    | 1439 | A    | C5-N7-C8   | 8.96  | 108.38      | 103.90   |
| 35  | BB    | 1989 | G    | O4'-C1'-N9 | 8.96  | 115.37      | 108.20   |
| 35  | BB    | 1368 | G    | N1-C6-O6   | 8.96  | 125.28      | 119.90   |
| 35  | BB    | 2645 | G    | N3-C2-N2   | 8.96  | 126.17      | 119.90   |
| 40  | BG    | 156  | TYR  | CB-CG-CD1  | -8.96 | 115.62      | 121.00   |
| 1   | AA    | 107  | G    | C5-C6-N1   | -8.96 | 107.02      | 111.50   |
| 1   | AA    | 255  | G    | C4-C5-C6   | 8.96  | 124.17      | 118.80   |
| 1   | AA    | 1447 | A    | C4-C5-C6   | 8.96  | 121.48      | 117.00   |
| 35  | BB    | 180  | G    | C8-N9-C4   | -8.96 | 102.82      | 106.40   |
| 35  | BB    | 1325 | U    | C5-C6-N1   | 8.96  | 127.18      | 122.70   |
| 35  | BB    | 1885 | A    | C2-N3-C4   | -8.96 | 106.12      | 110.60   |
| 1   | AA    | 62   | U    | C5-C4-O4   | -8.96 | 120.53      | 125.90   |
| 35  | BB    | 268  | C    | O4'-C1'-N1 | 8.96  | 115.36      | 108.20   |
| 35  | BB    | 1147 | A    | C4-C5-C6   | 8.96  | 121.48      | 117.00   |
| 35  | BB    | 2710 | C    | N3-C4-C5   | -8.96 | 118.32      | 121.90   |
| 35  | BB    | 818  | G    | O4'-C1'-N9 | 8.95  | 115.36      | 108.20   |
| 35  | BB    | 1967 | C    | O4'-C1'-N1 | 8.96  | 115.36      | 108.20   |
| 1   | AA    | 658  | C    | C6-N1-C2   | -8.95 | 116.72      | 120.30   |
| 1   | AA    | 1127 | G    | C8-N9-C4   | -8.95 | 102.82      | 106.40   |
| 22  | AV    | 42   | G    | N1-C6-O6   | 8.95  | 125.27      | 119.90   |
| 35  | BB    | 1635 | A    | C5-C6-N6   | -8.95 | 116.54      | 123.70   |
| 35  | BB    | 1053 | C    | N3-C4-C5   | -8.95 | 118.32      | 121.90   |
| 35  | BB    | 1070 | A    | N1-C6-N6   | 8.95  | 123.97      | 118.60   |
| 35  | BB    | 1268 | A    | C8-N9-C4   | 8.95  | 109.38      | 105.80   |
| 35  | BB    | 1950 | G    | N1-C6-O6   | 8.95  | 125.27      | 119.90   |
| 35  | BB    | 361  | G    | C6-C5-N7   | -8.95 | 125.03      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1447 | C    | C6-N1-C2    | -8.95 | 116.72      | 120.30   |
| 35  | BB    | 1814 | G    | N3-C2-N2    | 8.95  | 126.16      | 119.90   |
| 35  | BB    | 2819 | G    | C6-C5-N7    | -8.95 | 125.03      | 130.40   |
| 1   | AA    | 424  | G    | C6-C5-N7    | -8.95 | 125.03      | 130.40   |
| 1   | AA    | 645  | G    | N1-C2-N3    | -8.95 | 118.53      | 123.90   |
| 35  | BB    | 950  | G    | N3-C4-C5    | 8.95  | 133.07      | 128.60   |
| 35  | BB    | 1873 | G    | O4'-C1'-N9  | 8.95  | 115.36      | 108.20   |
| 1   | AA    | 167  | A    | C5-C6-N6    | -8.94 | 116.54      | 123.70   |
| 1   | AA    | 1186 | G    | O4'-C1'-N9  | 8.94  | 115.36      | 108.20   |
| 35  | BB    | 2281 | A    | C5-C6-N6    | -8.95 | 116.54      | 123.70   |
| 35  | BB    | 599  | A    | N1-C2-N3    | 8.94  | 133.77      | 129.30   |
| 1   | AA    | 106  | C    | C2-N3-C4    | 8.94  | 124.37      | 119.90   |
| 35  | BB    | 161  | A    | C8-N9-C4    | -8.94 | 102.22      | 105.80   |
| 35  | BB    | 654  | A    | C4-C5-N7    | -8.94 | 106.23      | 110.70   |
| 35  | BB    | 696  | G    | C4-C5-C6    | 8.94  | 124.17      | 118.80   |
| 1   | AA    | 1404 | C    | N3-C4-N4    | 8.94  | 124.26      | 118.00   |
| 19  | AS    | 36   | ARG  | NE-CZ-NH2   | -8.94 | 115.83      | 120.30   |
| 34  | BA    | 118  | C    | C4-C5-C6    | 8.94  | 121.87      | 117.40   |
| 35  | BB    | 2501 | C    | N3-C4-C5    | -8.94 | 118.32      | 121.90   |
| 35  | BB    | 68   | G    | C3'-C2'-C1' | 8.94  | 108.65      | 101.50   |
| 35  | BB    | 2107 | G    | N3-C2-N2    | 8.94  | 126.16      | 119.90   |
| 35  | BB    | 15   | G    | N1-C2-N3    | -8.94 | 118.54      | 123.90   |
| 1   | AA    | 517  | G    | C6-C5-N7    | -8.94 | 125.04      | 130.40   |
| 35  | BB    | 800  | A    | C5-C6-N1    | -8.94 | 113.23      | 117.70   |
| 35  | BB    | 1253 | A    | C5-N7-C8    | 8.94  | 108.37      | 103.90   |
| 35  | BB    | 1644 | C    | N3-C4-N4    | 8.94  | 124.25      | 118.00   |
| 35  | BB    | 1704 | C    | N3-C4-C5    | -8.94 | 118.33      | 121.90   |
| 38  | BE    | 172  | ALA  | N-CA-CB     | 8.94  | 122.61      | 110.10   |
| 35  | BB    | 1797 | G    | C5-C6-O6    | -8.94 | 123.24      | 128.60   |
| 35  | BB    | 2341 | G    | N1-C6-O6    | 8.94  | 125.26      | 119.90   |
| 35  | BB    | 2503 | A    | C5-N7-C8    | 8.94  | 108.37      | 103.90   |
| 3   | AC    | 10   | ARG  | NE-CZ-NH1   | 8.93  | 124.77      | 120.30   |
| 35  | BB    | 1443 | U    | N3-C2-O2    | 8.93  | 128.45      | 122.20   |
| 35  | BB    | 1927 | A    | C5-C6-N6    | -8.93 | 116.55      | 123.70   |
| 35  | BB    | 84   | A    | C4-C5-N7    | -8.93 | 106.23      | 110.70   |
| 35  | BB    | 1544 | A    | N9-C4-C5    | -8.93 | 102.23      | 105.80   |
| 35  | BB    | 1885 | A    | N1-C2-N3    | 8.93  | 133.77      | 129.30   |
| 35  | BB    | 2140 | G    | N1-C6-O6    | 8.93  | 125.26      | 119.90   |
| 35  | BB    | 2623 | G    | N1-C6-O6    | 8.93  | 125.26      | 119.90   |
| 35  | BB    | 2781 | A    | C5-C6-N1    | -8.93 | 113.23      | 117.70   |
| 35  | BB    | 1969 | A    | C4-C5-N7    | -8.93 | 106.23      | 110.70   |
| 35  | BB    | 2671 | G    | C5-C6-O6    | -8.93 | 123.24      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 553  | A    | C4-C5-C6    | 8.93  | 121.46      | 117.00   |
| 35  | BB    | 819  | A    | C8-N9-C4    | -8.93 | 102.23      | 105.80   |
| 35  | BB    | 2407 | A    | C4-C5-N7    | -8.93 | 106.24      | 110.70   |
| 35  | BB    | 1756 | G    | C6-C5-N7    | -8.93 | 125.04      | 130.40   |
| 35  | BB    | 2230 | G    | C5-C6-O6    | -8.93 | 123.24      | 128.60   |
| 35  | BB    | 313  | G    | C2-N3-C4    | 8.92  | 116.36      | 111.90   |
| 35  | BB    | 539  | G    | N3-C4-C5    | 8.92  | 133.06      | 128.60   |
| 35  | BB    | 214  | G    | N3-C2-N2    | 8.92  | 126.15      | 119.90   |
| 35  | BB    | 1150 | C    | C2-N3-C4    | 8.92  | 124.36      | 119.90   |
| 1   | AA    | 299  | G    | N3-C4-C5    | 8.92  | 133.06      | 128.60   |
| 1   | AA    | 315  | A    | N7-C8-N9    | -8.92 | 109.34      | 113.80   |
| 1   | AA    | 1261 | A    | N1-C6-N6    | 8.92  | 123.95      | 118.60   |
| 35  | BB    | 1710 | G    | N1-C2-N3    | -8.92 | 118.55      | 123.90   |
| 35  | BB    | 2038 | G    | N1-C6-O6    | 8.92  | 125.25      | 119.90   |
| 1   | AA    | 474  | G    | N1-C6-O6    | 8.92  | 125.25      | 119.90   |
| 1   | AA    | 528  | C    | C5-C6-N1    | -8.92 | 116.54      | 121.00   |
| 1   | AA    | 538  | G    | N1-C2-N3    | -8.92 | 118.55      | 123.90   |
| 1   | AA    | 812  | G    | C5-C6-O6    | -8.92 | 123.25      | 128.60   |
| 35  | BB    | 725  | G    | O4'-C1'-N9  | 8.92  | 115.33      | 108.20   |
| 35  | BB    | 954  | G    | O4'-C1'-N9  | 8.92  | 115.33      | 108.20   |
| 35  | BB    | 1035 | U    | O4'-C1'-N1  | 8.92  | 115.33      | 108.20   |
| 35  | BB    | 1424 | G    | C4'-C3'-C2' | -8.92 | 93.68       | 102.60   |
| 35  | BB    | 1328 | A    | C4-C5-N7    | -8.92 | 106.24      | 110.70   |
| 35  | BB    | 1366 | A    | C4-C5-C6    | 8.92  | 121.46      | 117.00   |
| 35  | BB    | 2669 | G    | C6-C5-N7    | -8.92 | 125.05      | 130.40   |
| 51  | BR    | 84   | ARG  | NE-CZ-NH1   | -8.92 | 115.84      | 120.30   |
| 1   | AA    | 336  | A    | N1-C2-N3    | -8.91 | 124.84      | 129.30   |
| 1   | AA    | 954  | G    | C5-C6-N1    | -8.91 | 107.04      | 111.50   |
| 35  | BB    | 2023 | C    | N3-C2-O2    | -8.91 | 115.66      | 121.90   |
| 35  | BB    | 2057 | G    | C6-N1-C2    | 8.91  | 130.45      | 125.10   |
| 1   | AA    | 533  | A    | N1-C6-N6    | 8.91  | 123.95      | 118.60   |
| 34  | BA    | 16   | G    | C6-C5-N7    | -8.91 | 125.05      | 130.40   |
| 35  | BB    | 1295 | C    | N3-C4-N4    | 8.91  | 124.24      | 118.00   |
| 35  | BB    | 2697 | G    | C5-C6-O6    | -8.91 | 123.25      | 128.60   |
| 1   | AA    | 1490 | U    | N1-C2-N3    | 8.91  | 120.25      | 114.90   |
| 35  | BB    | 778  | G    | N9-C4-C5    | -8.91 | 101.83      | 105.40   |
| 35  | BB    | 1291 | C    | C5-C6-N1    | 8.91  | 125.46      | 121.00   |
| 35  | BB    | 1655 | A    | C5-C6-N1    | -8.91 | 113.24      | 117.70   |
| 35  | BB    | 1973 | G    | N1-C2-N3    | -8.91 | 118.55      | 123.90   |
| 35  | BB    | 2341 | G    | C5-N7-C8    | -8.91 | 99.84       | 104.30   |
| 35  | BB    | 2896 | C    | N3-C4-C5    | -8.91 | 118.33      | 121.90   |
| 45  | BL    | 60   | ARG  | NE-CZ-NH1   | 8.91  | 124.76      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 85   | U    | N1-C2-N3   | -8.91 | 109.55      | 114.90   |
| 1   | AA    | 603  | U    | N1-C2-N3   | 8.91  | 120.25      | 114.90   |
| 1   | AA    | 668  | G    | C5-C6-O6   | -8.91 | 123.25      | 128.60   |
| 1   | AA    | 949  | A    | C8-N9-C4   | -8.91 | 102.24      | 105.80   |
| 3   | AC    | 163  | ARG  | NE-CZ-NH1  | 8.91  | 124.75      | 120.30   |
| 35  | BB    | 2068 | U    | N3-C4-C5   | -8.91 | 109.25      | 114.60   |
| 35  | BB    | 2083 | G    | N1-C2-N3   | -8.91 | 118.55      | 123.90   |
| 35  | BB    | 2643 | G    | C8-N9-C4   | -8.91 | 102.84      | 106.40   |
| 55  | BW    | 45   | ASP  | CB-CG-OD1  | -8.91 | 110.28      | 118.30   |
| 3   | AC    | 41   | TYR  | CB-CG-CD1  | 8.91  | 126.34      | 121.00   |
| 35  | BB    | 881  | G    | C8-N9-C4   | -8.91 | 102.84      | 106.40   |
| 35  | BB    | 1182 | G    | C5-C6-O6   | -8.91 | 123.25      | 128.60   |
| 35  | BB    | 1697 | G    | O4'-C1'-N9 | 8.91  | 115.33      | 108.20   |
| 35  | BB    | 1848 | A    | N1-C6-N6   | 8.91  | 123.94      | 118.60   |
| 35  | BB    | 2471 | A    | C6-C5-N7   | -8.91 | 126.06      | 132.30   |
| 35  | BB    | 2758 | A    | C8-N9-C4   | 8.91  | 109.36      | 105.80   |
| 56  | BY    | 38   | ARG  | NE-CZ-NH2  | -8.91 | 115.85      | 120.30   |
| 1   | AA    | 997  | U    | O4'-C1'-N1 | 8.90  | 115.32      | 108.20   |
| 1   | AA    | 1252 | A    | C5-C6-N1   | -8.90 | 113.25      | 117.70   |
| 35  | BB    | 64   | A    | O4'-C1'-N9 | 8.90  | 115.32      | 108.20   |
| 35  | BB    | 437  | U    | C5-C6-N1   | 8.90  | 127.15      | 122.70   |
| 35  | BB    | 1126 | A    | C6-N1-C2   | 8.90  | 123.94      | 118.60   |
| 35  | BB    | 1551 | A    | O4'-C1'-N9 | 8.90  | 115.32      | 108.20   |
| 1   | AA    | 1398 | A    | C4-C5-N7   | -8.90 | 106.25      | 110.70   |
| 35  | BB    | 229  | C    | O4'-C1'-N1 | 8.90  | 115.32      | 108.20   |
| 35  | BB    | 598  | U    | O4'-C1'-N1 | 8.90  | 115.32      | 108.20   |
| 35  | BB    | 1260 | A    | N1-C6-N6   | 8.90  | 123.94      | 118.60   |
| 35  | BB    | 1291 | C    | N1-C2-O2   | -8.90 | 113.56      | 118.90   |
| 35  | BB    | 1564 | C    | N3-C4-N4   | 8.90  | 124.23      | 118.00   |
| 35  | BB    | 2361 | G    | N3-C2-N2   | 8.90  | 126.13      | 119.90   |
| 1   | AA    | 314  | C    | N3-C4-C5   | -8.90 | 118.34      | 121.90   |
| 21  | AU    | 44   | ARG  | NE-CZ-NH1  | 8.90  | 124.75      | 120.30   |
| 1   | AA    | 147  | G    | N1-C6-O6   | 8.90  | 125.24      | 119.90   |
| 1   | AA    | 768  | A    | N1-C6-N6   | 8.90  | 123.94      | 118.60   |
| 1   | AA    | 1370 | G    | N3-C2-N2   | 8.90  | 126.13      | 119.90   |
| 35  | BB    | 513  | A    | N1-C6-N6   | 8.90  | 123.94      | 118.60   |
| 35  | BB    | 1690 | A    | C5-C6-N6   | -8.90 | 116.58      | 123.70   |
| 1   | AA    | 785  | G    | C4-C5-N7   | 8.89  | 114.36      | 110.80   |
| 1   | AA    | 798  | U    | O4'-C1'-N1 | 8.89  | 115.31      | 108.20   |
| 1   | AA    | 889  | A    | N1-C6-N6   | 8.89  | 123.94      | 118.60   |
| 1   | AA    | 1347 | G    | N3-C2-N2   | 8.89  | 126.12      | 119.90   |
| 35  | BB    | 1307 | A    | N1-C6-N6   | 8.89  | 123.94      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1443 | U    | C5-C6-N1   | 8.89  | 127.15      | 122.70   |
| 35  | BB    | 1966 | A    | N1-C2-N3   | 8.89  | 133.75      | 129.30   |
| 35  | BB    | 2008 | C    | O4'-C1'-N1 | 8.89  | 115.31      | 108.20   |
| 35  | BB    | 2317 | A    | C5-C6-N1   | -8.89 | 113.25      | 117.70   |
| 35  | BB    | 2624 | G    | N1-C6-O6   | 8.89  | 125.24      | 119.90   |
| 1   | AA    | 323  | U    | C5-C6-N1   | 8.89  | 127.15      | 122.70   |
| 35  | BB    | 1493 | C    | O4'-C1'-N1 | 8.89  | 115.31      | 108.20   |
| 35  | BB    | 2207 | C    | O4'-C1'-N1 | 8.89  | 115.31      | 108.20   |
| 1   | AA    | 910  | C    | N3-C4-C5   | -8.89 | 118.34      | 121.90   |
| 35  | BB    | 838  | C    | N3-C4-C5   | -8.89 | 118.34      | 121.90   |
| 35  | BB    | 2867 | G    | O4'-C1'-N9 | 8.89  | 115.31      | 108.20   |
| 1   | AA    | 523  | A    | N1-C6-N6   | 8.89  | 123.93      | 118.60   |
| 1   | AA    | 40   | C    | N3-C4-N4   | 8.89  | 124.22      | 118.00   |
| 1   | AA    | 636  | U    | C5-C4-O4   | -8.89 | 120.57      | 125.90   |
| 35  | BB    | 985  | C    | N3-C4-C5   | -8.89 | 118.34      | 121.90   |
| 35  | BB    | 1188 | U    | C4-C5-C6   | -8.89 | 114.37      | 119.70   |
| 35  | BB    | 1233 | C    | N3-C4-N4   | 8.89  | 124.22      | 118.00   |
| 1   | AA    | 162  | A    | C5-C6-N6   | -8.89 | 116.59      | 123.70   |
| 1   | AA    | 1345 | U    | C2-N3-C4   | -8.89 | 121.67      | 127.00   |
| 35  | BB    | 19   | A    | C5-C6-N1   | -8.89 | 113.26      | 117.70   |
| 35  | BB    | 1045 | C    | C5-C6-N1   | 8.89  | 125.44      | 121.00   |
| 35  | BB    | 1332 | G    | C6-C5-N7   | -8.89 | 125.07      | 130.40   |
| 1   | AA    | 1305 | G    | O4'-C1'-N9 | 8.88  | 115.31      | 108.20   |
| 34  | BA    | 101  | A    | C5-C6-N6   | -8.88 | 116.59      | 123.70   |
| 35  | BB    | 1059 | G    | N9-C4-C5   | -8.88 | 101.85      | 105.40   |
| 35  | BB    | 1157 | G    | C4-C5-C6   | 8.88  | 124.13      | 118.80   |
| 35  | BB    | 2861 | U    | O4'-C1'-N1 | 8.88  | 115.31      | 108.20   |
| 1   | AA    | 1141 | C    | N3-C4-N4   | 8.88  | 124.22      | 118.00   |
| 35  | BB    | 306  | U    | N3-C4-O4   | 8.88  | 125.62      | 119.40   |
| 35  | BB    | 325  | G    | N3-C2-N2   | 8.88  | 126.12      | 119.90   |
| 35  | BB    | 1805 | A    | O4'-C1'-N9 | 8.88  | 115.31      | 108.20   |
| 1   | AA    | 355  | C    | N3-C2-O2   | 8.88  | 128.12      | 121.90   |
| 1   | AA    | 496  | A    | O4'-C1'-N9 | 8.88  | 115.30      | 108.20   |
| 1   | AA    | 1028 | C    | N1-C2-N3   | -8.88 | 112.98      | 119.20   |
| 1   | AA    | 1500 | A    | O4'-C1'-N9 | 8.88  | 115.31      | 108.20   |
| 35  | BB    | 2685 | G    | C5-C6-N1   | 8.88  | 115.94      | 111.50   |
| 34  | BA    | 112  | G    | C8-N9-C4   | -8.88 | 102.85      | 106.40   |
| 35  | BB    | 1003 | G    | N1-C6-O6   | 8.88  | 125.23      | 119.90   |
| 35  | BB    | 1528 | A    | C5-C6-N6   | -8.88 | 116.60      | 123.70   |
| 35  | BB    | 2853 | C    | N3-C4-C5   | -8.88 | 118.35      | 121.90   |
| 35  | BB    | 758  | C    | N3-C4-C5   | -8.88 | 118.35      | 121.90   |
| 35  | BB    | 876  | C    | N3-C4-N4   | 8.88  | 124.21      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 945  | A    | N3-C4-C5    | -8.88 | 120.59      | 126.80   |
| 1   | AA    | 752  | G    | N1-C6-O6    | 8.88  | 125.22      | 119.90   |
| 1   | AA    | 816  | A    | N1-C6-N6    | 8.87  | 123.92      | 118.60   |
| 1   | AA    | 1230 | C    | C5-C4-N4    | -8.87 | 113.99      | 120.20   |
| 1   | AA    | 1442 | G    | C8-N9-C4    | -8.88 | 102.85      | 106.40   |
| 35  | BB    | 1919 | A    | C5-C6-N1    | -8.88 | 113.26      | 117.70   |
| 35  | BB    | 449  | A    | C4-C5-C6    | 8.87  | 121.44      | 117.00   |
| 52  | BS    | 5    | ALA  | N-CA-CB     | 8.88  | 122.53      | 110.10   |
| 1   | AA    | 633  | G    | N3-C2-N2    | 8.87  | 126.11      | 119.90   |
| 1   | AA    | 759  | A    | N7-C8-N9    | 8.87  | 118.24      | 113.80   |
| 1   | AA    | 1184 | G    | O4'-C1'-N9  | 8.87  | 115.30      | 108.20   |
| 1   | AA    | 1281 | C    | C6-N1-C2    | -8.87 | 116.75      | 120.30   |
| 22  | AV    | 39   | G    | C6-C5-N7    | -8.87 | 125.08      | 130.40   |
| 34  | BA    | 16   | G    | C5-C6-O6    | -8.87 | 123.28      | 128.60   |
| 35  | BB    | 80   | G    | C4-C5-C6    | 8.87  | 124.12      | 118.80   |
| 35  | BB    | 283  | G    | C2-N3-C4    | 8.87  | 116.34      | 111.90   |
| 35  | BB    | 1665 | A    | N1-C6-N6    | 8.87  | 123.92      | 118.60   |
| 35  | BB    | 977  | G    | O4'-C1'-N9  | 8.87  | 115.30      | 108.20   |
| 35  | BB    | 2221 | G    | O4'-C1'-N9  | 8.87  | 115.30      | 108.20   |
| 35  | BB    | 2777 | G    | C2-N3-C4    | 8.87  | 116.34      | 111.90   |
| 1   | AA    | 608  | A    | N1-C6-N6    | 8.87  | 123.92      | 118.60   |
| 1   | AA    | 1207 | G    | N3-C4-N9    | 8.87  | 131.32      | 126.00   |
| 1   | AA    | 1375 | A    | N1-C6-N6    | 8.87  | 123.92      | 118.60   |
| 35  | BB    | 39   | G    | C5-C6-O6    | -8.87 | 123.28      | 128.60   |
| 35  | BB    | 149  | A    | O4'-C1'-N9  | 8.87  | 115.29      | 108.20   |
| 35  | BB    | 218  | A    | C5-N7-C8    | 8.87  | 108.33      | 103.90   |
| 35  | BB    | 230  | G    | O4'-C1'-N9  | 8.87  | 115.29      | 108.20   |
| 35  | BB    | 766  | U    | N3-C4-C5    | -8.87 | 109.28      | 114.60   |
| 35  | BB    | 2526 | G    | C8-N9-C4    | 8.87  | 109.95      | 106.40   |
| 1   | AA    | 1032 | G    | N1-C2-N3    | -8.87 | 118.58      | 123.90   |
| 1   | AA    | 1289 | A    | C5-C6-N1    | -8.87 | 113.27      | 117.70   |
| 35  | BB    | 1561 | C    | C1'-O4'-C4' | 8.86  | 116.99      | 109.90   |
| 35  | BB    | 1702 | G    | O4'-C1'-N9  | 8.86  | 115.29      | 108.20   |
| 35  | BB    | 2009 | A    | C5-C6-N6    | -8.87 | 116.61      | 123.70   |
| 1   | AA    | 337  | G    | C2-N3-C4    | 8.86  | 116.33      | 111.90   |
| 35  | BB    | 2155 | U    | O4'-C1'-N1  | 8.86  | 115.29      | 108.20   |
| 35  | BB    | 2617 | U    | O4'-C1'-N1  | 8.86  | 115.29      | 108.20   |
| 1   | AA    | 50   | A    | C4-C5-C6    | 8.86  | 121.43      | 117.00   |
| 1   | AA    | 1502 | A    | N1-C6-N6    | 8.86  | 123.92      | 118.60   |
| 35  | BB    | 2183 | A    | C4-C5-C6    | 8.86  | 121.43      | 117.00   |
| 35  | BB    | 735  | A    | C2-N3-C4    | -8.86 | 106.17      | 110.60   |
| 35  | BB    | 1503 | A    | O4'-C1'-N9  | 8.86  | 115.29      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1616 | A    | C6-N1-C2   | -8.86 | 113.28      | 118.60   |
| 56  | BY    | 44   | PHE  | CB-CG-CD2  | -8.86 | 114.60      | 120.80   |
| 1   | AA    | 107  | G    | C8-N9-C4   | -8.86 | 102.86      | 106.40   |
| 35  | BB    | 201  | C    | O4'-C1'-N1 | 8.86  | 115.28      | 108.20   |
| 35  | BB    | 2006 | C    | N3-C4-N4   | 8.86  | 124.20      | 118.00   |
| 35  | BB    | 2389 | G    | N1-C6-O6   | 8.86  | 125.21      | 119.90   |
| 35  | BB    | 2869 | G    | N1-C6-O6   | 8.86  | 125.21      | 119.90   |
| 1   | AA    | 550  | G    | C4-C5-C6   | 8.85  | 124.11      | 118.80   |
| 35  | BB    | 1207 | C    | N1-C2-O2   | 8.85  | 124.21      | 118.90   |
| 52  | BS    | 95   | ARG  | NE-CZ-NH2  | 8.85  | 124.73      | 120.30   |
| 1   | AA    | 1039 | G    | C5-C6-N1   | 8.85  | 115.93      | 111.50   |
| 35  | BB    | 211  | C    | N1-C2-O2   | 8.85  | 124.21      | 118.90   |
| 35  | BB    | 2012 | G    | N3-C2-N2   | 8.85  | 126.10      | 119.90   |
| 35  | BB    | 985  | C    | O4'-C1'-N1 | 8.85  | 115.28      | 108.20   |
| 1   | AA    | 1273 | C    | N3-C4-N4   | 8.85  | 124.19      | 118.00   |
| 22  | AV    | 29   | G    | N1-C6-O6   | 8.85  | 125.21      | 119.90   |
| 35  | BB    | 477  | A    | C4-C5-C6   | 8.85  | 121.42      | 117.00   |
| 35  | BB    | 2468 | A    | N3-C4-C5   | -8.85 | 120.61      | 126.80   |
| 35  | BB    | 2500 | U    | C5-C4-O4   | -8.85 | 120.59      | 125.90   |
| 1   | AA    | 1127 | G    | N9-C4-C5   | 8.85  | 108.94      | 105.40   |
| 35  | BB    | 250  | G    | C6-C5-N7   | -8.85 | 125.09      | 130.40   |
| 35  | BB    | 822  | G    | C4-C5-C6   | 8.85  | 124.11      | 118.80   |
| 35  | BB    | 2024 | G    | C6-C5-N7   | -8.85 | 125.09      | 130.40   |
| 35  | BB    | 2705 | A    | O4'-C1'-N9 | 8.84  | 115.27      | 108.20   |
| 1   | AA    | 66   | A    | C2-N3-C4   | -8.84 | 106.18      | 110.60   |
| 35  | BB    | 121  | G    | C5-C6-O6   | -8.84 | 123.30      | 128.60   |
| 35  | BB    | 631  | A    | O4'-C1'-N9 | 8.84  | 115.27      | 108.20   |
| 1   | AA    | 674  | G    | N3-C2-N2   | 8.84  | 126.09      | 119.90   |
| 1   | AA    | 1037 | C    | O4'-C1'-N1 | 8.84  | 115.27      | 108.20   |
| 35  | BB    | 366  | C    | N3-C4-C5   | -8.84 | 118.36      | 121.90   |
| 35  | BB    | 983  | A    | O4'-C1'-N9 | 8.84  | 115.27      | 108.20   |
| 35  | BB    | 1080 | A    | C4-C5-N7   | -8.84 | 106.28      | 110.70   |
| 1   | AA    | 196  | A    | C4-C5-N7   | -8.84 | 106.28      | 110.70   |
| 1   | AA    | 295  | C    | C5-C4-N4   | -8.84 | 114.01      | 120.20   |
| 1   | AA    | 1138 | G    | C6-C5-N7   | -8.84 | 125.10      | 130.40   |
| 35  | BB    | 959  | A    | N1-C6-N6   | 8.84  | 123.90      | 118.60   |
| 35  | BB    | 2039 | U    | N3-C4-O4   | 8.84  | 125.59      | 119.40   |
| 1   | AA    | 853  | C    | N1-C1'-C2' | -8.84 | 102.28      | 112.00   |
| 1   | AA    | 1527 | U    | C2-N3-C4   | -8.84 | 121.70      | 127.00   |
| 35  | BB    | 1472 | C    | N3-C4-N4   | 8.84  | 124.19      | 118.00   |
| 34  | BA    | 50   | A    | C5-C6-N6   | -8.84 | 116.63      | 123.70   |
| 35  | BB    | 376  | G    | C5-C6-O6   | -8.84 | 123.30      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1611 | C    | O4'-C1'-N1  | 8.84  | 115.27      | 108.20   |
| 35  | BB    | 2429 | G    | N1-C6-O6    | 8.84  | 125.20      | 119.90   |
| 1   | AA    | 176  | C    | O4'-C1'-N1  | 8.83  | 115.27      | 108.20   |
| 1   | AA    | 1050 | G    | N1-C6-O6    | 8.83  | 125.20      | 119.90   |
| 1   | AA    | 718  | A    | C5-C6-N6    | -8.83 | 116.63      | 123.70   |
| 35  | BB    | 339  | U    | N3-C4-O4    | 8.83  | 125.58      | 119.40   |
| 35  | BB    | 636  | G    | N1-C2-N3    | -8.83 | 118.60      | 123.90   |
| 1   | AA    | 138  | G    | O4'-C1'-N9  | 8.83  | 115.27      | 108.20   |
| 1   | AA    | 764  | C    | O4'-C1'-N1  | 8.83  | 115.27      | 108.20   |
| 34  | BA    | 49   | C    | C6-N1-C2    | -8.83 | 116.77      | 120.30   |
| 35  | BB    | 352  | A    | C5-C6-N6    | -8.83 | 116.64      | 123.70   |
| 35  | BB    | 417  | C    | C5-C6-N1    | 8.83  | 125.42      | 121.00   |
| 1   | AA    | 283  | U    | C1'-O4'-C4' | 8.83  | 116.96      | 109.90   |
| 1   | AA    | 318  | G    | C5-C6-O6    | -8.83 | 123.30      | 128.60   |
| 1   | AA    | 551  | U    | O4'-C1'-N1  | 8.83  | 115.26      | 108.20   |
| 1   | AA    | 556  | C    | C5-C4-N4    | -8.83 | 114.02      | 120.20   |
| 1   | AA    | 890  | G    | P-O3'-C3'   | 8.83  | 130.29      | 119.70   |
| 1   | AA    | 1427 | C    | N3-C4-C5    | -8.83 | 118.37      | 121.90   |
| 35  | BB    | 237  | C    | N3-C4-N4    | 8.83  | 124.18      | 118.00   |
| 35  | BB    | 1566 | A    | C5-N7-C8    | 8.83  | 108.31      | 103.90   |
| 35  | BB    | 780  | G    | N9-C4-C5    | 8.83  | 108.93      | 105.40   |
| 35  | BB    | 1588 | G    | C4-C5-C6    | 8.83  | 124.10      | 118.80   |
| 35  | BB    | 2001 | C    | C5-C4-N4    | -8.83 | 114.02      | 120.20   |
| 35  | BB    | 146  | A    | C4-C5-C6    | 8.82  | 121.41      | 117.00   |
| 35  | BB    | 2115 | G    | N3-C2-N2    | 8.82  | 126.08      | 119.90   |
| 35  | BB    | 2157 | G    | C5-C6-O6    | -8.82 | 123.31      | 128.60   |
| 35  | BB    | 2304 | G    | O4'-C1'-N9  | 8.82  | 115.26      | 108.20   |
| 1   | AA    | 1017 | U    | O4'-C1'-N1  | 8.82  | 115.26      | 108.20   |
| 1   | AA    | 1092 | A    | C4-C5-C6    | 8.82  | 121.41      | 117.00   |
| 35  | BB    | 90   | U    | P-O3'-C3'   | 8.82  | 130.29      | 119.70   |
| 35  | BB    | 294  | A    | O4'-C1'-N9  | 8.82  | 115.26      | 108.20   |
| 35  | BB    | 1308 | A    | N1-C6-N6    | 8.82  | 123.89      | 118.60   |
| 35  | BB    | 2040 | G    | N3-C4-C5    | 8.82  | 133.01      | 128.60   |
| 35  | BB    | 2131 | U    | C5-C6-N1    | 8.82  | 127.11      | 122.70   |
| 35  | BB    | 2176 | A    | C5-N7-C8    | 8.82  | 108.31      | 103.90   |
| 1   | AA    | 790  | A    | C4-C5-C6    | 8.82  | 121.41      | 117.00   |
| 1   | AA    | 1385 | G    | N1-C2-N2    | 8.82  | 124.14      | 116.20   |
| 35  | BB    | 47   | C    | P-O3'-C3'   | 8.82  | 130.28      | 119.70   |
| 35  | BB    | 1862 | G    | C4-C5-C6    | 8.82  | 124.09      | 118.80   |
| 35  | BB    | 2843 | G    | N3-C2-N2    | 8.82  | 126.07      | 119.90   |
| 1   | AA    | 42   | G    | P-O5'-C5'   | 8.82  | 135.01      | 120.90   |
| 1   | AA    | 711  | G    | N3-C2-N2    | 8.82  | 126.07      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 731  | G    | C5-C6-N1    | -8.82 | 107.09      | 111.50   |
| 1   | AA    | 824  | G    | O4'-C1'-N9  | 8.82  | 115.25      | 108.20   |
| 1   | AA    | 943  | U    | O4'-C1'-N1  | 8.82  | 115.25      | 108.20   |
| 15  | AO    | 63   | ARG  | NE-CZ-NH1   | 8.82  | 124.71      | 120.30   |
| 35  | BB    | 1378 | A    | P-O5'-C5'   | -8.82 | 106.79      | 120.90   |
| 35  | BB    | 2858 | C    | O4'-C1'-N1  | 8.82  | 115.25      | 108.20   |
| 1   | AA    | 43   | C    | N3-C4-N4    | 8.81  | 124.17      | 118.00   |
| 1   | AA    | 1149 | C    | O4'-C1'-N1  | 8.81  | 115.25      | 108.20   |
| 35  | BB    | 668  | A    | N9-C4-C5    | 8.81  | 109.33      | 105.80   |
| 1   | AA    | 401  | C    | O4'-C1'-N1  | 8.81  | 115.25      | 108.20   |
| 35  | BB    | 1143 | A    | N3-C4-C5    | -8.81 | 120.63      | 126.80   |
| 35  | BB    | 1307 | A    | O4'-C1'-N9  | 8.81  | 115.25      | 108.20   |
| 35  | BB    | 2071 | A    | N7-C8-N9    | 8.81  | 118.21      | 113.80   |
| 1   | AA    | 926  | G    | C5-C6-N1    | -8.81 | 107.09      | 111.50   |
| 1   | AA    | 1128 | C    | N3-C4-C5    | -8.81 | 118.38      | 121.90   |
| 35  | BB    | 911  | A    | N1-C6-N6    | 8.81  | 123.89      | 118.60   |
| 35  | BB    | 1062 | G    | C6-C5-N7    | -8.81 | 125.11      | 130.40   |
| 35  | BB    | 1335 | C    | N3-C4-C5    | -8.81 | 118.38      | 121.90   |
| 35  | BB    | 1341 | G    | C6-C5-N7    | -8.81 | 125.11      | 130.40   |
| 35  | BB    | 2184 | A    | C6-N1-C2    | 8.81  | 123.89      | 118.60   |
| 1   | AA    | 874  | G    | O4'-C1'-N9  | 8.81  | 115.25      | 108.20   |
| 1   | AA    | 1127 | G    | C6-C5-N7    | -8.81 | 125.12      | 130.40   |
| 22  | AV    | 74   | C    | O4'-C1'-N1  | 8.81  | 115.25      | 108.20   |
| 34  | BA    | 43   | C    | N3-C4-N4    | 8.81  | 124.17      | 118.00   |
| 35  | BB    | 566  | U    | O4'-C1'-N1  | 8.81  | 115.25      | 108.20   |
| 35  | BB    | 1652 | A    | N9-C4-C5    | 8.81  | 109.32      | 105.80   |
| 35  | BB    | 1909 | C    | C6-N1-C2    | -8.81 | 116.78      | 120.30   |
| 1   | AA    | 33   | A    | N1-C6-N6    | 8.80  | 123.88      | 118.60   |
| 1   | AA    | 208  | U    | O4'-C1'-N1  | 8.80  | 115.24      | 108.20   |
| 1   | AA    | 1482 | G    | C8-N9-C4    | -8.81 | 102.88      | 106.40   |
| 35  | BB    | 1783 | A    | N1-C6-N6    | 8.81  | 123.88      | 118.60   |
| 35  | BB    | 1884 | G    | C3'-C2'-C1' | 8.81  | 108.54      | 101.50   |
| 35  | BB    | 2759 | G    | N3-C2-N2    | 8.81  | 126.06      | 119.90   |
| 35  | BB    | 1223 | G    | C5-C6-O6    | -8.80 | 123.32      | 128.60   |
| 35  | BB    | 1650 | A    | O4'-C1'-N9  | 8.80  | 115.24      | 108.20   |
| 35  | BB    | 1997 | C    | N3-C4-C5    | -8.80 | 118.38      | 121.90   |
| 35  | BB    | 2268 | A    | C2-N3-C4    | 8.80  | 115.00      | 110.60   |
| 35  | BB    | 2810 | A    | O4'-C1'-N9  | 8.80  | 115.24      | 108.20   |
| 35  | BB    | 1113 | U    | N1-C2-N3    | 8.80  | 120.18      | 114.90   |
| 35  | BB    | 2204 | G    | C5-C6-O6    | -8.80 | 123.32      | 128.60   |
| 1   | AA    | 221  | C    | C2-N3-C4    | 8.80  | 124.30      | 119.90   |
| 1   | AA    | 450  | G    | C4-C5-C6    | 8.80  | 124.08      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1105 | A    | C8-N9-C4    | 8.80  | 109.32      | 105.80   |
| 35  | BB    | 422  | A    | N1-C6-N6    | 8.80  | 123.88      | 118.60   |
| 35  | BB    | 2247 | A    | N7-C8-N9    | -8.80 | 109.40      | 113.80   |
| 1   | AA    | 860  | A    | O4'-C1'-N9  | 8.80  | 115.24      | 108.20   |
| 22  | AV    | 37   | G    | O4'-C1'-N9  | 8.80  | 115.24      | 108.20   |
| 1   | AA    | 1244 | G    | O4'-C1'-N9  | 8.80  | 115.24      | 108.20   |
| 35  | BB    | 640  | C    | O4'-C1'-N1  | 8.80  | 115.24      | 108.20   |
| 35  | BB    | 807  | U    | P-O3'-C3'   | -8.80 | 109.14      | 119.70   |
| 35  | BB    | 887  | U    | C5-C6-N1    | 8.80  | 127.10      | 122.70   |
| 35  | BB    | 1416 | G    | C5-C6-N1    | -8.80 | 107.10      | 111.50   |
| 35  | BB    | 1874 | C    | N3-C4-N4    | 8.80  | 124.16      | 118.00   |
| 35  | BB    | 1968 | G    | C4-C5-N7    | 8.80  | 114.32      | 110.80   |
| 1   | AA    | 690  | G    | N1-C6-O6    | 8.80  | 125.18      | 119.90   |
| 1   | AA    | 1014 | A    | C4-C5-C6    | 8.80  | 121.40      | 117.00   |
| 35  | BB    | 19   | A    | C4-C5-C6    | 8.79  | 121.40      | 117.00   |
| 35  | BB    | 966  | G    | C5-C6-O6    | -8.79 | 123.32      | 128.60   |
| 35  | BB    | 1809 | A    | N1-C6-N6    | 8.79  | 123.88      | 118.60   |
| 1   | AA    | 523  | A    | C5-C6-N6    | -8.79 | 116.67      | 123.70   |
| 1   | AA    | 802  | A    | C6-N1-C2    | -8.79 | 113.33      | 118.60   |
| 34  | BA    | 34   | A    | C4-C5-C6    | 8.79  | 121.40      | 117.00   |
| 35  | BB    | 10   | A    | C5-N7-C8    | 8.79  | 108.30      | 103.90   |
| 35  | BB    | 262  | A    | C5-C6-N1    | -8.79 | 113.30      | 117.70   |
| 35  | BB    | 981  | A    | C5-C6-N6    | -8.79 | 116.67      | 123.70   |
| 35  | BB    | 2899 | A    | C3'-C2'-C1' | 8.79  | 108.53      | 101.50   |
| 1   | AA    | 599  | C    | C6-N1-C2    | 8.79  | 123.82      | 120.30   |
| 1   | AA    | 757  | U    | O4'-C1'-N1  | 8.79  | 115.23      | 108.20   |
| 35  | BB    | 1815 | A    | C5-N7-C8    | 8.79  | 108.30      | 103.90   |
| 35  | BB    | 2693 | G    | C6-C5-N7    | -8.79 | 125.13      | 130.40   |
| 1   | AA    | 931  | C    | C5-C4-N4    | -8.79 | 114.05      | 120.20   |
| 1   | AA    | 1068 | G    | C8-N9-C4    | 8.79  | 109.92      | 106.40   |
| 35  | BB    | 98   | G    | N1-C6-O6    | 8.79  | 125.17      | 119.90   |
| 35  | BB    | 111  | A    | N1-C6-N6    | 8.79  | 123.87      | 118.60   |
| 35  | BB    | 774  | G    | N7-C8-N9    | 8.79  | 117.49      | 113.10   |
| 35  | BB    | 2744 | G    | C6-C5-N7    | -8.79 | 125.13      | 130.40   |
| 1   | AA    | 47   | C    | C2-N1-C1'   | 8.79  | 128.46      | 118.80   |
| 35  | BB    | 1113 | U    | C2-N3-C4    | -8.79 | 121.73      | 127.00   |
| 35  | BB    | 1217 | U    | O4'-C1'-N1  | 8.79  | 115.23      | 108.20   |
| 35  | BB    | 963  | U    | N3-C2-O2    | 8.78  | 128.35      | 122.20   |
| 35  | BB    | 2114 | A    | C8-N9-C4    | -8.78 | 102.29      | 105.80   |
| 35  | BB    | 2494 | G    | O4'-C1'-N9  | 8.79  | 115.23      | 108.20   |
| 35  | BB    | 2799 | A    | O4'-C1'-N9  | 8.79  | 115.23      | 108.20   |
| 1   | AA    | 1242 | G    | N1-C6-O6    | 8.78  | 125.17      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 653  | U    | C2-N3-C4   | 8.78  | 132.27      | 127.00   |
| 35  | BB    | 1895 | C    | N3-C4-C5   | -8.78 | 118.39      | 121.90   |
| 39  | BF    | 17   | THR  | CA-CB-CG2  | -8.78 | 100.10      | 112.40   |
| 34  | BA    | 111  | U    | O4'-C1'-N1 | 8.78  | 115.22      | 108.20   |
| 35  | BB    | 400  | G    | N3-C2-N2   | 8.78  | 126.05      | 119.90   |
| 35  | BB    | 583  | G    | C5-C6-N1   | 8.78  | 115.89      | 111.50   |
| 35  | BB    | 719  | C    | O4'-C1'-N1 | 8.78  | 115.23      | 108.20   |
| 35  | BB    | 1243 | C    | C6-N1-C2   | -8.78 | 116.79      | 120.30   |
| 35  | BB    | 1945 | G    | C5-C6-O6   | -8.78 | 123.33      | 128.60   |
| 35  | BB    | 2575 | C    | C5-C4-N4   | -8.78 | 114.05      | 120.20   |
| 1   | AA    | 26   | A    | N7-C8-N9   | -8.78 | 109.41      | 113.80   |
| 1   | AA    | 1334 | G    | C6-C5-N7   | -8.78 | 125.13      | 130.40   |
| 35  | BB    | 2128 | G    | C5-C6-O6   | -8.78 | 123.33      | 128.60   |
| 35  | BB    | 43   | G    | C5-C6-N1   | -8.78 | 107.11      | 111.50   |
| 35  | BB    | 48   | G    | O4'-C1'-N9 | 8.78  | 115.22      | 108.20   |
| 35  | BB    | 254  | G    | C5-C6-O6   | -8.78 | 123.33      | 128.60   |
| 35  | BB    | 643  | A    | N1-C6-N6   | 8.78  | 123.87      | 118.60   |
| 35  | BB    | 289  | G    | C5-C6-O6   | -8.78 | 123.33      | 128.60   |
| 35  | BB    | 1237 | A    | C5-C6-N6   | -8.78 | 116.68      | 123.70   |
| 35  | BB    | 1473 | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 35  | BB    | 2544 | G    | N3-C2-N2   | 8.78  | 126.04      | 119.90   |
| 35  | BB    | 2808 | G    | O4'-C1'-N9 | 8.78  | 115.22      | 108.20   |
| 1   | AA    | 866  | C    | O4'-C1'-N1 | 8.78  | 115.22      | 108.20   |
| 35  | BB    | 1652 | A    | C8-N9-C4   | -8.78 | 102.29      | 105.80   |
| 35  | BB    | 2006 | C    | O4'-C1'-N1 | 8.78  | 115.22      | 108.20   |
| 35  | BB    | 522  | A    | N1-C6-N6   | 8.77  | 123.86      | 118.60   |
| 35  | BB    | 1620 | G    | C5-C6-O6   | -8.77 | 123.34      | 128.60   |
| 1   | AA    | 36   | C    | N3-C4-N4   | 8.77  | 124.14      | 118.00   |
| 35  | BB    | 259  | G    | C5-C6-O6   | -8.77 | 123.34      | 128.60   |
| 35  | BB    | 751  | A    | C5-C6-N1   | -8.77 | 113.31      | 117.70   |
| 35  | BB    | 1518 | C    | N3-C4-C5   | -8.77 | 118.39      | 121.90   |
| 35  | BB    | 1624 | U    | O4'-C1'-N1 | 8.77  | 115.22      | 108.20   |
| 35  | BB    | 1947 | C    | N3-C4-C5   | -8.77 | 118.39      | 121.90   |
| 35  | BB    | 2251 | G    | O4'-C1'-N9 | 8.77  | 115.22      | 108.20   |
| 35  | BB    | 1425 | G    | C8-N9-C4   | -8.77 | 102.89      | 106.40   |
| 35  | BB    | 2046 | G    | N1-C2-N3   | -8.77 | 118.64      | 123.90   |
| 35  | BB    | 2058 | A    | N7-C8-N9   | 8.77  | 118.18      | 113.80   |
| 35  | BB    | 661  | A    | C4-C5-C6   | 8.77  | 121.38      | 117.00   |
| 35  | BB    | 1049 | C    | C6-N1-C2   | -8.77 | 116.79      | 120.30   |
| 35  | BB    | 1138 | G    | C5-C6-O6   | -8.77 | 123.34      | 128.60   |
| 1   | AA    | 108  | G    | C6-C5-N7   | -8.76 | 125.14      | 130.40   |
| 1   | AA    | 155  | A    | N1-C6-N6   | 8.76  | 123.86      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 279  | A    | O4'-C1'-N9  | 8.76  | 115.21      | 108.20   |
| 1   | AA    | 1110 | A    | C6-C5-N7    | -8.76 | 126.17      | 132.30   |
| 34  | BA    | 59   | A    | N3-C4-C5    | -8.76 | 120.67      | 126.80   |
| 35  | BB    | 19   | A    | O4'-C1'-N9  | 8.76  | 115.21      | 108.20   |
| 35  | BB    | 1904 | G    | C4-C5-C6    | 8.76  | 124.06      | 118.80   |
| 35  | BB    | 2171 | A    | P-O3'-C3'   | 8.76  | 130.22      | 119.70   |
| 1   | AA    | 1419 | G    | N9-C4-C5    | -8.76 | 101.89      | 105.40   |
| 35  | BB    | 155  | A    | N7-C8-N9    | 8.76  | 118.18      | 113.80   |
| 35  | BB    | 266  | G    | N1-C6-O6    | 8.76  | 125.16      | 119.90   |
| 35  | BB    | 2409 | G    | N3-C2-N2    | 8.76  | 126.03      | 119.90   |
| 35  | BB    | 2860 | A    | N1-C6-N6    | 8.76  | 123.86      | 118.60   |
| 1   | AA    | 754  | C    | N3-C4-N4    | 8.76  | 124.13      | 118.00   |
| 1   | AA    | 771  | G    | N3-C4-C5    | -8.76 | 124.22      | 128.60   |
| 35  | BB    | 4    | U    | N3-C4-O4    | 8.76  | 125.53      | 119.40   |
| 35  | BB    | 24   | G    | N3-C4-N9    | -8.76 | 120.74      | 126.00   |
| 35  | BB    | 55   | G    | C5-N7-C8    | 8.76  | 108.68      | 104.30   |
| 35  | BB    | 430  | A    | C4-C5-C6    | 8.76  | 121.38      | 117.00   |
| 35  | BB    | 482  | A    | C5-C6-N6    | -8.76 | 116.69      | 123.70   |
| 35  | BB    | 1401 | G    | N1-C6-O6    | 8.76  | 125.15      | 119.90   |
| 35  | BB    | 1637 | A    | C5-C6-N6    | -8.76 | 116.69      | 123.70   |
| 35  | BB    | 1533 | C    | C6-N1-C2    | -8.76 | 116.80      | 120.30   |
| 35  | BB    | 1884 | G    | C5-C6-O6    | -8.76 | 123.35      | 128.60   |
| 35  | BB    | 2180 | U    | O4'-C1'-N1  | 8.76  | 115.20      | 108.20   |
| 35  | BB    | 2186 | G    | N9-C4-C5    | -8.76 | 101.90      | 105.40   |
| 35  | BB    | 2227 | A    | N1-C2-N3    | 8.76  | 133.68      | 129.30   |
| 35  | BB    | 1717 | A    | C6-C5-N7    | -8.76 | 126.17      | 132.30   |
| 35  | BB    | 1900 | A    | N1-C2-N3    | -8.76 | 124.92      | 129.30   |
| 35  | BB    | 2305 | U    | O4'-C1'-N1  | 8.76  | 115.20      | 108.20   |
| 1   | AA    | 242  | G    | P-O3'-C3'   | 8.75  | 130.20      | 119.70   |
| 35  | BB    | 1897 | G    | N9-C4-C5    | -8.75 | 101.90      | 105.40   |
| 1   | AA    | 590  | U    | N3-C4-O4    | 8.75  | 125.53      | 119.40   |
| 1   | AA    | 1509 | C    | O4'-C1'-N1  | 8.75  | 115.20      | 108.20   |
| 35  | BB    | 654  | A    | C4-C5-C6    | 8.75  | 121.38      | 117.00   |
| 35  | BB    | 1304 | A    | C5-C6-N6    | -8.75 | 116.70      | 123.70   |
| 35  | BB    | 1508 | A    | C5-C6-N6    | -8.75 | 116.70      | 123.70   |
| 1   | AA    | 983  | A    | O4'-C1'-N9  | 8.75  | 115.20      | 108.20   |
| 35  | BB    | 1802 | A    | N7-C8-N9    | -8.75 | 109.42      | 113.80   |
| 35  | BB    | 2117 | A    | O4'-C1'-N9  | 8.75  | 115.20      | 108.20   |
| 1   | AA    | 257  | G    | C3'-C2'-C1' | 8.75  | 108.50      | 101.50   |
| 1   | AA    | 558  | G    | C4-C5-C6    | 8.75  | 124.05      | 118.80   |
| 35  | BB    | 315  | G    | O4'-C1'-N9  | 8.75  | 115.20      | 108.20   |
| 35  | BB    | 1996 | C    | C6-N1-C2    | -8.75 | 116.80      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1429 | A    | C5-C6-N1   | -8.75 | 113.33      | 117.70   |
| 35  | BB    | 2173 | A    | C8-N9-C4   | -8.75 | 102.30      | 105.80   |
| 1   | AA    | 1276 | G    | C8-N9-C4   | -8.75 | 102.90      | 106.40   |
| 35  | BB    | 2901 | C    | C5-C4-N4   | -8.75 | 114.08      | 120.20   |
| 1   | AA    | 312  | C    | N3-C4-N4   | 8.74  | 124.12      | 118.00   |
| 1   | AA    | 402  | G    | C4-C5-N7   | -8.74 | 107.30      | 110.80   |
| 34  | BA    | 98   | G    | N3-C2-N2   | 8.74  | 126.02      | 119.90   |
| 35  | BB    | 551  | G    | C4-C5-N7   | -8.74 | 107.30      | 110.80   |
| 35  | BB    | 722  | A    | C5-N7-C8   | 8.74  | 108.27      | 103.90   |
| 35  | BB    | 966  | G    | O4'-C1'-N9 | 8.74  | 115.20      | 108.20   |
| 1   | AA    | 885  | G    | C5-C6-O6   | -8.74 | 123.36      | 128.60   |
| 35  | BB    | 722  | A    | C4-C5-C6   | 8.74  | 121.37      | 117.00   |
| 35  | BB    | 1500 | G    | N7-C8-N9   | 8.74  | 117.47      | 113.10   |
| 35  | BB    | 1725 | U    | O4'-C1'-N1 | 8.74  | 115.19      | 108.20   |
| 35  | BB    | 1904 | G    | N3-C4-C5   | -8.74 | 124.23      | 128.60   |
| 35  | BB    | 2397 | G    | N1-C6-O6   | 8.74  | 125.14      | 119.90   |
| 35  | BB    | 2426 | A    | C5-C6-N1   | -8.74 | 113.33      | 117.70   |
| 1   | AA    | 614  | C    | C6-N1-C2   | -8.74 | 116.80      | 120.30   |
| 1   | AA    | 390  | U    | C6-N1-C2   | -8.74 | 115.76      | 121.00   |
| 1   | AA    | 1453 | G    | C4-C5-C6   | 8.74  | 124.04      | 118.80   |
| 35  | BB    | 718  | A    | C5-C6-N1   | -8.74 | 113.33      | 117.70   |
| 35  | BB    | 1014 | A    | C4-C5-C6   | 8.74  | 121.37      | 117.00   |
| 11  | AK    | 55   | ARG  | NE-CZ-NH2  | -8.74 | 115.93      | 120.30   |
| 35  | BB    | 614  | A    | O4'-C1'-N9 | 8.74  | 115.19      | 108.20   |
| 1   | AA    | 189  | A    | N7-C8-N9   | -8.74 | 109.43      | 113.80   |
| 35  | BB    | 788  | A    | O4'-C1'-N9 | 8.74  | 115.19      | 108.20   |
| 35  | BB    | 2142 | A    | N1-C2-N3   | 8.74  | 133.67      | 129.30   |
| 1   | AA    | 929  | G    | N3-C2-N2   | 8.74  | 126.02      | 119.90   |
| 1   | AA    | 1079 | G    | N3-C2-N2   | 8.74  | 126.02      | 119.90   |
| 1   | AA    | 1402 | C    | C5-C6-N1   | 8.74  | 125.37      | 121.00   |
| 35  | BB    | 1760 | C    | C6-N1-C2   | -8.74 | 116.81      | 120.30   |
| 35  | BB    | 2592 | G    | O4'-C1'-N9 | 8.74  | 115.19      | 108.20   |
| 35  | BB    | 2771 | C    | N3-C4-N4   | 8.74  | 124.12      | 118.00   |
| 1   | AA    | 948  | C    | C2-N3-C4   | 8.73  | 124.27      | 119.90   |
| 35  | BB    | 2701 | U    | C5-C6-N1   | 8.73  | 127.07      | 122.70   |
| 1   | AA    | 846  | G    | C5-C6-O6   | -8.73 | 123.36      | 128.60   |
| 35  | BB    | 266  | G    | C5-N7-C8   | 8.73  | 108.67      | 104.30   |
| 35  | BB    | 1744 | A    | C5-C6-N6   | -8.73 | 116.71      | 123.70   |
| 1   | AA    | 1398 | A    | C5-C6-N6   | -8.73 | 116.71      | 123.70   |
| 35  | BB    | 349  | U    | O4'-C1'-N1 | 8.73  | 115.19      | 108.20   |
| 35  | BB    | 2274 | A    | C6-C5-N7   | -8.73 | 126.19      | 132.30   |
| 1   | AA    | 439  | U    | N1-C2-N3   | -8.73 | 109.66      | 114.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 585  | G    | C8-N9-C4    | -8.73 | 102.91      | 106.40   |
| 35  | BB    | 892  | A    | C5-C6-N6    | -8.73 | 116.72      | 123.70   |
| 35  | BB    | 986  | C    | O4'-C1'-N1  | 8.73  | 115.19      | 108.20   |
| 35  | BB    | 1050 | A    | C4-C5-C6    | 8.73  | 121.37      | 117.00   |
| 35  | BB    | 1074 | G    | C4-C5-C6    | 8.73  | 124.04      | 118.80   |
| 1   | AA    | 1305 | G    | C5-C6-N1    | -8.73 | 107.14      | 111.50   |
| 35  | BB    | 89   | A    | C5-N7-C8    | 8.73  | 108.26      | 103.90   |
| 1   | AA    | 5    | U    | O4'-C1'-N1  | 8.73  | 115.18      | 108.20   |
| 1   | AA    | 7    | A    | O4'-C1'-N9  | 8.73  | 115.18      | 108.20   |
| 1   | AA    | 63   | C    | C5-C4-N4    | -8.73 | 114.09      | 120.20   |
| 1   | AA    | 671  | G    | C8-N9-C4    | -8.73 | 102.91      | 106.40   |
| 35  | BB    | 173  | A    | C8-N9-C4    | 8.73  | 109.29      | 105.80   |
| 35  | BB    | 1323 | C    | N3-C4-C5    | -8.73 | 118.41      | 121.90   |
| 35  | BB    | 1745 | A    | C4-C5-C6    | 8.73  | 121.36      | 117.00   |
| 44  | BK    | 105  | ARG  | NE-CZ-NH1   | 8.73  | 124.66      | 120.30   |
| 35  | BB    | 886  | A    | C4-C5-C6    | 8.73  | 121.36      | 117.00   |
| 35  | BB    | 1705 | A    | C2-N3-C4    | -8.73 | 106.24      | 110.60   |
| 35  | BB    | 2159 | G    | C1'-O4'-C4' | 8.73  | 116.88      | 109.90   |
| 35  | BB    | 2683 | C    | O4'-C1'-N1  | 8.73  | 115.18      | 108.20   |
| 1   | AA    | 315  | A    | C5-C6-N1    | -8.72 | 113.34      | 117.70   |
| 1   | AA    | 460  | A    | N9-C4-C5    | -8.72 | 102.31      | 105.80   |
| 1   | AA    | 1109 | C    | N3-C4-C5    | -8.72 | 118.41      | 121.90   |
| 35  | BB    | 2549 | G    | N1-C2-N3    | -8.72 | 118.67      | 123.90   |
| 35  | BB    | 376  | G    | P-O5'-C5'   | 8.72  | 134.86      | 120.90   |
| 35  | BB    | 608  | A    | N1-C2-N3    | 8.72  | 133.66      | 129.30   |
| 35  | BB    | 766  | U    | N3-C4-O4    | 8.72  | 125.51      | 119.40   |
| 35  | BB    | 1236 | G    | C5-C6-O6    | -8.72 | 123.37      | 128.60   |
| 35  | BB    | 2188 | U    | O4'-C1'-N1  | 8.72  | 115.18      | 108.20   |
| 35  | BB    | 2682 | A    | N9-C4-C5    | 8.72  | 109.29      | 105.80   |
| 1   | AA    | 413  | G    | N1-C2-N3    | -8.72 | 118.67      | 123.90   |
| 1   | AA    | 1287 | A    | C8-N9-C4    | -8.72 | 102.31      | 105.80   |
| 1   | AA    | 510  | A    | C5-N7-C8    | 8.72  | 108.26      | 103.90   |
| 35  | BB    | 161  | A    | C4-C5-C6    | 8.72  | 121.36      | 117.00   |
| 35  | BB    | 950  | G    | C2-N3-C4    | -8.72 | 107.54      | 111.90   |
| 35  | BB    | 2303 | G    | C5-C6-O6    | -8.72 | 123.37      | 128.60   |
| 35  | BB    | 2374 | C    | P-O3'-C3'   | -8.72 | 109.23      | 119.70   |
| 1   | AA    | 621  | A    | C5-C6-N1    | -8.72 | 113.34      | 117.70   |
| 1   | AA    | 1263 | C    | C5-C6-N1    | 8.72  | 125.36      | 121.00   |
| 1   | AA    | 1278 | G    | C5-C6-N1    | 8.72  | 115.86      | 111.50   |
| 1   | AA    | 1331 | G    | C5-C6-O6    | -8.72 | 123.37      | 128.60   |
| 35  | BB    | 215  | G    | N3-C2-N2    | 8.72  | 126.00      | 119.90   |
| 35  | BB    | 670  | A    | C4-C5-C6    | 8.72  | 121.36      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 780  | G    | N3-C2-N2    | 8.72  | 126.00      | 119.90   |
| 35  | BB    | 1262 | A    | C2-N3-C4    | -8.72 | 106.24      | 110.60   |
| 35  | BB    | 1500 | G    | C2-N3-C4    | 8.72  | 116.26      | 111.90   |
| 35  | BB    | 2298 | A    | C5-N7-C8    | 8.72  | 108.26      | 103.90   |
| 35  | BB    | 2531 | A    | C4'-C3'-C2' | -8.72 | 93.88       | 102.60   |
| 1   | AA    | 1184 | G    | C5-C6-O6    | -8.72 | 123.37      | 128.60   |
| 35  | BB    | 558  | U    | N1-C2-O2    | -8.72 | 116.70      | 122.80   |
| 35  | BB    | 798  | G    | C5-C6-O6    | -8.71 | 123.37      | 128.60   |
| 1   | AA    | 109  | A    | C8-N9-C4    | -8.71 | 102.32      | 105.80   |
| 1   | AA    | 847  | G    | O4'-C1'-N9  | 8.71  | 115.17      | 108.20   |
| 35  | BB    | 1092 | C    | O4'-C1'-N1  | 8.71  | 115.17      | 108.20   |
| 1   | AA    | 859  | G    | N1-C6-O6    | 8.71  | 125.13      | 119.90   |
| 1   | AA    | 1042 | A    | C8-N9-C4    | -8.71 | 102.32      | 105.80   |
| 1   | AA    | 1279 | G    | N7-C8-N9    | 8.71  | 117.46      | 113.10   |
| 35  | BB    | 1155 | A    | C4-C5-C6    | 8.71  | 121.36      | 117.00   |
| 35  | BB    | 747  | U    | O4'-C1'-N1  | 8.71  | 115.17      | 108.20   |
| 35  | BB    | 2215 | C    | C4-C5-C6    | 8.71  | 121.75      | 117.40   |
| 35  | BB    | 311  | A    | N1-C6-N6    | 8.71  | 123.83      | 118.60   |
| 35  | BB    | 404  | A    | C8-N9-C4    | 8.71  | 109.28      | 105.80   |
| 35  | BB    | 821  | A    | N1-C6-N6    | 8.71  | 123.83      | 118.60   |
| 35  | BB    | 1310 | G    | C4-C5-C6    | 8.71  | 124.03      | 118.80   |
| 35  | BB    | 1767 | G    | C6-N1-C2    | 8.71  | 130.32      | 125.10   |
| 35  | BB    | 466  | A    | C5-C6-N1    | -8.71 | 113.35      | 117.70   |
| 35  | BB    | 1107 | G    | N1-C2-N3    | -8.71 | 118.68      | 123.90   |
| 35  | BB    | 1871 | A    | C4-C5-C6    | 8.71  | 121.35      | 117.00   |
| 1   | AA    | 502  | A    | O4'-C1'-N9  | 8.71  | 115.16      | 108.20   |
| 35  | BB    | 1204 | A    | N9-C4-C5    | -8.71 | 102.32      | 105.80   |
| 35  | BB    | 1966 | A    | C5-C6-N1    | -8.71 | 113.35      | 117.70   |
| 22  | AV    | 52   | G    | N1-C6-O6    | 8.70  | 125.12      | 119.90   |
| 35  | BB    | 332  | A    | C4-C5-C6    | 8.70  | 121.35      | 117.00   |
| 35  | BB    | 1484 | U    | N3-C2-O2    | 8.70  | 128.29      | 122.20   |
| 35  | BB    | 1600 | C    | O4'-C1'-N1  | 8.70  | 115.16      | 108.20   |
| 35  | BB    | 1693 | U    | N3-C4-C5    | -8.70 | 109.38      | 114.60   |
| 35  | BB    | 1746 | A    | C8-N9-C4    | -8.71 | 102.32      | 105.80   |
| 35  | BB    | 2073 | C    | N1-C2-O2    | 8.70  | 124.12      | 118.90   |
| 35  | BB    | 2572 | A    | O4'-C1'-N9  | 8.71  | 115.16      | 108.20   |
| 1   | AA    | 549  | C    | C6-N1-C2    | -8.70 | 116.82      | 120.30   |
| 35  | BB    | 557  | C    | N3-C4-C5    | -8.70 | 118.42      | 121.90   |
| 1   | AA    | 508  | U    | N3-C4-C5    | -8.70 | 109.38      | 114.60   |
| 1   | AA    | 771  | G    | N3-C2-N2    | 8.70  | 125.99      | 119.90   |
| 15  | AO    | 79   | ARG  | NE-CZ-NH1   | 8.70  | 124.65      | 120.30   |
| 35  | BB    | 804  | A    | C5-C6-N6    | -8.70 | 116.74      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2283 | C    | O4'-C1'-N1  | 8.70  | 115.16      | 108.20   |
| 35  | BB    | 549  | G    | C8-N9-C4    | -8.70 | 102.92      | 106.40   |
| 35  | BB    | 689  | A    | C4-C5-C6    | 8.70  | 121.35      | 117.00   |
| 1   | AA    | 621  | A    | N1-C6-N6    | 8.70  | 123.82      | 118.60   |
| 35  | BB    | 219  | A    | C8-N9-C4    | -8.70 | 102.32      | 105.80   |
| 35  | BB    | 851  | C    | O4'-C1'-N1  | 8.70  | 115.16      | 108.20   |
| 35  | BB    | 1675 | C    | C4-C5-C6    | -8.70 | 113.05      | 117.40   |
| 35  | BB    | 2061 | G    | C5-C6-O6    | -8.70 | 123.38      | 128.60   |
| 35  | BB    | 1706 | C    | N3-C4-N4    | 8.70  | 124.09      | 118.00   |
| 35  | BB    | 1762 | A    | C4-C5-C6    | 8.70  | 121.35      | 117.00   |
| 35  | BB    | 2490 | G    | C5-C6-O6    | -8.70 | 123.38      | 128.60   |
| 35  | BB    | 2700 | A    | C6-C5-N7    | -8.70 | 126.21      | 132.30   |
| 1   | AA    | 796  | C    | C2-N3-C4    | 8.70  | 124.25      | 119.90   |
| 1   | AA    | 1235 | U    | O4'-C1'-N1  | 8.70  | 115.16      | 108.20   |
| 34  | BA    | 16   | G    | O4'-C1'-N9  | 8.70  | 115.16      | 108.20   |
| 35  | BB    | 906  | U    | N3-C4-O4    | 8.70  | 125.49      | 119.40   |
| 35  | BB    | 287  | G    | O4'-C1'-N9  | 8.69  | 115.16      | 108.20   |
| 35  | BB    | 480  | A    | O4'-C1'-N9  | 8.70  | 115.16      | 108.20   |
| 35  | BB    | 2037 | A    | C5-C6-N6    | -8.70 | 116.74      | 123.70   |
| 35  | BB    | 491  | G    | N1-C2-N3    | -8.69 | 118.68      | 123.90   |
| 1   | AA    | 1245 | C    | C5-C6-N1    | 8.69  | 125.35      | 121.00   |
| 34  | BA    | 28   | C    | C6-N1-C2    | -8.69 | 116.82      | 120.30   |
| 35  | BB    | 565  | C    | N3-C4-C5    | -8.69 | 118.42      | 121.90   |
| 1   | AA    | 533  | A    | C4-C5-C6    | 8.69  | 121.35      | 117.00   |
| 1   | AA    | 1279 | G    | N1-C6-O6    | 8.69  | 125.11      | 119.90   |
| 1   | AA    | 781  | A    | N9-C4-C5    | 8.69  | 109.28      | 105.80   |
| 35  | BB    | 1042 | G    | C4-C5-N7    | -8.69 | 107.33      | 110.80   |
| 35  | BB    | 2382 | G    | C6-C5-N7    | -8.69 | 125.19      | 130.40   |
| 1   | AA    | 571  | U    | O4'-C1'-N1  | 8.69  | 115.15      | 108.20   |
| 35  | BB    | 324  | A    | C5-N7-C8    | 8.69  | 108.24      | 103.90   |
| 1   | AA    | 1281 | C    | C2-N1-C1'   | 8.69  | 128.35      | 118.80   |
| 35  | BB    | 57   | C    | C5-C4-N4    | -8.69 | 114.12      | 120.20   |
| 35  | BB    | 887  | U    | N1-C2-N3    | 8.69  | 120.11      | 114.90   |
| 35  | BB    | 1679 | A    | C5-C6-N6    | -8.69 | 116.75      | 123.70   |
| 35  | BB    | 1378 | A    | N9-C4-C5    | 8.69  | 109.27      | 105.80   |
| 35  | BB    | 1788 | C    | C5-C6-N1    | 8.69  | 125.34      | 121.00   |
| 35  | BB    | 1875 | G    | C5-N7-C8    | -8.69 | 99.96       | 104.30   |
| 35  | BB    | 2168 | G    | C5-N7-C8    | -8.69 | 99.96       | 104.30   |
| 35  | BB    | 2615 | U    | C4'-C3'-C2' | -8.69 | 93.91       | 102.60   |
| 35  | BB    | 2383 | G    | C5-C6-N1    | -8.69 | 107.16      | 111.50   |
| 35  | BB    | 2755 | C    | O4'-C1'-N1  | 8.69  | 115.15      | 108.20   |
| 1   | AA    | 85   | U    | N3-C4-O4    | 8.68  | 125.48      | 119.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 573  | A    | C5-N7-C8   | 8.68  | 108.24      | 103.90   |
| 1   | AA    | 646  | G    | C8-N9-C4   | -8.68 | 102.93      | 106.40   |
| 35  | BB    | 159  | G    | C4-C5-C6   | 8.68  | 124.01      | 118.80   |
| 35  | BB    | 307  | G    | N3-C2-N2   | 8.68  | 125.98      | 119.90   |
| 35  | BB    | 1272 | A    | C5-C6-N6   | -8.68 | 116.75      | 123.70   |
| 35  | BB    | 1398 | C    | N3-C2-O2   | -8.68 | 115.82      | 121.90   |
| 1   | AA    | 262  | A    | C5-C6-N1   | -8.68 | 113.36      | 117.70   |
| 10  | AJ    | 89   | ARG  | NE-CZ-NH2  | 8.68  | 124.64      | 120.30   |
| 35  | BB    | 386  | G    | C6-C5-N7   | -8.68 | 125.19      | 130.40   |
| 35  | BB    | 551  | G    | N9-C4-C5   | 8.68  | 108.87      | 105.40   |
| 35  | BB    | 677  | A    | C4-C5-C6   | 8.68  | 121.34      | 117.00   |
| 35  | BB    | 2594 | C    | N3-C4-C5   | -8.68 | 118.43      | 121.90   |
| 35  | BB    | 375  | G    | N1-C2-N3   | -8.68 | 118.69      | 123.90   |
| 35  | BB    | 869  | G    | N3-C2-N2   | 8.68  | 125.97      | 119.90   |
| 35  | BB    | 2283 | C    | N1-C2-N3   | 8.68  | 125.28      | 119.20   |
| 1   | AA    | 277  | C    | N3-C4-N4   | 8.68  | 124.07      | 118.00   |
| 35  | BB    | 14   | A    | C8-N9-C4   | -8.68 | 102.33      | 105.80   |
| 35  | BB    | 1068 | G    | N1-C6-O6   | 8.68  | 125.11      | 119.90   |
| 35  | BB    | 1149 | G    | N1-C6-O6   | 8.68  | 125.11      | 119.90   |
| 35  | BB    | 1455 | G    | C5-C6-O6   | -8.68 | 123.39      | 128.60   |
| 35  | BB    | 2055 | C    | N1-C2-O2   | -8.68 | 113.69      | 118.90   |
| 35  | BB    | 1547 | C    | N3-C4-N4   | 8.67  | 124.07      | 118.00   |
| 35  | BB    | 1631 | G    | C4-C5-C6   | 8.67  | 124.00      | 118.80   |
| 35  | BB    | 2634 | A    | C5-C6-N1   | -8.67 | 113.36      | 117.70   |
| 36  | BC    | 220  | ARG  | NE-CZ-NH1  | 8.67  | 124.64      | 120.30   |
| 22  | AV    | 12   | G    | N1-C6-O6   | 8.67  | 125.10      | 119.90   |
| 34  | BA    | 45   | A    | C4-C5-C6   | 8.67  | 121.33      | 117.00   |
| 35  | BB    | 259  | G    | N1-C2-N3   | -8.67 | 118.70      | 123.90   |
| 35  | BB    | 452  | G    | N3-C2-N2   | 8.67  | 125.97      | 119.90   |
| 35  | BB    | 590  | A    | O4'-C1'-N9 | 8.67  | 115.14      | 108.20   |
| 35  | BB    | 794  | A    | O4'-C1'-N9 | 8.67  | 115.14      | 108.20   |
| 35  | BB    | 2078 | C    | C5-C4-N4   | -8.67 | 114.13      | 120.20   |
| 35  | BB    | 390  | U    | O4'-C1'-N1 | 8.67  | 115.14      | 108.20   |
| 1   | AA    | 936  | C    | C5-C6-N1   | 8.67  | 125.33      | 121.00   |
| 35  | BB    | 688  | U    | N3-C2-O2   | 8.67  | 128.27      | 122.20   |
| 35  | BB    | 902  | C    | O4'-C1'-N1 | 8.67  | 115.13      | 108.20   |
| 35  | BB    | 2524 | G    | N9-C4-C5   | 8.67  | 108.87      | 105.40   |
| 35  | BB    | 2573 | C    | C6-N1-C2   | -8.67 | 116.83      | 120.30   |
| 35  | BB    | 2600 | A    | C5-N7-C8   | 8.67  | 108.23      | 103.90   |
| 35  | BB    | 2642 | G    | N7-C8-N9   | 8.67  | 117.43      | 113.10   |
| 35  | BB    | 2742 | G    | C4-C5-C6   | 8.67  | 124.00      | 118.80   |
| 1   | AA    | 1349 | A    | C2-N3-C4   | -8.66 | 106.27      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1487 | G    | O4'-C1'-N9  | 8.66  | 115.13      | 108.20   |
| 35  | BB    | 2814 | A    | O4'-C1'-N9  | 8.66  | 115.13      | 108.20   |
| 35  | BB    | 225  | C    | O4'-C1'-N1  | 8.66  | 115.13      | 108.20   |
| 35  | BB    | 292  | U    | C5-C4-O4    | -8.66 | 120.70      | 125.90   |
| 35  | BB    | 797  | G    | O4'-C1'-N9  | 8.66  | 115.13      | 108.20   |
| 35  | BB    | 1857 | G    | C6-C5-N7    | -8.66 | 125.20      | 130.40   |
| 35  | BB    | 2440 | C    | N3-C4-C5    | -8.66 | 118.43      | 121.90   |
| 1   | AA    | 148  | G    | C6-C5-N7    | -8.66 | 125.20      | 130.40   |
| 1   | AA    | 328  | C    | C2-N3-C4    | 8.66  | 124.23      | 119.90   |
| 1   | AA    | 752  | G    | N1-C2-N3    | -8.66 | 118.70      | 123.90   |
| 1   | AA    | 329  | A    | N9-C4-C5    | -8.66 | 102.34      | 105.80   |
| 1   | AA    | 421  | U    | N3-C2-O2    | -8.66 | 116.14      | 122.20   |
| 1   | AA    | 861  | G    | C5-C6-O6    | -8.66 | 123.40      | 128.60   |
| 1   | AA    | 1386 | G    | N3-C4-C5    | -8.66 | 124.27      | 128.60   |
| 35  | BB    | 1297 | C    | C5-C4-N4    | -8.66 | 114.14      | 120.20   |
| 35  | BB    | 2082 | A    | C6-C5-N7    | -8.66 | 126.24      | 132.30   |
| 35  | BB    | 2213 | U    | C5-C4-O4    | -8.66 | 120.70      | 125.90   |
| 35  | BB    | 339  | U    | C4-C5-C6    | 8.66  | 124.89      | 119.70   |
| 35  | BB    | 1061 | U    | C5'-C4'-O4' | 8.66  | 119.49      | 109.10   |
| 35  | BB    | 1303 | G    | N1-C6-O6    | 8.66  | 125.10      | 119.90   |
| 35  | BB    | 2362 | C    | N3-C4-N4    | 8.66  | 124.06      | 118.00   |
| 35  | BB    | 2588 | G    | O4'-C1'-N9  | 8.66  | 115.13      | 108.20   |
| 35  | BB    | 2599 | G    | N3-C2-N2    | 8.66  | 125.96      | 119.90   |
| 1   | AA    | 1357 | A    | C4-C5-C6    | 8.66  | 121.33      | 117.00   |
| 35  | BB    | 1580 | A    | C2-N3-C4    | -8.66 | 106.27      | 110.60   |
| 1   | AA    | 115  | G    | N1-C6-O6    | 8.66  | 125.09      | 119.90   |
| 1   | AA    | 950  | U    | C5-C6-N1    | 8.66  | 127.03      | 122.70   |
| 35  | BB    | 2183 | A    | C5-C6-N1    | -8.66 | 113.37      | 117.70   |
| 35  | BB    | 527  | C    | C5-C4-N4    | -8.65 | 114.14      | 120.20   |
| 1   | AA    | 1225 | A    | C5-C6-N6    | -8.65 | 116.78      | 123.70   |
| 35  | BB    | 155  | A    | N1-C6-N6    | 8.65  | 123.79      | 118.60   |
| 35  | BB    | 891  | G    | O4'-C1'-N9  | 8.65  | 115.12      | 108.20   |
| 35  | BB    | 1048 | A    | O4'-C1'-N9  | 8.65  | 115.12      | 108.20   |
| 35  | BB    | 1154 | G    | N3-C2-N2    | 8.65  | 125.96      | 119.90   |
| 35  | BB    | 1422 | G    | C5-C6-O6    | -8.65 | 123.41      | 128.60   |
| 35  | BB    | 1877 | A    | C5-C6-N1    | -8.65 | 113.37      | 117.70   |
| 35  | BB    | 2140 | G    | C5-C6-O6    | -8.65 | 123.41      | 128.60   |
| 35  | BB    | 2659 | G    | C5-C6-O6    | -8.65 | 123.41      | 128.60   |
| 35  | BB    | 104  | A    | C2-N3-C4    | -8.65 | 106.27      | 110.60   |
| 35  | BB    | 1816 | C    | N3-C4-N4    | 8.65  | 124.06      | 118.00   |
| 35  | BB    | 2219 | U    | C6-N1-C2    | 8.65  | 126.19      | 121.00   |
| 35  | BB    | 2293 | G    | N9-C4-C5    | -8.65 | 101.94      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 923  | A    | C5-N7-C8   | 8.65  | 108.22      | 103.90   |
| 1   | AA    | 533  | A    | C8-N9-C4   | -8.65 | 102.34      | 105.80   |
| 1   | AA    | 790  | A    | C6-C5-N7   | -8.65 | 126.25      | 132.30   |
| 1   | AA    | 1340 | A    | N1-C6-N6   | 8.65  | 123.79      | 118.60   |
| 1   | AA    | 1020 | G    | C5-C6-N1   | -8.65 | 107.18      | 111.50   |
| 35  | BB    | 863  | A    | C5-C6-N6   | -8.65 | 116.78      | 123.70   |
| 35  | BB    | 1309 | G    | C4-C5-N7   | -8.65 | 107.34      | 110.80   |
| 35  | BB    | 1516 | G    | N1-C6-O6   | 8.65  | 125.09      | 119.90   |
| 35  | BB    | 2439 | A    | C5-C6-N6   | -8.65 | 116.78      | 123.70   |
| 35  | BB    | 2536 | G    | N3-C2-N2   | 8.65  | 125.95      | 119.90   |
| 1   | AA    | 321  | A    | C5-C6-N1   | -8.64 | 113.38      | 117.70   |
| 1   | AA    | 561  | U    | C2-N3-C4   | -8.64 | 121.81      | 127.00   |
| 1   | AA    | 720  | C    | C6-N1-C2   | -8.64 | 116.84      | 120.30   |
| 1   | AA    | 1349 | A    | O4'-C1'-N9 | 8.64  | 115.12      | 108.20   |
| 35  | BB    | 301  | G    | N1-C2-N3   | -8.64 | 118.71      | 123.90   |
| 1   | AA    | 60   | A    | P-O3'-C3'  | 8.64  | 130.07      | 119.70   |
| 1   | AA    | 131  | A    | N1-C6-N6   | 8.64  | 123.79      | 118.60   |
| 1   | AA    | 858  | G    | N1-C6-O6   | 8.64  | 125.09      | 119.90   |
| 1   | AA    | 1046 | A    | C4-C5-C6   | 8.64  | 121.32      | 117.00   |
| 1   | AA    | 1132 | C    | O4'-C1'-N1 | 8.64  | 115.11      | 108.20   |
| 1   | AA    | 1433 | A    | C5-C6-N6   | -8.64 | 116.78      | 123.70   |
| 35  | BB    | 1071 | G    | C8-N9-C4   | -8.64 | 102.94      | 106.40   |
| 35  | BB    | 1109 | C    | N3-C4-N4   | 8.64  | 124.05      | 118.00   |
| 35  | BB    | 1171 | G    | N1-C6-O6   | 8.64  | 125.09      | 119.90   |
| 35  | BB    | 1810 | A    | C4-C5-N7   | -8.64 | 106.38      | 110.70   |
| 35  | BB    | 1110 | G    | N7-C8-N9   | 8.64  | 117.42      | 113.10   |
| 1   | AA    | 106  | C    | N3-C4-N4   | 8.64  | 124.05      | 118.00   |
| 1   | AA    | 447  | G    | C6-C5-N7   | -8.64 | 125.22      | 130.40   |
| 35  | BB    | 277  | G    | C8-N9-C4   | 8.64  | 109.86      | 106.40   |
| 35  | BB    | 1177 | G    | N3-C2-N2   | 8.64  | 125.95      | 119.90   |
| 35  | BB    | 1328 | A    | C5-N7-C8   | 8.64  | 108.22      | 103.90   |
| 35  | BB    | 2596 | U    | C5-C4-O4   | -8.64 | 120.72      | 125.90   |
| 1   | AA    | 142  | G    | O4'-C1'-N9 | 8.64  | 115.11      | 108.20   |
| 1   | AA    | 179  | A    | C5-C6-N1   | -8.64 | 113.38      | 117.70   |
| 35  | BB    | 759  | G    | N3-C4-C5   | -8.64 | 124.28      | 128.60   |
| 1   | AA    | 356  | A    | C5-N7-C8   | 8.64  | 108.22      | 103.90   |
| 1   | AA    | 1191 | A    | N3-C4-C5   | -8.64 | 120.75      | 126.80   |
| 1   | AA    | 1512 | U    | N3-C4-O4   | 8.64  | 125.44      | 119.40   |
| 35  | BB    | 44   | A    | C2-N3-C4   | -8.63 | 106.28      | 110.60   |
| 35  | BB    | 255  | A    | O4'-C1'-N9 | 8.64  | 115.11      | 108.20   |
| 35  | BB    | 1059 | G    | N1-C6-O6   | 8.64  | 125.08      | 119.90   |
| 35  | BB    | 540  | C    | N3-C4-N4   | 8.63  | 124.04      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 984  | A    | C6-C5-N7    | -8.63 | 126.26      | 132.30   |
| 35  | BB    | 1164 | C    | N3-C4-N4    | 8.63  | 124.04      | 118.00   |
| 35  | BB    | 1341 | G    | C4-C5-C6    | 8.63  | 123.98      | 118.80   |
| 1   | AA    | 560  | A    | O4'-C1'-N9  | 8.63  | 115.11      | 108.20   |
| 35  | BB    | 941  | A    | N1-C6-N6    | 8.63  | 123.78      | 118.60   |
| 1   | AA    | 154  | U    | O4'-C1'-N1  | 8.63  | 115.10      | 108.20   |
| 35  | BB    | 638  | G    | C4-C5-C6    | 8.63  | 123.98      | 118.80   |
| 35  | BB    | 806  | C    | O4'-C1'-N1  | 8.63  | 115.11      | 108.20   |
| 35  | BB    | 1251 | C    | N3-C4-N4    | 8.63  | 124.04      | 118.00   |
| 35  | BB    | 2061 | G    | O4'-C1'-N9  | 8.63  | 115.11      | 108.20   |
| 35  | BB    | 2301 | C    | O4'-C1'-N1  | 8.63  | 115.10      | 108.20   |
| 35  | BB    | 1213 | A    | C5-C6-N6    | -8.63 | 116.80      | 123.70   |
| 35  | BB    | 1665 | A    | C6-N1-C2    | -8.63 | 113.42      | 118.60   |
| 1   | AA    | 1358 | U    | N3-C4-O4    | 8.63  | 125.44      | 119.40   |
| 22  | AV    | 45   | G    | N1-C6-O6    | 8.63  | 125.08      | 119.90   |
| 35  | BB    | 964  | C    | C5-C4-N4    | -8.63 | 114.16      | 120.20   |
| 35  | BB    | 1270 | C    | N3-C4-N4    | 8.63  | 124.04      | 118.00   |
| 35  | BB    | 2421 | G    | C4-C5-C6    | 8.63  | 123.98      | 118.80   |
| 35  | BB    | 2442 | C    | O4'-C1'-N1  | 8.63  | 115.10      | 108.20   |
| 50  | BQ    | 5    | ARG  | NE-CZ-NH1   | 8.63  | 124.61      | 120.30   |
| 35  | BB    | 1805 | A    | C5-C6-N6    | -8.63 | 116.80      | 123.70   |
| 1   | AA    | 1337 | G    | C5-C6-O6    | -8.63 | 123.42      | 128.60   |
| 1   | AA    | 136  | C    | N1-C2-O2    | -8.62 | 113.73      | 118.90   |
| 1   | AA    | 1281 | C    | O4'-C1'-N1  | 8.62  | 115.10      | 108.20   |
| 35  | BB    | 29   | U    | O4'-C1'-N1  | 8.62  | 115.10      | 108.20   |
| 35  | BB    | 70   | G    | C5-C6-O6    | -8.62 | 123.43      | 128.60   |
| 35  | BB    | 1252 | G    | C6-C5-N7    | -8.62 | 125.22      | 130.40   |
| 35  | BB    | 1728 | C    | C5-C6-N1    | -8.63 | 116.69      | 121.00   |
| 35  | BB    | 1978 | A    | OP1-P-OP2   | -8.62 | 106.66      | 119.60   |
| 1   | AA    | 38   | G    | C6-N1-C2    | 8.62  | 130.27      | 125.10   |
| 1   | AA    | 1312 | G    | O4'-C1'-N9  | 8.62  | 115.10      | 108.20   |
| 1   | AA    | 1518 | A    | C5-C6-N1    | -8.62 | 113.39      | 117.70   |
| 35  | BB    | 407  | G    | C5-C6-O6    | -8.62 | 123.43      | 128.60   |
| 35  | BB    | 1659 | G    | C4'-C3'-C2' | -8.62 | 93.98       | 102.60   |
| 35  | BB    | 2094 | A    | C5-C6-N6    | -8.62 | 116.80      | 123.70   |
| 35  | BB    | 532  | A    | N1-C6-N6    | 8.62  | 123.77      | 118.60   |
| 35  | BB    | 785  | G    | C5-N7-C8    | 8.62  | 108.61      | 104.30   |
| 35  | BB    | 1012 | U    | C3'-C2'-C1' | -8.62 | 94.60       | 101.50   |
| 35  | BB    | 2775 | G    | C5-C6-O6    | -8.62 | 123.43      | 128.60   |
| 35  | BB    | 1138 | G    | N1-C6-O6    | 8.62  | 125.07      | 119.90   |
| 35  | BB    | 1619 | G    | N3-C2-N2    | 8.62  | 125.93      | 119.90   |
| 35  | BB    | 31   | C    | C5-C6-N1    | 8.62  | 125.31      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 316  | C    | O4'-C1'-N1  | 8.62  | 115.10      | 108.20   |
| 1   | AA    | 53   | A    | C5-C6-N6    | -8.62 | 116.81      | 123.70   |
| 1   | AA    | 1101 | A    | C5-C6-N6    | -8.62 | 116.81      | 123.70   |
| 1   | AA    | 1476 | A    | C5-N7-C8    | 8.62  | 108.21      | 103.90   |
| 35  | BB    | 365  | U    | C5-C4-O4    | -8.62 | 120.73      | 125.90   |
| 35  | BB    | 2488 | G    | C4-C5-C6    | 8.62  | 123.97      | 118.80   |
| 1   | AA    | 423  | G    | N1-C6-O6    | 8.62  | 125.07      | 119.90   |
| 1   | AA    | 770  | C    | N3-C4-C5    | -8.61 | 118.45      | 121.90   |
| 1   | AA    | 1035 | A    | C5-C6-N6    | -8.61 | 116.81      | 123.70   |
| 35  | BB    | 921  | C    | N3-C4-N4    | 8.62  | 124.03      | 118.00   |
| 35  | BB    | 2310 | C    | C4-C5-C6    | 8.61  | 121.71      | 117.40   |
| 35  | BB    | 2314 | A    | C4-C5-C6    | 8.62  | 121.31      | 117.00   |
| 35  | BB    | 2488 | G    | N9-C4-C5    | 8.62  | 108.85      | 105.40   |
| 35  | BB    | 2425 | A    | C5-C6-N1    | -8.61 | 113.39      | 117.70   |
| 1   | AA    | 768  | A    | C2-N3-C4    | 8.61  | 114.91      | 110.60   |
| 1   | AA    | 993  | G    | N9-C4-C5    | -8.61 | 101.95      | 105.40   |
| 30  | B5    | 111  | PHE  | CB-CG-CD1   | 8.61  | 126.83      | 120.80   |
| 34  | BA    | 64   | G    | O4'-C1'-N9  | 8.61  | 115.09      | 108.20   |
| 35  | BB    | 980  | A    | C4-C5-C6    | 8.61  | 121.31      | 117.00   |
| 35  | BB    | 1512 | C    | C6-N1-C2    | -8.61 | 116.86      | 120.30   |
| 35  | BB    | 1188 | U    | P-O3'-C3'   | -8.61 | 109.37      | 119.70   |
| 35  | BB    | 2030 | A    | C5-C6-N1    | -8.61 | 113.39      | 117.70   |
| 35  | BB    | 2110 | G    | N3-C4-C5    | 8.61  | 132.91      | 128.60   |
| 1   | AA    | 579  | A    | N1-C6-N6    | 8.61  | 123.77      | 118.60   |
| 1   | AA    | 1508 | A    | C8-N9-C4    | -8.61 | 102.36      | 105.80   |
| 35  | BB    | 235  | U    | C5-C4-O4    | -8.61 | 120.73      | 125.90   |
| 35  | BB    | 592  | A    | C2-N3-C4    | -8.61 | 106.30      | 110.60   |
| 35  | BB    | 2255 | G    | C1'-O4'-C4' | -8.61 | 103.01      | 109.90   |
| 35  | BB    | 2899 | A    | C6-C5-N7    | -8.61 | 126.28      | 132.30   |
| 1   | AA    | 1517 | G    | N7-C8-N9    | 8.61  | 117.40      | 113.10   |
| 35  | BB    | 415  | A    | C8-N9-C4    | -8.61 | 102.36      | 105.80   |
| 1   | AA    | 657  | U    | N1-C2-N3    | -8.61 | 109.74      | 114.90   |
| 1   | AA    | 778  | G    | C5-N7-C8    | -8.61 | 100.00      | 104.30   |
| 34  | BA    | 13   | G    | C4-C5-C6    | 8.61  | 123.96      | 118.80   |
| 35  | BB    | 216  | A    | C5-C6-N1    | -8.61 | 113.40      | 117.70   |
| 35  | BB    | 2060 | A    | C4-C5-C6    | 8.61  | 121.30      | 117.00   |
| 35  | BB    | 2729 | G    | N9-C4-C5    | -8.61 | 101.96      | 105.40   |
| 1   | AA    | 538  | G    | N3-C2-N2    | 8.60  | 125.92      | 119.90   |
| 1   | AA    | 567  | G    | C5-N7-C8    | -8.60 | 100.00      | 104.30   |
| 1   | AA    | 830  | G    | C5-C6-O6    | -8.60 | 123.44      | 128.60   |
| 35  | BB    | 460  | A    | N1-C6-N6    | 8.60  | 123.76      | 118.60   |
| 35  | BB    | 551  | G    | C8-N9-C4    | -8.60 | 102.96      | 106.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 998  | C    | C5-C6-N1    | 8.60  | 125.30      | 121.00   |
| 35  | BB    | 1115 | G    | N1-C6-O6    | 8.60  | 125.06      | 119.90   |
| 1   | AA    | 1267 | C    | C2-N3-C4    | 8.60  | 124.20      | 119.90   |
| 35  | BB    | 1448 | G    | N3-C4-N9    | -8.60 | 120.84      | 126.00   |
| 35  | BB    | 1718 | G    | N1-C2-N3    | -8.60 | 118.74      | 123.90   |
| 35  | BB    | 1961 | C    | C5-C6-N1    | 8.60  | 125.30      | 121.00   |
| 1   | AA    | 1525 | G    | N1-C6-O6    | 8.60  | 125.06      | 119.90   |
| 35  | BB    | 2343 | U    | C5-C6-N1    | 8.60  | 127.00      | 122.70   |
| 35  | BB    | 206  | U    | C5-C6-N1    | -8.60 | 118.40      | 122.70   |
| 35  | BB    | 969  | G    | C6-N1-C2    | 8.60  | 130.26      | 125.10   |
| 35  | BB    | 1993 | U    | N3-C4-C5    | 8.60  | 119.76      | 114.60   |
| 35  | BB    | 2829 | A    | N7-C8-N9    | -8.60 | 109.50      | 113.80   |
| 35  | BB    | 2024 | G    | C4-C5-C6    | 8.60  | 123.96      | 118.80   |
| 35  | BB    | 473  | G    | C5-C6-O6    | -8.60 | 123.44      | 128.60   |
| 1   | AA    | 774  | G    | N1-C6-O6    | 8.60  | 125.06      | 119.90   |
| 1   | AA    | 779  | C    | N1-C2-O2    | -8.60 | 113.74      | 118.90   |
| 35  | BB    | 212  | G    | C8-N9-C4    | 8.60  | 109.84      | 106.40   |
| 35  | BB    | 608  | A    | N1-C6-N6    | 8.60  | 123.76      | 118.60   |
| 35  | BB    | 1899 | A    | C5-C6-N6    | -8.60 | 116.82      | 123.70   |
| 35  | BB    | 1163 | G    | N9-C4-C5    | -8.59 | 101.96      | 105.40   |
| 1   | AA    | 221  | C    | N1-C2-O2    | -8.59 | 113.75      | 118.90   |
| 1   | AA    | 1392 | G    | N3-C2-N2    | 8.59  | 125.91      | 119.90   |
| 35  | BB    | 801  | G    | C6-C5-N7    | -8.59 | 125.25      | 130.40   |
| 35  | BB    | 2057 | G    | N9-C4-C5    | -8.59 | 101.96      | 105.40   |
| 22  | AV    | 73   | A    | C5'-C4'-C3' | 8.59  | 129.75      | 116.00   |
| 22  | AV    | 44   | G    | N1-C6-O6    | 8.59  | 125.05      | 119.90   |
| 35  | BB    | 1137 | G    | N7-C8-N9    | 8.59  | 117.39      | 113.10   |
| 35  | BB    | 2326 | C    | O4'-C1'-N1  | 8.59  | 115.07      | 108.20   |
| 35  | BB    | 2387 | U    | N3-C2-O2    | -8.59 | 116.19      | 122.20   |
| 1   | AA    | 129  | A    | N1-C6-N6    | 8.59  | 123.75      | 118.60   |
| 1   | AA    | 1457 | G    | C4-C5-N7    | 8.59  | 114.23      | 110.80   |
| 1   | AA    | 1509 | C    | N3-C4-C5    | -8.59 | 118.47      | 121.90   |
| 35  | BB    | 705  | A    | P-O5'-C5'   | 8.59  | 134.63      | 120.90   |
| 35  | BB    | 1189 | A    | C5-C6-N1    | -8.59 | 113.41      | 117.70   |
| 35  | BB    | 1873 | G    | N9-C4-C5    | 8.59  | 108.83      | 105.40   |
| 35  | BB    | 1975 | G    | N1-C2-N3    | -8.59 | 118.75      | 123.90   |
| 35  | BB    | 2097 | A    | C5-C6-N1    | -8.59 | 113.41      | 117.70   |
| 35  | BB    | 2228 | G    | C8-N9-C4    | -8.59 | 102.97      | 106.40   |
| 35  | BB    | 2327 | A    | C6-C5-N7    | -8.59 | 126.29      | 132.30   |
| 35  | BB    | 2737 | G    | O4'-C1'-N9  | 8.59  | 115.07      | 108.20   |
| 1   | AA    | 592  | G    | N1-C2-N2    | 8.58  | 123.92      | 116.20   |
| 1   | AA    | 1071 | C    | C5-C6-N1    | 8.58  | 125.29      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 34  | BA    | 4    | C    | N3-C4-N4   | 8.58  | 124.01      | 118.00   |
| 35  | BB    | 311  | A    | C5-C6-N1   | -8.58 | 113.41      | 117.70   |
| 35  | BB    | 857  | G    | C5-C6-O6   | -8.58 | 123.45      | 128.60   |
| 1   | AA    | 287  | U    | C2-N3-C4   | 8.58  | 132.15      | 127.00   |
| 1   | AA    | 878  | A    | O4'-C1'-N9 | 8.58  | 115.06      | 108.20   |
| 9   | AI    | 94   | ARG  | NE-CZ-NH1  | 8.58  | 124.59      | 120.30   |
| 35  | BB    | 189  | G    | C2-N3-C4   | 8.58  | 116.19      | 111.90   |
| 35  | BB    | 1465 | G    | N3-C4-C5   | 8.58  | 132.89      | 128.60   |
| 35  | BB    | 2539 | C    | N3-C4-C5   | -8.58 | 118.47      | 121.90   |
| 1   | AA    | 731  | G    | O4'-C1'-N9 | 8.58  | 115.06      | 108.20   |
| 1   | AA    | 1042 | A    | O4'-C1'-N9 | 8.58  | 115.06      | 108.20   |
| 1   | AA    | 1473 | G    | N7-C8-N9   | 8.58  | 117.39      | 113.10   |
| 35  | BB    | 305  | C    | N3-C4-N4   | 8.58  | 124.00      | 118.00   |
| 35  | BB    | 637  | A    | C4-C5-C6   | 8.58  | 121.29      | 117.00   |
| 35  | BB    | 901  | C    | C6-N1-C2   | -8.58 | 116.87      | 120.30   |
| 35  | BB    | 1131 | G    | C2-N3-C4   | 8.58  | 116.19      | 111.90   |
| 35  | BB    | 1469 | A    | O4'-C1'-N9 | 8.58  | 115.06      | 108.20   |
| 35  | BB    | 1715 | G    | C2-N3-C4   | 8.58  | 116.19      | 111.90   |
| 35  | BB    | 2451 | A    | C5-C6-N1   | -8.58 | 113.41      | 117.70   |
| 1   | AA    | 704  | A    | N7-C8-N9   | -8.58 | 109.51      | 113.80   |
| 35  | BB    | 2660 | A    | C5-C6-N1   | -8.58 | 113.41      | 117.70   |
| 1   | AA    | 258  | G    | N3-C2-N2   | 8.58  | 125.90      | 119.90   |
| 35  | BB    | 452  | G    | O4'-C1'-N9 | 8.58  | 115.06      | 108.20   |
| 35  | BB    | 1013 | C    | C5-C4-N4   | -8.58 | 114.20      | 120.20   |
| 35  | BB    | 2683 | C    | C4-C5-C6   | 8.58  | 121.69      | 117.40   |
| 35  | BB    | 1411 | U    | O4'-C1'-N1 | 8.58  | 115.06      | 108.20   |
| 56  | BY    | 75   | ASN  | N-CA-CB    | 8.58  | 126.04      | 110.60   |
| 1   | AA    | 275  | G    | N7-C8-N9   | -8.57 | 108.81      | 113.10   |
| 1   | AA    | 470  | C    | C2-N3-C4   | 8.57  | 124.19      | 119.90   |
| 1   | AA    | 619  | U    | N3-C4-C5   | -8.57 | 109.46      | 114.60   |
| 35  | BB    | 614  | A    | N1-C6-N6   | 8.57  | 123.74      | 118.60   |
| 35  | BB    | 2213 | U    | N3-C4-O4   | 8.57  | 125.40      | 119.40   |
| 35  | BB    | 2740 | A    | C2-N3-C4   | 8.57  | 114.89      | 110.60   |
| 1   | AA    | 1188 | A    | N1-C6-N6   | 8.57  | 123.74      | 118.60   |
| 1   | AA    | 1201 | A    | P-O3'-C3'  | 8.57  | 129.99      | 119.70   |
| 35  | BB    | 993  | G    | N9-C4-C5   | 8.57  | 108.83      | 105.40   |
| 35  | BB    | 1371 | G    | C6-C5-N7   | -8.57 | 125.26      | 130.40   |
| 35  | BB    | 1473 | G    | O4'-C1'-N9 | 8.57  | 115.06      | 108.20   |
| 1   | AA    | 644  | U    | C5-C4-O4   | -8.57 | 120.76      | 125.90   |
| 34  | BA    | 26   | C    | C5-C4-N4   | -8.57 | 114.20      | 120.20   |
| 34  | BA    | 66   | A    | P-O3'-C3'  | 8.57  | 129.99      | 119.70   |
| 35  | BB    | 1329 | U    | N3-C4-C5   | -8.57 | 109.46      | 114.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1780 | A    | C4-C5-C6   | 8.57  | 121.28      | 117.00   |
| 35  | BB    | 2856 | A    | C8-N9-C4   | 8.57  | 109.23      | 105.80   |
| 35  | BB    | 320  | A    | C8-N9-C4   | -8.57 | 102.37      | 105.80   |
| 35  | BB    | 2251 | G    | C2-N3-C4   | -8.57 | 107.62      | 111.90   |
| 35  | BB    | 2584 | U    | C5-C4-O4   | -8.57 | 120.76      | 125.90   |
| 1   | AA    | 1343 | G    | C4-C5-C6   | 8.57  | 123.94      | 118.80   |
| 1   | AA    | 1373 | G    | O4'-C1'-N9 | 8.57  | 115.05      | 108.20   |
| 1   | AA    | 1417 | G    | N1-C2-N3   | -8.57 | 118.76      | 123.90   |
| 35  | BB    | 25   | U    | N3-C4-O4   | 8.57  | 125.40      | 119.40   |
| 35  | BB    | 84   | A    | N1-C2-N3   | 8.57  | 133.58      | 129.30   |
| 35  | BB    | 1181 | U    | O4'-C1'-N1 | 8.57  | 115.05      | 108.20   |
| 35  | BB    | 2709 | G    | C5-N7-C8   | 8.57  | 108.58      | 104.30   |
| 35  | BB    | 1355 | G    | C5-C6-O6   | -8.57 | 123.46      | 128.60   |
| 1   | AA    | 767  | A    | O4'-C1'-N9 | 8.56  | 115.05      | 108.20   |
| 35  | BB    | 899  | A    | O4'-C1'-N9 | 8.56  | 115.05      | 108.20   |
| 35  | BB    | 1748 | C    | O4'-C1'-N1 | 8.56  | 115.05      | 108.20   |
| 1   | AA    | 224  | U    | N3-C2-O2   | 8.56  | 128.19      | 122.20   |
| 1   | AA    | 837  | U    | C5-C6-N1   | 8.56  | 126.98      | 122.70   |
| 35  | BB    | 17   | G    | N1-C6-O6   | 8.56  | 125.04      | 119.90   |
| 35  | BB    | 1171 | G    | C5-C6-O6   | -8.56 | 123.46      | 128.60   |
| 35  | BB    | 1974 | C    | N3-C4-N4   | 8.56  | 123.99      | 118.00   |
| 35  | BB    | 2340 | A    | P-O3'-C3'  | -8.56 | 109.42      | 119.70   |
| 35  | BB    | 2628 | C    | N3-C2-O2   | 8.56  | 127.89      | 121.90   |
| 1   | AA    | 1385 | G    | C4-C5-C6   | 8.56  | 123.94      | 118.80   |
| 1   | AA    | 201  | G    | N3-C4-C5   | -8.56 | 124.32      | 128.60   |
| 1   | AA    | 1398 | A    | C4-C5-C6   | 8.56  | 121.28      | 117.00   |
| 35  | BB    | 279  | A    | N1-C6-N6   | 8.56  | 123.74      | 118.60   |
| 35  | BB    | 1379 | U    | C2-N3-C4   | 8.56  | 132.14      | 127.00   |
| 35  | BB    | 2642 | G    | N9-C4-C5   | 8.56  | 108.83      | 105.40   |
| 1   | AA    | 1429 | A    | C4-C5-C6   | 8.56  | 121.28      | 117.00   |
| 22  | AV    | 39   | G    | O4'-C1'-N9 | 8.56  | 115.05      | 108.20   |
| 35  | BB    | 82   | U    | O4'-C1'-N1 | 8.56  | 115.05      | 108.20   |
| 35  | BB    | 294  | A    | C4-C5-C6   | 8.56  | 121.28      | 117.00   |
| 35  | BB    | 325  | G    | N1-C2-N3   | -8.56 | 118.77      | 123.90   |
| 35  | BB    | 2054 | A    | O4'-C1'-N9 | 8.56  | 115.05      | 108.20   |
| 35  | BB    | 2744 | G    | N1-C2-N3   | -8.56 | 118.77      | 123.90   |
| 1   | AA    | 217  | C    | N3-C4-C5   | -8.56 | 118.48      | 121.90   |
| 1   | AA    | 230  | G    | C8-N9-C4   | -8.55 | 102.98      | 106.40   |
| 1   | AA    | 1012 | A    | O4'-C1'-N9 | 8.55  | 115.04      | 108.20   |
| 43  | BJ    | 119  | PHE  | CB-CG-CD2  | -8.56 | 114.81      | 120.80   |
| 35  | BB    | 299  | A    | N1-C6-N6   | 8.55  | 123.73      | 118.60   |
| 35  | BB    | 368  | A    | C4-C5-N7   | -8.55 | 106.42      | 110.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 550  | C    | O4'-C1'-N1  | 8.55  | 115.04      | 108.20   |
| 35  | BB    | 1463 | C    | N3-C4-N4    | 8.55  | 123.99      | 118.00   |
| 35  | BB    | 74   | A    | O4'-C1'-N9  | 8.55  | 115.04      | 108.20   |
| 35  | BB    | 2012 | G    | C5-C6-N1    | -8.55 | 107.22      | 111.50   |
| 1   | AA    | 313  | A    | C2-N3-C4    | -8.55 | 106.33      | 110.60   |
| 1   | AA    | 698  | G    | C5-C6-O6    | -8.55 | 123.47      | 128.60   |
| 28  | B3    | 49   | ARG  | NE-CZ-NH1   | 8.55  | 124.58      | 120.30   |
| 35  | BB    | 1601 | G    | N9-C4-C5    | -8.55 | 101.98      | 105.40   |
| 35  | BB    | 1731 | G    | C4-C5-C6    | 8.55  | 123.93      | 118.80   |
| 35  | BB    | 1981 | A    | N1-C6-N6    | 8.55  | 123.73      | 118.60   |
| 1   | AA    | 778  | G    | N3-C2-N2    | 8.55  | 125.88      | 119.90   |
| 1   | AA    | 386  | C    | N3-C4-N4    | 8.55  | 123.98      | 118.00   |
| 1   | AA    | 494  | G    | C3'-C2'-C1' | 8.55  | 108.34      | 101.50   |
| 35  | BB    | 86   | G    | O4'-C1'-N9  | 8.55  | 115.04      | 108.20   |
| 35  | BB    | 400  | G    | O4'-C1'-N9  | 8.55  | 115.04      | 108.20   |
| 35  | BB    | 1370 | C    | O4'-C1'-N1  | 8.55  | 115.04      | 108.20   |
| 35  | BB    | 1446 | C    | N3-C4-N4    | 8.55  | 123.98      | 118.00   |
| 35  | BB    | 1863 | G    | C6-C5-N7    | -8.55 | 125.27      | 130.40   |
| 35  | BB    | 2360 | G    | O4'-C1'-N9  | 8.55  | 115.04      | 108.20   |
| 35  | BB    | 2583 | G    | C6-N1-C2    | 8.55  | 130.23      | 125.10   |
| 1   | AA    | 248  | C    | O4'-C1'-N1  | 8.54  | 115.04      | 108.20   |
| 1   | AA    | 379  | C    | N1-C2-O2    | 8.54  | 124.03      | 118.90   |
| 35  | BB    | 230  | G    | C5-C6-O6    | -8.55 | 123.47      | 128.60   |
| 35  | BB    | 1685 | C    | C6-N1-C2    | -8.55 | 116.88      | 120.30   |
| 1   | AA    | 571  | U    | C5-C4-O4    | -8.54 | 120.77      | 125.90   |
| 1   | AA    | 1019 | A    | C5-C6-N6    | -8.54 | 116.86      | 123.70   |
| 35  | BB    | 1731 | G    | C5-C6-N1    | -8.55 | 107.23      | 111.50   |
| 1   | AA    | 1343 | G    | N3-C4-C5    | -8.54 | 124.33      | 128.60   |
| 1   | AA    | 1421 | G    | C6-N1-C2    | 8.54  | 130.23      | 125.10   |
| 1   | AA    | 1491 | G    | C5-C6-O6    | -8.54 | 123.47      | 128.60   |
| 35  | BB    | 2215 | C    | N1-C2-O2    | 8.54  | 124.03      | 118.90   |
| 1   | AA    | 413  | G    | C2-N3-C4    | 8.54  | 116.17      | 111.90   |
| 35  | BB    | 114  | U    | O4'-C1'-N1  | 8.54  | 115.03      | 108.20   |
| 35  | BB    | 866  | A    | C5-C6-N1    | -8.54 | 113.43      | 117.70   |
| 35  | BB    | 2330 | G    | N3-C4-N9    | 8.54  | 131.12      | 126.00   |
| 35  | BB    | 2631 | G    | O4'-C1'-N9  | 8.54  | 115.03      | 108.20   |
| 1   | AA    | 215  | C    | C4'-C3'-C2' | -8.54 | 94.06       | 102.60   |
| 1   | AA    | 250  | A    | O4'-C1'-N9  | 8.54  | 115.03      | 108.20   |
| 35  | BB    | 248  | G    | N1-C6-O6    | 8.54  | 125.02      | 119.90   |
| 35  | BB    | 483  | A    | N1-C6-N6    | 8.54  | 123.72      | 118.60   |
| 35  | BB    | 1803 | A    | N3-C4-C5    | -8.54 | 120.82      | 126.80   |
| 1   | AA    | 716  | A    | C5-C6-N1    | -8.54 | 113.43      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1299 | A    | N1-C6-N6    | 8.54  | 123.72      | 118.60   |
| 35  | BB    | 385  | C    | O4'-C1'-N1  | 8.54  | 115.03      | 108.20   |
| 35  | BB    | 713  | G    | N3-C2-N2    | 8.54  | 125.88      | 119.90   |
| 35  | BB    | 1055 | G    | C1'-O4'-C4' | -8.54 | 103.07      | 109.90   |
| 35  | BB    | 1135 | C    | N3-C4-N4    | 8.54  | 123.98      | 118.00   |
| 35  | BB    | 1983 | G    | O4'-C1'-N9  | 8.54  | 115.03      | 108.20   |
| 35  | BB    | 2284 | A    | C5-C6-N1    | -8.54 | 113.43      | 117.70   |
| 35  | BB    | 2598 | A    | N7-C8-N9    | -8.54 | 109.53      | 113.80   |
| 1   | AA    | 435  | A    | O4'-C1'-N9  | 8.54  | 115.03      | 108.20   |
| 1   | AA    | 611  | C    | C5-C6-N1    | 8.53  | 125.27      | 121.00   |
| 1   | AA    | 765  | G    | C6-C5-N7    | -8.53 | 125.28      | 130.40   |
| 1   | AA    | 902  | G    | P-O3'-C3'   | -8.53 | 109.46      | 119.70   |
| 34  | BA    | 37   | C    | O4'-C1'-N1  | 8.53  | 115.03      | 108.20   |
| 35  | BB    | 319  | G    | C2-N3-C4    | 8.53  | 116.17      | 111.90   |
| 35  | BB    | 679  | C    | N3-C4-N4    | 8.54  | 123.97      | 118.00   |
| 35  | BB    | 887  | U    | C3'-C2'-C1' | -8.54 | 94.67       | 101.50   |
| 35  | BB    | 1429 | G    | O4'-C1'-N9  | 8.54  | 115.03      | 108.20   |
| 35  | BB    | 1609 | A    | O4'-C1'-N9  | 8.54  | 115.03      | 108.20   |
| 35  | BB    | 2436 | G    | C5-C6-O6    | -8.54 | 123.48      | 128.60   |
| 43  | BJ    | 75   | TYR  | CG-CD2-CE2  | 8.54  | 128.13      | 121.30   |
| 1   | AA    | 338  | A    | C5-C6-N6    | -8.53 | 116.87      | 123.70   |
| 35  | BB    | 575  | A    | C2-N3-C4    | 8.53  | 114.87      | 110.60   |
| 35  | BB    | 1423 | G    | N1-C6-O6    | 8.53  | 125.02      | 119.90   |
| 35  | BB    | 1653 | G    | C6-C5-N7    | -8.53 | 125.28      | 130.40   |
| 35  | BB    | 1665 | A    | N1-C2-N3    | 8.53  | 133.57      | 129.30   |
| 35  | BB    | 1918 | A    | C6-C5-N7    | -8.53 | 126.33      | 132.30   |
| 35  | BB    | 2795 | C    | N3-C4-N4    | 8.53  | 123.97      | 118.00   |
| 1   | AA    | 985  | C    | N3-C4-N4    | 8.53  | 123.97      | 118.00   |
| 1   | AA    | 1002 | G    | C5-C6-O6    | -8.53 | 123.48      | 128.60   |
| 1   | AA    | 1068 | G    | N9-C4-C5    | -8.53 | 101.99      | 105.40   |
| 35  | BB    | 1264 | A    | N1-C6-N6    | 8.53  | 123.72      | 118.60   |
| 35  | BB    | 1288 | G    | N3-C4-N9    | 8.53  | 131.12      | 126.00   |
| 35  | BB    | 1612 | C    | C5-C4-N4    | -8.53 | 114.23      | 120.20   |
| 35  | BB    | 2049 | G    | O4'-C1'-N9  | 8.53  | 115.02      | 108.20   |
| 1   | AA    | 208  | U    | N3-C2-O2    | 8.53  | 128.17      | 122.20   |
| 1   | AA    | 596  | A    | C4-C5-C6    | 8.53  | 121.26      | 117.00   |
| 35  | BB    | 908  | C    | P-O5'-C5'   | 8.53  | 134.54      | 120.90   |
| 35  | BB    | 1586 | A    | O4'-C1'-N9  | 8.53  | 115.02      | 108.20   |
| 22  | AV    | 2    | G    | C5-C6-O6    | -8.53 | 123.48      | 128.60   |
| 34  | BA    | 75   | G    | C5-C6-O6    | -8.53 | 123.48      | 128.60   |
| 35  | BB    | 1332 | G    | N1-C6-O6    | 8.53  | 125.02      | 119.90   |
| 35  | BB    | 2193 | G    | O4'-C4'-C3' | -8.53 | 95.47       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2654 | A    | C4-C5-C6    | 8.53  | 121.26      | 117.00   |
| 1   | AA    | 435  | A    | C2-N3-C4    | 8.52  | 114.86      | 110.60   |
| 35  | BB    | 15   | G    | N1-C6-O6    | 8.52  | 125.01      | 119.90   |
| 35  | BB    | 375  | G    | N1-C6-O6    | 8.52  | 125.01      | 119.90   |
| 35  | BB    | 420  | C    | C6-N1-C2    | -8.52 | 116.89      | 120.30   |
| 35  | BB    | 726  | G    | N1-C6-O6    | 8.52  | 125.01      | 119.90   |
| 35  | BB    | 1096 | A    | C3'-C2'-C1' | 8.52  | 108.32      | 101.50   |
| 1   | AA    | 1303 | C    | C6-N1-C2    | -8.52 | 116.89      | 120.30   |
| 1   | AA    | 357  | G    | N3-C4-C5    | -8.52 | 124.34      | 128.60   |
| 1   | AA    | 1074 | G    | C6-C5-N7    | -8.52 | 125.29      | 130.40   |
| 35  | BB    | 283  | G    | C4-C5-C6    | 8.52  | 123.91      | 118.80   |
| 35  | BB    | 820  | A    | C5-C6-N6    | -8.52 | 116.89      | 123.70   |
| 35  | BB    | 990  | A    | C6-C5-N7    | -8.52 | 126.34      | 132.30   |
| 1   | AA    | 321  | A    | N9-C4-C5    | 8.52  | 109.21      | 105.80   |
| 1   | AA    | 448  | A    | C6-C5-N7    | -8.52 | 126.34      | 132.30   |
| 1   | AA    | 729  | A    | C5-C6-N6    | -8.52 | 116.89      | 123.70   |
| 1   | AA    | 1002 | G    | N9-C4-C5    | 8.52  | 108.81      | 105.40   |
| 35  | BB    | 319  | G    | C5-C6-O6    | -8.52 | 123.49      | 128.60   |
| 35  | BB    | 474  | G    | C4-C5-N7    | 8.52  | 114.21      | 110.80   |
| 35  | BB    | 662  | G    | N7-C8-N9    | -8.52 | 108.84      | 113.10   |
| 44  | BK    | 17   | ARG  | NE-CZ-NH1   | 8.51  | 124.56      | 120.30   |
| 1   | AA    | 443  | C    | C2-N3-C4    | 8.51  | 124.16      | 119.90   |
| 1   | AA    | 1385 | G    | C5-C6-N1    | -8.51 | 107.24      | 111.50   |
| 35  | BB    | 209  | C    | C4-C5-C6    | 8.51  | 121.66      | 117.40   |
| 35  | BB    | 428  | A    | C4-C5-C6    | 8.51  | 121.26      | 117.00   |
| 35  | BB    | 524  | G    | N1-C6-O6    | 8.51  | 125.01      | 119.90   |
| 35  | BB    | 589  | U    | C2-N3-C4    | 8.51  | 132.11      | 127.00   |
| 1   | AA    | 950  | U    | C2-N3-C4    | -8.51 | 121.89      | 127.00   |
| 1   | AA    | 1123 | U    | O4'-C1'-N1  | 8.51  | 115.01      | 108.20   |
| 35  | BB    | 402  | A    | N1-C6-N6    | 8.51  | 123.71      | 118.60   |
| 35  | BB    | 992  | C    | C6-N1-C2    | -8.51 | 116.90      | 120.30   |
| 35  | BB    | 2610 | C    | N1-C2-N3    | -8.51 | 113.24      | 119.20   |
| 35  | BB    | 1146 | C    | N3-C4-N4    | 8.51  | 123.96      | 118.00   |
| 35  | BB    | 1899 | A    | C4-C5-N7    | -8.51 | 106.44      | 110.70   |
| 35  | BB    | 2019 | A    | C5-C6-N6    | -8.51 | 116.89      | 123.70   |
| 35  | BB    | 2512 | C    | C4-C5-C6    | 8.51  | 121.66      | 117.40   |
| 35  | BB    | 2182 | U    | C5'-C4'-O4' | 8.51  | 119.31      | 109.10   |
| 1   | AA    | 1392 | G    | N1-C6-O6    | 8.51  | 125.00      | 119.90   |
| 35  | BB    | 815  | C    | N3-C4-N4    | 8.51  | 123.96      | 118.00   |
| 1   | AA    | 482  | A    | N3-C4-C5    | -8.51 | 120.85      | 126.80   |
| 1   | AA    | 1000 | A    | N1-C6-N6    | 8.51  | 123.70      | 118.60   |
| 1   | AA    | 1533 | C    | C2-N1-C1'   | 8.51  | 128.16      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 2842 | G    | N3-C2-N2   | 8.51  | 125.86      | 119.90   |
| 1   | AA    | 1047 | G    | N1-C2-N3   | -8.51 | 118.80      | 123.90   |
| 35  | BB    | 452  | G    | C8-N9-C4   | -8.51 | 103.00      | 106.40   |
| 35  | BB    | 916  | G    | N1-C6-O6   | 8.51  | 125.00      | 119.90   |
| 35  | BB    | 1062 | G    | O4'-C1'-N9 | 8.51  | 115.00      | 108.20   |
| 35  | BB    | 1204 | A    | N1-C6-N6   | 8.51  | 123.70      | 118.60   |
| 34  | BA    | 85   | G    | C6-C5-N7   | -8.50 | 125.30      | 130.40   |
| 35  | BB    | 272  | A    | C5-C6-N6   | -8.50 | 116.90      | 123.70   |
| 35  | BB    | 543  | G    | N3-C2-N2   | 8.50  | 125.85      | 119.90   |
| 35  | BB    | 810  | U    | O4'-C1'-N1 | 8.50  | 115.00      | 108.20   |
| 35  | BB    | 1436 | G    | O4'-C1'-N9 | 8.50  | 115.00      | 108.20   |
| 35  | BB    | 1882 | U    | O4'-C1'-N1 | 8.50  | 115.00      | 108.20   |
| 35  | BB    | 2016 | U    | C6-N1-C2   | -8.50 | 115.90      | 121.00   |
| 35  | BB    | 2140 | G    | C2-N3-C4   | 8.50  | 116.15      | 111.90   |
| 1   | AA    | 210  | C    | N3-C4-N4   | 8.50  | 123.95      | 118.00   |
| 1   | AA    | 1297 | G    | O4'-C1'-N9 | 8.50  | 115.00      | 108.20   |
| 1   | AA    | 693  | G    | C2-N3-C4   | -8.50 | 107.65      | 111.90   |
| 1   | AA    | 1259 | C    | N3-C4-N4   | 8.50  | 123.95      | 118.00   |
| 1   | AA    | 1264 | U    | O4'-C1'-N1 | 8.50  | 115.00      | 108.20   |
| 35  | BB    | 2452 | C    | C5-C6-N1   | -8.50 | 116.75      | 121.00   |
| 35  | BB    | 2588 | G    | N7-C8-N9   | -8.50 | 108.85      | 113.10   |
| 1   | AA    | 1405 | G    | C8-N9-C4   | -8.50 | 103.00      | 106.40   |
| 1   | AA    | 1055 | A    | C2-N3-C4   | -8.50 | 106.35      | 110.60   |
| 1   | AA    | 1266 | G    | N9-C4-C5   | 8.50  | 108.80      | 105.40   |
| 35  | BB    | 40   | U    | O4'-C1'-N1 | 8.50  | 115.00      | 108.20   |
| 35  | BB    | 58   | G    | C6-C5-N7   | -8.50 | 125.30      | 130.40   |
| 35  | BB    | 348  | A    | O4'-C1'-N9 | 8.50  | 115.00      | 108.20   |
| 35  | BB    | 163  | C    | C6-N1-C1'  | -8.50 | 110.61      | 120.80   |
| 35  | BB    | 1684 | G    | C8-N9-C1'  | 8.50  | 138.04      | 127.00   |
| 35  | BB    | 2485 | G    | O5'-P-OP2  | -8.50 | 98.05       | 105.70   |
| 35  | BB    | 2727 | A    | N1-C6-N6   | 8.50  | 123.70      | 118.60   |
| 1   | AA    | 220  | G    | N1-C6-O6   | 8.49  | 125.00      | 119.90   |
| 35  | BB    | 1800 | C    | C4-C5-C6   | 8.49  | 121.65      | 117.40   |
| 35  | BB    | 1817 | G    | N1-C6-O6   | 8.49  | 125.00      | 119.90   |
| 1   | AA    | 143  | A    | C5-C6-N1   | -8.49 | 113.45      | 117.70   |
| 35  | BB    | 2378 | A    | N3-C4-C5   | -8.49 | 120.85      | 126.80   |
| 35  | BB    | 435  | C    | O4'-C1'-N1 | 8.49  | 114.99      | 108.20   |
| 35  | BB    | 650  | C    | C5-C4-N4   | -8.49 | 114.25      | 120.20   |
| 35  | BB    | 1016 | G    | N1-C6-O6   | 8.49  | 125.00      | 119.90   |
| 35  | BB    | 1953 | A    | C6-N1-C2   | 8.49  | 123.69      | 118.60   |
| 35  | BB    | 2624 | G    | N3-C2-N2   | 8.49  | 125.84      | 119.90   |
| 1   | AA    | 186  | C    | O4'-C1'-N1 | 8.49  | 114.99      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 399  | G    | C5-C6-O6   | -8.49 | 123.51      | 128.60   |
| 1   | AA    | 615  | G    | N1-C2-N3   | -8.49 | 118.81      | 123.90   |
| 35  | BB    | 2297 | A    | N1-C6-N6   | 8.49  | 123.69      | 118.60   |
| 35  | BB    | 2435 | A    | C4-C5-C6   | 8.49  | 121.25      | 117.00   |
| 1   | AA    | 897  | C    | N3-C4-N4   | 8.49  | 123.94      | 118.00   |
| 35  | BB    | 1758 | U    | C2-N1-C1'  | 8.49  | 127.89      | 117.70   |
| 35  | BB    | 2662 | A    | N1-C6-N6   | 8.49  | 123.69      | 118.60   |
| 1   | AA    | 513  | C    | O4'-C1'-N1 | 8.49  | 114.99      | 108.20   |
| 35  | BB    | 366  | C    | C4-C5-C6   | 8.49  | 121.64      | 117.40   |
| 35  | BB    | 482  | A    | C4-C5-C6   | 8.49  | 121.24      | 117.00   |
| 1   | AA    | 847  | G    | N1-C6-O6   | 8.49  | 124.99      | 119.90   |
| 35  | BB    | 671  | C    | C4-C5-C6   | -8.49 | 113.16      | 117.40   |
| 35  | BB    | 1619 | G    | C6-C5-N7   | -8.49 | 125.31      | 130.40   |
| 35  | BB    | 2129 | C    | C2-N1-C1'  | 8.49  | 128.14      | 118.80   |
| 35  | BB    | 2879 | A    | C5-N7-C8   | 8.49  | 108.14      | 103.90   |
| 1   | AA    | 64   | G    | N1-C6-O6   | 8.48  | 124.99      | 119.90   |
| 1   | AA    | 186  | C    | N3-C4-N4   | 8.48  | 123.94      | 118.00   |
| 1   | AA    | 776  | G    | O4'-C1'-N9 | 8.48  | 114.99      | 108.20   |
| 1   | AA    | 1180 | A    | C5-C6-N6   | -8.48 | 116.91      | 123.70   |
| 1   | AA    | 1331 | G    | N3-C2-N2   | 8.48  | 125.84      | 119.90   |
| 35  | BB    | 642  | U    | N3-C2-O2   | 8.48  | 128.14      | 122.20   |
| 35  | BB    | 1986 | C    | N3-C4-N4   | 8.48  | 123.94      | 118.00   |
| 1   | AA    | 985  | C    | N3-C4-C5   | -8.48 | 118.51      | 121.90   |
| 1   | AA    | 1422 | G    | N3-C2-N2   | 8.48  | 125.84      | 119.90   |
| 35  | BB    | 280  | U    | N3-C2-O2   | 8.48  | 128.14      | 122.20   |
| 35  | BB    | 1839 | G    | C2-N3-C4   | -8.48 | 107.66      | 111.90   |
| 35  | BB    | 1004 | U    | C5-C4-O4   | -8.48 | 120.81      | 125.90   |
| 35  | BB    | 2041 | U    | N3-C2-O2   | 8.48  | 128.14      | 122.20   |
| 35  | BB    | 2846 | G    | C8-N9-C4   | 8.48  | 109.79      | 106.40   |
| 1   | AA    | 1302 | C    | C6-N1-C2   | -8.48 | 116.91      | 120.30   |
| 35  | BB    | 960  | A    | C8-N9-C4   | -8.48 | 102.41      | 105.80   |
| 35  | BB    | 1465 | G    | N3-C4-N9   | -8.48 | 120.91      | 126.00   |
| 35  | BB    | 1531 | C    | C2-N1-C1'  | 8.48  | 128.13      | 118.80   |
| 35  | BB    | 1925 | C    | C5-C4-N4   | -8.48 | 114.27      | 120.20   |
| 1   | AA    | 1268 | G    | O4'-C1'-N9 | 8.48  | 114.98      | 108.20   |
| 35  | BB    | 327  | G    | C4-C5-N7   | -8.48 | 107.41      | 110.80   |
| 1   | AA    | 654  | G    | O4'-C1'-N9 | 8.47  | 114.98      | 108.20   |
| 1   | AA    | 824  | G    | N1-C2-N3   | -8.47 | 118.81      | 123.90   |
| 35  | BB    | 1265 | A    | N1-C6-N6   | 8.47  | 123.69      | 118.60   |
| 1   | AA    | 431  | A    | C5-C6-N6   | -8.47 | 116.92      | 123.70   |
| 35  | BB    | 876  | C    | N1-C2-O2   | -8.47 | 113.82      | 118.90   |
| 35  | BB    | 1902 | C    | C4-C5-C6   | -8.47 | 113.16      | 117.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 103  | U    | C5-C6-N1    | 8.47  | 126.94      | 122.70   |
| 1   | AA    | 617  | G    | N3-C4-C5    | 8.47  | 132.84      | 128.60   |
| 35  | BB    | 168  | G    | C5-C6-N1    | -8.47 | 107.26      | 111.50   |
| 35  | BB    | 279  | A    | C8-N9-C4    | -8.47 | 102.41      | 105.80   |
| 35  | BB    | 391  | A    | C5-N7-C8    | 8.47  | 108.14      | 103.90   |
| 1   | AA    | 243  | A    | C5-C6-N6    | -8.47 | 116.92      | 123.70   |
| 1   | AA    | 328  | C    | O4'-C1'-N1  | 8.47  | 114.98      | 108.20   |
| 1   | AA    | 707  | U    | O4'-C1'-N1  | 8.47  | 114.98      | 108.20   |
| 35  | BB    | 2342 | C    | O4'-C1'-N1  | 8.47  | 114.98      | 108.20   |
| 35  | BB    | 2409 | G    | C5-N7-C8    | -8.47 | 100.06      | 104.30   |
| 35  | BB    | 2505 | G    | C5-N7-C8    | 8.47  | 108.53      | 104.30   |
| 1   | AA    | 145  | G    | N3-C2-N2    | 8.47  | 125.83      | 119.90   |
| 1   | AA    | 694  | A    | C5-C6-N1    | -8.47 | 113.47      | 117.70   |
| 1   | AA    | 1039 | G    | N3-C4-C5    | -8.47 | 124.37      | 128.60   |
| 1   | AA    | 1241 | G    | P-O5'-C5'   | 8.47  | 134.45      | 120.90   |
| 35  | BB    | 24   | G    | N3-C4-C5    | 8.47  | 132.83      | 128.60   |
| 35  | BB    | 330  | A    | N9-C4-C5    | -8.47 | 102.41      | 105.80   |
| 35  | BB    | 689  | A    | C2-N3-C4    | -8.47 | 106.37      | 110.60   |
| 35  | BB    | 1044 | C    | O4'-C1'-N1  | 8.47  | 114.97      | 108.20   |
| 35  | BB    | 1047 | G    | P-O3'-C3'   | 8.47  | 129.86      | 119.70   |
| 35  | BB    | 1178 | C    | C5-C4-N4    | -8.47 | 114.27      | 120.20   |
| 1   | AA    | 620  | C    | O4'-C1'-N1  | 8.47  | 114.97      | 108.20   |
| 1   | AA    | 1237 | C    | P-O3'-C3'   | 8.47  | 129.86      | 119.70   |
| 35  | BB    | 356  | G    | O4'-C1'-N9  | 8.47  | 114.97      | 108.20   |
| 35  | BB    | 2742 | G    | C5-C6-O6    | -8.47 | 123.52      | 128.60   |
| 1   | AA    | 224  | U    | C5-C4-O4    | -8.46 | 120.82      | 125.90   |
| 1   | AA    | 992  | U    | N3-C4-O4    | 8.46  | 125.33      | 119.40   |
| 1   | AA    | 1149 | C    | N3-C4-N4    | 8.46  | 123.93      | 118.00   |
| 35  | BB    | 2439 | A    | C5-N7-C8    | -8.47 | 99.67       | 103.90   |
| 35  | BB    | 2523 | G    | C8-N9-C4    | -8.47 | 103.01      | 106.40   |
| 1   | AA    | 1317 | C    | O4'-C1'-N1  | 8.46  | 114.97      | 108.20   |
| 35  | BB    | 1383 | A    | C4-C5-N7    | -8.46 | 106.47      | 110.70   |
| 35  | BB    | 1589 | U    | O4'-C1'-N1  | 8.46  | 114.97      | 108.20   |
| 37  | BD    | 184  | ARG  | NE-CZ-NH1   | -8.46 | 116.07      | 120.30   |
| 1   | AA    | 393  | A    | C5-C6-N6    | -8.46 | 116.93      | 123.70   |
| 1   | AA    | 574  | A    | C5-C6-N1    | -8.46 | 113.47      | 117.70   |
| 35  | BB    | 22   | C    | C2-N3-C4    | 8.46  | 124.13      | 119.90   |
| 35  | BB    | 579  | G    | C4-C5-C6    | 8.46  | 123.88      | 118.80   |
| 35  | BB    | 663  | G    | N1-C2-N3    | -8.46 | 118.82      | 123.90   |
| 35  | BB    | 770  | G    | N1-C6-O6    | 8.46  | 124.98      | 119.90   |
| 35  | BB    | 1017 | G    | N1-C6-O6    | 8.46  | 124.98      | 119.90   |
| 35  | BB    | 1079 | C    | C5'-C4'-C3' | -8.46 | 102.46      | 116.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1172 | C    | N3-C4-C5    | -8.46 | 118.52      | 121.90   |
| 35  | BB    | 1628 | G    | N1-C2-N3    | -8.46 | 118.82      | 123.90   |
| 35  | BB    | 1938 | A    | P-O3'-C3'   | 8.46  | 129.85      | 119.70   |
| 1   | AA    | 1133 | G    | N1-C2-N3    | -8.46 | 118.82      | 123.90   |
| 35  | BB    | 443  | A    | C5-C6-N1    | -8.46 | 113.47      | 117.70   |
| 35  | BB    | 845  | A    | N1-C6-N6    | 8.46  | 123.68      | 118.60   |
| 35  | BB    | 2572 | A    | P-O3'-C3'   | 8.46  | 129.85      | 119.70   |
| 35  | BB    | 2583 | G    | N3-C4-C5    | 8.46  | 132.83      | 128.60   |
| 35  | BB    | 2686 | G    | N3-C2-N2    | 8.46  | 125.82      | 119.90   |
| 35  | BB    | 278  | A    | C6-N1-C2    | 8.46  | 123.67      | 118.60   |
| 1   | AA    | 20   | U    | O4'-C1'-N1  | 8.46  | 114.97      | 108.20   |
| 1   | AA    | 381  | C    | O4'-C1'-N1  | 8.46  | 114.97      | 108.20   |
| 34  | BA    | 51   | G    | O4'-C1'-N9  | 8.46  | 114.97      | 108.20   |
| 35  | BB    | 716  | A    | N1-C6-N6    | 8.46  | 123.67      | 118.60   |
| 35  | BB    | 1990 | C    | C6-N1-C2    | 8.46  | 123.68      | 120.30   |
| 35  | BB    | 2292 | U    | C4-C5-C6    | 8.46  | 124.78      | 119.70   |
| 1   | AA    | 226  | G    | N3-C2-N2    | 8.46  | 125.82      | 119.90   |
| 35  | BB    | 2574 | G    | C5-C6-O6    | -8.46 | 123.53      | 128.60   |
| 35  | BB    | 2576 | G    | C5-C6-O6    | -8.46 | 123.53      | 128.60   |
| 35  | BB    | 2667 | C    | N3-C4-C5    | -8.46 | 118.52      | 121.90   |
| 35  | BB    | 2155 | U    | N1-C2-O2    | -8.45 | 116.88      | 122.80   |
| 1   | AA    | 39   | G    | N7-C8-N9    | -8.45 | 108.87      | 113.10   |
| 1   | AA    | 236  | A    | C4-C5-C6    | 8.45  | 121.23      | 117.00   |
| 35  | BB    | 554  | U    | O4'-C1'-N1  | 8.45  | 114.96      | 108.20   |
| 35  | BB    | 927  | A    | C6-C5-N7    | -8.45 | 126.38      | 132.30   |
| 35  | BB    | 2779 | U    | O4'-C1'-N1  | 8.45  | 114.96      | 108.20   |
| 35  | BB    | 1889 | A    | C5-C6-N1    | -8.45 | 113.47      | 117.70   |
| 35  | BB    | 2743 | U    | C5-C6-N1    | 8.45  | 126.92      | 122.70   |
| 56  | BY    | 40   | ARG  | NE-CZ-NH2   | -8.45 | 116.07      | 120.30   |
| 1   | AA    | 272  | C    | N3-C4-C5    | -8.45 | 118.52      | 121.90   |
| 1   | AA    | 1361 | G    | C1'-O4'-C4' | -8.45 | 103.14      | 109.90   |
| 35  | BB    | 73   | A    | C5-C6-N6    | -8.45 | 116.94      | 123.70   |
| 1   | AA    | 1423 | G    | O4'-C1'-N9  | 8.45  | 114.96      | 108.20   |
| 35  | BB    | 304  | U    | O4'-C1'-N1  | 8.45  | 114.96      | 108.20   |
| 35  | BB    | 939  | G    | N1-C2-N3    | -8.45 | 118.83      | 123.90   |
| 35  | BB    | 1573 | G    | N3-C2-N2    | 8.45  | 125.81      | 119.90   |
| 35  | BB    | 2313 | C    | N1-C2-O2    | -8.45 | 113.83      | 118.90   |
| 1   | AA    | 175  | C    | C6-N1-C2    | -8.45 | 116.92      | 120.30   |
| 1   | AA    | 875  | U    | C2-N3-C4    | -8.45 | 121.93      | 127.00   |
| 37  | BD    | 179  | ARG  | NE-CZ-NH2   | -8.45 | 116.08      | 120.30   |
| 1   | AA    | 136  | C    | N3-C2-O2    | 8.44  | 127.81      | 121.90   |
| 35  | BB    | 267  | C    | N3-C4-C5    | -8.45 | 118.52      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1972 | G    | C6-C5-N7   | -8.45 | 125.33      | 130.40   |
| 30  | B5    | 121  | MET  | CG-SD-CE   | -8.44 | 86.69       | 100.20   |
| 1   | AA    | 173  | U    | O4'-C1'-N1 | 8.44  | 114.95      | 108.20   |
| 1   | AA    | 597  | G    | C2-N3-C4   | -8.44 | 107.68      | 111.90   |
| 35  | BB    | 250  | G    | C4-C5-C6   | 8.44  | 123.86      | 118.80   |
| 35  | BB    | 540  | C    | O4'-C1'-N1 | 8.44  | 114.95      | 108.20   |
| 35  | BB    | 917  | A    | C4-C5-C6   | 8.44  | 121.22      | 117.00   |
| 35  | BB    | 1128 | G    | C5-N7-C8   | 8.44  | 108.52      | 104.30   |
| 35  | BB    | 1540 | G    | N1-C6-O6   | 8.44  | 124.97      | 119.90   |
| 35  | BB    | 1796 | U    | C5-C6-N1   | 8.44  | 126.92      | 122.70   |
| 35  | BB    | 1826 | G    | N3-C2-N2   | 8.44  | 125.81      | 119.90   |
| 35  | BB    | 2382 | G    | C5-C6-O6   | -8.44 | 123.53      | 128.60   |
| 35  | BB    | 2497 | A    | P-O3'-C3'  | 8.44  | 129.83      | 119.70   |
| 35  | BB    | 2591 | C    | O4'-C1'-N1 | 8.44  | 114.95      | 108.20   |
| 35  | BB    | 2632 | A    | C4-C5-C6   | 8.44  | 121.22      | 117.00   |
| 35  | BB    | 1482 | G    | C5-N7-C8   | 8.44  | 108.52      | 104.30   |
| 1   | AA    | 397  | A    | N1-C6-N6   | 8.44  | 123.66      | 118.60   |
| 1   | AA    | 1022 | A    | C4-C5-C6   | 8.44  | 121.22      | 117.00   |
| 35  | BB    | 53   | A    | C5-N7-C8   | 8.44  | 108.12      | 103.90   |
| 35  | BB    | 147  | C    | C4-C5-C6   | 8.44  | 121.62      | 117.40   |
| 35  | BB    | 2618 | G    | C6-C5-N7   | -8.44 | 125.34      | 130.40   |
| 35  | BB    | 2810 | A    | C4-C5-C6   | 8.44  | 121.22      | 117.00   |
| 35  | BB    | 578  | G    | C5-C6-N1   | -8.44 | 107.28      | 111.50   |
| 35  | BB    | 589  | U    | N3-C4-O4   | 8.44  | 125.31      | 119.40   |
| 35  | BB    | 2061 | G    | C4-C5-N7   | -8.44 | 107.42      | 110.80   |
| 1   | AA    | 93   | U    | N3-C4-O4   | 8.44  | 125.30      | 119.40   |
| 1   | AA    | 693  | G    | C5-C6-N1   | -8.44 | 107.28      | 111.50   |
| 1   | AA    | 963  | G    | O4'-C1'-N9 | 8.44  | 114.95      | 108.20   |
| 35  | BB    | 141  | G    | N3-C2-N2   | 8.44  | 125.81      | 119.90   |
| 35  | BB    | 939  | G    | C5-C6-O6   | -8.44 | 123.54      | 128.60   |
| 35  | BB    | 985  | C    | N3-C4-N4   | 8.44  | 123.91      | 118.00   |
| 35  | BB    | 1719 | G    | C5-C6-O6   | -8.44 | 123.54      | 128.60   |
| 46  | BM    | 91   | TYR  | CB-CG-CD2  | -8.44 | 115.94      | 121.00   |
| 1   | AA    | 710  | G    | C4-C5-C6   | 8.43  | 123.86      | 118.80   |
| 7   | AG    | 19   | SER  | N-CA-CB    | 8.43  | 123.15      | 110.50   |
| 28  | B3    | 49   | ARG  | NE-CZ-NH2  | -8.43 | 116.08      | 120.30   |
| 29  | B4    | 5    | ARG  | N-CA-CB    | 8.43  | 125.78      | 110.60   |
| 34  | BA    | 73   | A    | N1-C6-N6   | 8.43  | 123.66      | 118.60   |
| 35  | BB    | 799  | G    | C4-C5-N7   | 8.43  | 114.17      | 110.80   |
| 35  | BB    | 881  | G    | O4'-C1'-N9 | 8.43  | 114.95      | 108.20   |
| 35  | BB    | 1186 | G    | O4'-C1'-N9 | 8.43  | 114.95      | 108.20   |
| 35  | BB    | 2018 | G    | C4-C5-N7   | -8.43 | 107.43      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2497 | A    | C5-C6-N6    | -8.43 | 116.95      | 123.70   |
| 1   | AA    | 589  | U    | N1-C2-N3    | 8.43  | 119.96      | 114.90   |
| 1   | AA    | 1076 | U    | N3-C4-O4    | 8.43  | 125.30      | 119.40   |
| 35  | BB    | 1740 | G    | O4'-C1'-N9  | 8.43  | 114.94      | 108.20   |
| 35  | BB    | 2368 | C    | C5-C6-N1    | 8.43  | 125.22      | 121.00   |
| 1   | AA    | 50   | A    | C6-C5-N7    | -8.43 | 126.40      | 132.30   |
| 1   | AA    | 1013 | G    | C5-C6-O6    | -8.43 | 123.54      | 128.60   |
| 1   | AA    | 1505 | G    | N3-C2-N2    | 8.43  | 125.80      | 119.90   |
| 35  | BB    | 129  | C    | N3-C4-N4    | 8.43  | 123.90      | 118.00   |
| 35  | BB    | 278  | A    | N1-C6-N6    | 8.43  | 123.66      | 118.60   |
| 35  | BB    | 1597 | A    | C4-C5-C6    | 8.43  | 121.22      | 117.00   |
| 35  | BB    | 2542 | A    | C5-N7-C8    | 8.43  | 108.11      | 103.90   |
| 1   | AA    | 462  | G    | N1-C6-O6    | 8.43  | 124.96      | 119.90   |
| 1   | AA    | 567  | G    | N3-C2-N2    | 8.43  | 125.80      | 119.90   |
| 1   | AA    | 1468 | A    | O4'-C1'-N9  | 8.43  | 114.94      | 108.20   |
| 22  | AV    | 18   | G    | N1-C6-O6    | 8.43  | 124.96      | 119.90   |
| 35  | BB    | 445  | C    | O4'-C1'-N1  | 8.43  | 114.94      | 108.20   |
| 35  | BB    | 690  | G    | N1-C6-O6    | 8.43  | 124.96      | 119.90   |
| 35  | BB    | 1549 | A    | C4-C5-C6    | 8.43  | 121.21      | 117.00   |
| 35  | BB    | 2232 | C    | N3-C4-C5    | 8.43  | 125.27      | 121.90   |
| 1   | AA    | 19   | A    | C5-C6-N6    | -8.42 | 116.96      | 123.70   |
| 1   | AA    | 235  | C    | N3-C4-C5    | -8.42 | 118.53      | 121.90   |
| 35  | BB    | 725  | G    | C6-C5-N7    | -8.42 | 125.35      | 130.40   |
| 35  | BB    | 2027 | G    | N3-C2-N2    | 8.42  | 125.80      | 119.90   |
| 1   | AA    | 79   | G    | N3-C4-C5    | -8.42 | 124.39      | 128.60   |
| 35  | BB    | 66   | C    | C2-N3-C4    | 8.42  | 124.11      | 119.90   |
| 35  | BB    | 543  | G    | C6-N1-C2    | 8.42  | 130.15      | 125.10   |
| 35  | BB    | 1346 | G    | N1-C6-O6    | 8.42  | 124.95      | 119.90   |
| 35  | BB    | 1695 | G    | C6-C5-N7    | -8.42 | 125.35      | 130.40   |
| 35  | BB    | 2361 | G    | C4-C5-N7    | -8.42 | 107.43      | 110.80   |
| 1   | AA    | 420  | U    | N3-C4-C5    | -8.42 | 109.55      | 114.60   |
| 1   | AA    | 1039 | G    | C6-N1-C2    | -8.42 | 120.05      | 125.10   |
| 34  | BA    | 87   | U    | C5-C4-O4    | -8.42 | 120.85      | 125.90   |
| 35  | BB    | 2768 | U    | C2-N3-C4    | -8.42 | 121.95      | 127.00   |
| 1   | AA    | 336  | A    | N1-C6-N6    | 8.42  | 123.65      | 118.60   |
| 1   | AA    | 379  | C    | N3-C2-O2    | -8.42 | 116.01      | 121.90   |
| 35  | BB    | 1711 | A    | O4'-C1'-N9  | 8.42  | 114.93      | 108.20   |
| 1   | AA    | 1069 | C    | N3-C4-N4    | 8.42  | 123.89      | 118.00   |
| 1   | AA    | 1365 | G    | C6-C5-N7    | -8.42 | 125.35      | 130.40   |
| 34  | BA    | 36   | C    | C4-C5-C6    | 8.42  | 121.61      | 117.40   |
| 35  | BB    | 125  | A    | C4-C5-C6    | 8.42  | 121.21      | 117.00   |
| 35  | BB    | 1240 | U    | C1'-O4'-C4' | 8.42  | 116.63      | 109.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 2872 | A    | C4-C5-N7   | -8.42 | 106.49      | 110.70   |
| 1   | AA    | 327  | A    | C4-C5-C6   | 8.41  | 121.21      | 117.00   |
| 34  | BA    | 88   | C    | C4-C5-C6   | 8.41  | 121.61      | 117.40   |
| 35  | BB    | 310  | A    | C6-N1-C2   | 8.41  | 123.65      | 118.60   |
| 35  | BB    | 1873 | G    | N1-C6-O6   | 8.41  | 124.95      | 119.90   |
| 35  | BB    | 925  | A    | O4'-C1'-N9 | 8.41  | 114.93      | 108.20   |
| 1   | AA    | 593  | U    | C5-C4-O4   | -8.41 | 120.85      | 125.90   |
| 1   | AA    | 745  | G    | C8-N9-C1'  | 8.41  | 137.93      | 127.00   |
| 1   | AA    | 1395 | C    | N1-C2-N3   | -8.41 | 113.31      | 119.20   |
| 5   | AE    | 44   | ARG  | NE-CZ-NH2  | 8.41  | 124.50      | 120.30   |
| 35  | BB    | 582  | A    | C4-C5-C6   | 8.41  | 121.20      | 117.00   |
| 35  | BB    | 837  | C    | N3-C4-C5   | -8.41 | 118.54      | 121.90   |
| 35  | BB    | 1565 | C    | N3-C4-C5   | -8.41 | 118.54      | 121.90   |
| 38  | BE    | 184  | ASP  | CB-CG-OD1  | -8.41 | 110.73      | 118.30   |
| 35  | BB    | 6    | A    | O4'-C1'-N9 | 8.41  | 114.93      | 108.20   |
| 35  | BB    | 746  | U    | O4'-C1'-N1 | 8.41  | 114.93      | 108.20   |
| 35  | BB    | 1951 | U    | C6-N1-C2   | 8.41  | 126.05      | 121.00   |
| 35  | BB    | 2485 | G    | C6-C5-N7   | -8.41 | 125.36      | 130.40   |
| 1   | AA    | 432  | A    | C5-C6-N6   | -8.41 | 116.97      | 123.70   |
| 1   | AA    | 925  | G    | O4'-C1'-N9 | 8.41  | 114.92      | 108.20   |
| 35  | BB    | 466  | A    | C4-C5-C6   | 8.41  | 121.20      | 117.00   |
| 35  | BB    | 1384 | A    | C5-C6-N6   | -8.41 | 116.97      | 123.70   |
| 35  | BB    | 2607 | G    | O4'-C1'-N9 | 8.41  | 114.92      | 108.20   |
| 1   | AA    | 450  | G    | C5-C6-N1   | -8.40 | 107.30      | 111.50   |
| 35  | BB    | 1878 | G    | C8-N9-C4   | -8.40 | 103.04      | 106.40   |
| 35  | BB    | 274  | C    | N3-C4-C5   | -8.40 | 118.54      | 121.90   |
| 35  | BB    | 734  | A    | C5-C6-N6   | -8.40 | 116.98      | 123.70   |
| 35  | BB    | 2577 | A    | C5-C6-N1   | -8.40 | 113.50      | 117.70   |
| 35  | BB    | 2706 | A    | C5-C6-N1   | -8.40 | 113.50      | 117.70   |
| 35  | BB    | 2900 | A    | C4-C5-N7   | 8.40  | 114.90      | 110.70   |
| 1   | AA    | 994  | A    | C5-C6-N6   | -8.40 | 116.98      | 123.70   |
| 1   | AA    | 1145 | A    | N1-C6-N6   | 8.40  | 123.64      | 118.60   |
| 35  | BB    | 489  | G    | C5-C6-O6   | -8.40 | 123.56      | 128.60   |
| 35  | BB    | 1924 | C    | C2-N3-C4   | 8.40  | 124.10      | 119.90   |
| 35  | BB    | 2268 | A    | C8-N9-C4   | -8.40 | 102.44      | 105.80   |
| 1   | AA    | 842  | U    | N1-C2-O2   | 8.40  | 128.68      | 122.80   |
| 1   | AA    | 1433 | A    | N1-C2-N3   | 8.40  | 133.50      | 129.30   |
| 35  | BB    | 974  | G    | C4-C5-C6   | 8.40  | 123.84      | 118.80   |
| 35  | BB    | 1745 | A    | P-O3'-C3'  | -8.40 | 109.62      | 119.70   |
| 35  | BB    | 2040 | G    | N1-C6-O6   | 8.40  | 124.94      | 119.90   |
| 35  | BB    | 2272 | U    | O4'-C1'-N1 | 8.40  | 114.92      | 108.20   |
| 35  | BB    | 623  | C    | O4'-C1'-N1 | 8.40  | 114.92      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 966  | G    | N1-C2-N3   | -8.40 | 118.86      | 123.90   |
| 45  | BL    | 60   | ARG  | NE-CZ-NH2  | -8.40 | 116.10      | 120.30   |
| 35  | BB    | 1464 | G    | N1-C6-O6   | 8.40  | 124.94      | 119.90   |
| 1   | AA    | 516  | U    | N3-C4-O4   | -8.39 | 113.52      | 119.40   |
| 1   | AA    | 926  | G    | C2-N3-C4   | -8.39 | 107.70      | 111.90   |
| 1   | AA    | 1213 | A    | N7-C8-N9   | -8.39 | 109.60      | 113.80   |
| 1   | AA    | 1298 | U    | N3-C4-O4   | 8.39  | 125.28      | 119.40   |
| 35  | BB    | 2013 | A    | N3-C4-C5   | 8.39  | 132.68      | 126.80   |
| 35  | BB    | 2014 | A    | C5-C6-N1   | -8.39 | 113.50      | 117.70   |
| 35  | BB    | 662  | G    | C8-N9-C4   | 8.39  | 109.76      | 106.40   |
| 35  | BB    | 2149 | U    | C5-C6-N1   | 8.39  | 126.90      | 122.70   |
| 35  | BB    | 2463 | C    | C6-N1-C2   | -8.39 | 116.94      | 120.30   |
| 35  | BB    | 2549 | G    | N1-C6-O6   | 8.39  | 124.94      | 119.90   |
| 35  | BB    | 2814 | A    | C5-C6-N1   | -8.39 | 113.50      | 117.70   |
| 1   | AA    | 652  | U    | C5-C4-O4   | -8.39 | 120.86      | 125.90   |
| 1   | AA    | 1361 | G    | O4'-C1'-N9 | 8.39  | 114.91      | 108.20   |
| 35  | BB    | 327  | G    | N1-C2-N3   | -8.39 | 118.86      | 123.90   |
| 35  | BB    | 1318 | U    | O4'-C1'-N1 | 8.39  | 114.91      | 108.20   |
| 35  | BB    | 2320 | U    | C5-C4-O4   | -8.39 | 120.86      | 125.90   |
| 45  | BL    | 21   | ARG  | NE-CZ-NH2  | 8.39  | 124.50      | 120.30   |
| 1   | AA    | 63   | C    | O4'-C1'-N1 | 8.39  | 114.91      | 108.20   |
| 1   | AA    | 74   | A    | C5-N7-C8   | 8.39  | 108.09      | 103.90   |
| 35  | BB    | 1641 | A    | C5-C6-N6   | -8.39 | 116.99      | 123.70   |
| 1   | AA    | 124  | C    | C2-N3-C4   | 8.39  | 124.09      | 119.90   |
| 1   | AA    | 290  | C    | O4'-C1'-N1 | 8.39  | 114.91      | 108.20   |
| 1   | AA    | 1224 | U    | O4'-C1'-N1 | 8.39  | 114.91      | 108.20   |
| 22  | AV    | 19   | G    | N1-C6-O6   | 8.39  | 124.93      | 119.90   |
| 35  | BB    | 457  | A    | C5-C6-N6   | -8.39 | 116.99      | 123.70   |
| 35  | BB    | 1699 | G    | N3-C2-N2   | 8.39  | 125.77      | 119.90   |
| 35  | BB    | 2096 | C    | C5-C4-N4   | -8.39 | 114.33      | 120.20   |
| 35  | BB    | 2777 | G    | C5-C6-O6   | -8.39 | 123.57      | 128.60   |
| 35  | BB    | 2857 | G    | N3-C2-N2   | 8.39  | 125.77      | 119.90   |
| 35  | BB    | 2894 | G    | N1-C6-O6   | 8.39  | 124.93      | 119.90   |
| 1   | AA    | 773  | G    | N3-C2-N2   | 8.38  | 125.77      | 119.90   |
| 51  | BR    | 5    | PHE  | CB-CG-CD1  | 8.39  | 126.67      | 120.80   |
| 1   | AA    | 781  | A    | C5-C6-N1   | -8.38 | 113.51      | 117.70   |
| 2   | AB    | 161  | PHE  | CB-CG-CD2  | 8.38  | 126.67      | 120.80   |
| 34  | BA    | 83   | G    | C5-C6-N1   | 8.38  | 115.69      | 111.50   |
| 35  | BB    | 781  | A    | C8-N9-C4   | -8.38 | 102.45      | 105.80   |
| 35  | BB    | 785  | G    | N7-C8-N9   | -8.38 | 108.91      | 113.10   |
| 35  | BB    | 1934 | C    | C6-N1-C2   | -8.38 | 116.95      | 120.30   |
| 35  | BB    | 2857 | G    | C5-C6-N1   | -8.38 | 107.31      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 777  | A    | C5-C6-N6    | -8.38 | 116.99      | 123.70   |
| 35  | BB    | 332  | A    | C8-N9-C4    | -8.38 | 102.45      | 105.80   |
| 1   | AA    | 95   | C    | C6-N1-C2    | -8.38 | 116.95      | 120.30   |
| 1   | AA    | 138  | G    | C6-C5-N7    | -8.38 | 125.37      | 130.40   |
| 35  | BB    | 835  | C    | C2-N3-C4    | 8.38  | 124.09      | 119.90   |
| 35  | BB    | 888  | C    | O4'-C4'-C3' | -8.38 | 95.62       | 104.00   |
| 35  | BB    | 1579 | A    | C5-C6-N1    | -8.38 | 113.51      | 117.70   |
| 35  | BB    | 2775 | G    | O4'-C1'-N9  | 8.38  | 114.91      | 108.20   |
| 35  | BB    | 1269 | A    | C5-C6-N6    | -8.38 | 117.00      | 123.70   |
| 35  | BB    | 1877 | A    | N1-C2-N3    | 8.38  | 133.49      | 129.30   |
| 35  | BB    | 1879 | C    | N3-C4-N4    | 8.38  | 123.87      | 118.00   |
| 35  | BB    | 2569 | G    | C8-N9-C4    | -8.38 | 103.05      | 106.40   |
| 1   | AA    | 100  | G    | C5-C6-O6    | -8.38 | 123.57      | 128.60   |
| 1   | AA    | 1070 | U    | N3-C4-O4    | 8.38  | 125.27      | 119.40   |
| 1   | AA    | 9    | G    | C8-N9-C4    | 8.38  | 109.75      | 106.40   |
| 1   | AA    | 243  | A    | C2'-C3'-O3' | 8.38  | 127.93      | 109.50   |
| 35  | BB    | 1401 | G    | O4'-C1'-N9  | 8.38  | 114.90      | 108.20   |
| 39  | BF    | 19   | PHE  | CB-CG-CD1   | -8.38 | 114.94      | 120.80   |
| 1   | AA    | 254  | G    | C6-N1-C2    | 8.38  | 130.13      | 125.10   |
| 35  | BB    | 918  | A    | C4-C5-C6    | 8.38  | 121.19      | 117.00   |
| 35  | BB    | 1342 | A    | C5-C6-N6    | -8.38 | 117.00      | 123.70   |
| 35  | BB    | 2218 | G    | N1-C2-N3    | -8.38 | 118.87      | 123.90   |
| 1   | AA    | 778  | G    | C8-N9-C4    | -8.38 | 103.05      | 106.40   |
| 1   | AA    | 1419 | G    | N7-C8-N9    | -8.38 | 108.91      | 113.10   |
| 1   | AA    | 1531 | A    | C5-C6-N1    | -8.38 | 113.51      | 117.70   |
| 16  | AP    | 32   | PHE  | CB-CG-CD1   | -8.38 | 114.94      | 120.80   |
| 35  | BB    | 211  | C    | N3-C4-C5    | -8.38 | 118.55      | 121.90   |
| 35  | BB    | 634  | C    | C5-C4-N4    | -8.37 | 114.34      | 120.20   |
| 35  | BB    | 1103 | A    | C8-N9-C4    | -8.37 | 102.45      | 105.80   |
| 35  | BB    | 1186 | G    | C5-C6-O6    | -8.38 | 123.58      | 128.60   |
| 1   | AA    | 397  | A    | O4'-C1'-N9  | 8.37  | 114.90      | 108.20   |
| 35  | BB    | 1131 | G    | N3-C2-N2    | 8.37  | 125.76      | 119.90   |
| 35  | BB    | 2028 | U    | C6-N1-C2    | -8.37 | 115.98      | 121.00   |
| 35  | BB    | 2753 | A    | C5-C6-N6    | -8.37 | 117.00      | 123.70   |
| 34  | BA    | 92   | C    | C6-N1-C2    | -8.37 | 116.95      | 120.30   |
| 35  | BB    | 823  | C    | C4-C5-C6    | 8.37  | 121.58      | 117.40   |
| 1   | AA    | 228  | A    | C5-C6-N1    | -8.37 | 113.52      | 117.70   |
| 1   | AA    | 1037 | C    | P-O3'-C3'   | -8.37 | 109.66      | 119.70   |
| 35  | BB    | 1398 | C    | N3-C4-N4    | 8.37  | 123.86      | 118.00   |
| 35  | BB    | 1927 | A    | C5-C6-N1    | -8.37 | 113.52      | 117.70   |
| 35  | BB    | 2087 | G    | C4-C5-C6    | 8.37  | 123.82      | 118.80   |
| 22  | AV    | 34   | G    | OP1-P-OP2   | -8.37 | 107.05      | 119.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1598 | A    | C4-C5-N7    | -8.37 | 106.52      | 110.70   |
| 35  | BB    | 1911 | U    | O4'-C1'-N1  | 8.37  | 114.89      | 108.20   |
| 1   | AA    | 115  | G    | C2-N3-C4    | 8.37  | 116.08      | 111.90   |
| 1   | AA    | 1016 | A    | C5-C6-N6    | -8.37 | 117.01      | 123.70   |
| 35  | BB    | 428  | A    | N1-C2-N3    | 8.37  | 133.48      | 129.30   |
| 35  | BB    | 1624 | U    | N3-C4-C5    | -8.37 | 109.58      | 114.60   |
| 1   | AA    | 303  | A    | C6-C5-N7    | -8.36 | 126.44      | 132.30   |
| 1   | AA    | 906  | A    | C4-C5-C6    | 8.36  | 121.18      | 117.00   |
| 35  | BB    | 1179 | G    | C5-C6-O6    | -8.36 | 123.58      | 128.60   |
| 35  | BB    | 2746 | U    | O4'-C1'-N1  | 8.36  | 114.89      | 108.20   |
| 1   | AA    | 915  | A    | O4'-C1'-N9  | 8.36  | 114.89      | 108.20   |
| 1   | AA    | 1281 | C    | N3-C4-N4    | 8.36  | 123.85      | 118.00   |
| 1   | AA    | 1314 | C    | C5-C4-N4    | -8.36 | 114.35      | 120.20   |
| 35  | BB    | 753  | A    | C4-C5-N7    | -8.36 | 106.52      | 110.70   |
| 35  | BB    | 1057 | A    | O4'-C4'-C3' | 8.36  | 112.79      | 106.10   |
| 35  | BB    | 1551 | A    | N1-C6-N6    | 8.36  | 123.62      | 118.60   |
| 35  | BB    | 1653 | G    | C5-C6-N1    | -8.36 | 107.32      | 111.50   |
| 1   | AA    | 649  | A    | C5-N7-C8    | 8.36  | 108.08      | 103.90   |
| 1   | AA    | 1400 | C    | C6-N1-C1'   | -8.36 | 110.77      | 120.80   |
| 4   | AD    | 55   | ARG  | NE-CZ-NH2   | -8.36 | 116.12      | 120.30   |
| 35  | BB    | 422  | A    | C5-C6-N6    | -8.36 | 117.01      | 123.70   |
| 35  | BB    | 1367 | A    | N1-C6-N6    | 8.36  | 123.62      | 118.60   |
| 35  | BB    | 2813 | A    | O4'-C1'-N9  | 8.36  | 114.89      | 108.20   |
| 35  | BB    | 681  | G    | C8-N9-C4    | -8.36 | 103.06      | 106.40   |
| 35  | BB    | 1598 | A    | N7-C8-N9    | 8.36  | 117.98      | 113.80   |
| 35  | BB    | 2573 | C    | C5-C6-N1    | 8.36  | 125.18      | 121.00   |
| 1   | AA    | 1391 | U    | C2-N3-C4    | 8.36  | 132.01      | 127.00   |
| 1   | AA    | 1515 | G    | C6-C5-N7    | -8.36 | 125.39      | 130.40   |
| 35  | BB    | 333  | G    | N1-C6-O6    | 8.36  | 124.91      | 119.90   |
| 35  | BB    | 1365 | A    | P-O3'-C3'   | 8.36  | 129.73      | 119.70   |
| 35  | BB    | 2569 | G    | N1-C6-O6    | 8.36  | 124.91      | 119.90   |
| 35  | BB    | 1908 | C    | C5-C4-N4    | -8.36 | 114.35      | 120.20   |
| 35  | BB    | 2573 | C    | C2-N1-C1'   | 8.36  | 127.99      | 118.80   |
| 1   | AA    | 169  | C    | O4'-C1'-N1  | 8.35  | 114.88      | 108.20   |
| 1   | AA    | 694  | A    | N1-C6-N6    | 8.35  | 123.61      | 118.60   |
| 1   | AA    | 936  | C    | O4'-C1'-N1  | 8.35  | 114.88      | 108.20   |
| 1   | AA    | 1079 | G    | C4-C5-C6    | 8.35  | 123.81      | 118.80   |
| 35  | BB    | 2848 | G    | N1-C2-N3    | -8.35 | 118.89      | 123.90   |
| 35  | BB    | 1294 | U    | N3-C4-O4    | -8.35 | 113.56      | 119.40   |
| 35  | BB    | 1511 | G    | O4'-C1'-N9  | 8.35  | 114.88      | 108.20   |
| 35  | BB    | 1858 | A    | C5-C6-N1    | -8.35 | 113.53      | 117.70   |
| 35  | BB    | 2309 | A    | C5-C6-N6    | -8.35 | 117.02      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 2403 | C    | P-O3'-C3'  | -8.35 | 109.68      | 119.70   |
| 1   | AA    | 440  | C    | O4'-C1'-N1 | 8.35  | 114.88      | 108.20   |
| 1   | AA    | 1083 | U    | O4'-C1'-N1 | 8.35  | 114.88      | 108.20   |
| 1   | AA    | 1462 | C    | O4'-C1'-N1 | 8.35  | 114.88      | 108.20   |
| 35  | BB    | 39   | G    | N3-C2-N2   | 8.35  | 125.74      | 119.90   |
| 35  | BB    | 345  | A    | C4-C5-N7   | -8.35 | 106.53      | 110.70   |
| 35  | BB    | 926  | G    | C8-N9-C4   | -8.35 | 103.06      | 106.40   |
| 35  | BB    | 1543 | G    | C4-C5-C6   | 8.35  | 123.81      | 118.80   |
| 35  | BB    | 1838 | C    | N3-C4-C5   | -8.35 | 118.56      | 121.90   |
| 35  | BB    | 2424 | C    | N3-C4-C5   | -8.35 | 118.56      | 121.90   |
| 35  | BB    | 2479 | U    | O4'-C1'-N1 | 8.35  | 114.88      | 108.20   |
| 35  | BB    | 2850 | A    | C5-C6-N6   | -8.35 | 117.02      | 123.70   |
| 1   | AA    | 428  | G    | P-O3'-C3'  | 8.35  | 129.72      | 119.70   |
| 1   | AA    | 830  | G    | N1-C2-N3   | -8.35 | 118.89      | 123.90   |
| 1   | AA    | 1262 | C    | C5-C4-N4   | -8.35 | 114.36      | 120.20   |
| 1   | AA    | 1404 | C    | C6-N1-C2   | -8.35 | 116.96      | 120.30   |
| 35  | BB    | 1681 | G    | O4'-C1'-N9 | 8.35  | 114.88      | 108.20   |
| 1   | AA    | 73   | C    | C5-C6-N1   | 8.35  | 125.17      | 121.00   |
| 1   | AA    | 1188 | A    | N7-C8-N9   | -8.35 | 109.63      | 113.80   |
| 35  | BB    | 1535 | A    | C8-N9-C4   | -8.35 | 102.46      | 105.80   |
| 35  | BB    | 1573 | G    | O4'-C1'-N9 | 8.35  | 114.88      | 108.20   |
| 35  | BB    | 1964 | G    | C5-C6-O6   | -8.35 | 123.59      | 128.60   |
| 35  | BB    | 2376 | A    | N1-C6-N6   | 8.35  | 123.61      | 118.60   |
| 35  | BB    | 2379 | G    | C4-C5-C6   | 8.35  | 123.81      | 118.80   |
| 1   | AA    | 351  | G    | N1-C2-N3   | -8.34 | 118.89      | 123.90   |
| 1   | AA    | 738  | C    | O4'-C1'-N1 | 8.34  | 114.87      | 108.20   |
| 34  | BA    | 96   | G    | O4'-C1'-N9 | 8.34  | 114.87      | 108.20   |
| 35  | BB    | 2497 | A    | C8-N9-C4   | 8.34  | 109.14      | 105.80   |
| 1   | AA    | 253  | A    | O4'-C1'-N9 | 8.34  | 114.87      | 108.20   |
| 1   | AA    | 456  | A    | O4'-C1'-N9 | 8.34  | 114.87      | 108.20   |
| 1   | AA    | 943  | U    | C4-C5-C6   | -8.34 | 114.70      | 119.70   |
| 2   | AB    | 212  | TYR  | CB-CG-CD1  | 8.34  | 126.00      | 121.00   |
| 35  | BB    | 1663 | G    | O5'-P-OP2  | 8.34  | 120.71      | 110.70   |
| 35  | BB    | 2121 | G    | O4'-C1'-N9 | 8.34  | 114.87      | 108.20   |
| 35  | BB    | 2861 | U    | C2-N3-C4   | -8.34 | 122.00      | 127.00   |
| 1   | AA    | 66   | A    | N1-C2-N3   | 8.34  | 133.47      | 129.30   |
| 1   | AA    | 874  | G    | C2-N3-C4   | 8.34  | 116.07      | 111.90   |
| 1   | AA    | 1448 | C    | O4'-C1'-N1 | 8.34  | 114.87      | 108.20   |
| 35  | BB    | 2295 | C    | C5-C6-N1   | 8.34  | 125.17      | 121.00   |
| 1   | AA    | 702  | A    | C4-C5-C6   | 8.34  | 121.17      | 117.00   |
| 35  | BB    | 502  | A    | C5-C6-N6   | -8.34 | 117.03      | 123.70   |
| 35  | BB    | 2399 | G    | C6-C5-N7   | -8.34 | 125.40      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 894  | G    | N1-C6-O6    | 8.33  | 124.90      | 119.90   |
| 35  | BB    | 39   | G    | N1-C6-O6    | 8.33  | 124.90      | 119.90   |
| 35  | BB    | 1060 | U    | O4'-C1'-N1  | 8.33  | 114.87      | 108.20   |
| 35  | BB    | 2318 | G    | C4-C5-N7    | -8.33 | 107.47      | 110.80   |
| 1   | AA    | 110  | C    | O4'-C1'-N1  | 8.33  | 114.87      | 108.20   |
| 1   | AA    | 935  | A    | N1-C2-N3    | 8.33  | 133.47      | 129.30   |
| 35  | BB    | 38   | A    | O4'-C1'-N9  | 8.33  | 114.87      | 108.20   |
| 35  | BB    | 1302 | A    | C8-N9-C4    | -8.33 | 102.47      | 105.80   |
| 35  | BB    | 1649 | G    | C2-N3-C4    | 8.33  | 116.07      | 111.90   |
| 35  | BB    | 1762 | A    | C5-C6-N1    | -8.33 | 113.53      | 117.70   |
| 35  | BB    | 2855 | C    | C5-C4-N4    | -8.33 | 114.37      | 120.20   |
| 41  | BH    | 50   | ARG  | NE-CZ-NH2   | -8.33 | 116.13      | 120.30   |
| 54  | BU    | 80   | ASP  | CB-CG-OD2   | -8.33 | 110.80      | 118.30   |
| 1   | AA    | 183  | C    | O4'-C4'-C3' | -8.33 | 95.67       | 104.00   |
| 1   | AA    | 254  | G    | O4'-C1'-N9  | 8.33  | 114.86      | 108.20   |
| 35  | BB    | 97   | C    | N3-C4-N4    | 8.33  | 123.83      | 118.00   |
| 35  | BB    | 1392 | A    | N7-C8-N9    | -8.33 | 109.63      | 113.80   |
| 1   | AA    | 306  | A    | N1-C6-N6    | 8.33  | 123.60      | 118.60   |
| 1   | AA    | 711  | G    | O4'-C1'-N9  | 8.33  | 114.86      | 108.20   |
| 34  | BA    | 24   | G    | N1-C6-O6    | 8.33  | 124.90      | 119.90   |
| 35  | BB    | 173  | A    | C5-C6-N6    | -8.33 | 117.04      | 123.70   |
| 35  | BB    | 2504 | U    | O4'-C1'-N1  | 8.33  | 114.86      | 108.20   |
| 35  | BB    | 2603 | G    | C5-N7-C8    | 8.33  | 108.46      | 104.30   |
| 1   | AA    | 1118 | U    | O4'-C1'-N1  | 8.33  | 114.86      | 108.20   |
| 1   | AA    | 1179 | A    | N3-C4-C5    | -8.33 | 120.97      | 126.80   |
| 35  | BB    | 1237 | A    | C5-C6-N1    | -8.33 | 113.54      | 117.70   |
| 1   | AA    | 1500 | A    | C5-C6-N1    | -8.33 | 113.54      | 117.70   |
| 35  | BB    | 1486 | U    | C5-C6-N1    | 8.33  | 126.86      | 122.70   |
| 35  | BB    | 1633 | G    | C5-C6-O6    | -8.33 | 123.60      | 128.60   |
| 1   | AA    | 282  | A    | C5-C6-N6    | -8.32 | 117.04      | 123.70   |
| 1   | AA    | 1004 | A    | C5-C6-N6    | -8.32 | 117.04      | 123.70   |
| 35  | BB    | 380  | G    | N1-C6-O6    | 8.32  | 124.89      | 119.90   |
| 35  | BB    | 1205 | A    | O4'-C1'-N9  | 8.32  | 114.86      | 108.20   |
| 35  | BB    | 2186 | G    | C5-C6-O6    | -8.32 | 123.61      | 128.60   |
| 1   | AA    | 160  | A    | O4'-C1'-N9  | 8.32  | 114.86      | 108.20   |
| 35  | BB    | 407  | G    | N1-C2-N3    | -8.32 | 118.91      | 123.90   |
| 35  | BB    | 662  | G    | C5-C6-O6    | -8.32 | 123.61      | 128.60   |
| 35  | BB    | 678  | C    | O4'-C1'-N1  | 8.32  | 114.86      | 108.20   |
| 35  | BB    | 1099 | G    | C5-C6-O6    | -8.32 | 123.61      | 128.60   |
| 35  | BB    | 1115 | G    | C4-C5-C6    | 8.32  | 123.79      | 118.80   |
| 35  | BB    | 1485 | U    | C2-N3-C4    | -8.32 | 122.01      | 127.00   |
| 35  | BB    | 2370 | G    | N1-C2-N3    | -8.32 | 118.91      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2534 | A    | C8-N9-C4    | 8.32  | 109.13      | 105.80   |
| 35  | BB    | 2771 | C    | N3-C4-C5    | -8.32 | 118.57      | 121.90   |
| 1   | AA    | 79   | G    | C8-N9-C4    | -8.32 | 103.07      | 106.40   |
| 1   | AA    | 391  | G    | O4'-C1'-N9  | 8.32  | 114.86      | 108.20   |
| 1   | AA    | 1375 | A    | O4'-C1'-N9  | 8.32  | 114.86      | 108.20   |
| 34  | BA    | 68   | C    | N3-C4-C5    | -8.32 | 118.57      | 121.90   |
| 35  | BB    | 2645 | G    | C5-C6-O6    | -8.32 | 123.61      | 128.60   |
| 1   | AA    | 577  | G    | N3-C4-C5    | -8.32 | 124.44      | 128.60   |
| 1   | AA    | 840  | C    | N3-C4-N4    | 8.32  | 123.82      | 118.00   |
| 35  | BB    | 106  | C    | N3-C4-C5    | -8.32 | 118.57      | 121.90   |
| 35  | BB    | 253  | C    | N3-C4-N4    | 8.32  | 123.82      | 118.00   |
| 35  | BB    | 346  | A    | C5-C6-N1    | -8.32 | 113.54      | 117.70   |
| 35  | BB    | 389  | G    | C2-N3-C4    | 8.32  | 116.06      | 111.90   |
| 35  | BB    | 579  | G    | C6-C5-N7    | -8.32 | 125.41      | 130.40   |
| 35  | BB    | 2418 | A    | C5-C6-N1    | -8.32 | 113.54      | 117.70   |
| 35  | BB    | 1432 | G    | N3-C2-N2    | 8.32  | 125.72      | 119.90   |
| 35  | BB    | 1796 | U    | C2-N3-C4    | 8.32  | 131.99      | 127.00   |
| 34  | BA    | 102  | G    | N3-C2-N2    | 8.32  | 125.72      | 119.90   |
| 35  | BB    | 205  | G    | C4-C5-C6    | 8.32  | 123.79      | 118.80   |
| 35  | BB    | 393  | C    | N3-C4-N4    | 8.32  | 123.82      | 118.00   |
| 35  | BB    | 301  | G    | N3-C4-N9    | -8.32 | 121.01      | 126.00   |
| 35  | BB    | 721  | A    | N9-C4-C5    | 8.32  | 109.13      | 105.80   |
| 35  | BB    | 2488 | G    | C2-N3-C4    | 8.32  | 116.06      | 111.90   |
| 35  | BB    | 2868 | A    | C4-C5-C6    | 8.32  | 121.16      | 117.00   |
| 1   | AA    | 400  | C    | C4-C5-C6    | -8.31 | 113.24      | 117.40   |
| 1   | AA    | 1021 | A    | C5-C6-N1    | -8.31 | 113.54      | 117.70   |
| 35  | BB    | 282  | A    | N9-C4-C5    | 8.31  | 109.13      | 105.80   |
| 35  | BB    | 504  | A    | N1-C6-N6    | 8.31  | 123.59      | 118.60   |
| 35  | BB    | 1301 | A    | N1-C2-N3    | 8.31  | 133.46      | 129.30   |
| 35  | BB    | 2172 | U    | C1'-O4'-C4' | -8.31 | 103.25      | 109.90   |
| 1   | AA    | 205  | A    | O4'-C1'-N9  | 8.31  | 114.85      | 108.20   |
| 1   | AA    | 1377 | A    | C4-C5-N7    | -8.31 | 106.54      | 110.70   |
| 35  | BB    | 1305 | C    | N3-C4-C5    | -8.31 | 118.58      | 121.90   |
| 35  | BB    | 1443 | U    | O4'-C1'-N1  | 8.31  | 114.85      | 108.20   |
| 35  | BB    | 2605 | U    | O4'-C1'-N1  | 8.31  | 114.85      | 108.20   |
| 1   | AA    | 563  | A    | C5-C6-N1    | -8.31 | 113.55      | 117.70   |
| 1   | AA    | 841  | C    | C6-N1-C2    | 8.31  | 123.62      | 120.30   |
| 5   | AE    | 102  | THR  | CA-CB-CG2   | -8.31 | 100.77      | 112.40   |
| 22  | AV    | 3    | G    | N1-C2-N3    | -8.31 | 118.91      | 123.90   |
| 35  | BB    | 1925 | C    | N3-C4-N4    | 8.31  | 123.82      | 118.00   |
| 1   | AA    | 129  | A    | N7-C8-N9    | 8.31  | 117.95      | 113.80   |
| 1   | AA    | 337  | G    | N1-C2-N3    | -8.31 | 118.92      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 347  | G    | C3'-C2'-C1' | 8.31  | 108.15      | 101.50   |
| 1   | AA    | 553  | A    | C6-N1-C2    | -8.31 | 113.61      | 118.60   |
| 1   | AA    | 602  | A    | C1'-O4'-C4' | -8.31 | 103.25      | 109.90   |
| 35  | BB    | 855  | G    | C6-C5-N7    | -8.31 | 125.42      | 130.40   |
| 35  | BB    | 1096 | A    | O4'-C1'-N9  | 8.31  | 114.85      | 108.20   |
| 35  | BB    | 1601 | G    | C6-C5-N7    | -8.31 | 125.42      | 130.40   |
| 35  | BB    | 2282 | G    | C5-C6-O6    | -8.31 | 123.62      | 128.60   |
| 35  | BB    | 2429 | G    | O4'-C1'-N9  | -8.31 | 101.55      | 108.20   |
| 1   | AA    | 347  | G    | O4'-C1'-N9  | 8.30  | 114.84      | 108.20   |
| 1   | AA    | 1463 | U    | O4'-C1'-N1  | 8.30  | 114.84      | 108.20   |
| 35  | BB    | 188  | G    | C6-C5-N7    | 8.30  | 135.38      | 130.40   |
| 35  | BB    | 250  | G    | C2-N3-C4    | -8.30 | 107.75      | 111.90   |
| 35  | BB    | 368  | A    | C6-N1-C2    | -8.31 | 113.62      | 118.60   |
| 35  | BB    | 729  | G    | C6-C5-N7    | -8.30 | 125.42      | 130.40   |
| 35  | BB    | 851  | C    | C2-N3-C4    | 8.30  | 124.05      | 119.90   |
| 35  | BB    | 44   | A    | C8-N9-C4    | 8.30  | 109.12      | 105.80   |
| 35  | BB    | 1289 | C    | C2-N3-C4    | -8.30 | 115.75      | 119.90   |
| 35  | BB    | 2154 | A    | C5-C6-N6    | -8.30 | 117.06      | 123.70   |
| 35  | BB    | 2369 | A    | C4-C5-C6    | 8.30  | 121.15      | 117.00   |
| 41  | BH    | 91   | PHE  | CB-CG-CD1   | 8.30  | 126.61      | 120.80   |
| 35  | BB    | 789  | A    | C5-C6-N6    | -8.30 | 117.06      | 123.70   |
| 35  | BB    | 2781 | A    | C5-C6-N6    | -8.30 | 117.06      | 123.70   |
| 1   | AA    | 62   | U    | C6-N1-C2    | 8.30  | 125.98      | 121.00   |
| 1   | AA    | 168  | G    | N3-C2-N2    | 8.30  | 125.71      | 119.90   |
| 1   | AA    | 411  | A    | C4-C5-C6    | 8.30  | 121.15      | 117.00   |
| 1   | AA    | 765  | G    | C5-C6-N1    | -8.30 | 107.35      | 111.50   |
| 1   | AA    | 1157 | A    | C8-N9-C4    | -8.30 | 102.48      | 105.80   |
| 35  | BB    | 891  | G    | C5'-C4'-O4' | 8.30  | 119.06      | 109.10   |
| 1   | AA    | 1435 | G    | C4-C5-C6    | 8.30  | 123.78      | 118.80   |
| 22  | AV    | 56   | C    | O4'-C1'-N1  | 8.30  | 114.84      | 108.20   |
| 34  | BA    | 79   | G    | C8-N9-C4    | -8.30 | 103.08      | 106.40   |
| 35  | BB    | 1071 | G    | C4-C5-C6    | 8.30  | 123.78      | 118.80   |
| 35  | BB    | 1312 | U    | P-O3'-C3'   | 8.30  | 129.66      | 119.70   |
| 35  | BB    | 1415 | U    | O4'-C1'-N1  | 8.30  | 114.84      | 108.20   |
| 35  | BB    | 1528 | A    | O4'-C1'-N9  | 8.30  | 114.84      | 108.20   |
| 35  | BB    | 2027 | G    | C6-C5-N7    | -8.30 | 125.42      | 130.40   |
| 35  | BB    | 2470 | G    | N7-C8-N9    | -8.30 | 108.95      | 113.10   |
| 35  | BB    | 2500 | U    | N3-C4-O4    | 8.30  | 125.21      | 119.40   |
| 35  | BB    | 2533 | U    | C2-N3-C4    | -8.30 | 122.02      | 127.00   |
| 35  | BB    | 2705 | A    | C8-N9-C4    | -8.30 | 102.48      | 105.80   |
| 1   | AA    | 9    | G    | O4'-C1'-N9  | 8.30  | 114.84      | 108.20   |
| 1   | AA    | 699  | C    | N3-C4-N4    | 8.30  | 123.81      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1282 | C    | O4'-C1'-N1 | 8.30  | 114.84      | 108.20   |
| 19  | AS    | 35   | ARG  | NE-CZ-NH2  | -8.30 | 116.15      | 120.30   |
| 22  | AV    | 39   | G    | C6-N1-C2   | -8.30 | 120.12      | 125.10   |
| 35  | BB    | 2738 | A    | C5-C6-N6   | -8.30 | 117.06      | 123.70   |
| 35  | BB    | 410  | G    | C8-N9-C4   | -8.30 | 103.08      | 106.40   |
| 35  | BB    | 470  | A    | N1-C6-N6   | 8.30  | 123.58      | 118.60   |
| 35  | BB    | 764  | A    | C4-C5-N7   | -8.30 | 106.55      | 110.70   |
| 35  | BB    | 1560 | G    | C8-N9-C4   | -8.30 | 103.08      | 106.40   |
| 35  | BB    | 1803 | A    | C4-C5-C6   | 8.30  | 121.15      | 117.00   |
| 35  | BB    | 2830 | C    | O4'-C1'-N1 | 8.30  | 114.84      | 108.20   |
| 1   | AA    | 274  | A    | O4'-C1'-N9 | 8.30  | 114.84      | 108.20   |
| 1   | AA    | 952  | U    | O4'-C1'-N1 | 8.30  | 114.84      | 108.20   |
| 35  | BB    | 2096 | C    | N3-C4-N4   | 8.30  | 123.81      | 118.00   |
| 1   | AA    | 1026 | G    | O4'-C1'-N9 | 8.29  | 114.83      | 108.20   |
| 35  | BB    | 84   | A    | C2-N3-C4   | -8.29 | 106.45      | 110.60   |
| 35  | BB    | 405  | U    | C5-C6-N1   | -8.29 | 118.55      | 122.70   |
| 35  | BB    | 855  | G    | N3-C4-C5   | 8.29  | 132.75      | 128.60   |
| 35  | BB    | 2053 | G    | P-O3'-C3'  | -8.29 | 109.75      | 119.70   |
| 35  | BB    | 2156 | G    | N3-C4-C5   | 8.29  | 132.75      | 128.60   |
| 35  | BB    | 2760 | C    | C2-N3-C4   | 8.29  | 124.05      | 119.90   |
| 1   | AA    | 625  | U    | C2-N3-C4   | -8.29 | 122.03      | 127.00   |
| 1   | AA    | 1114 | C    | N3-C4-C5   | -8.29 | 118.58      | 121.90   |
| 21  | AU    | 18   | PHE  | CB-CG-CD1  | -8.29 | 115.00      | 120.80   |
| 34  | BA    | 56   | G    | N3-C4-C5   | -8.29 | 124.45      | 128.60   |
| 35  | BB    | 1181 | U    | N3-C2-O2   | 8.29  | 128.00      | 122.20   |
| 35  | BB    | 1676 | A    | C6-C5-N7   | -8.29 | 126.50      | 132.30   |
| 35  | BB    | 2510 | C    | O4'-C1'-N1 | 8.29  | 114.83      | 108.20   |
| 25  | B0    | 73   | ARG  | NE-CZ-NH1  | -8.29 | 116.16      | 120.30   |
| 35  | BB    | 1191 | G    | C8-N9-C4   | -8.29 | 103.08      | 106.40   |
| 35  | BB    | 1465 | G    | O4'-C1'-N9 | 8.29  | 114.83      | 108.20   |
| 35  | BB    | 2101 | A    | C4-C5-C6   | 8.29  | 121.14      | 117.00   |
| 35  | BB    | 1795 | C    | C6-N1-C2   | -8.29 | 116.98      | 120.30   |
| 1   | AA    | 336  | A    | C8-N9-C4   | 8.29  | 109.11      | 105.80   |
| 1   | AA    | 945  | G    | C6-C5-N7   | -8.29 | 125.43      | 130.40   |
| 35  | BB    | 720  | U    | C4-C5-C6   | -8.29 | 114.73      | 119.70   |
| 35  | BB    | 1117 | C    | N3-C4-N4   | 8.29  | 123.80      | 118.00   |
| 35  | BB    | 1891 | G    | N9-C4-C5   | 8.29  | 108.72      | 105.40   |
| 35  | BB    | 2026 | U    | C5-C6-N1   | 8.29  | 126.84      | 122.70   |
| 1   | AA    | 1122 | U    | N3-C4-C5   | -8.28 | 109.63      | 114.60   |
| 1   | AA    | 1327 | C    | O4'-C1'-N1 | 8.28  | 114.83      | 108.20   |
| 35  | BB    | 1039 | A    | C4-C5-C6   | 8.28  | 121.14      | 117.00   |
| 35  | BB    | 1064 | C    | N3-C2-O2   | -8.28 | 116.10      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1901 | A    | C4-C5-N7    | -8.29 | 106.56      | 110.70   |
| 35  | BB    | 2432 | A    | C2-N3-C4    | -8.28 | 106.46      | 110.60   |
| 1   | AA    | 134  | G    | P-O3'-C3'   | 8.28  | 129.64      | 119.70   |
| 1   | AA    | 366  | A    | C5-N7-C8    | 8.28  | 108.04      | 103.90   |
| 1   | AA    | 470  | C    | N3-C4-N4    | 8.28  | 123.80      | 118.00   |
| 1   | AA    | 774  | G    | C4-C5-N7    | -8.28 | 107.49      | 110.80   |
| 1   | AA    | 1179 | A    | C4-C5-N7    | -8.28 | 106.56      | 110.70   |
| 1   | AA    | 1467 | C    | O4'-C1'-N1  | 8.28  | 114.83      | 108.20   |
| 35  | BB    | 144  | A    | C8-N9-C4    | -8.28 | 102.49      | 105.80   |
| 35  | BB    | 841  | G    | O4'-C1'-N9  | 8.28  | 114.83      | 108.20   |
| 35  | BB    | 844  | A    | C6-C5-N7    | -8.28 | 126.50      | 132.30   |
| 35  | BB    | 2026 | U    | O4'-C1'-N1  | 8.28  | 114.83      | 108.20   |
| 35  | BB    | 2456 | C    | C4-C5-C6    | 8.28  | 121.54      | 117.40   |
| 1   | AA    | 734  | G    | N7-C8-N9    | 8.28  | 117.24      | 113.10   |
| 1   | AA    | 753  | A    | N1-C2-N3    | -8.28 | 125.16      | 129.30   |
| 35  | BB    | 89   | A    | C5-C6-N1    | -8.28 | 113.56      | 117.70   |
| 35  | BB    | 2357 | G    | C5-C6-O6    | -8.28 | 123.63      | 128.60   |
| 1   | AA    | 1492 | A    | N9-C4-C5    | 8.28  | 109.11      | 105.80   |
| 34  | BA    | 64   | G    | C5-N7-C8    | 8.28  | 108.44      | 104.30   |
| 35  | BB    | 2715 | C    | O4'-C1'-N1  | 8.28  | 114.82      | 108.20   |
| 35  | BB    | 1531 | C    | O4'-C1'-N1  | 8.28  | 114.82      | 108.20   |
| 35  | BB    | 2391 | G    | N7-C8-N9    | -8.28 | 108.96      | 113.10   |
| 35  | BB    | 2497 | A    | N7-C8-N9    | -8.28 | 109.66      | 113.80   |
| 1   | AA    | 832  | G    | N3-C2-N2    | 8.28  | 125.69      | 119.90   |
| 1   | AA    | 1066 | C    | C6-N1-C2    | -8.28 | 116.99      | 120.30   |
| 34  | BA    | 19   | C    | O4'-C1'-N1  | 8.28  | 114.82      | 108.20   |
| 35  | BB    | 1395 | A    | C8-N9-C4    | -8.28 | 102.49      | 105.80   |
| 35  | BB    | 578  | G    | O4'-C1'-N9  | 8.28  | 114.82      | 108.20   |
| 35  | BB    | 1155 | A    | O4'-C1'-N9  | 8.28  | 114.82      | 108.20   |
| 35  | BB    | 1269 | A    | N7-C8-N9    | -8.28 | 109.66      | 113.80   |
| 35  | BB    | 1339 | G    | O4'-C1'-N9  | 8.28  | 114.82      | 108.20   |
| 35  | BB    | 2254 | C    | C4-C5-C6    | 8.28  | 121.54      | 117.40   |
| 20  | AT    | 9    | ARG  | NE-CZ-NH2   | -8.27 | 116.16      | 120.30   |
| 35  | BB    | 314  | C    | C2-N3-C4    | 8.27  | 124.04      | 119.90   |
| 35  | BB    | 497  | A    | C5-C6-N6    | -8.27 | 117.08      | 123.70   |
| 35  | BB    | 703  | U    | C5-C4-O4    | -8.27 | 120.94      | 125.90   |
| 35  | BB    | 860  | U    | O4'-C1'-N1  | 8.27  | 114.82      | 108.20   |
| 35  | BB    | 2584 | U    | C3'-C2'-C1' | 8.27  | 108.12      | 101.50   |
| 35  | BB    | 2489 | U    | N3-C4-O4    | 8.27  | 125.19      | 119.40   |
| 35  | BB    | 2655 | G    | O4'-C1'-N9  | 8.27  | 114.82      | 108.20   |
| 9   | AI    | 118  | ARG  | NE-CZ-NH1   | 8.27  | 124.44      | 120.30   |
| 35  | BB    | 485  | C    | N3-C4-N4    | 8.27  | 123.79      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 772  | U    | O4'-C1'-N1  | 8.27  | 114.81      | 108.20   |
| 1   | AA    | 1020 | G    | C4-C5-C6    | 8.27  | 123.76      | 118.80   |
| 1   | AA    | 1250 | A    | C8-N9-C4    | -8.27 | 102.49      | 105.80   |
| 35  | BB    | 1358 | G    | N9-C4-C5    | -8.27 | 102.09      | 105.40   |
| 1   | AA    | 346  | G    | O4'-C1'-N9  | 8.27  | 114.81      | 108.20   |
| 1   | AA    | 1476 | A    | N1-C6-N6    | 8.27  | 123.56      | 118.60   |
| 35  | BB    | 510  | C    | N3-C4-N4    | 8.27  | 123.79      | 118.00   |
| 35  | BB    | 976  | G    | C8-N9-C4    | -8.27 | 103.09      | 106.40   |
| 35  | BB    | 991  | C    | N3-C2-O2    | 8.27  | 127.69      | 121.90   |
| 35  | BB    | 2666 | C    | C6-N1-C1'   | -8.27 | 110.88      | 120.80   |
| 35  | BB    | 1027 | A    | P-O3'-C3'   | 8.27  | 129.62      | 119.70   |
| 35  | BB    | 1169 | A    | O4'-C1'-N9  | 8.27  | 114.81      | 108.20   |
| 1   | AA    | 36   | C    | O4'-C1'-N1  | 8.26  | 114.81      | 108.20   |
| 34  | BA    | 49   | C    | C4-C5-C6    | -8.26 | 113.27      | 117.40   |
| 34  | BA    | 75   | G    | C2-N3-C4    | 8.26  | 116.03      | 111.90   |
| 35  | BB    | 352  | A    | N9-C4-C5    | 8.26  | 109.11      | 105.80   |
| 35  | BB    | 564  | C    | C4-C5-C6    | 8.26  | 121.53      | 117.40   |
| 35  | BB    | 2186 | G    | O4'-C1'-N9  | 8.26  | 114.81      | 108.20   |
| 35  | BB    | 1661 | G    | N1-C6-O6    | 8.26  | 124.86      | 119.90   |
| 1   | AA    | 778  | G    | C6-C5-N7    | -8.26 | 125.44      | 130.40   |
| 1   | AA    | 812  | G    | N1-C2-N3    | -8.26 | 118.94      | 123.90   |
| 1   | AA    | 980  | C    | O4'-C1'-N1  | 8.26  | 114.81      | 108.20   |
| 35  | BB    | 434  | U    | O4'-C1'-N1  | 8.26  | 114.81      | 108.20   |
| 35  | BB    | 2221 | G    | C5-C6-O6    | -8.26 | 123.64      | 128.60   |
| 1   | AA    | 1305 | G    | N9-C4-C5    | 8.26  | 108.70      | 105.40   |
| 1   | AA    | 1338 | G    | C4-C5-N7    | -8.26 | 107.50      | 110.80   |
| 35  | BB    | 117  | G    | N7-C8-N9    | 8.26  | 117.23      | 113.10   |
| 35  | BB    | 829  | A    | N9-C4-C5    | -8.26 | 102.50      | 105.80   |
| 1   | AA    | 127  | G    | C6-C5-N7    | -8.26 | 125.45      | 130.40   |
| 1   | AA    | 225  | C    | C6-N1-C2    | 8.26  | 123.60      | 120.30   |
| 1   | AA    | 521  | G    | C5-N7-C8    | -8.26 | 100.17      | 104.30   |
| 1   | AA    | 1025 | U    | P-O5'-C5'   | 8.26  | 134.11      | 120.90   |
| 35  | BB    | 947  | A    | C3'-C2'-C1' | -8.26 | 94.89       | 101.50   |
| 1   | AA    | 193  | C    | N3-C4-N4    | 8.26  | 123.78      | 118.00   |
| 1   | AA    | 893  | C    | N1-C2-O2    | 8.26  | 123.85      | 118.90   |
| 1   | AA    | 1305 | G    | C4-C5-C6    | 8.26  | 123.75      | 118.80   |
| 1   | AA    | 1346 | A    | N1-C6-N6    | 8.26  | 123.55      | 118.60   |
| 35  | BB    | 1338 | G    | C6-N1-C2    | 8.26  | 130.05      | 125.10   |
| 35  | BB    | 1750 | G    | C2-N3-C4    | 8.26  | 116.03      | 111.90   |
| 35  | BB    | 2105 | U    | O4'-C1'-N1  | 8.26  | 114.81      | 108.20   |
| 35  | BB    | 2527 | C    | N3-C4-C5    | -8.26 | 118.60      | 121.90   |
| 35  | BB    | 2083 | G    | C2-N3-C4    | 8.25  | 116.03      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 173  | U    | N3-C2-O2   | 8.25  | 127.98      | 122.20   |
| 1   | AA    | 415  | A    | P-O3'-C3'  | 8.25  | 129.60      | 119.70   |
| 1   | AA    | 610  | U    | O4'-C1'-N1 | 8.25  | 114.80      | 108.20   |
| 35  | BB    | 1508 | A    | C2-N3-C4   | -8.25 | 106.47      | 110.60   |
| 34  | BA    | 23   | G    | C4-C5-N7   | 8.25  | 114.10      | 110.80   |
| 35  | BB    | 1906 | G    | C4-C5-N7   | 8.25  | 114.10      | 110.80   |
| 1   | AA    | 149  | A    | N3-C4-C5   | -8.25 | 121.03      | 126.80   |
| 35  | BB    | 1916 | A    | C5-C6-N6   | -8.25 | 117.10      | 123.70   |
| 1   | AA    | 1293 | C    | O4'-C1'-N1 | 8.25  | 114.80      | 108.20   |
| 35  | BB    | 2283 | C    | P-O5'-C5'  | 8.25  | 134.10      | 120.90   |
| 1   | AA    | 325  | A    | C4-C5-C6   | 8.25  | 121.12      | 117.00   |
| 35  | BB    | 888  | C    | O4'-C1'-N1 | 8.25  | 114.80      | 108.20   |
| 1   | AA    | 115  | G    | C4-C5-C6   | 8.25  | 123.75      | 118.80   |
| 1   | AA    | 370  | C    | O4'-C1'-N1 | 8.25  | 114.80      | 108.20   |
| 35  | BB    | 1598 | A    | C4-C5-C6   | 8.25  | 121.12      | 117.00   |
| 1   | AA    | 101  | A    | C5-C6-N6   | -8.24 | 117.11      | 123.70   |
| 1   | AA    | 427  | U    | N1-C2-N3   | -8.24 | 109.95      | 114.90   |
| 1   | AA    | 998  | C    | C5-C4-N4   | -8.24 | 114.43      | 120.20   |
| 35  | BB    | 881  | G    | C6-N1-C2   | 8.24  | 130.05      | 125.10   |
| 35  | BB    | 2067 | G    | C5-C6-N1   | -8.24 | 107.38      | 111.50   |
| 1   | AA    | 1137 | C    | C5-C6-N1   | 8.24  | 125.12      | 121.00   |
| 35  | BB    | 983  | A    | N1-C2-N3   | -8.24 | 125.18      | 129.30   |
| 35  | BB    | 1362 | C    | O4'-C1'-N1 | 8.24  | 114.80      | 108.20   |
| 35  | BB    | 1433 | A    | C4-C5-C6   | 8.24  | 121.12      | 117.00   |
| 35  | BB    | 1651 | G    | N7-C8-N9   | -8.24 | 108.98      | 113.10   |
| 35  | BB    | 2101 | A    | C6-N1-C2   | 8.24  | 123.55      | 118.60   |
| 35  | BB    | 2531 | A    | C5-C6-N6   | -8.24 | 117.10      | 123.70   |
| 1   | AA    | 1410 | A    | C5-C6-N6   | -8.24 | 117.11      | 123.70   |
| 35  | BB    | 49   | A    | C4-C5-C6   | 8.24  | 121.12      | 117.00   |
| 35  | BB    | 2406 | A    | C4-C5-C6   | 8.24  | 121.12      | 117.00   |
| 1   | AA    | 60   | A    | N7-C8-N9   | 8.24  | 117.92      | 113.80   |
| 1   | AA    | 76   | G    | N1-C6-O6   | 8.24  | 124.84      | 119.90   |
| 1   | AA    | 559  | A    | C8-N9-C4   | -8.24 | 102.50      | 105.80   |
| 35  | BB    | 1241 | A    | O4'-C1'-N9 | 8.24  | 114.79      | 108.20   |
| 35  | BB    | 2417 | C    | N3-C4-C5   | -8.24 | 118.60      | 121.90   |
| 35  | BB    | 1229 | C    | C5-C6-N1   | 8.24  | 125.12      | 121.00   |
| 1   | AA    | 78   | A    | C4-C5-C6   | 8.24  | 121.12      | 117.00   |
| 1   | AA    | 486  | U    | C2-N3-C4   | -8.24 | 122.06      | 127.00   |
| 1   | AA    | 1278 | G    | OP1-P-OP2  | -8.24 | 107.25      | 119.60   |
| 1   | AA    | 1477 | U    | O4'-C1'-N1 | 8.24  | 114.79      | 108.20   |
| 1   | AA    | 1509 | C    | C6-N1-C2   | -8.24 | 117.00      | 120.30   |
| 35  | BB    | 344  | A    | O4'-C1'-N9 | 8.24  | 114.79      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 795  | C    | C5-C4-N4   | -8.24 | 114.43      | 120.20   |
| 35  | BB    | 388  | G    | C5-C6-O6   | -8.23 | 123.66      | 128.60   |
| 35  | BB    | 1114 | C    | C5-C6-N1   | -8.23 | 116.88      | 121.00   |
| 35  | BB    | 2346 | A    | C4-C5-C6   | 8.23  | 121.12      | 117.00   |
| 35  | BB    | 2419 | U    | O4'-C1'-N1 | 8.23  | 114.79      | 108.20   |
| 35  | BB    | 2356 | U    | O4'-C1'-N1 | 8.23  | 114.79      | 108.20   |
| 35  | BB    | 2871 | U    | O4'-C1'-N1 | 8.23  | 114.79      | 108.20   |
| 55  | BW    | 19   | ARG  | NE-CZ-NH1  | 8.23  | 124.42      | 120.30   |
| 34  | BA    | 20   | G    | N1-C6-O6   | 8.23  | 124.84      | 119.90   |
| 35  | BB    | 1317 | G    | O4'-C1'-N9 | 8.23  | 114.78      | 108.20   |
| 35  | BB    | 2677 | G    | N7-C8-N9   | -8.23 | 108.98      | 113.10   |
| 52  | BS    | 22   | ASP  | CB-CG-OD2  | -8.23 | 110.89      | 118.30   |
| 1   | AA    | 893  | C    | O4'-C1'-N1 | 8.23  | 114.78      | 108.20   |
| 35  | BB    | 128  | C    | O4'-C1'-N1 | 8.23  | 114.78      | 108.20   |
| 35  | BB    | 800  | A    | C4-C5-C6   | 8.23  | 121.11      | 117.00   |
| 35  | BB    | 1979 | U    | O4'-C1'-N1 | 8.23  | 114.78      | 108.20   |
| 1   | AA    | 399  | G    | N1-C6-O6   | 8.23  | 124.83      | 119.90   |
| 1   | AA    | 833  | G    | O4'-C1'-N9 | 8.23  | 114.78      | 108.20   |
| 34  | BA    | 93   | C    | N3-C4-C5   | -8.23 | 118.61      | 121.90   |
| 35  | BB    | 1337 | G    | N1-C2-N3   | -8.23 | 118.96      | 123.90   |
| 35  | BB    | 2061 | G    | C4-N9-C1'  | 8.23  | 137.19      | 126.50   |
| 35  | BB    | 917  | A    | N1-C6-N6   | 8.22  | 123.53      | 118.60   |
| 35  | BB    | 2266 | A    | C5-C6-N1   | -8.22 | 113.59      | 117.70   |
| 35  | BB    | 2471 | A    | C5-C6-N6   | -8.22 | 117.12      | 123.70   |
| 48  | BO    | 30   | ARG  | NE-CZ-NH2  | -8.22 | 116.19      | 120.30   |
| 1   | AA    | 189  | A    | C5-N7-C8   | 8.22  | 108.01      | 103.90   |
| 1   | AA    | 966  | G    | N1-C6-O6   | 8.22  | 124.83      | 119.90   |
| 35  | BB    | 295  | G    | C4-C5-N7   | 8.22  | 114.09      | 110.80   |
| 35  | BB    | 1018 | U    | C2-N3-C4   | -8.22 | 122.07      | 127.00   |
| 35  | BB    | 1913 | A    | C4-C5-N7   | -8.22 | 106.59      | 110.70   |
| 35  | BB    | 474  | G    | C5-C6-O6   | -8.22 | 123.67      | 128.60   |
| 35  | BB    | 1438 | U    | N3-C4-C5   | -8.22 | 109.67      | 114.60   |
| 35  | BB    | 2151 | U    | C2-N3-C4   | -8.22 | 122.07      | 127.00   |
| 35  | BB    | 2512 | C    | C6-N1-C2   | 8.22  | 123.59      | 120.30   |
| 1   | AA    | 713  | G    | C6-C5-N7   | -8.22 | 125.47      | 130.40   |
| 1   | AA    | 767  | A    | C4-C5-C6   | 8.22  | 121.11      | 117.00   |
| 1   | AA    | 831  | A    | N1-C6-N6   | 8.22  | 123.53      | 118.60   |
| 1   | AA    | 1242 | G    | C5-C6-N1   | -8.22 | 107.39      | 111.50   |
| 1   | AA    | 1383 | C    | C6-N1-C2   | -8.22 | 117.01      | 120.30   |
| 22  | AV    | 53   | G    | C5-C6-O6   | -8.22 | 123.67      | 128.60   |
| 34  | BA    | 31   | C    | N3-C4-C5   | -8.22 | 118.61      | 121.90   |
| 34  | BA    | 100  | G    | C5-C6-O6   | -8.22 | 123.67      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 259  | G    | N1-C6-O6    | 8.22  | 124.83      | 119.90   |
| 35  | BB    | 500  | G    | N3-C2-N2    | 8.22  | 125.65      | 119.90   |
| 35  | BB    | 2025 | C    | C5-C6-N1    | 8.22  | 125.11      | 121.00   |
| 35  | BB    | 634  | C    | O4'-C1'-N1  | 8.22  | 114.77      | 108.20   |
| 35  | BB    | 1194 | A    | C4-C5-C6    | 8.22  | 121.11      | 117.00   |
| 35  | BB    | 1756 | G    | N3-C2-N2    | 8.22  | 125.65      | 119.90   |
| 35  | BB    | 2088 | A    | C5-C6-N6    | -8.22 | 117.13      | 123.70   |
| 49  | BP    | 19   | PHE  | CB-CG-CD1   | -8.22 | 115.05      | 120.80   |
| 52  | BS    | 61   | ASN  | N-CA-CB     | 8.22  | 125.39      | 110.60   |
| 1   | AA    | 998  | C    | N3-C4-C5    | 8.22  | 125.19      | 121.90   |
| 1   | AA    | 1238 | A    | C2-N3-C4    | 8.22  | 114.71      | 110.60   |
| 35  | BB    | 595  | C    | N3-C4-C5    | -8.22 | 118.61      | 121.90   |
| 1   | AA    | 247  | G    | C5-C6-O6    | -8.21 | 123.67      | 128.60   |
| 1   | AA    | 724  | G    | C5-C6-O6    | -8.21 | 123.67      | 128.60   |
| 35  | BB    | 96   | C    | N3-C4-N4    | 8.21  | 123.75      | 118.00   |
| 35  | BB    | 722  | A    | C5-C6-N1    | -8.21 | 113.59      | 117.70   |
| 35  | BB    | 1569 | A    | C8-N9-C4    | -8.21 | 102.51      | 105.80   |
| 35  | BB    | 1743 | G    | N1-C2-N3    | -8.22 | 118.97      | 123.90   |
| 35  | BB    | 1873 | G    | C5-N7-C8    | 8.22  | 108.41      | 104.30   |
| 1   | AA    | 330  | C    | C4-C5-C6    | 8.21  | 121.50      | 117.40   |
| 1   | AA    | 1295 | U    | C1'-O4'-C4' | 8.21  | 116.47      | 109.90   |
| 1   | AA    | 1237 | C    | O4'-C1'-N1  | 8.21  | 114.77      | 108.20   |
| 34  | BA    | 34   | A    | C5-C6-N6    | -8.21 | 117.13      | 123.70   |
| 34  | BA    | 87   | U    | C6-N1-C2    | 8.21  | 125.93      | 121.00   |
| 35  | BB    | 734  | A    | C4-C5-C6    | 8.21  | 121.11      | 117.00   |
| 35  | BB    | 1342 | A    | C4-C5-C6    | 8.21  | 121.11      | 117.00   |
| 35  | BB    | 2730 | C    | C5-C4-N4    | -8.21 | 114.45      | 120.20   |
| 35  | BB    | 2772 | C    | N3-C4-N4    | 8.21  | 123.75      | 118.00   |
| 1   | AA    | 510  | A    | C8-N9-C4    | -8.21 | 102.52      | 105.80   |
| 34  | BA    | 97   | C    | C3'-C2'-C1' | -8.21 | 94.93       | 101.50   |
| 35  | BB    | 136  | G    | C6-C5-N7    | -8.21 | 125.47      | 130.40   |
| 35  | BB    | 1945 | G    | N1-C6-O6    | 8.21  | 124.83      | 119.90   |
| 35  | BB    | 463  | G    | N1-C6-O6    | 8.21  | 124.82      | 119.90   |
| 35  | BB    | 2089 | C    | C4-C5-C6    | 8.21  | 121.50      | 117.40   |
| 35  | BB    | 2796 | U    | C5-C4-O4    | -8.21 | 120.98      | 125.90   |
| 1   | AA    | 67   | C    | N3-C4-C5    | -8.21 | 118.62      | 121.90   |
| 1   | AA    | 774  | G    | P-O3'-C3'   | -8.21 | 109.85      | 119.70   |
| 1   | AA    | 844  | G    | N3-C4-C5    | -8.20 | 124.50      | 128.60   |
| 1   | AA    | 1055 | A    | N7-C8-N9    | 8.21  | 117.90      | 113.80   |
| 1   | AA    | 1339 | A    | N1-C6-N6    | 8.20  | 123.52      | 118.60   |
| 35  | BB    | 96   | C    | N1-C2-N3    | -8.21 | 113.46      | 119.20   |
| 35  | BB    | 244  | A    | N1-C2-N3    | 8.21  | 133.40      | 129.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 761  | A    | C5-C6-N1   | -8.20 | 113.60      | 117.70   |
| 35  | BB    | 1434 | A    | O4'-C1'-N9 | 8.20  | 114.76      | 108.20   |
| 35  | BB    | 1480 | C    | N3-C4-N4   | 8.20  | 123.74      | 118.00   |
| 35  | BB    | 1858 | A    | C5-N7-C8   | 8.20  | 108.00      | 103.90   |
| 1   | AA    | 155  | A    | N7-C8-N9   | 8.20  | 117.90      | 113.80   |
| 35  | BB    | 1884 | G    | N1-C6-O6   | 8.20  | 124.82      | 119.90   |
| 1   | AA    | 197  | A    | C5-C6-N6   | -8.20 | 117.14      | 123.70   |
| 34  | BA    | 62   | C    | N3-C4-N4   | 8.20  | 123.74      | 118.00   |
| 35  | BB    | 76   | C    | C6-N1-C2   | -8.20 | 117.02      | 120.30   |
| 35  | BB    | 467  | G    | O4'-C1'-N9 | 8.20  | 114.76      | 108.20   |
| 35  | BB    | 836  | G    | N1-C6-O6   | 8.20  | 124.82      | 119.90   |
| 35  | BB    | 1543 | G    | C5-C6-N1   | -8.20 | 107.40      | 111.50   |
| 35  | BB    | 1949 | G    | C5-N7-C8   | 8.20  | 108.40      | 104.30   |
| 35  | BB    | 2240 | U    | O4'-C1'-N1 | 8.20  | 114.76      | 108.20   |
| 1   | AA    | 1470 | U    | N3-C4-O4   | 8.20  | 125.14      | 119.40   |
| 29  | B4    | 20   | TYR  | CB-CG-CD2  | 8.20  | 125.92      | 121.00   |
| 1   | AA    | 164  | G    | N7-C8-N9   | 8.20  | 117.20      | 113.10   |
| 1   | AA    | 877  | G    | N3-C4-C5   | 8.20  | 132.70      | 128.60   |
| 1   | AA    | 1240 | U    | P-O5'-C5'  | -8.20 | 107.78      | 120.90   |
| 1   | AA    | 1251 | A    | C4-C5-C6   | 8.20  | 121.10      | 117.00   |
| 34  | BA    | 45   | A    | N7-C8-N9   | -8.20 | 109.70      | 113.80   |
| 35  | BB    | 122  | G    | C6-C5-N7   | -8.20 | 125.48      | 130.40   |
| 35  | BB    | 2216 | G    | C5-C6-O6   | -8.20 | 123.68      | 128.60   |
| 35  | BB    | 69   | C    | C6-N1-C2   | -8.20 | 117.02      | 120.30   |
| 35  | BB    | 490  | C    | O4'-C1'-N1 | 8.20  | 114.76      | 108.20   |
| 35  | BB    | 1999 | C    | C6-N1-C2   | 8.20  | 123.58      | 120.30   |
| 35  | BB    | 2620 | C    | C2-N3-C4   | 8.20  | 124.00      | 119.90   |
| 1   | AA    | 98   | A    | C5-C6-N6   | -8.20 | 117.14      | 123.70   |
| 1   | AA    | 428  | G    | N9-C4-C5   | -8.20 | 102.12      | 105.40   |
| 1   | AA    | 1179 | A    | C5-N7-C8   | 8.20  | 108.00      | 103.90   |
| 35  | BB    | 777  | G    | C5-C6-O6   | -8.20 | 123.68      | 128.60   |
| 1   | AA    | 141  | G    | C6-C5-N7   | -8.20 | 125.48      | 130.40   |
| 1   | AA    | 366  | A    | C4-C5-N7   | -8.19 | 106.60      | 110.70   |
| 1   | AA    | 953  | G    | C6-C5-N7   | -8.20 | 125.48      | 130.40   |
| 3   | AC    | 87   | ARG  | NE-CZ-NH1  | -8.19 | 116.20      | 120.30   |
| 10  | AJ    | 62   | ARG  | NE-CZ-NH2  | 8.20  | 124.40      | 120.30   |
| 35  | BB    | 681  | G    | N1-C6-O6   | 8.20  | 124.82      | 119.90   |
| 35  | BB    | 764  | A    | N9-C4-C5   | 8.20  | 109.08      | 105.80   |
| 34  | BA    | 56   | G    | N9-C4-C5   | 8.19  | 108.68      | 105.40   |
| 35  | BB    | 173  | A    | C5-N7-C8   | 8.19  | 108.00      | 103.90   |
| 35  | BB    | 339  | U    | N3-C4-C5   | -8.19 | 109.68      | 114.60   |
| 35  | BB    | 1689 | A    | C5-C6-N1   | -8.20 | 113.60      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 2021 | C    | N3-C4-C5   | -8.19 | 118.62      | 121.90   |
| 35  | BB    | 2092 | U    | O4'-C1'-N1 | 8.20  | 114.76      | 108.20   |
| 35  | BB    | 2626 | C    | C5-C6-N1   | 8.19  | 125.10      | 121.00   |
| 35  | BB    | 2775 | G    | N3-C2-N2   | 8.20  | 125.64      | 119.90   |
| 35  | BB    | 2856 | A    | N1-C6-N6   | 8.19  | 123.52      | 118.60   |
| 1   | AA    | 830  | G    | N1-C6-O6   | 8.19  | 124.82      | 119.90   |
| 35  | BB    | 1861 | G    | C5-C6-O6   | -8.19 | 123.68      | 128.60   |
| 1   | AA    | 318  | G    | O4'-C1'-N9 | 8.19  | 114.75      | 108.20   |
| 35  | BB    | 1157 | G    | C6-C5-N7   | -8.19 | 125.48      | 130.40   |
| 35  | BB    | 2407 | A    | N9-C4-C5   | 8.19  | 109.08      | 105.80   |
| 40  | BG    | 54   | ARG  | NE-CZ-NH2  | -8.19 | 116.20      | 120.30   |
| 1   | AA    | 666  | G    | N1-C2-N3   | -8.19 | 118.99      | 123.90   |
| 1   | AA    | 857  | C    | C4-C5-C6   | 8.19  | 121.49      | 117.40   |
| 1   | AA    | 1303 | C    | C4-C5-C6   | 8.19  | 121.50      | 117.40   |
| 35  | BB    | 557  | C    | O4'-C1'-N1 | 8.19  | 114.75      | 108.20   |
| 1   | AA    | 1338 | G    | C5-C6-O6   | -8.19 | 123.69      | 128.60   |
| 35  | BB    | 289  | G    | N1-C6-O6   | 8.19  | 124.81      | 119.90   |
| 35  | BB    | 315  | G    | C4-C5-N7   | -8.19 | 107.53      | 110.80   |
| 35  | BB    | 700  | G    | C2-N3-C4   | 8.19  | 115.99      | 111.90   |
| 35  | BB    | 2797 | U    | C2-N1-C1'  | 8.19  | 127.53      | 117.70   |
| 34  | BA    | 108  | A    | N1-C6-N6   | 8.19  | 123.51      | 118.60   |
| 1   | AA    | 1142 | G    | O4'-C1'-N9 | 8.19  | 114.75      | 108.20   |
| 35  | BB    | 1514 | G    | N3-C4-C5   | -8.19 | 124.51      | 128.60   |
| 35  | BB    | 2043 | C    | C4-C5-C6   | 8.19  | 121.49      | 117.40   |
| 35  | BB    | 2640 | G    | O4'-C1'-N9 | 8.19  | 114.75      | 108.20   |
| 35  | BB    | 2147 | A    | P-O3'-C3'  | 8.19  | 129.52      | 119.70   |
| 35  | BB    | 2798 | U    | C6-N1-C2   | -8.19 | 116.09      | 121.00   |
| 1   | AA    | 754  | C    | C6-N1-C1'  | -8.18 | 110.98      | 120.80   |
| 1   | AA    | 1146 | A    | N1-C6-N6   | 8.18  | 123.51      | 118.60   |
| 1   | AA    | 1416 | G    | C5-C6-N1   | -8.18 | 107.41      | 111.50   |
| 22  | AV    | 49   | G    | N1-C6-O6   | 8.18  | 124.81      | 119.90   |
| 35  | BB    | 751  | A    | C5-N7-C8   | 8.18  | 107.99      | 103.90   |
| 35  | BB    | 1218 | G    | N3-C2-N2   | 8.18  | 125.63      | 119.90   |
| 35  | BB    | 1343 | G    | N1-C6-O6   | 8.18  | 124.81      | 119.90   |
| 35  | BB    | 2450 | A    | C5-C6-N6   | -8.18 | 117.15      | 123.70   |
| 35  | BB    | 2657 | A    | N1-C6-N6   | 8.18  | 123.51      | 118.60   |
| 1   | AA    | 514  | C    | N3-C4-C5   | -8.18 | 118.63      | 121.90   |
| 1   | AA    | 422  | C    | N3-C4-N4   | 8.18  | 123.72      | 118.00   |
| 1   | AA    | 974  | A    | C6-C5-N7   | -8.18 | 126.58      | 132.30   |
| 1   | AA    | 1526 | G    | C4-C5-C6   | 8.18  | 123.71      | 118.80   |
| 35  | BB    | 191  | A    | C5-C6-N1   | -8.18 | 113.61      | 117.70   |
| 35  | BB    | 930  | G    | N1-C6-O6   | 8.18  | 124.81      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1085 | A    | C5-C6-N6    | -8.18 | 117.16      | 123.70   |
| 35  | BB    | 2411 | A    | N9-C4-C5    | 8.18  | 109.07      | 105.80   |
| 1   | AA    | 929  | G    | C4-C5-N7    | -8.18 | 107.53      | 110.80   |
| 1   | AA    | 950  | U    | C4-C5-C6    | -8.18 | 114.79      | 119.70   |
| 8   | AH    | 44   | PHE  | CB-CG-CD2   | 8.18  | 126.52      | 120.80   |
| 35  | BB    | 151  | C    | C2-N3-C4    | 8.18  | 123.99      | 119.90   |
| 35  | BB    | 334  | C    | C4'-C3'-C2' | -8.18 | 94.42       | 102.60   |
| 35  | BB    | 1014 | A    | N9-C4-C5    | 8.18  | 109.07      | 105.80   |
| 35  | BB    | 1361 | G    | C8-N9-C4    | -8.18 | 103.13      | 106.40   |
| 35  | BB    | 1770 | G    | C6-C5-N7    | -8.18 | 125.50      | 130.40   |
| 35  | BB    | 2841 | C    | O4'-C1'-N1  | 8.18  | 114.74      | 108.20   |
| 35  | BB    | 2872 | A    | C5-C6-N6    | -8.18 | 117.16      | 123.70   |
| 35  | BB    | 1881 | C    | N3-C4-C5    | -8.17 | 118.63      | 121.90   |
| 1   | AA    | 139  | A    | C4-C5-C6    | 8.17  | 121.09      | 117.00   |
| 1   | AA    | 681  | A    | N1-C6-N6    | 8.17  | 123.50      | 118.60   |
| 1   | AA    | 793  | U    | C5-C4-O4    | -8.17 | 121.00      | 125.90   |
| 35  | BB    | 514  | A    | C5-C6-N1    | -8.17 | 113.61      | 117.70   |
| 35  | BB    | 578  | G    | C5-N7-C8    | -8.17 | 100.21      | 104.30   |
| 35  | BB    | 683  | U    | C6-N1-C2    | -8.17 | 116.10      | 121.00   |
| 35  | BB    | 884  | U    | N3-C4-O4    | 8.17  | 125.12      | 119.40   |
| 35  | BB    | 1231 | U    | C6-N1-C2    | -8.17 | 116.10      | 121.00   |
| 35  | BB    | 1253 | A    | O4'-C1'-N9  | 8.17  | 114.74      | 108.20   |
| 35  | BB    | 2620 | C    | N3-C4-C5    | -8.17 | 118.63      | 121.90   |
| 35  | BB    | 1311 | G    | C5-C6-O6    | -8.17 | 123.70      | 128.60   |
| 35  | BB    | 1965 | C    | N3-C4-C5    | -8.17 | 118.63      | 121.90   |
| 35  | BB    | 2193 | G    | C5-C6-O6    | -8.17 | 123.70      | 128.60   |
| 35  | BB    | 2301 | C    | C6-N1-C2    | 8.17  | 123.57      | 120.30   |
| 35  | BB    | 2330 | G    | C3'-C2'-C1' | -8.17 | 94.96       | 101.50   |
| 35  | BB    | 2570 | G    | O4'-C1'-N9  | 8.17  | 114.74      | 108.20   |
| 1   | AA    | 1119 | C    | O4'-C1'-N1  | 8.17  | 114.74      | 108.20   |
| 35  | BB    | 274  | C    | O4'-C1'-N1  | 8.17  | 114.74      | 108.20   |
| 35  | BB    | 1038 | G    | N3-C2-N2    | 8.17  | 125.62      | 119.90   |
| 1   | AA    | 621  | A    | C8-N9-C4    | -8.17 | 102.53      | 105.80   |
| 1   | AA    | 742  | G    | N1-C6-O6    | 8.17  | 124.80      | 119.90   |
| 1   | AA    | 1194 | U    | C4-C5-C6    | -8.17 | 114.80      | 119.70   |
| 35  | BB    | 1139 | G    | O4'-C1'-N9  | 8.17  | 114.74      | 108.20   |
| 35  | BB    | 1393 | A    | C4'-C3'-C2' | -8.17 | 94.43       | 102.60   |
| 35  | BB    | 1574 | C    | O4'-C1'-N1  | 8.17  | 114.74      | 108.20   |
| 35  | BB    | 1743 | G    | C4-C5-N7    | 8.17  | 114.07      | 110.80   |
| 35  | BB    | 2423 | U    | C3'-C2'-C1' | -8.17 | 94.96       | 101.50   |
| 35  | BB    | 2829 | A    | C6-C5-N7    | -8.17 | 126.58      | 132.30   |
| 1   | AA    | 522  | C    | N3-C4-C5    | -8.17 | 118.63      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 845  | A    | C2-N3-C4    | 8.17  | 114.68      | 110.60   |
| 1   | AA    | 1196 | A    | C6-C5-N7    | -8.17 | 126.58      | 132.30   |
| 1   | AA    | 1243 | C    | N3-C4-C5    | -8.17 | 118.63      | 121.90   |
| 34  | BA    | 94   | A    | O4'-C1'-N9  | 8.17  | 114.73      | 108.20   |
| 34  | BA    | 116  | G    | O4'-C1'-N9  | 8.17  | 114.73      | 108.20   |
| 35  | BB    | 85   | G    | C4-C5-N7    | -8.17 | 107.53      | 110.80   |
| 35  | BB    | 527  | C    | C2-N1-C1'   | 8.17  | 127.78      | 118.80   |
| 35  | BB    | 1102 | C    | C2-N3-C4    | 8.17  | 123.98      | 119.90   |
| 35  | BB    | 1137 | G    | C5-C6-O6    | -8.17 | 123.70      | 128.60   |
| 35  | BB    | 1387 | A    | N9-C4-C5    | 8.17  | 109.07      | 105.80   |
| 35  | BB    | 1580 | A    | N1-C6-N6    | 8.17  | 123.50      | 118.60   |
| 35  | BB    | 1813 | G    | C5-C6-O6    | -8.17 | 123.70      | 128.60   |
| 35  | BB    | 1845 | G    | N1-C6-O6    | 8.17  | 124.80      | 119.90   |
| 35  | BB    | 1918 | A    | N9-C4-C5    | 8.17  | 109.07      | 105.80   |
| 35  | BB    | 2531 | A    | O4'-C1'-N9  | 8.17  | 114.73      | 108.20   |
| 1   | AA    | 339  | C    | C4-C5-C6    | 8.16  | 121.48      | 117.40   |
| 1   | AA    | 1350 | A    | N1-C2-N3    | 8.16  | 133.38      | 129.30   |
| 35  | BB    | 15   | G    | C5-C6-O6    | -8.16 | 123.70      | 128.60   |
| 35  | BB    | 941  | A    | C5-N7-C8    | 8.16  | 107.98      | 103.90   |
| 35  | BB    | 1737 | G    | P-O3'-C3'   | 8.16  | 129.50      | 119.70   |
| 35  | BB    | 701  | G    | C5-C6-N1    | -8.16 | 107.42      | 111.50   |
| 35  | BB    | 761  | A    | C2-N3-C4    | -8.16 | 106.52      | 110.60   |
| 35  | BB    | 1016 | G    | O4'-C1'-N9  | 8.16  | 114.73      | 108.20   |
| 35  | BB    | 1788 | C    | C5-C4-N4    | -8.16 | 114.49      | 120.20   |
| 35  | BB    | 1822 | C    | N3-C4-C5    | -8.16 | 118.64      | 121.90   |
| 35  | BB    | 2164 | C    | O4'-C1'-N1  | 8.16  | 114.73      | 108.20   |
| 41  | BH    | 27   | ARG  | NE-CZ-NH2   | -8.16 | 116.22      | 120.30   |
| 35  | BB    | 175  | G    | N1-C2-N2    | -8.16 | 108.86      | 116.20   |
| 35  | BB    | 361  | G    | C6-N1-C2    | -8.16 | 120.20      | 125.10   |
| 35  | BB    | 2648 | G    | N3-C4-N9    | 8.16  | 130.90      | 126.00   |
| 1   | AA    | 320  | A    | C5-C6-N1    | -8.16 | 113.62      | 117.70   |
| 1   | AA    | 419  | C    | N1-C2-O2    | -8.16 | 114.00      | 118.90   |
| 1   | AA    | 1316 | G    | N3-C2-N2    | 8.16  | 125.61      | 119.90   |
| 35  | BB    | 380  | G    | C5-C6-N1    | -8.16 | 107.42      | 111.50   |
| 35  | BB    | 973  | A    | C5'-C4'-O4' | 8.16  | 118.89      | 109.10   |
| 35  | BB    | 2251 | G    | N3-C4-C5    | 8.16  | 132.68      | 128.60   |
| 35  | BB    | 1114 | C    | N3-C4-C5    | -8.16 | 118.64      | 121.90   |
| 35  | BB    | 1477 | A    | N1-C6-N6    | 8.16  | 123.50      | 118.60   |
| 35  | BB    | 1674 | G    | N3-C2-N2    | 8.16  | 125.61      | 119.90   |
| 35  | BB    | 270  | A    | O4'-C1'-N9  | 8.16  | 114.73      | 108.20   |
| 1   | AA    | 402  | G    | C5-C6-O6    | -8.16 | 123.71      | 128.60   |
| 1   | AA    | 1274 | A    | N3-C4-C5    | -8.16 | 121.09      | 126.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1303 | C    | O4'-C1'-N1  | 8.16  | 114.72      | 108.20   |
| 35  | BB    | 1120 | G    | C2-N3-C4    | -8.16 | 107.82      | 111.90   |
| 35  | BB    | 847  | U    | O4'-C1'-N1  | 8.15  | 114.72      | 108.20   |
| 35  | BB    | 2900 | A    | C5-N7-C8    | -8.15 | 99.82       | 103.90   |
| 1   | AA    | 53   | A    | O4'-C1'-N9  | 8.15  | 114.72      | 108.20   |
| 1   | AA    | 444  | G    | C4-C5-C6    | 8.15  | 123.69      | 118.80   |
| 1   | AA    | 763  | G    | C8-N9-C4    | -8.15 | 103.14      | 106.40   |
| 1   | AA    | 952  | U    | C5-C6-N1    | 8.15  | 126.78      | 122.70   |
| 35  | BB    | 1779 | U    | C6-N1-C2    | -8.15 | 116.11      | 121.00   |
| 35  | BB    | 2484 | G    | O4'-C1'-N9  | 8.15  | 114.72      | 108.20   |
| 1   | AA    | 1009 | U    | O4'-C1'-N1  | 8.15  | 114.72      | 108.20   |
| 35  | BB    | 36   | G    | C8-N9-C4    | -8.15 | 103.14      | 106.40   |
| 35  | BB    | 95   | A    | C5'-C4'-O4' | 8.15  | 118.88      | 109.10   |
| 35  | BB    | 2503 | A    | C4-C5-N7    | -8.15 | 106.62      | 110.70   |
| 1   | AA    | 79   | G    | N3-C2-N2    | 8.15  | 125.61      | 119.90   |
| 1   | AA    | 491  | G    | N3-C4-C5    | -8.15 | 124.52      | 128.60   |
| 1   | AA    | 1197 | A    | N1-C6-N6    | 8.15  | 123.49      | 118.60   |
| 1   | AA    | 1342 | C    | O4'-C1'-N1  | 8.15  | 114.72      | 108.20   |
| 35  | BB    | 733  | G    | N3-C2-N2    | 8.15  | 125.61      | 119.90   |
| 35  | BB    | 2348 | U    | C1'-O4'-C4' | -8.15 | 103.38      | 109.90   |
| 35  | BB    | 2444 | G    | C5-C6-O6    | -8.15 | 123.71      | 128.60   |
| 1   | AA    | 293  | G    | C4-C5-C6    | 8.15  | 123.69      | 118.80   |
| 1   | AA    | 725  | G    | N7-C8-N9    | -8.15 | 109.03      | 113.10   |
| 35  | BB    | 1004 | U    | N3-C4-O4    | 8.15  | 125.11      | 119.40   |
| 35  | BB    | 1428 | C    | O4'-C1'-N1  | 8.15  | 114.72      | 108.20   |
| 1   | AA    | 377  | G    | C2-N3-C4    | -8.15 | 107.83      | 111.90   |
| 35  | BB    | 1526 | C    | C5-C6-N1    | 8.15  | 125.07      | 121.00   |
| 35  | BB    | 1824 | G    | O4'-C1'-N9  | 8.15  | 114.72      | 108.20   |
| 1   | AA    | 757  | U    | C2-N3-C4    | -8.15 | 122.11      | 127.00   |
| 1   | AA    | 948  | C    | C4-C5-C6    | 8.15  | 121.47      | 117.40   |
| 35  | BB    | 180  | G    | C5-C6-O6    | -8.15 | 123.71      | 128.60   |
| 35  | BB    | 791  | C    | O4'-C1'-N1  | 8.15  | 114.72      | 108.20   |
| 35  | BB    | 998  | C    | O4'-C1'-N1  | 8.15  | 114.72      | 108.20   |
| 35  | BB    | 1485 | U    | N3-C4-O4    | 8.15  | 125.10      | 119.40   |
| 35  | BB    | 1206 | G    | C5-C6-N1    | -8.15 | 107.43      | 111.50   |
| 35  | BB    | 2671 | G    | O4'-C1'-N9  | 8.15  | 114.72      | 108.20   |
| 35  | BB    | 2868 | A    | C5-C6-N1    | -8.15 | 113.63      | 117.70   |
| 1   | AA    | 81   | A    | N1-C6-N6    | 8.14  | 123.49      | 118.60   |
| 35  | BB    | 1222 | U    | N3-C2-O2    | 8.14  | 127.90      | 122.20   |
| 1   | AA    | 439  | U    | C2-N3-C4    | 8.14  | 131.89      | 127.00   |
| 1   | AA    | 588  | G    | C5-C6-O6    | -8.14 | 123.71      | 128.60   |
| 35  | BB    | 896  | A    | O4'-C1'-N9  | 8.14  | 114.72      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1517 | G    | C5-C6-O6   | 8.14  | 133.49      | 128.60   |
| 35  | BB    | 1556 | C    | N3-C4-N4   | 8.14  | 123.70      | 118.00   |
| 35  | BB    | 2144 | G    | C5-C6-O6   | -8.14 | 123.71      | 128.60   |
| 35  | BB    | 2735 | G    | C2-N3-C4   | -8.14 | 107.83      | 111.90   |
| 1   | AA    | 495  | A    | C6-C5-N7   | -8.14 | 126.60      | 132.30   |
| 1   | AA    | 713  | G    | C4-C5-N7   | 8.14  | 114.06      | 110.80   |
| 35  | BB    | 1284 | A    | C5-N7-C8   | 8.14  | 107.97      | 103.90   |
| 1   | AA    | 894  | G    | C5-C6-O6   | -8.14 | 123.72      | 128.60   |
| 35  | BB    | 83   | A    | N1-C6-N6   | 8.14  | 123.48      | 118.60   |
| 35  | BB    | 1314 | C    | C5-C4-N4   | -8.14 | 114.50      | 120.20   |
| 35  | BB    | 1403 | A    | C5-N7-C8   | 8.14  | 107.97      | 103.90   |
| 35  | BB    | 1999 | C    | N3-C4-N4   | 8.14  | 123.70      | 118.00   |
| 1   | AA    | 371  | A    | C5-C6-N1   | -8.14 | 113.63      | 117.70   |
| 1   | AA    | 515  | G    | N1-C6-O6   | 8.14  | 124.78      | 119.90   |
| 1   | AA    | 200  | G    | N3-C2-N2   | 8.14  | 125.60      | 119.90   |
| 1   | AA    | 968  | A    | C6-N1-C2   | 8.14  | 123.48      | 118.60   |
| 1   | AA    | 980  | C    | P-O3'-C3'  | 8.14  | 129.47      | 119.70   |
| 1   | AA    | 1517 | G    | C5-C6-N1   | -8.14 | 107.43      | 111.50   |
| 34  | BA    | 108  | A    | O4'-C1'-N9 | 8.14  | 114.71      | 108.20   |
| 34  | BA    | 113  | C    | N3-C4-N4   | 8.14  | 123.70      | 118.00   |
| 35  | BB    | 13   | A    | C4-C5-C6   | 8.14  | 121.07      | 117.00   |
| 35  | BB    | 185  | G    | C5-C6-N1   | -8.14 | 107.43      | 111.50   |
| 35  | BB    | 1560 | G    | N1-C6-O6   | 8.14  | 124.78      | 119.90   |
| 35  | BB    | 2487 | G    | C2-N3-C4   | -8.14 | 107.83      | 111.90   |
| 35  | BB    | 2128 | G    | C6-N1-C2   | 8.14  | 129.98      | 125.10   |
| 35  | BB    | 2831 | G    | C5-C6-O6   | -8.14 | 123.72      | 128.60   |
| 1   | AA    | 306  | A    | C5-C6-N1   | -8.14 | 113.63      | 117.70   |
| 1   | AA    | 357  | G    | N3-C4-N9   | 8.14  | 130.88      | 126.00   |
| 1   | AA    | 447  | G    | C4-C5-C6   | 8.13  | 123.68      | 118.80   |
| 1   | AA    | 547  | A    | C8-N9-C4   | 8.13  | 109.05      | 105.80   |
| 1   | AA    | 695  | A    | O4'-C1'-N9 | 8.13  | 114.71      | 108.20   |
| 1   | AA    | 862  | C    | O4'-C1'-N1 | 8.13  | 114.71      | 108.20   |
| 1   | AA    | 1243 | C    | N3-C4-N4   | 8.13  | 123.69      | 118.00   |
| 14  | AN    | 80   | ARG  | NE-CZ-NH1  | -8.13 | 116.23      | 120.30   |
| 35  | BB    | 1863 | G    | C4-C5-C6   | 8.13  | 123.68      | 118.80   |
| 35  | BB    | 1937 | A    | O4'-C1'-N9 | 8.13  | 114.71      | 108.20   |
| 35  | BB    | 2145 | C    | O4'-C1'-N1 | 8.13  | 114.71      | 108.20   |
| 35  | BB    | 2660 | A    | N1-C6-N6   | 8.13  | 123.48      | 118.60   |
| 1   | AA    | 730  | G    | C2-N3-C4   | 8.13  | 115.97      | 111.90   |
| 1   | AA    | 1137 | C    | C5-C4-N4   | -8.13 | 114.51      | 120.20   |
| 1   | AA    | 1331 | G    | P-O5'-C5'  | 8.13  | 133.91      | 120.90   |
| 1   | AA    | 1441 | A    | N3-C4-C5   | -8.13 | 121.11      | 126.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 585  | G    | C2-N3-C4    | 8.13  | 115.97      | 111.90   |
| 35  | BB    | 736  | C    | O4'-C1'-N1  | 8.13  | 114.70      | 108.20   |
| 35  | BB    | 1107 | G    | C5'-C4'-C3' | 8.13  | 129.01      | 116.00   |
| 35  | BB    | 1702 | G    | C8-N9-C4    | -8.13 | 103.15      | 106.40   |
| 1   | AA    | 829  | G    | N1-C2-N3    | -8.13 | 119.02      | 123.90   |
| 1   | AA    | 1459 | G    | N1-C6-O6    | 8.13  | 124.78      | 119.90   |
| 35  | BB    | 818  | G    | N1-C2-N3    | -8.13 | 119.02      | 123.90   |
| 35  | BB    | 2340 | A    | C8-N9-C4    | -8.13 | 102.55      | 105.80   |
| 35  | BB    | 218  | A    | N7-C8-N9    | -8.13 | 109.73      | 113.80   |
| 35  | BB    | 1936 | A    | C8-N9-C4    | -8.13 | 102.55      | 105.80   |
| 35  | BB    | 2039 | U    | O4'-C1'-N1  | 8.13  | 114.70      | 108.20   |
| 35  | BB    | 2767 | C    | N3-C4-N4    | 8.13  | 123.69      | 118.00   |
| 35  | BB    | 2792 | A    | C8-N9-C4    | -8.13 | 102.55      | 105.80   |
| 1   | AA    | 444  | G    | C6-C5-N7    | -8.13 | 125.52      | 130.40   |
| 1   | AA    | 1290 | G    | N9-C4-C5    | -8.13 | 102.15      | 105.40   |
| 1   | AA    | 1294 | G    | N7-C8-N9    | 8.13  | 117.17      | 113.10   |
| 1   | AA    | 1511 | G    | C5-C6-O6    | -8.13 | 123.72      | 128.60   |
| 34  | BA    | 47   | C    | C6-N1-C2    | -8.13 | 117.05      | 120.30   |
| 35  | BB    | 184  | C    | C2-N3-C4    | 8.13  | 123.96      | 119.90   |
| 35  | BB    | 291  | G    | O4'-C1'-N9  | 8.13  | 114.70      | 108.20   |
| 35  | BB    | 649  | G    | C8-N9-C4    | -8.13 | 103.15      | 106.40   |
| 35  | BB    | 1116 | G    | O4'-C1'-N9  | 8.13  | 114.70      | 108.20   |
| 35  | BB    | 2159 | G    | C6-N1-C2    | 8.13  | 129.98      | 125.10   |
| 35  | BB    | 2192 | U    | O4'-C1'-N1  | 8.13  | 114.70      | 108.20   |
| 35  | BB    | 2867 | G    | C2-N3-C4    | 8.13  | 115.96      | 111.90   |
| 35  | BB    | 94   | A    | P-O3'-C3'   | 8.13  | 129.45      | 119.70   |
| 35  | BB    | 1483 | G    | N3-C2-N2    | 8.13  | 125.59      | 119.90   |
| 35  | BB    | 1783 | A    | N9-C4-C5    | -8.13 | 102.55      | 105.80   |
| 1   | AA    | 315  | A    | C5-N7-C8    | 8.12  | 107.96      | 103.90   |
| 1   | AA    | 478  | A    | C5-C6-N1    | -8.12 | 113.64      | 117.70   |
| 9   | AI    | 122  | ARG  | NE-CZ-NH1   | -8.12 | 116.24      | 120.30   |
| 35  | BB    | 1256 | G    | N9-C4-C5    | 8.12  | 108.65      | 105.40   |
| 35  | BB    | 1420 | A    | C2-N3-C4    | -8.12 | 106.54      | 110.60   |
| 35  | BB    | 627  | A    | N1-C6-N6    | 8.12  | 123.47      | 118.60   |
| 1   | AA    | 305  | G    | O4'-C1'-N9  | 8.12  | 114.70      | 108.20   |
| 1   | AA    | 439  | U    | N3-C4-C5    | -8.12 | 109.73      | 114.60   |
| 1   | AA    | 1487 | G    | C5-C6-O6    | -8.12 | 123.73      | 128.60   |
| 1   | AA    | 42   | G    | O4'-C1'-N9  | 8.12  | 114.70      | 108.20   |
| 1   | AA    | 457  | G    | C4-C5-C6    | 8.12  | 123.67      | 118.80   |
| 1   | AA    | 609  | A    | C1'-O4'-C4' | 8.12  | 116.39      | 109.90   |
| 1   | AA    | 1242 | G    | C4-C5-C6    | 8.12  | 123.67      | 118.80   |
| 1   | AA    | 1106 | G    | N3-C2-N2    | 8.12  | 125.58      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2884 | U    | N3-C4-C5    | -8.12 | 109.73      | 114.60   |
| 1   | AA    | 1138 | G    | N7-C8-N9    | 8.12  | 117.16      | 113.10   |
| 35  | BB    | 668  | A    | C4-C5-C6    | 8.12  | 121.06      | 117.00   |
| 35  | BB    | 961  | C    | N3-C4-C5    | -8.12 | 118.65      | 121.90   |
| 1   | AA    | 1238 | A    | C5-N7-C8    | 8.12  | 107.96      | 103.90   |
| 1   | AA    | 1476 | A    | C5-C6-N1    | -8.12 | 113.64      | 117.70   |
| 35  | BB    | 2094 | A    | C6-C5-N7    | -8.12 | 126.62      | 132.30   |
| 35  | BB    | 2096 | C    | O4'-C1'-N1  | 8.12  | 114.69      | 108.20   |
| 35  | BB    | 324  | A    | C5-C6-N6    | -8.11 | 117.21      | 123.70   |
| 35  | BB    | 1640 | A    | C5-C6-N1    | -8.11 | 113.64      | 117.70   |
| 35  | BB    | 2136 | G    | C4'-C3'-C2' | -8.12 | 94.48       | 102.60   |
| 39  | BF    | 127  | TYR  | CB-CG-CD2   | -8.12 | 116.13      | 121.00   |
| 1   | AA    | 566  | G    | C5-C6-N1    | -8.11 | 107.44      | 111.50   |
| 35  | BB    | 2365 | G    | O4'-C1'-N9  | 8.11  | 114.69      | 108.20   |
| 34  | BA    | 99   | A    | N1-C2-N3    | 8.11  | 133.36      | 129.30   |
| 34  | BA    | 113  | C    | C5-C4-N4    | -8.11 | 114.52      | 120.20   |
| 35  | BB    | 1034 | G    | N1-C2-N3    | -8.11 | 119.03      | 123.90   |
| 35  | BB    | 1768 | C    | C2-N3-C4    | 8.11  | 123.96      | 119.90   |
| 35  | BB    | 119  | A    | N1-C6-N6    | 8.11  | 123.47      | 118.60   |
| 35  | BB    | 1151 | A    | O4'-C1'-N9  | 8.11  | 114.69      | 108.20   |
| 35  | BB    | 1999 | C    | C5-C6-N1    | -8.11 | 116.94      | 121.00   |
| 1   | AA    | 974  | A    | C5-C6-N1    | -8.11 | 113.65      | 117.70   |
| 1   | AA    | 1237 | C    | N3-C4-N4    | 8.11  | 123.68      | 118.00   |
| 35  | BB    | 76   | C    | N3-C4-C5    | -8.11 | 118.66      | 121.90   |
| 35  | BB    | 708  | G    | C5-C6-O6    | -8.11 | 123.73      | 128.60   |
| 35  | BB    | 354  | A    | O5'-P-OP1   | 8.11  | 120.43      | 110.70   |
| 35  | BB    | 510  | C    | C3'-C2'-C1' | 8.11  | 107.99      | 101.50   |
| 35  | BB    | 920  | A    | O4'-C1'-N9  | 8.11  | 114.69      | 108.20   |
| 35  | BB    | 1129 | A    | C5-C6-N1    | -8.11 | 113.65      | 117.70   |
| 35  | BB    | 1407 | G    | N3-C4-C5    | -8.11 | 124.55      | 128.60   |
| 35  | BB    | 1708 | C    | N3-C4-C5    | -8.11 | 118.66      | 121.90   |
| 35  | BB    | 2088 | A    | N7-C8-N9    | -8.11 | 109.75      | 113.80   |
| 1   | AA    | 1241 | G    | N1-C2-N3    | -8.11 | 119.04      | 123.90   |
| 35  | BB    | 843  | G    | N9-C4-C5    | -8.11 | 102.16      | 105.40   |
| 35  | BB    | 2846 | G    | N3-C4-C5    | 8.11  | 132.65      | 128.60   |
| 1   | AA    | 167  | A    | C5-C6-N1    | -8.11 | 113.65      | 117.70   |
| 1   | AA    | 386  | C    | P-O3'-C3'   | -8.11 | 109.97      | 119.70   |
| 35  | BB    | 122  | G    | N3-C4-C5    | -8.11 | 124.55      | 128.60   |
| 35  | BB    | 627  | A    | C8-N9-C4    | -8.11 | 102.56      | 105.80   |
| 43  | BJ    | 119  | PHE  | CB-CG-CD1   | 8.11  | 126.47      | 120.80   |
| 1   | AA    | 580  | C    | C5-C4-N4    | -8.10 | 114.53      | 120.20   |
| 35  | BB    | 888  | C    | N3-C4-N4    | 8.10  | 123.67      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1941 | C    | O4'-C1'-N1  | 8.10  | 114.68      | 108.20   |
| 1   | AA    | 51   | A    | N3-C4-C5    | -8.10 | 121.13      | 126.80   |
| 1   | AA    | 448  | A    | N7-C8-N9    | -8.10 | 109.75      | 113.80   |
| 34  | BA    | 41   | G    | N3-C2-N2    | 8.10  | 125.57      | 119.90   |
| 35  | BB    | 151  | C    | O4'-C1'-N1  | 8.10  | 114.68      | 108.20   |
| 35  | BB    | 207  | A    | O4'-C1'-N9  | 8.10  | 114.68      | 108.20   |
| 35  | BB    | 924  | G    | N3-C4-C5    | -8.10 | 124.55      | 128.60   |
| 35  | BB    | 1071 | G    | C5-C6-N1    | -8.10 | 107.45      | 111.50   |
| 35  | BB    | 1877 | A    | C5-N7-C8    | 8.10  | 107.95      | 103.90   |
| 35  | BB    | 2366 | A    | C5-N7-C8    | 8.10  | 107.95      | 103.90   |
| 35  | BB    | 2774 | C    | C5-C6-N1    | -8.10 | 116.95      | 121.00   |
| 1   | AA    | 627  | G    | O4'-C1'-N9  | 8.10  | 114.68      | 108.20   |
| 1   | AA    | 640  | A    | O4'-C1'-N9  | 8.10  | 114.68      | 108.20   |
| 35  | BB    | 250  | G    | N3-C2-N2    | 8.10  | 125.57      | 119.90   |
| 22  | AV    | 25   | C    | O4'-C1'-N1  | 8.10  | 114.68      | 108.20   |
| 34  | BA    | 66   | A    | C5-C6-N6    | -8.10 | 117.22      | 123.70   |
| 35  | BB    | 307  | G    | C2-N3-C4    | 8.10  | 115.95      | 111.90   |
| 35  | BB    | 1731 | G    | C4-C5-N7    | -8.10 | 107.56      | 110.80   |
| 35  | BB    | 2495 | G    | C5-C6-O6    | -8.10 | 123.74      | 128.60   |
| 1   | AA    | 182  | A    | N1-C6-N6    | 8.10  | 123.46      | 118.60   |
| 1   | AA    | 736  | C    | P-O5'-C5'   | -8.10 | 107.95      | 120.90   |
| 1   | AA    | 770  | C    | O4'-C1'-N1  | 8.10  | 114.68      | 108.20   |
| 1   | AA    | 1054 | C    | O4'-C1'-N1  | 8.10  | 114.68      | 108.20   |
| 1   | AA    | 1508 | A    | C5-C6-N6    | -8.10 | 117.22      | 123.70   |
| 23  | AX    | 19   | A    | C6-C5-N7    | -8.10 | 126.63      | 132.30   |
| 35  | BB    | 568  | U    | C5-C6-N1    | -8.10 | 118.65      | 122.70   |
| 35  | BB    | 823  | C    | O4'-C1'-N1  | 8.10  | 114.68      | 108.20   |
| 35  | BB    | 1526 | C    | C2-N3-C4    | 8.10  | 123.95      | 119.90   |
| 35  | BB    | 1887 | C    | C6-N1-C2    | 8.10  | 123.54      | 120.30   |
| 35  | BB    | 2141 | G    | O4'-C1'-N9  | 8.10  | 114.68      | 108.20   |
| 1   | AA    | 1392 | G    | N1-C2-N3    | -8.10 | 119.04      | 123.90   |
| 35  | BB    | 1110 | G    | N1-C6-O6    | 8.10  | 124.76      | 119.90   |
| 35  | BB    | 1939 | U    | C4-C5-C6    | 8.10  | 124.56      | 119.70   |
| 35  | BB    | 2090 | A    | P-O5'-C5'   | -8.10 | 107.95      | 120.90   |
| 35  | BB    | 2179 | C    | O4'-C1'-N1  | 8.10  | 114.68      | 108.20   |
| 35  | BB    | 2901 | C    | N3-C4-N4    | 8.10  | 123.67      | 118.00   |
| 35  | BB    | 183  | C    | C1'-O4'-C4' | -8.09 | 103.42      | 109.90   |
| 1   | AA    | 269  | C    | N3-C4-N4    | 8.09  | 123.66      | 118.00   |
| 1   | AA    | 748  | G    | N1-C6-O6    | 8.09  | 124.76      | 119.90   |
| 1   | AA    | 1099 | G    | N1-C2-N3    | -8.09 | 119.04      | 123.90   |
| 35  | BB    | 473  | G    | C5-C6-N1    | -8.09 | 107.45      | 111.50   |
| 35  | BB    | 869  | G    | N1-C6-O6    | 8.09  | 124.76      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2537 | U    | C2-N3-C4    | 8.09  | 131.86      | 127.00   |
| 35  | BB    | 618  | G    | N1-C2-N3    | -8.09 | 119.05      | 123.90   |
| 35  | BB    | 701  | G    | N3-C2-N2    | 8.09  | 125.56      | 119.90   |
| 35  | BB    | 1059 | G    | C8-N9-C4    | 8.09  | 109.64      | 106.40   |
| 35  | BB    | 1069 | A    | C6-C5-N7    | -8.09 | 126.64      | 132.30   |
| 35  | BB    | 1782 | U    | O4'-C1'-N1  | 8.09  | 114.67      | 108.20   |
| 1   | AA    | 815  | A    | C4-C5-C6    | 8.09  | 121.05      | 117.00   |
| 35  | BB    | 219  | A    | O4'-C1'-N9  | 8.09  | 114.67      | 108.20   |
| 34  | BA    | 94   | A    | C4-C5-C6    | 8.09  | 121.05      | 117.00   |
| 35  | BB    | 178  | G    | N1-C6-O6    | 8.09  | 124.75      | 119.90   |
| 35  | BB    | 498  | G    | C5-C6-O6    | -8.09 | 123.75      | 128.60   |
| 35  | BB    | 947  | A    | N1-C2-N3    | 8.09  | 133.34      | 129.30   |
| 35  | BB    | 968  | C    | C5-C6-N1    | -8.09 | 116.96      | 121.00   |
| 35  | BB    | 2270 | A    | N1-C2-N3    | 8.09  | 133.34      | 129.30   |
| 35  | BB    | 2478 | A    | C5-N7-C8    | 8.09  | 107.94      | 103.90   |
| 35  | BB    | 689  | A    | C5-C6-N1    | -8.09 | 113.66      | 117.70   |
| 35  | BB    | 1118 | C    | C1'-O4'-C4' | 8.09  | 116.37      | 109.90   |
| 1   | AA    | 844  | G    | N3-C4-N9    | 8.09  | 130.85      | 126.00   |
| 35  | BB    | 1494 | A    | O4'-C1'-N9  | 8.09  | 114.67      | 108.20   |
| 35  | BB    | 2229 | U    | C6-N1-C2    | -8.09 | 116.15      | 121.00   |
| 37  | BD    | 31   | ALA  | N-CA-CB     | 8.09  | 121.42      | 110.10   |
| 1   | AA    | 1441 | A    | C2-N3-C4    | 8.09  | 114.64      | 110.60   |
| 35  | BB    | 312  | G    | N9-C4-C5    | -8.09 | 102.17      | 105.40   |
| 35  | BB    | 463  | G    | C5-C6-O6    | -8.09 | 123.75      | 128.60   |
| 35  | BB    | 1543 | G    | N9-C4-C5    | 8.09  | 108.63      | 105.40   |
| 35  | BB    | 2199 | A    | C6-N1-C2    | 8.09  | 123.45      | 118.60   |
| 39  | BF    | 101  | ARG  | NE-CZ-NH2   | 8.09  | 124.34      | 120.30   |
| 1   | AA    | 821  | G    | N3-C2-N2    | 8.08  | 125.56      | 119.90   |
| 35  | BB    | 867  | C    | N3-C4-N4    | 8.08  | 123.66      | 118.00   |
| 35  | BB    | 995  | C    | N3-C4-C5    | -8.08 | 118.67      | 121.90   |
| 35  | BB    | 1428 | C    | N1-C2-N3    | -8.08 | 113.54      | 119.20   |
| 35  | BB    | 2235 | G    | N3-C2-N2    | 8.08  | 125.56      | 119.90   |
| 35  | BB    | 2581 | G    | N1-C2-N3    | -8.08 | 119.05      | 123.90   |
| 35  | BB    | 1493 | C    | C4-C5-C6    | 8.08  | 121.44      | 117.40   |
| 35  | BB    | 2838 | G    | O4'-C1'-N9  | 8.08  | 114.67      | 108.20   |
| 1   | AA    | 51   | A    | C4-C5-C6    | 8.08  | 121.04      | 117.00   |
| 1   | AA    | 1441 | A    | C5-C6-N1    | -8.08 | 113.66      | 117.70   |
| 35  | BB    | 91   | A    | C5-C6-N6    | -8.08 | 117.24      | 123.70   |
| 35  | BB    | 786  | C    | P-O3'-C3'   | -8.08 | 110.00      | 119.70   |
| 35  | BB    | 218  | A    | C4'-C3'-C2' | -8.08 | 94.52       | 102.60   |
| 35  | BB    | 679  | C    | C5-C6-N1    | 8.08  | 125.04      | 121.00   |
| 35  | BB    | 1250 | G    | C4-C5-N7    | -8.08 | 107.57      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1280 | G    | C5-C6-O6   | -8.08 | 123.75      | 128.60   |
| 35  | BB    | 1449 | G    | N1-C2-N3   | -8.08 | 119.05      | 123.90   |
| 35  | BB    | 220  | G    | O4'-C1'-N9 | 8.08  | 114.66      | 108.20   |
| 1   | AA    | 275  | G    | C6-C5-N7   | -8.08 | 125.56      | 130.40   |
| 1   | AA    | 581  | G    | N3-C2-N2   | 8.08  | 125.55      | 119.90   |
| 34  | BA    | 41   | G    | N3-C4-C5   | -8.08 | 124.56      | 128.60   |
| 35  | BB    | 696  | G    | C6-N1-C2   | 8.08  | 129.95      | 125.10   |
| 35  | BB    | 833  | A    | C5-C6-N1   | -8.08 | 113.66      | 117.70   |
| 35  | BB    | 937  | C    | O4'-C1'-N1 | 8.08  | 114.66      | 108.20   |
| 35  | BB    | 1095 | A    | C5-C6-N1   | -8.08 | 113.66      | 117.70   |
| 35  | BB    | 1644 | C    | C6-N1-C2   | -8.08 | 117.07      | 120.30   |
| 1   | AA    | 275  | G    | N1-C6-O6   | 8.07  | 124.74      | 119.90   |
| 1   | AA    | 1189 | U    | N1-C2-O2   | -8.07 | 117.15      | 122.80   |
| 35  | BB    | 384  | A    | C5-C6-N1   | -8.07 | 113.66      | 117.70   |
| 35  | BB    | 1661 | G    | O4'-C1'-N9 | 8.07  | 114.66      | 108.20   |
| 35  | BB    | 2439 | A    | C8-N9-C4   | -8.07 | 102.57      | 105.80   |
| 35  | BB    | 2800 | A    | C6-C5-N7   | -8.07 | 126.65      | 132.30   |
| 1   | AA    | 246  | A    | C4-C5-C6   | 8.07  | 121.04      | 117.00   |
| 1   | AA    | 454  | G    | N1-C2-N3   | -8.07 | 119.06      | 123.90   |
| 1   | AA    | 755  | G    | N1-C6-O6   | 8.07  | 124.74      | 119.90   |
| 35  | BB    | 858  | G    | N1-C2-N3   | -8.07 | 119.06      | 123.90   |
| 35  | BB    | 2497 | A    | C2-N3-C4   | -8.07 | 106.56      | 110.60   |
| 35  | BB    | 2787 | C    | N3-C4-N4   | 8.07  | 123.65      | 118.00   |
| 1   | AA    | 1232 | U    | C5-C6-N1   | 8.07  | 126.73      | 122.70   |
| 28  | B3    | 51   | ARG  | N-CA-CB    | 8.07  | 125.12      | 110.60   |
| 35  | BB    | 1537 | G    | C5-N7-C8   | 8.07  | 108.33      | 104.30   |
| 35  | BB    | 1886 | U    | N1-C2-N3   | -8.07 | 110.06      | 114.90   |
| 1   | AA    | 754  | C    | C5-C4-N4   | -8.07 | 114.55      | 120.20   |
| 1   | AA    | 885  | G    | N1-C6-O6   | 8.07  | 124.74      | 119.90   |
| 35  | BB    | 685  | A    | C5-C6-N6   | -8.07 | 117.25      | 123.70   |
| 34  | BA    | 4    | C    | C6-N1-C2   | 8.07  | 123.53      | 120.30   |
| 34  | BA    | 71   | C    | C4-C5-C6   | 8.07  | 121.43      | 117.40   |
| 35  | BB    | 26   | G    | C6-C5-N7   | -8.07 | 125.56      | 130.40   |
| 35  | BB    | 69   | C    | C2-N3-C4   | 8.07  | 123.93      | 119.90   |
| 35  | BB    | 699  | A    | N3-C4-C5   | -8.07 | 121.15      | 126.80   |
| 35  | BB    | 1910 | G    | N3-C2-N2   | 8.07  | 125.55      | 119.90   |
| 35  | BB    | 2252 | G    | O4'-C1'-N9 | 8.07  | 114.65      | 108.20   |
| 35  | BB    | 2529 | G    | N1-C2-N3   | -8.07 | 119.06      | 123.90   |
| 1   | AA    | 108  | G    | O4'-C1'-N9 | 8.06  | 114.65      | 108.20   |
| 35  | BB    | 395  | U    | C5-C4-O4   | -8.06 | 121.06      | 125.90   |
| 35  | BB    | 2895 | G    | N3-C4-C5   | -8.06 | 124.57      | 128.60   |
| 1   | AA    | 166  | U    | C5-C4-O4   | -8.06 | 121.06      | 125.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1369 | C    | O4'-C1'-N1  | 8.06  | 114.65      | 108.20   |
| 35  | BB    | 298  | G    | C4-C5-C6    | 8.06  | 123.64      | 118.80   |
| 35  | BB    | 621  | A    | C6-C5-N7    | -8.06 | 126.66      | 132.30   |
| 35  | BB    | 2083 | G    | N7-C8-N9    | 8.06  | 117.13      | 113.10   |
| 35  | BB    | 2668 | G    | C4-C5-C6    | 8.06  | 123.64      | 118.80   |
| 35  | BB    | 2771 | C    | O4'-C1'-N1  | 8.06  | 114.65      | 108.20   |
| 1   | AA    | 362  | G    | O4'-C1'-N9  | 8.06  | 114.65      | 108.20   |
| 1   | AA    | 1453 | G    | C5-C6-N1    | -8.06 | 107.47      | 111.50   |
| 35  | BB    | 29   | U    | N3-C4-O4    | 8.06  | 125.04      | 119.40   |
| 35  | BB    | 1168 | G    | C8-N9-C4    | -8.06 | 103.17      | 106.40   |
| 1   | AA    | 1253 | G    | C8-N9-C4    | 8.06  | 109.62      | 106.40   |
| 35  | BB    | 708  | G    | N7-C8-N9    | -8.06 | 109.07      | 113.10   |
| 35  | BB    | 921  | C    | C2-N3-C4    | 8.06  | 123.93      | 119.90   |
| 35  | BB    | 1455 | G    | N1-C6-O6    | 8.06  | 124.74      | 119.90   |
| 35  | BB    | 1890 | A    | C6-C5-N7    | -8.06 | 126.66      | 132.30   |
| 1   | AA    | 1298 | U    | C5'-C4'-O4' | 8.06  | 118.77      | 109.10   |
| 35  | BB    | 24   | G    | O4'-C1'-N9  | 8.06  | 114.65      | 108.20   |
| 35  | BB    | 2144 | G    | O4'-C1'-N9  | 8.06  | 114.65      | 108.20   |
| 1   | AA    | 205  | A    | C5-C6-N6    | -8.05 | 117.26      | 123.70   |
| 1   | AA    | 890  | G    | C6-N1-C2    | 8.05  | 129.93      | 125.10   |
| 35  | BB    | 696  | G    | C6-C5-N7    | -8.06 | 125.57      | 130.40   |
| 35  | BB    | 1913 | A    | N3-C4-C5    | -8.06 | 121.16      | 126.80   |
| 1   | AA    | 228  | A    | C4-C5-C6    | 8.05  | 121.03      | 117.00   |
| 1   | AA    | 433  | G    | O4'-C1'-N9  | 8.05  | 114.64      | 108.20   |
| 1   | AA    | 1394 | A    | N1-C6-N6    | 8.05  | 123.43      | 118.60   |
| 35  | BB    | 214  | G    | O4'-C1'-N9  | 8.05  | 114.64      | 108.20   |
| 35  | BB    | 1661 | G    | C2-N3-C4    | 8.05  | 115.93      | 111.90   |
| 35  | BB    | 2034 | U    | N1-C2-O2    | 8.05  | 128.44      | 122.80   |
| 1   | AA    | 1340 | A    | C5-C6-N6    | -8.05 | 117.26      | 123.70   |
| 1   | AA    | 1080 | A    | C4-C5-N7    | 8.05  | 114.72      | 110.70   |
| 2   | AB    | 136  | ARG  | NE-CZ-NH1   | 8.05  | 124.33      | 120.30   |
| 35  | BB    | 864  | G    | N1-C6-O6    | 8.05  | 124.73      | 119.90   |
| 35  | BB    | 891  | G    | N1-C6-O6    | 8.05  | 124.73      | 119.90   |
| 34  | BA    | 39   | A    | C2-N3-C4    | 8.05  | 114.62      | 110.60   |
| 35  | BB    | 455  | C    | N3-C4-C5    | -8.05 | 118.68      | 121.90   |
| 35  | BB    | 892  | A    | N3-C4-C5    | -8.05 | 121.16      | 126.80   |
| 35  | BB    | 2317 | A    | N3-C4-C5    | -8.05 | 121.16      | 126.80   |
| 35  | BB    | 2391 | G    | C5-N7-C8    | 8.05  | 108.33      | 104.30   |
| 1   | AA    | 922  | G    | C6-C5-N7    | -8.05 | 125.57      | 130.40   |
| 1   | AA    | 38   | G    | C5-C6-N1    | -8.05 | 107.48      | 111.50   |
| 1   | AA    | 39   | G    | C5-C6-O6    | -8.05 | 123.77      | 128.60   |
| 1   | AA    | 1058 | G    | N1-C6-O6    | 8.05  | 124.73      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1192 | C    | N3-C4-N4    | 8.05  | 123.63      | 118.00   |
| 1   | AA    | 1488 | G    | N3-C2-N2    | 8.05  | 125.53      | 119.90   |
| 35  | BB    | 1816 | C    | C2-N1-C1'   | 8.05  | 127.65      | 118.80   |
| 35  | BB    | 1921 | G    | N9-C4-C5    | 8.05  | 108.62      | 105.40   |
| 1   | AA    | 136  | C    | C5-C4-N4    | -8.04 | 114.57      | 120.20   |
| 1   | AA    | 293  | G    | C5-N7-C8    | 8.04  | 108.32      | 104.30   |
| 35  | BB    | 1552 | A    | P-O3'-C3'   | -8.05 | 110.05      | 119.70   |
| 1   | AA    | 305  | G    | C5'-C4'-O4' | 8.04  | 118.75      | 109.10   |
| 1   | AA    | 540  | G    | N1-C6-O6    | 8.04  | 124.73      | 119.90   |
| 9   | AI    | 108  | ARG  | NE-CZ-NH1   | 8.05  | 124.32      | 120.30   |
| 35  | BB    | 947  | A    | C6-C5-N7    | -8.05 | 126.67      | 132.30   |
| 1   | AA    | 1170 | A    | C4'-C3'-C2' | -8.04 | 94.56       | 102.60   |
| 22  | AV    | 61   | C    | O4'-C1'-N1  | 8.04  | 114.64      | 108.20   |
| 35  | BB    | 1040 | A    | C2-N3-C4    | -8.04 | 106.58      | 110.60   |
| 35  | BB    | 1421 | G    | C5-C6-O6    | -8.05 | 123.77      | 128.60   |
| 35  | BB    | 1310 | G    | C5-C6-N1    | -8.04 | 107.48      | 111.50   |
| 35  | BB    | 1461 | C    | N3-C4-N4    | 8.04  | 123.63      | 118.00   |
| 35  | BB    | 2597 | G    | O4'-C1'-N9  | 8.04  | 114.64      | 108.20   |
| 1   | AA    | 1112 | C    | C6-N1-C2    | -8.04 | 117.08      | 120.30   |
| 1   | AA    | 1260 | G    | N1-C6-O6    | 8.04  | 124.72      | 119.90   |
| 1   | AA    | 1314 | C    | N3-C4-C5    | -8.04 | 118.68      | 121.90   |
| 8   | AH    | 127  | TYR  | CB-CG-CD2   | 8.04  | 125.83      | 121.00   |
| 35  | BB    | 35   | G    | C5-C6-O6    | -8.04 | 123.78      | 128.60   |
| 35  | BB    | 968  | C    | N3-C4-N4    | 8.04  | 123.63      | 118.00   |
| 35  | BB    | 1764 | C    | O4'-C1'-N1  | 8.04  | 114.63      | 108.20   |
| 35  | BB    | 230  | G    | N9-C4-C5    | -8.04 | 102.18      | 105.40   |
| 35  | BB    | 282  | A    | C5-N7-C8    | 8.04  | 107.92      | 103.90   |
| 35  | BB    | 737  | C    | N3-C4-C5    | -8.04 | 118.68      | 121.90   |
| 35  | BB    | 906  | U    | N3-C4-C5    | -8.04 | 109.78      | 114.60   |
| 35  | BB    | 1633 | G    | C5-N7-C8    | 8.04  | 108.32      | 104.30   |
| 35  | BB    | 2027 | G    | C8-N9-C4    | 8.04  | 109.62      | 106.40   |
| 1   | AA    | 632  | U    | P-O3'-C3'   | 8.04  | 129.34      | 119.70   |
| 35  | BB    | 1300 | G    | C6-C5-N7    | -8.04 | 125.58      | 130.40   |
| 35  | BB    | 2839 | G    | N1-C2-N3    | -8.04 | 119.08      | 123.90   |
| 40  | BG    | 108  | PHE  | CB-CG-CD1   | -8.04 | 115.17      | 120.80   |
| 35  | BB    | 1786 | A    | C5-N7-C8    | 8.04  | 107.92      | 103.90   |
| 35  | BB    | 1811 | G    | N1-C6-O6    | 8.04  | 124.72      | 119.90   |
| 54  | BU    | 79   | ALA  | N-CA-CB     | 8.04  | 121.35      | 110.10   |
| 1   | AA    | 85   | U    | C2-N3-C4    | 8.03  | 131.82      | 127.00   |
| 35  | BB    | 112  | U    | O4'-C1'-N1  | 8.03  | 114.63      | 108.20   |
| 35  | BB    | 474  | G    | N9-C4-C5    | -8.03 | 102.19      | 105.40   |
| 35  | BB    | 516  | C    | O4'-C1'-N1  | 8.03  | 114.63      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1172 | C    | O4'-C1'-N1  | 8.04  | 114.63      | 108.20   |
| 35  | BB    | 1527 | G    | N1-C2-N3    | -8.04 | 119.08      | 123.90   |
| 35  | BB    | 1569 | A    | C5'-C4'-C3' | -8.04 | 103.14      | 116.00   |
| 1   | AA    | 204  | G    | O4'-C1'-N9  | 8.03  | 114.62      | 108.20   |
| 1   | AA    | 686  | U    | C4-C5-C6    | 8.03  | 124.52      | 119.70   |
| 1   | AA    | 732  | C    | O4'-C1'-N1  | 8.03  | 114.63      | 108.20   |
| 35  | BB    | 1632 | A    | N1-C6-N6    | 8.03  | 123.42      | 118.60   |
| 35  | BB    | 2069 | G    | N9-C4-C5    | -8.03 | 102.19      | 105.40   |
| 35  | BB    | 4    | U    | C5-C4-O4    | -8.03 | 121.08      | 125.90   |
| 35  | BB    | 683  | U    | N1-C2-N3    | 8.03  | 119.72      | 114.90   |
| 35  | BB    | 1058 | U    | N1-C2-O2    | -8.03 | 117.18      | 122.80   |
| 35  | BB    | 1107 | G    | C2-N3-C4    | 8.03  | 115.92      | 111.90   |
| 35  | BB    | 2013 | A    | C5-C6-N1    | -8.03 | 113.69      | 117.70   |
| 35  | BB    | 2274 | A    | C5-C6-N1    | -8.03 | 113.68      | 117.70   |
| 35  | BB    | 2397 | G    | C4-C5-N7    | 8.03  | 114.01      | 110.80   |
| 35  | BB    | 2509 | G    | C5-C6-O6    | -8.03 | 123.78      | 128.60   |
| 1   | AA    | 151  | A    | C2-N3-C4    | 8.03  | 114.61      | 110.60   |
| 1   | AA    | 1400 | C    | C2-N1-C1'   | 8.03  | 127.63      | 118.80   |
| 1   | AA    | 1534 | A    | C2-N3-C4    | -8.03 | 106.58      | 110.60   |
| 35  | BB    | 345  | A    | O4'-C1'-N9  | 8.03  | 114.62      | 108.20   |
| 35  | BB    | 1420 | A    | C4-C5-C6    | 8.03  | 121.02      | 117.00   |
| 1   | AA    | 380  | G    | N1-C2-N3    | -8.03 | 119.08      | 123.90   |
| 35  | BB    | 449  | A    | C6-C5-N7    | -8.03 | 126.68      | 132.30   |
| 35  | BB    | 2128 | G    | N1-C6-O6    | 8.03  | 124.72      | 119.90   |
| 1   | AA    | 1151 | A    | N3-C4-N9    | 8.03  | 133.82      | 127.40   |
| 26  | B1    | 7    | ARG  | NE-CZ-NH2   | -8.03 | 116.29      | 120.30   |
| 35  | BB    | 186  | G    | N3-C2-N2    | 8.03  | 125.52      | 119.90   |
| 35  | BB    | 78   | U    | C2-N3-C4    | -8.03 | 122.19      | 127.00   |
| 35  | BB    | 924  | G    | N1-C2-N3    | -8.03 | 119.08      | 123.90   |
| 35  | BB    | 1498 | C    | O4'-C4'-C3' | -8.03 | 95.97       | 104.00   |
| 35  | BB    | 2445 | G    | O4'-C1'-N9  | 8.03  | 114.62      | 108.20   |
| 35  | BB    | 1080 | A    | C5-N7-C8    | 8.03  | 107.91      | 103.90   |
| 37  | BD    | 128  | ARG  | NE-CZ-NH1   | 8.03  | 124.31      | 120.30   |
| 41  | BH    | 132  | PHE  | CB-CG-CD2   | -8.03 | 115.18      | 120.80   |
| 1   | AA    | 55   | A    | C8-N9-C4    | -8.02 | 102.59      | 105.80   |
| 1   | AA    | 271  | C    | O4'-C1'-N1  | 8.02  | 114.62      | 108.20   |
| 1   | AA    | 733  | G    | N3-C2-N2    | 8.02  | 125.52      | 119.90   |
| 1   | AA    | 1060 | U    | O4'-C1'-N1  | 8.02  | 114.62      | 108.20   |
| 35  | BB    | 2865 | U    | O4'-C1'-N1  | 8.02  | 114.62      | 108.20   |
| 1   | AA    | 1299 | A    | N3-C4-C5    | -8.02 | 121.19      | 126.80   |
| 35  | BB    | 539  | G    | N9-C4-C5    | -8.02 | 102.19      | 105.40   |
| 35  | BB    | 1307 | A    | C5-C6-N6    | -8.02 | 117.28      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1328 | A    | O4'-C1'-N9  | 8.02  | 114.62      | 108.20   |
| 35  | BB    | 1751 | U    | C5-C4-O4    | -8.02 | 121.09      | 125.90   |
| 35  | BB    | 1925 | C    | P-O5'-C5'   | 8.02  | 133.74      | 120.90   |
| 35  | BB    | 1960 | A    | O4'-C1'-N9  | 8.02  | 114.62      | 108.20   |
| 35  | BB    | 2485 | G    | C4-C5-C6    | 8.02  | 123.61      | 118.80   |
| 52  | BS    | 8    | ARG  | NE-CZ-NH1   | 8.02  | 124.31      | 120.30   |
| 1   | AA    | 298  | A    | N9-C4-C5    | 8.02  | 109.01      | 105.80   |
| 1   | AA    | 1099 | G    | C6-N1-C2    | 8.02  | 129.91      | 125.10   |
| 1   | AA    | 1138 | G    | N9-C4-C5    | 8.02  | 108.61      | 105.40   |
| 1   | AA    | 1181 | G    | N9-C1'-C2'  | -8.02 | 103.18      | 112.00   |
| 35  | BB    | 53   | A    | N1-C6-N6    | 8.02  | 123.41      | 118.60   |
| 35  | BB    | 2609 | U    | C5'-C4'-O4' | 8.02  | 118.72      | 109.10   |
| 1   | AA    | 1461 | G    | N1-C6-O6    | 8.02  | 124.71      | 119.90   |
| 35  | BB    | 53   | A    | C4-C5-N7    | -8.02 | 106.69      | 110.70   |
| 35  | BB    | 117  | G    | N1-C6-O6    | 8.02  | 124.71      | 119.90   |
| 35  | BB    | 512  | G    | N3-C2-N2    | 8.02  | 125.51      | 119.90   |
| 35  | BB    | 1392 | A    | C4-C5-C6    | 8.02  | 121.01      | 117.00   |
| 35  | BB    | 2226 | C    | O4'-C1'-N1  | 8.02  | 114.62      | 108.20   |
| 35  | BB    | 2701 | U    | C6-N1-C2    | -8.02 | 116.19      | 121.00   |
| 1   | AA    | 770  | C    | N3-C2-O2    | 8.02  | 127.51      | 121.90   |
| 21  | AU    | 34   | ARG  | NE-CZ-NH1   | 8.02  | 124.31      | 120.30   |
| 35  | BB    | 170  | U    | C5-C4-O4    | -8.02 | 121.09      | 125.90   |
| 35  | BB    | 389  | G    | N3-C2-N2    | 8.02  | 125.51      | 119.90   |
| 35  | BB    | 615  | U    | N3-C4-O4    | 8.02  | 125.01      | 119.40   |
| 35  | BB    | 1483 | G    | N7-C8-N9    | -8.02 | 109.09      | 113.10   |
| 35  | BB    | 2396 | G    | O4'-C1'-N9  | 8.02  | 114.61      | 108.20   |
| 1   | AA    | 386  | C    | C2-N1-C1'   | 8.02  | 127.62      | 118.80   |
| 1   | AA    | 895  | G    | N3-C2-N2    | 8.02  | 125.51      | 119.90   |
| 25  | B0    | 56   | ARG  | NE-CZ-NH2   | -8.02 | 116.29      | 120.30   |
| 35  | BB    | 2432 | A    | C4-C5-C6    | 8.02  | 121.01      | 117.00   |
| 35  | BB    | 2832 | U    | P-O3'-C3'   | 8.02  | 129.32      | 119.70   |
| 40  | BG    | 74   | MET  | CG-SD-CE    | -8.02 | 87.38       | 100.20   |
| 1   | AA    | 104  | G    | O4'-C1'-N9  | 8.01  | 114.61      | 108.20   |
| 26  | B1    | 52   | ARG  | NE-CZ-NH2   | 8.01  | 124.31      | 120.30   |
| 35  | BB    | 74   | A    | N1-C6-N6    | 8.01  | 123.41      | 118.60   |
| 35  | BB    | 2800 | A    | O4'-C1'-N9  | 8.01  | 114.61      | 108.20   |
| 34  | BA    | 35   | C    | O4'-C1'-N1  | 8.01  | 114.61      | 108.20   |
| 35  | BB    | 179  | C    | O4'-C1'-N1  | 8.01  | 114.61      | 108.20   |
| 35  | BB    | 1101 | U    | N1-C2-O2    | -8.01 | 117.19      | 122.80   |
| 35  | BB    | 2043 | C    | N3-C4-N4    | 8.01  | 123.61      | 118.00   |
| 35  | BB    | 2236 | U    | N3-C4-C5    | -8.01 | 109.79      | 114.60   |
| 36  | BC    | 211  | ARG  | NE-CZ-NH1   | 8.01  | 124.31      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 14   | U    | N3-C4-O4    | 8.01  | 125.01      | 119.40   |
| 1   | AA    | 465  | A    | N7-C8-N9    | -8.01 | 109.80      | 113.80   |
| 1   | AA    | 169  | C    | N3-C4-N4    | 8.01  | 123.60      | 118.00   |
| 34  | BA    | 85   | G    | N9-C4-C5    | -8.01 | 102.20      | 105.40   |
| 35  | BB    | 131  | A    | C5-N7-C8    | 8.01  | 107.90      | 103.90   |
| 35  | BB    | 492  | A    | C5-C6-N1    | -8.01 | 113.70      | 117.70   |
| 35  | BB    | 619  | G    | C6-C5-N7    | -8.01 | 125.60      | 130.40   |
| 35  | BB    | 1566 | A    | C1'-O4'-C4' | 8.01  | 116.31      | 109.90   |
| 35  | BB    | 2345 | G    | C4-C5-C6    | 8.01  | 123.60      | 118.80   |
| 1   | AA    | 76   | G    | N1-C2-N3    | -8.00 | 119.10      | 123.90   |
| 1   | AA    | 204  | G    | C4-C5-N7    | -8.00 | 107.60      | 110.80   |
| 1   | AA    | 1235 | U    | C4-C5-C6    | 8.00  | 124.50      | 119.70   |
| 1   | AA    | 1288 | A    | C4-C5-C6    | 8.00  | 121.00      | 117.00   |
| 1   | AA    | 1484 | C    | N3-C4-C5    | -8.00 | 118.70      | 121.90   |
| 35  | BB    | 189  | G    | N1-C2-N2    | -8.00 | 109.00      | 116.20   |
| 35  | BB    | 276  | U    | N3-C4-O4    | 8.00  | 125.00      | 119.40   |
| 35  | BB    | 1365 | A    | N7-C8-N9    | 8.00  | 117.80      | 113.80   |
| 35  | BB    | 1846 | G    | O4'-C1'-N9  | 8.00  | 114.60      | 108.20   |
| 35  | BB    | 261  | G    | O4'-C1'-N9  | 8.00  | 114.60      | 108.20   |
| 35  | BB    | 947  | A    | C5-C6-N6    | -8.00 | 117.30      | 123.70   |
| 1   | AA    | 351  | G    | C6-C5-N7    | -8.00 | 125.60      | 130.40   |
| 35  | BB    | 906  | U    | O4'-C1'-N1  | 8.00  | 114.60      | 108.20   |
| 35  | BB    | 2312 | U    | N1-C2-N3    | -8.00 | 110.10      | 114.90   |
| 35  | BB    | 2683 | C    | C4'-C3'-C2' | -8.00 | 94.60       | 102.60   |
| 37  | BD    | 118  | PHE  | CB-CG-CD2   | 8.00  | 126.40      | 120.80   |
| 1   | AA    | 392  | C    | O4'-C1'-N1  | 8.00  | 114.60      | 108.20   |
| 1   | AA    | 568  | G    | N9-C4-C5    | -8.00 | 102.20      | 105.40   |
| 35  | BB    | 2125 | G    | N1-C6-O6    | 8.00  | 124.70      | 119.90   |
| 35  | BB    | 64   | A    | C2-N3-C4    | -8.00 | 106.60      | 110.60   |
| 35  | BB    | 293  | U    | O4'-C1'-N1  | 8.00  | 114.60      | 108.20   |
| 35  | BB    | 661  | A    | N1-C6-N6    | 8.00  | 123.40      | 118.60   |
| 35  | BB    | 734  | A    | C5-C6-N1    | -8.00 | 113.70      | 117.70   |
| 35  | BB    | 864  | G    | C6-N1-C2    | 8.00  | 129.90      | 125.10   |
| 1   | AA    | 150  | U    | O4'-C1'-N1  | 8.00  | 114.60      | 108.20   |
| 34  | BA    | 87   | U    | P-O3'-C3'   | 8.00  | 129.29      | 119.70   |
| 35  | BB    | 1370 | C    | C5-C6-N1    | 7.99  | 125.00      | 121.00   |
| 35  | BB    | 1513 | U    | O4'-C1'-N1  | 7.99  | 114.59      | 108.20   |
| 35  | BB    | 2109 | U    | O4'-C1'-N1  | 7.99  | 114.59      | 108.20   |
| 35  | BB    | 2506 | U    | C5-C6-N1    | 7.99  | 126.70      | 122.70   |
| 1   | AA    | 1148 | U    | O4'-C1'-N1  | 7.99  | 114.59      | 108.20   |
| 34  | BA    | 30   | C    | O4'-C1'-N1  | 7.99  | 114.59      | 108.20   |
| 35  | BB    | 563  | A    | C5-C6-N1    | -7.99 | 113.70      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 701  | G    | C6-C5-N7    | -7.99 | 125.61      | 130.40   |
| 35  | BB    | 1112 | G    | O4'-C1'-N9  | 7.99  | 114.59      | 108.20   |
| 35  | BB    | 1705 | A    | C5-C6-N6    | -7.99 | 117.31      | 123.70   |
| 1   | AA    | 298  | A    | C4-C5-C6    | 7.99  | 121.00      | 117.00   |
| 1   | AA    | 391  | G    | C2-N3-C4    | 7.99  | 115.90      | 111.90   |
| 35  | BB    | 285  | G    | C6-C5-N7    | -7.99 | 125.61      | 130.40   |
| 35  | BB    | 342  | A    | O4'-C1'-N9  | 7.99  | 114.59      | 108.20   |
| 35  | BB    | 675  | A    | C5-C6-N1    | -7.99 | 113.70      | 117.70   |
| 35  | BB    | 1247 | A    | C4-C5-C6    | 7.99  | 121.00      | 117.00   |
| 35  | BB    | 2544 | G    | N1-C6-O6    | 7.99  | 124.69      | 119.90   |
| 1   | AA    | 168  | G    | C4-C5-C6    | 7.99  | 123.59      | 118.80   |
| 1   | AA    | 263  | A    | C6-C5-N7    | -7.99 | 126.71      | 132.30   |
| 35  | BB    | 743  | A    | N7-C8-N9    | -7.99 | 109.81      | 113.80   |
| 35  | BB    | 303  | G    | O4'-C1'-N9  | 7.99  | 114.59      | 108.20   |
| 35  | BB    | 835  | C    | O4'-C1'-N1  | 7.99  | 114.59      | 108.20   |
| 35  | BB    | 2268 | A    | C4-C5-N7    | -7.99 | 106.71      | 110.70   |
| 1   | AA    | 72   | A    | P-O5'-C5'   | 7.99  | 133.68      | 120.90   |
| 1   | AA    | 140  | U    | P-O3'-C3'   | -7.99 | 110.12      | 119.70   |
| 1   | AA    | 1306 | A    | N1-C2-N3    | -7.99 | 125.31      | 129.30   |
| 1   | AA    | 1414 | U    | C5-C6-N1    | 7.99  | 126.69      | 122.70   |
| 35  | BB    | 778  | G    | N7-C8-N9    | 7.99  | 117.09      | 113.10   |
| 35  | BB    | 2866 | U    | C4-C5-C6    | 7.99  | 124.49      | 119.70   |
| 51  | BR    | 21   | ARG  | NE-CZ-NH1   | -7.99 | 116.31      | 120.30   |
| 1   | AA    | 633  | G    | O4'-C1'-N9  | 7.98  | 114.59      | 108.20   |
| 1   | AA    | 1140 | C    | O4'-C1'-N1  | 7.98  | 114.59      | 108.20   |
| 35  | BB    | 1406 | U    | O4'-C1'-N1  | 7.98  | 114.59      | 108.20   |
| 35  | BB    | 2495 | G    | C5-N7-C8    | 7.98  | 108.29      | 104.30   |
| 1   | AA    | 1157 | A    | C4-C5-C6    | 7.98  | 120.99      | 117.00   |
| 34  | BA    | 72   | G    | N3-C2-N2    | 7.98  | 125.49      | 119.90   |
| 35  | BB    | 1037 | G    | O4'-C1'-N9  | 7.98  | 114.59      | 108.20   |
| 35  | BB    | 2173 | A    | C5-C6-N6    | -7.98 | 117.31      | 123.70   |
| 1   | AA    | 299  | G    | C8-N9-C4    | 7.98  | 109.59      | 106.40   |
| 1   | AA    | 526  | C    | N3-C4-N4    | 7.98  | 123.59      | 118.00   |
| 35  | BB    | 183  | C    | N3-C4-C5    | -7.98 | 118.71      | 121.90   |
| 35  | BB    | 205  | G    | C4'-C3'-C2' | -7.98 | 94.62       | 102.60   |
| 35  | BB    | 248  | G    | N1-C2-N3    | -7.98 | 119.11      | 123.90   |
| 35  | BB    | 296  | U    | O4'-C1'-N1  | 7.98  | 114.58      | 108.20   |
| 35  | BB    | 157  | C    | C6-N1-C2    | -7.98 | 117.11      | 120.30   |
| 35  | BB    | 1279 | G    | N9-C4-C5    | 7.98  | 108.59      | 105.40   |
| 35  | BB    | 1604 | C    | C5-C4-N4    | -7.98 | 114.61      | 120.20   |
| 1   | AA    | 818  | G    | C2-N3-C4    | 7.98  | 115.89      | 111.90   |
| 1   | AA    | 900  | A    | O4'-C1'-N9  | 7.98  | 114.58      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 949  | A    | C5-C6-N1    | -7.98 | 113.71      | 117.70   |
| 35  | BB    | 445  | C    | N3-C4-N4    | 7.98  | 123.58      | 118.00   |
| 35  | BB    | 605  | G    | N7-C8-N9    | -7.98 | 109.11      | 113.10   |
| 35  | BB    | 1826 | G    | C4-C5-C6    | 7.98  | 123.59      | 118.80   |
| 35  | BB    | 2021 | C    | C5-C4-N4    | -7.98 | 114.62      | 120.20   |
| 35  | BB    | 825  | A    | C5-C6-N1    | -7.98 | 113.71      | 117.70   |
| 35  | BB    | 1067 | A    | C5-C6-N1    | -7.98 | 113.71      | 117.70   |
| 1   | AA    | 130  | A    | P-O3'-C3'   | 7.97  | 129.27      | 119.70   |
| 35  | BB    | 1803 | A    | C6-C5-N7    | -7.97 | 126.72      | 132.30   |
| 35  | BB    | 1833 | C    | O4'-C1'-N1  | 7.97  | 114.58      | 108.20   |
| 35  | BB    | 1847 | A    | C2-N3-C4    | -7.97 | 106.61      | 110.60   |
| 35  | BB    | 2452 | C    | P-O5'-C5'   | -7.97 | 108.14      | 120.90   |
| 35  | BB    | 2496 | C    | C4-C5-C6    | 7.97  | 121.39      | 117.40   |
| 35  | BB    | 2765 | A    | N1-C2-N3    | 7.97  | 133.29      | 129.30   |
| 1   | AA    | 35   | G    | N3-C2-N2    | 7.97  | 125.48      | 119.90   |
| 1   | AA    | 364  | A    | C1'-O4'-C4' | 7.97  | 116.28      | 109.90   |
| 1   | AA    | 540  | G    | C5-C6-O6    | -7.97 | 123.82      | 128.60   |
| 35  | BB    | 1596 | A    | N1-C6-N6    | 7.97  | 123.38      | 118.60   |
| 35  | BB    | 2082 | A    | O4'-C1'-N9  | 7.97  | 114.58      | 108.20   |
| 35  | BB    | 2161 | C    | O4'-C4'-C3' | -7.97 | 96.03       | 104.00   |
| 1   | AA    | 1368 | A    | C4-C5-C6    | 7.97  | 120.99      | 117.00   |
| 4   | AD    | 114  | ARG  | NE-CZ-NH1   | -7.97 | 116.31      | 120.30   |
| 1   | AA    | 384  | G    | C8-N9-C4    | -7.97 | 103.21      | 106.40   |
| 1   | AA    | 1340 | A    | N1-C2-N3    | 7.97  | 133.28      | 129.30   |
| 35  | BB    | 334  | C    | O4'-C1'-N1  | 7.97  | 114.58      | 108.20   |
| 35  | BB    | 1982 | U    | O4'-C1'-N1  | 7.97  | 114.58      | 108.20   |
| 35  | BB    | 2214 | C    | O4'-C1'-N1  | 7.97  | 114.58      | 108.20   |
| 35  | BB    | 610  | C    | C5-C6-N1    | 7.97  | 124.98      | 121.00   |
| 1   | AA    | 73   | C    | N3-C4-C5    | -7.97 | 118.71      | 121.90   |
| 1   | AA    | 228  | A    | N1-C6-N6    | 7.97  | 123.38      | 118.60   |
| 35  | BB    | 696  | G    | C4'-C3'-C2' | -7.97 | 94.63       | 102.60   |
| 48  | BO    | 16   | ARG  | NE-CZ-NH2   | -7.97 | 116.32      | 120.30   |
| 1   | AA    | 1269 | A    | C6-N1-C2    | 7.96  | 123.38      | 118.60   |
| 35  | BB    | 175  | G    | N3-C2-N2    | 7.96  | 125.47      | 119.90   |
| 35  | BB    | 442  | G    | C2-N3-C4    | 7.96  | 115.88      | 111.90   |
| 35  | BB    | 1277 | G    | C5-N7-C8    | -7.96 | 100.32      | 104.30   |
| 35  | BB    | 1547 | C    | C2-N3-C4    | 7.96  | 123.88      | 119.90   |
| 35  | BB    | 1583 | A    | N9-C4-C5    | 7.96  | 108.99      | 105.80   |
| 35  | BB    | 1603 | A    | C5-C6-N6    | -7.96 | 117.33      | 123.70   |
| 35  | BB    | 2039 | U    | C5-C4-O4    | -7.96 | 121.12      | 125.90   |
| 35  | BB    | 2368 | C    | C6-N1-C2    | -7.96 | 117.11      | 120.30   |
| 1   | AA    | 1300 | G    | N7-C8-N9    | -7.96 | 109.12      | 113.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1419 | A    | C5-C6-N6    | -7.96 | 117.33      | 123.70   |
| 35  | BB    | 2389 | G    | O4'-C1'-N9  | 7.96  | 114.57      | 108.20   |
| 1   | AA    | 904  | U    | C6-N1-C2    | 7.96  | 125.78      | 121.00   |
| 35  | BB    | 101  | A    | C5-C6-N6    | -7.96 | 117.33      | 123.70   |
| 35  | BB    | 1754 | A    | N7-C8-N9    | -7.96 | 109.82      | 113.80   |
| 50  | BQ    | 46   | TYR  | CG-CD2-CE2  | -7.96 | 114.93      | 121.30   |
| 34  | BA    | 13   | G    | N7-C8-N9    | 7.96  | 117.08      | 113.10   |
| 35  | BB    | 117  | G    | C5-N7-C8    | -7.96 | 100.32      | 104.30   |
| 35  | BB    | 824  | U    | C5-C4-O4    | 7.96  | 130.68      | 125.90   |
| 35  | BB    | 1618 | A    | N1-C2-N3    | 7.96  | 133.28      | 129.30   |
| 35  | BB    | 1711 | A    | C5-C6-N1    | -7.96 | 113.72      | 117.70   |
| 1   | AA    | 236  | A    | C5-C6-N1    | -7.96 | 113.72      | 117.70   |
| 1   | AA    | 1214 | C    | C2-N3-C4    | 7.96  | 123.88      | 119.90   |
| 35  | BB    | 596  | U    | C6-N1-C2    | -7.96 | 116.22      | 121.00   |
| 35  | BB    | 971  | G    | N1-C2-N3    | -7.96 | 119.12      | 123.90   |
| 35  | BB    | 1503 | A    | N1-C6-N6    | 7.96  | 123.38      | 118.60   |
| 35  | BB    | 2437 | G    | O4'-C1'-N9  | 7.96  | 114.57      | 108.20   |
| 1   | AA    | 903  | G    | C5-N7-C8    | 7.96  | 108.28      | 104.30   |
| 1   | AA    | 1491 | G    | N3-C2-N2    | 7.96  | 125.47      | 119.90   |
| 35  | BB    | 278  | A    | C4-C5-N7    | -7.96 | 106.72      | 110.70   |
| 35  | BB    | 256  | A    | C5-C6-N6    | -7.96 | 117.34      | 123.70   |
| 35  | BB    | 2474 | U    | O4'-C1'-N1  | 7.96  | 114.56      | 108.20   |
| 1   | AA    | 396  | C    | C2-N3-C4    | 7.95  | 123.88      | 119.90   |
| 35  | BB    | 175  | G    | O4'-C1'-N9  | 7.95  | 114.56      | 108.20   |
| 1   | AA    | 922  | G    | C5-C6-O6    | -7.95 | 123.83      | 128.60   |
| 35  | BB    | 505  | A    | C6-C5-N7    | -7.95 | 126.73      | 132.30   |
| 35  | BB    | 1807 | G    | N3-C4-N9    | -7.95 | 121.23      | 126.00   |
| 1   | AA    | 214  | C    | O4'-C1'-N1  | 7.95  | 114.56      | 108.20   |
| 1   | AA    | 599  | C    | O4'-C1'-N1  | 7.95  | 114.56      | 108.20   |
| 35  | BB    | 25   | U    | O4'-C1'-N1  | 7.95  | 114.56      | 108.20   |
| 35  | BB    | 1780 | A    | C6-C5-N7    | -7.95 | 126.73      | 132.30   |
| 35  | BB    | 2584 | U    | N3-C4-O4    | 7.95  | 124.97      | 119.40   |
| 35  | BB    | 2603 | G    | C5'-C4'-C3' | -7.95 | 103.28      | 116.00   |
| 55  | BW    | 57   | TYR  | CG-CD2-CE2  | -7.95 | 114.94      | 121.30   |
| 21  | AU    | 37   | TYR  | CB-CG-CD1   | 7.95  | 125.77      | 121.00   |
| 35  | BB    | 682  | G    | C6-C5-N7    | -7.95 | 125.63      | 130.40   |
| 35  | BB    | 957  | C    | C2-N3-C4    | 7.95  | 123.87      | 119.90   |
| 35  | BB    | 2088 | A    | O4'-C1'-N9  | 7.95  | 114.56      | 108.20   |
| 1   | AA    | 641  | U    | P-O3'-C3'   | 7.95  | 129.24      | 119.70   |
| 1   | AA    | 684  | U    | N3-C4-O4    | 7.95  | 124.96      | 119.40   |
| 1   | AA    | 281  | G    | N3-C2-N2    | 7.95  | 125.46      | 119.90   |
| 35  | BB    | 619  | G    | N1-C6-O6    | 7.95  | 124.67      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 905  | A    | N1-C6-N6    | 7.95  | 123.37      | 118.60   |
| 35  | BB    | 1609 | A    | C6-N1-C2    | 7.95  | 123.37      | 118.60   |
| 35  | BB    | 2124 | G    | N3-C2-N2    | 7.95  | 125.46      | 119.90   |
| 35  | BB    | 2879 | A    | C4-C5-C6    | 7.95  | 120.97      | 117.00   |
| 35  | BB    | 78   | U    | C5-C6-N1    | 7.94  | 126.67      | 122.70   |
| 35  | BB    | 2364 | C    | C6-N1-C2    | -7.94 | 117.12      | 120.30   |
| 1   | AA    | 1087 | G    | N3-C2-N2    | 7.94  | 125.46      | 119.90   |
| 35  | BB    | 2    | G    | N3-C2-N2    | 7.94  | 125.46      | 119.90   |
| 35  | BB    | 68   | G    | C5-C6-O6    | -7.94 | 123.83      | 128.60   |
| 35  | BB    | 89   | A    | C4-C5-C6    | 7.94  | 120.97      | 117.00   |
| 35  | BB    | 297  | G    | C5-C6-N1    | -7.94 | 107.53      | 111.50   |
| 35  | BB    | 1979 | U    | N3-C2-O2    | 7.94  | 127.76      | 122.20   |
| 35  | BB    | 2534 | A    | N9-C4-C5    | -7.94 | 102.62      | 105.80   |
| 1   | AA    | 644  | U    | N3-C4-O4    | 7.94  | 124.96      | 119.40   |
| 1   | AA    | 664  | G    | N1-C2-N3    | -7.94 | 119.14      | 123.90   |
| 1   | AA    | 950  | U    | N3-C4-C5    | 7.94  | 119.36      | 114.60   |
| 1   | AA    | 1470 | U    | N3-C4-C5    | -7.94 | 109.84      | 114.60   |
| 35  | BB    | 337  | C    | O4'-C1'-N1  | 7.94  | 114.55      | 108.20   |
| 35  | BB    | 2820 | A    | N3-C4-C5    | -7.94 | 121.24      | 126.80   |
| 1   | AA    | 494  | G    | C1'-O4'-C4' | 7.94  | 116.25      | 109.90   |
| 35  | BB    | 1714 | U    | C4-C5-C6    | 7.94  | 124.46      | 119.70   |
| 35  | BB    | 2730 | C    | O4'-C1'-N1  | 7.94  | 114.55      | 108.20   |
| 1   | AA    | 278  | G    | C5-C6-N1    | -7.94 | 107.53      | 111.50   |
| 1   | AA    | 799  | G    | C8-N9-C4    | -7.94 | 103.22      | 106.40   |
| 1   | AA    | 824  | G    | N1-C6-O6    | 7.94  | 124.66      | 119.90   |
| 1   | AA    | 1151 | A    | O4'-C1'-N9  | 7.94  | 114.55      | 108.20   |
| 35  | BB    | 771  | G    | C8-N9-C1'   | 7.94  | 137.32      | 127.00   |
| 35  | BB    | 1818 | U    | O4'-C4'-C3' | 7.94  | 112.45      | 106.10   |
| 35  | BB    | 2071 | A    | N1-C2-N3    | 7.94  | 133.27      | 129.30   |
| 1   | AA    | 1395 | C    | N1-C2-O2    | 7.94  | 123.66      | 118.90   |
| 35  | BB    | 2571 | U    | N3-C4-O4    | 7.94  | 124.95      | 119.40   |
| 1   | AA    | 31   | G    | C5-C6-N1    | -7.93 | 107.53      | 111.50   |
| 1   | AA    | 829  | G    | C4-C5-N7    | 7.93  | 113.97      | 110.80   |
| 35  | BB    | 418  | C    | C2-N3-C4    | 7.93  | 123.87      | 119.90   |
| 35  | BB    | 431  | U    | O4'-C1'-N1  | 7.93  | 114.55      | 108.20   |
| 35  | BB    | 607  | U    | C3'-C2'-C1' | 7.93  | 107.85      | 101.50   |
| 35  | BB    | 2336 | A    | C5-C6-N1    | -7.93 | 113.73      | 117.70   |
| 1   | AA    | 266  | G    | C5-N7-C8    | 7.93  | 108.27      | 104.30   |
| 1   | AA    | 281  | G    | O4'-C1'-N9  | 7.93  | 114.55      | 108.20   |
| 1   | AA    | 535  | A    | C8-N9-C4    | -7.93 | 102.63      | 105.80   |
| 1   | AA    | 1064 | G    | N1-C2-N3    | -7.93 | 119.14      | 123.90   |
| 35  | BB    | 279  | A    | C6-C5-N7    | -7.93 | 126.75      | 132.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 326  | G    | N1-C6-O6    | 7.93  | 124.66      | 119.90   |
| 35  | BB    | 798  | G    | N3-C4-N9    | -7.93 | 121.24      | 126.00   |
| 35  | BB    | 821  | A    | P-O3'-C3'   | 7.93  | 129.22      | 119.70   |
| 35  | BB    | 1202 | G    | C5-C6-O6    | -7.93 | 123.84      | 128.60   |
| 35  | BB    | 1679 | A    | C8-N9-C4    | -7.93 | 102.63      | 105.80   |
| 1   | AA    | 357  | G    | N1-C2-N3    | -7.93 | 119.14      | 123.90   |
| 1   | AA    | 574  | A    | P-O3'-C3'   | 7.93  | 129.22      | 119.70   |
| 1   | AA    | 847  | G    | C4-C5-N7    | 7.93  | 113.97      | 110.80   |
| 35  | BB    | 516  | C    | N3-C2-O2    | 7.93  | 127.45      | 121.90   |
| 35  | BB    | 2400 | G    | C5-C6-O6    | -7.93 | 123.84      | 128.60   |
| 1   | AA    | 59   | A    | C5-C6-N1    | -7.93 | 113.73      | 117.70   |
| 1   | AA    | 520  | A    | N9-C4-C5    | 7.93  | 108.97      | 105.80   |
| 1   | AA    | 896  | C    | C5-C4-N4    | -7.93 | 114.65      | 120.20   |
| 1   | AA    | 1013 | G    | O4'-C1'-N9  | 7.93  | 114.54      | 108.20   |
| 35  | BB    | 411  | G    | C5-C6-O6    | -7.93 | 123.84      | 128.60   |
| 35  | BB    | 1011 | G    | C2-N3-C4    | 7.93  | 115.86      | 111.90   |
| 35  | BB    | 2273 | A    | C4-C5-C6    | 7.93  | 120.97      | 117.00   |
| 35  | BB    | 2417 | C    | N3-C4-N4    | 7.93  | 123.55      | 118.00   |
| 35  | BB    | 2663 | G    | N1-C6-O6    | 7.93  | 124.66      | 119.90   |
| 35  | BB    | 1418 | G    | N3-C2-N2    | 7.93  | 125.45      | 119.90   |
| 35  | BB    | 2570 | G    | N1-C6-O6    | 7.93  | 124.66      | 119.90   |
| 1   | AA    | 1486 | G    | N1-C6-O6    | 7.93  | 124.66      | 119.90   |
| 22  | AV    | 39   | G    | C4-C5-C6    | 7.93  | 123.56      | 118.80   |
| 35  | BB    | 26   | G    | C1'-O4'-C4' | 7.93  | 116.24      | 109.90   |
| 35  | BB    | 1396 | U    | N3-C2-O2    | -7.93 | 116.65      | 122.20   |
| 35  | BB    | 1641 | A    | C5-C6-N1    | -7.93 | 113.74      | 117.70   |
| 35  | BB    | 1483 | G    | N1-C6-O6    | 7.92  | 124.66      | 119.90   |
| 35  | BB    | 1530 | G    | C5-C6-O6    | -7.92 | 123.84      | 128.60   |
| 35  | BB    | 2847 | U    | C6-N1-C2    | -7.92 | 116.25      | 121.00   |
| 1   | AA    | 222  | C    | N3-C4-N4    | 7.92  | 123.55      | 118.00   |
| 3   | AC    | 41   | TYR  | CB-CG-CD2   | -7.92 | 116.25      | 121.00   |
| 35  | BB    | 1502 | A    | C5-C6-N6    | -7.92 | 117.36      | 123.70   |
| 35  | BB    | 1821 | A    | C5-C6-N6    | -7.92 | 117.36      | 123.70   |
| 35  | BB    | 2639 | A    | C5-N7-C8    | 7.92  | 107.86      | 103.90   |
| 1   | AA    | 535  | A    | C4-C5-C6    | 7.92  | 120.96      | 117.00   |
| 1   | AA    | 596  | A    | C5-N7-C8    | 7.92  | 107.86      | 103.90   |
| 1   | AA    | 883  | C    | O4'-C1'-N1  | 7.92  | 114.54      | 108.20   |
| 34  | BA    | 51   | G    | C5-C6-O6    | -7.92 | 123.85      | 128.60   |
| 35  | BB    | 862  | G    | C4'-C3'-C2' | -7.92 | 94.68       | 102.60   |
| 35  | BB    | 873  | C    | C5-C4-N4    | -7.92 | 114.66      | 120.20   |
| 35  | BB    | 1161 | C    | C5-C4-N4    | -7.92 | 114.66      | 120.20   |
| 35  | BB    | 1170 | C    | O4'-C1'-N1  | 7.92  | 114.54      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1174 | U    | C2-N3-C4    | -7.92 | 122.25      | 127.00   |
| 35  | BB    | 1419 | A    | N1-C2-N3    | 7.92  | 133.26      | 129.30   |
| 35  | BB    | 1536 | C    | N3-C4-C5    | -7.92 | 118.73      | 121.90   |
| 35  | BB    | 2057 | G    | N1-C2-N3    | -7.92 | 119.15      | 123.90   |
| 25  | B0    | 49   | ARG  | NE-CZ-NH1   | -7.92 | 116.34      | 120.30   |
| 35  | BB    | 538  | A    | C5-N7-C8    | 7.92  | 107.86      | 103.90   |
| 1   | AA    | 600  | A    | C5-C6-N6    | -7.92 | 117.36      | 123.70   |
| 35  | BB    | 1298 | C    | C2-N3-C4    | 7.92  | 123.86      | 119.90   |
| 35  | BB    | 2454 | G    | C5-C6-O6    | -7.92 | 123.85      | 128.60   |
| 35  | BB    | 443  | A    | O4'-C1'-N9  | 7.92  | 114.53      | 108.20   |
| 35  | BB    | 451  | U    | C2-N3-C4    | -7.92 | 122.25      | 127.00   |
| 35  | BB    | 1057 | A    | P-O3'-C3'   | -7.92 | 110.20      | 119.70   |
| 35  | BB    | 1215 | G    | N3-C4-N9    | -7.92 | 121.25      | 126.00   |
| 35  | BB    | 1426 | G    | C5-C6-O6    | -7.92 | 123.85      | 128.60   |
| 35  | BB    | 2503 | A    | C2-N3-C4    | -7.92 | 106.64      | 110.60   |
| 35  | BB    | 2675 | A    | C8-N9-C4    | -7.92 | 102.63      | 105.80   |
| 46  | BM    | 44   | ARG  | NE-CZ-NH2   | 7.92  | 124.26      | 120.30   |
| 35  | BB    | 1449 | G    | O4'-C1'-N9  | 7.92  | 114.53      | 108.20   |
| 1   | AA    | 272  | C    | O4'-C1'-N1  | 7.91  | 114.53      | 108.20   |
| 1   | AA    | 1062 | U    | O4'-C1'-N1  | 7.91  | 114.53      | 108.20   |
| 1   | AA    | 1182 | G    | C5'-C4'-O4' | 7.91  | 118.59      | 109.10   |
| 1   | AA    | 1433 | A    | C5-C6-N1    | -7.91 | 113.74      | 117.70   |
| 35  | BB    | 309  | A    | C4-C5-N7    | -7.91 | 106.74      | 110.70   |
| 35  | BB    | 509  | C    | C3'-C2'-C1' | 7.91  | 107.83      | 101.50   |
| 35  | BB    | 2477 | U    | N1-C2-O2    | -7.91 | 117.26      | 122.80   |
| 35  | BB    | 2484 | G    | N1-C6-O6    | 7.91  | 124.65      | 119.90   |
| 1   | AA    | 278  | G    | N1-C2-N2    | -7.91 | 109.08      | 116.20   |
| 1   | AA    | 1035 | A    | C4-C5-C6    | 7.91  | 120.96      | 117.00   |
| 35  | BB    | 288  | U    | O4'-C1'-N1  | 7.91  | 114.53      | 108.20   |
| 35  | BB    | 329  | G    | N7-C8-N9    | 7.91  | 117.06      | 113.10   |
| 35  | BB    | 1801 | A    | C8-N9-C4    | -7.91 | 102.64      | 105.80   |
| 35  | BB    | 2150 | C    | O4'-C1'-N1  | 7.91  | 114.53      | 108.20   |
| 1   | AA    | 21   | G    | C5-C6-O6    | -7.91 | 123.85      | 128.60   |
| 1   | AA    | 228  | A    | C6-C5-N7    | -7.91 | 126.76      | 132.30   |
| 1   | AA    | 350  | G    | N1-C2-N3    | -7.91 | 119.15      | 123.90   |
| 1   | AA    | 700  | G    | N7-C8-N9    | -7.91 | 109.14      | 113.10   |
| 1   | AA    | 1164 | G    | C5-C6-N1    | -7.91 | 107.55      | 111.50   |
| 35  | BB    | 17   | G    | N3-C2-N2    | 7.91  | 125.44      | 119.90   |
| 35  | BB    | 1055 | G    | C5-C6-N1    | 7.91  | 115.45      | 111.50   |
| 1   | AA    | 222  | C    | C6-N1-C2    | -7.91 | 117.14      | 120.30   |
| 1   | AA    | 597  | G    | O4'-C1'-N9  | 7.91  | 114.53      | 108.20   |
| 34  | BA    | 2    | G    | N1-C6-O6    | 7.91  | 124.64      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 42   | A    | N1-C6-N6   | 7.91  | 123.34      | 118.60   |
| 35  | BB    | 158  | U    | O4'-C1'-N1 | 7.91  | 114.53      | 108.20   |
| 35  | BB    | 508  | A    | C6-C5-N7   | -7.91 | 126.76      | 132.30   |
| 35  | BB    | 909  | A    | N9-C4-C5   | -7.91 | 102.64      | 105.80   |
| 35  | BB    | 1564 | C    | C5-C4-N4   | -7.91 | 114.66      | 120.20   |
| 35  | BB    | 1566 | A    | C6-N1-C2   | 7.91  | 123.34      | 118.60   |
| 35  | BB    | 1631 | G    | C6-C5-N7   | -7.91 | 125.66      | 130.40   |
| 35  | BB    | 1854 | A    | C5-C6-N1   | -7.91 | 113.75      | 117.70   |
| 35  | BB    | 2360 | G    | N3-C2-N2   | 7.91  | 125.44      | 119.90   |
| 1   | AA    | 652  | U    | P-O3'-C3'  | -7.91 | 110.21      | 119.70   |
| 1   | AA    | 755  | G    | O4'-C1'-N9 | 7.91  | 114.53      | 108.20   |
| 1   | AA    | 888  | G    | C6-N1-C2   | 7.91  | 129.84      | 125.10   |
| 35  | BB    | 1482 | G    | C6-C5-N7   | -7.91 | 125.66      | 130.40   |
| 35  | BB    | 2750 | A    | N7-C8-N9   | -7.91 | 109.85      | 113.80   |
| 1   | AA    | 706  | A    | N9-C4-C5   | 7.91  | 108.96      | 105.80   |
| 1   | AA    | 777  | A    | C5-C6-N1   | -7.91 | 113.75      | 117.70   |
| 1   | AA    | 1053 | G    | C8-N9-C1'  | 7.91  | 137.28      | 127.00   |
| 34  | BA    | 32   | U    | C5-C6-N1   | 7.91  | 126.65      | 122.70   |
| 34  | BA    | 47   | C    | C5-C4-N4   | -7.91 | 114.67      | 120.20   |
| 35  | BB    | 646  | U    | N3-C4-C5   | -7.91 | 109.86      | 114.60   |
| 1   | AA    | 525  | C    | C4-C5-C6   | 7.90  | 121.35      | 117.40   |
| 1   | AA    | 749  | A    | N1-C2-N3   | 7.90  | 133.25      | 129.30   |
| 1   | AA    | 849  | G    | C5-C6-N1   | -7.90 | 107.55      | 111.50   |
| 1   | AA    | 462  | G    | C2-N3-C4   | 7.90  | 115.85      | 111.90   |
| 1   | AA    | 816  | A    | C6-N1-C2   | 7.90  | 123.34      | 118.60   |
| 1   | AA    | 1329 | A    | C5-C6-N6   | -7.90 | 117.38      | 123.70   |
| 35  | BB    | 85   | G    | O4'-C1'-N9 | 7.90  | 114.52      | 108.20   |
| 35  | BB    | 460  | A    | C5-C6-N1   | -7.90 | 113.75      | 117.70   |
| 35  | BB    | 1641 | A    | C4-C5-C6   | 7.90  | 120.95      | 117.00   |
| 38  | BE    | 117  | ARG  | NE-CZ-NH1  | 7.90  | 124.25      | 120.30   |
| 1   | AA    | 472  | U    | O4'-C1'-N1 | 7.90  | 114.52      | 108.20   |
| 1   | AA    | 701  | U    | O4'-C1'-N1 | 7.90  | 114.52      | 108.20   |
| 1   | AA    | 839  | C    | O4'-C1'-N1 | 7.90  | 114.52      | 108.20   |
| 1   | AA    | 931  | C    | C5-C6-N1   | 7.90  | 124.95      | 121.00   |
| 13  | AM    | 78   | ARG  | NE-CZ-NH2  | -7.90 | 116.35      | 120.30   |
| 35  | BB    | 653  | U    | N3-C4-C5   | -7.90 | 109.86      | 114.60   |
| 35  | BB    | 2099 | U    | N1-C2-O2   | -7.90 | 117.27      | 122.80   |
| 1   | AA    | 595  | A    | N1-C2-N3   | 7.90  | 133.25      | 129.30   |
| 12  | AL    | 65   | TYR  | CB-CG-CD2  | -7.90 | 116.26      | 121.00   |
| 35  | BB    | 1149 | G    | O4'-C1'-N9 | 7.90  | 114.52      | 108.20   |
| 35  | BB    | 1211 | C    | N3-C4-N4   | 7.90  | 123.53      | 118.00   |
| 35  | BB    | 2369 | A    | O4'-C1'-N9 | 7.90  | 114.52      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 507  | C    | P-O3'-C3'  | 7.90  | 129.18      | 119.70   |
| 1   | AA    | 593  | U    | O4'-C1'-N1 | 7.90  | 114.52      | 108.20   |
| 35  | BB    | 264  | C    | C5-C4-N4   | -7.90 | 114.67      | 120.20   |
| 35  | BB    | 1703 | G    | N1-C6-O6   | 7.90  | 124.64      | 119.90   |
| 35  | BB    | 2006 | C    | C6-N1-C2   | 7.90  | 123.46      | 120.30   |
| 35  | BB    | 2862 | G    | C6-C5-N7   | -7.90 | 125.66      | 130.40   |
| 1   | AA    | 833  | G    | C5-N7-C8   | 7.90  | 108.25      | 104.30   |
| 34  | BA    | 11   | C    | P-O3'-C3'  | 7.90  | 129.18      | 119.70   |
| 35  | BB    | 115  | C    | C5-C6-N1   | 7.90  | 124.95      | 121.00   |
| 35  | BB    | 1084 | A    | C5-N7-C8   | 7.90  | 107.85      | 103.90   |
| 35  | BB    | 1365 | A    | C8-N9-C4   | -7.90 | 102.64      | 105.80   |
| 35  | BB    | 1383 | A    | P-O3'-C3'  | 7.90  | 129.18      | 119.70   |
| 35  | BB    | 1952 | A    | C4-C5-C6   | 7.90  | 120.95      | 117.00   |
| 35  | BB    | 2254 | C    | C5-C6-N1   | -7.90 | 117.05      | 121.00   |
| 1   | AA    | 6    | G    | N1-C2-N3   | -7.89 | 119.16      | 123.90   |
| 22  | AV    | 65   | U    | O4'-C1'-N1 | 7.89  | 114.52      | 108.20   |
| 35  | BB    | 96   | C    | C5-C4-N4   | -7.89 | 114.67      | 120.20   |
| 35  | BB    | 642  | U    | C6-N1-C2   | 7.89  | 125.74      | 121.00   |
| 35  | BB    | 1054 | A    | O4'-C1'-N9 | 7.89  | 114.52      | 108.20   |
| 1   | AA    | 1166 | G    | N7-C8-N9   | -7.89 | 109.15      | 113.10   |
| 35  | BB    | 183  | C    | O4'-C1'-N1 | 7.89  | 114.51      | 108.20   |
| 35  | BB    | 1287 | A    | N1-C6-N6   | 7.89  | 123.33      | 118.60   |
| 1   | AA    | 1075 | U    | C5-C4-O4   | -7.89 | 121.17      | 125.90   |
| 35  | BB    | 2116 | G    | N3-C2-N2   | 7.89  | 125.42      | 119.90   |
| 35  | BB    | 2799 | A    | N1-C6-N6   | 7.89  | 123.33      | 118.60   |
| 1   | AA    | 98   | A    | O4'-C1'-N9 | 7.89  | 114.51      | 108.20   |
| 1   | AA    | 612  | C    | N3-C4-C5   | -7.89 | 118.74      | 121.90   |
| 35  | BB    | 1748 | C    | C2-N3-C4   | 7.89  | 123.84      | 119.90   |
| 35  | BB    | 2733 | A    | C2-N3-C4   | -7.89 | 106.66      | 110.60   |
| 35  | BB    | 980  | A    | C6-N1-C2   | -7.89 | 113.87      | 118.60   |
| 1   | AA    | 617  | G    | C2-N3-C4   | -7.89 | 107.96      | 111.90   |
| 1   | AA    | 1470 | U    | N3-C2-O2   | 7.89  | 127.72      | 122.20   |
| 35  | BB    | 13   | A    | C5-N7-C8   | 7.89  | 107.84      | 103.90   |
| 35  | BB    | 697  | G    | O4'-C1'-N9 | 7.89  | 114.51      | 108.20   |
| 35  | BB    | 1974 | C    | N3-C4-C5   | -7.89 | 118.75      | 121.90   |
| 35  | BB    | 202  | U    | P-O3'-C3'  | 7.88  | 129.16      | 119.70   |
| 35  | BB    | 752  | A    | C6-C5-N7   | -7.88 | 126.78      | 132.30   |
| 35  | BB    | 874  | G    | C5-C6-O6   | -7.88 | 123.87      | 128.60   |
| 35  | BB    | 1814 | G    | C2-N3-C4   | 7.88  | 115.84      | 111.90   |
| 35  | BB    | 2270 | A    | O4'-C1'-N9 | 7.88  | 114.51      | 108.20   |
| 35  | BB    | 2527 | C    | O4'-C1'-N1 | 7.88  | 114.51      | 108.20   |
| 34  | BA    | 59   | A    | C2-N3-C4   | 7.88  | 114.54      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 206  | C    | C5-C4-N4    | -7.88 | 114.68      | 120.20   |
| 1   | AA    | 1252 | A    | C4-C5-C6    | 7.88  | 120.94      | 117.00   |
| 1   | AA    | 1390 | U    | O4'-C1'-N1  | 7.88  | 114.51      | 108.20   |
| 1   | AA    | 1409 | C    | N3-C4-N4    | 7.88  | 123.52      | 118.00   |
| 9   | AI    | 11   | ARG  | NE-CZ-NH1   | 7.88  | 124.24      | 120.30   |
| 22  | AV    | 62   | C    | O4'-C1'-N1  | 7.88  | 114.50      | 108.20   |
| 35  | BB    | 1005 | C    | C2-N1-C1'   | 7.88  | 127.47      | 118.80   |
| 35  | BB    | 1158 | C    | N3-C4-N4    | 7.88  | 123.52      | 118.00   |
| 35  | BB    | 2080 | A    | C4-C5-C6    | 7.88  | 120.94      | 117.00   |
| 35  | BB    | 2154 | A    | C4-C5-C6    | 7.88  | 120.94      | 117.00   |
| 35  | BB    | 2281 | A    | C6-N1-C2    | -7.88 | 113.87      | 118.60   |
| 35  | BB    | 2426 | A    | C5-N7-C8    | 7.88  | 107.84      | 103.90   |
| 45  | BL    | 107  | PHE  | CB-CG-CD2   | -7.88 | 115.28      | 120.80   |
| 35  | BB    | 1470 | A    | C5-C6-N1    | -7.88 | 113.76      | 117.70   |
| 1   | AA    | 1280 | A    | C2-N3-C4    | -7.88 | 106.66      | 110.60   |
| 22  | AV    | 11   | C    | O4'-C1'-N1  | 7.88  | 114.50      | 108.20   |
| 35  | BB    | 830  | G    | C4-C5-C6    | 7.88  | 123.53      | 118.80   |
| 35  | BB    | 1475 | G    | N3-C4-C5    | -7.88 | 124.66      | 128.60   |
| 35  | BB    | 2129 | C    | O4'-C1'-N1  | 7.88  | 114.50      | 108.20   |
| 35  | BB    | 2275 | C    | C4-C5-C6    | 7.88  | 121.34      | 117.40   |
| 35  | BB    | 2334 | U    | P-O3'-C3'   | 7.88  | 129.15      | 119.70   |
| 35  | BB    | 2684 | U    | C3'-C2'-C1' | 7.88  | 107.80      | 101.50   |
| 1   | AA    | 1471 | U    | C1'-O4'-C4' | 7.88  | 116.20      | 109.90   |
| 35  | BB    | 548  | G    | O4'-C1'-N9  | 7.88  | 114.50      | 108.20   |
| 35  | BB    | 2160 | C    | C4-C5-C6    | -7.88 | 113.46      | 117.40   |
| 1   | AA    | 597  | G    | P-O3'-C3'   | -7.88 | 110.25      | 119.70   |
| 1   | AA    | 1421 | G    | C5-C6-N1    | -7.88 | 107.56      | 111.50   |
| 1   | AA    | 1530 | G    | O4'-C1'-N9  | 7.88  | 114.50      | 108.20   |
| 35  | BB    | 1311 | G    | C5-C6-N1    | -7.88 | 107.56      | 111.50   |
| 1   | AA    | 60   | A    | C8-N9-C4    | -7.87 | 102.65      | 105.80   |
| 1   | AA    | 529  | G    | N9-C4-C5    | -7.87 | 102.25      | 105.40   |
| 1   | AA    | 588  | G    | O4'-C1'-N9  | 7.87  | 114.50      | 108.20   |
| 35  | BB    | 536  | G    | C5-C6-O6    | -7.87 | 123.88      | 128.60   |
| 35  | BB    | 1284 | A    | N9-C4-C5    | 7.87  | 108.95      | 105.80   |
| 35  | BB    | 1509 | A    | P-O3'-C3'   | 7.87  | 129.15      | 119.70   |
| 35  | BB    | 1792 | G    | N7-C8-N9    | -7.87 | 109.16      | 113.10   |
| 35  | BB    | 2138 | G    | O4'-C1'-N9  | 7.87  | 114.50      | 108.20   |
| 35  | BB    | 2538 | C    | O4'-C1'-N1  | 7.87  | 114.50      | 108.20   |
| 35  | BB    | 2678 | C    | C6-N1-C2    | -7.87 | 117.15      | 120.30   |
| 1   | AA    | 669  | G    | O4'-C1'-N9  | 7.87  | 114.50      | 108.20   |
| 1   | AA    | 946  | A    | C4-C5-C6    | 7.87  | 120.94      | 117.00   |
| 22  | AV    | 64   | C    | O4'-C1'-N1  | 7.87  | 114.50      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 241  | A    | C2-N3-C4    | -7.87 | 106.66      | 110.60   |
| 35  | BB    | 458  | G    | C2-N3-C4    | 7.87  | 115.84      | 111.90   |
| 35  | BB    | 796  | C    | C1'-O4'-C4' | 7.87  | 116.20      | 109.90   |
| 35  | BB    | 1266 | G    | C6-C5-N7    | -7.87 | 125.68      | 130.40   |
| 35  | BB    | 1409 | U    | N1-C2-N3    | -7.87 | 110.18      | 114.90   |
| 35  | BB    | 2594 | C    | O4'-C1'-N1  | 7.87  | 114.50      | 108.20   |
| 1   | AA    | 1015 | G    | O4'-C1'-N9  | 7.87  | 114.50      | 108.20   |
| 1   | AA    | 1111 | A    | P-O3'-C3'   | 7.87  | 129.14      | 119.70   |
| 1   | AA    | 1253 | G    | C5-C6-O6    | -7.87 | 123.88      | 128.60   |
| 35  | BB    | 567  | U    | C4'-C3'-C2' | -7.87 | 94.73       | 102.60   |
| 35  | BB    | 833  | A    | C5-N7-C8    | 7.87  | 107.83      | 103.90   |
| 35  | BB    | 890  | C    | N3-C4-N4    | 7.87  | 123.51      | 118.00   |
| 35  | BB    | 1393 | A    | C5-C6-N1    | -7.87 | 113.77      | 117.70   |
| 35  | BB    | 1948 | G    | N1-C6-O6    | -7.87 | 115.18      | 119.90   |
| 35  | BB    | 2758 | A    | C5-C6-N1    | 7.87  | 121.63      | 117.70   |
| 46  | BM    | 103  | TYR  | CB-CG-CD1   | -7.87 | 116.28      | 121.00   |
| 1   | AA    | 1253 | G    | C1'-O4'-C4' | 7.87  | 116.19      | 109.90   |
| 35  | BB    | 398  | C    | N3-C4-C5    | -7.87 | 118.75      | 121.90   |
| 1   | AA    | 312  | C    | C5-C4-N4    | -7.87 | 114.69      | 120.20   |
| 1   | AA    | 774  | G    | C5-N7-C8    | 7.87  | 108.23      | 104.30   |
| 1   | AA    | 1205 | U    | P-O3'-C3'   | 7.87  | 129.14      | 119.70   |
| 35  | BB    | 207  | A    | C5-C6-N6    | -7.87 | 117.41      | 123.70   |
| 35  | BB    | 746  | U    | C1'-O4'-C4' | -7.87 | 103.61      | 109.90   |
| 35  | BB    | 1209 | U    | N3-C4-C5    | -7.87 | 109.88      | 114.60   |
| 1   | AA    | 616  | G    | N7-C8-N9    | 7.86  | 117.03      | 113.10   |
| 1   | AA    | 1266 | G    | N1-C2-N3    | -7.86 | 119.18      | 123.90   |
| 35  | BB    | 542  | C    | C6-N1-C2    | -7.86 | 117.16      | 120.30   |
| 35  | BB    | 2447 | G    | O4'-C1'-N9  | 7.86  | 114.49      | 108.20   |
| 1   | AA    | 1355 | G    | C6-C5-N7    | -7.86 | 125.68      | 130.40   |
| 35  | BB    | 297  | G    | C4-C5-N7    | -7.86 | 107.66      | 110.80   |
| 35  | BB    | 854  | C    | O4'-C1'-N1  | 7.86  | 114.49      | 108.20   |
| 35  | BB    | 2813 | A    | C5-C6-N1    | -7.86 | 113.77      | 117.70   |
| 1   | AA    | 222  | C    | O4'-C1'-N1  | 7.86  | 114.49      | 108.20   |
| 1   | AA    | 494  | G    | N1-C6-O6    | 7.86  | 124.62      | 119.90   |
| 35  | BB    | 1434 | A    | C8-N9-C4    | 7.86  | 108.94      | 105.80   |
| 35  | BB    | 1579 | A    | N7-C8-N9    | -7.86 | 109.87      | 113.80   |
| 1   | AA    | 157  | U    | O4'-C1'-N1  | 7.86  | 114.49      | 108.20   |
| 35  | BB    | 706  | A    | C5-C6-N1    | -7.86 | 113.77      | 117.70   |
| 35  | BB    | 1417 | C    | N3-C4-N4    | 7.86  | 123.50      | 118.00   |
| 35  | BB    | 2059 | A    | N1-C6-N6    | 7.86  | 123.31      | 118.60   |
| 35  | BB    | 161  | A    | N1-C6-N6    | 7.86  | 123.31      | 118.60   |
| 35  | BB    | 198  | C    | N3-C4-N4    | 7.86  | 123.50      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 435  | C    | N3-C4-C5    | -7.86 | 118.76      | 121.90   |
| 35  | BB    | 2075 | U    | C6-N1-C2    | -7.86 | 116.29      | 121.00   |
| 1   | AA    | 1197 | A    | N9-C4-C5    | -7.86 | 102.66      | 105.80   |
| 35  | BB    | 209  | C    | C6-N1-C2    | -7.86 | 117.16      | 120.30   |
| 35  | BB    | 880  | G    | O4'-C1'-N9  | 7.86  | 114.48      | 108.20   |
| 35  | BB    | 942  | G    | N1-C6-O6    | 7.86  | 124.61      | 119.90   |
| 35  | BB    | 1087 | G    | C5-N7-C8    | -7.86 | 100.37      | 104.30   |
| 35  | BB    | 1574 | C    | N3-C4-N4    | 7.86  | 123.50      | 118.00   |
| 35  | BB    | 2547 | A    | N1-C6-N6    | 7.86  | 123.31      | 118.60   |
| 1   | AA    | 714  | G    | N1-C2-N3    | -7.85 | 119.19      | 123.90   |
| 35  | BB    | 2279 | G    | C8-N9-C4    | -7.85 | 103.26      | 106.40   |
| 1   | AA    | 1280 | A    | C6-N1-C2    | -7.85 | 113.89      | 118.60   |
| 35  | BB    | 154  | U    | O4'-C1'-N1  | 7.85  | 114.48      | 108.20   |
| 35  | BB    | 1268 | A    | N1-C6-N6    | 7.85  | 123.31      | 118.60   |
| 35  | BB    | 1360 | G    | C5-C6-N1    | 7.85  | 115.43      | 111.50   |
| 35  | BB    | 2787 | C    | C2-N3-C4    | 7.85  | 123.83      | 119.90   |
| 1   | AA    | 83   | C    | C6-N1-C2    | -7.85 | 117.16      | 120.30   |
| 1   | AA    | 145  | G    | N1-C2-N3    | -7.85 | 119.19      | 123.90   |
| 35  | BB    | 331  | C    | C5-C6-N1    | 7.85  | 124.93      | 121.00   |
| 35  | BB    | 1499 | C    | C4-C5-C6    | 7.85  | 121.33      | 117.40   |
| 35  | BB    | 626  | A    | C4-C5-C6    | 7.85  | 120.92      | 117.00   |
| 35  | BB    | 1756 | G    | P-O3'-C3'   | 7.85  | 129.12      | 119.70   |
| 35  | BB    | 1918 | A    | C8-N9-C4    | -7.85 | 102.66      | 105.80   |
| 35  | BB    | 1996 | C    | N3-C4-N4    | 7.85  | 123.50      | 118.00   |
| 1   | AA    | 261  | U    | C5-C4-O4    | -7.85 | 121.19      | 125.90   |
| 1   | AA    | 1150 | A    | C6-C5-N7    | -7.85 | 126.81      | 132.30   |
| 35  | BB    | 295  | G    | C3'-C2'-C1' | 7.85  | 107.78      | 101.50   |
| 35  | BB    | 1807 | G    | N7-C8-N9    | 7.85  | 117.02      | 113.10   |
| 35  | BB    | 2826 | A    | C5-C6-N6    | -7.85 | 117.42      | 123.70   |
| 1   | AA    | 1406 | U    | C5-C6-N1    | -7.85 | 118.78      | 122.70   |
| 35  | BB    | 425  | G    | N3-C4-C5    | 7.85  | 132.52      | 128.60   |
| 35  | BB    | 1422 | G    | N3-C2-N2    | 7.85  | 125.39      | 119.90   |
| 35  | BB    | 2354 | C    | O4'-C1'-N1  | 7.85  | 114.48      | 108.20   |
| 35  | BB    | 2794 | C    | N3-C4-C5    | -7.85 | 118.76      | 121.90   |
| 1   | AA    | 1006 | G    | C5-C6-O6    | -7.84 | 123.89      | 128.60   |
| 35  | BB    | 992  | C    | O4'-C1'-N1  | 7.84  | 114.48      | 108.20   |
| 35  | BB    | 1922 | G    | C1'-O4'-C4' | -7.84 | 103.62      | 109.90   |
| 35  | BB    | 2288 | A    | C5-C6-N6    | -7.84 | 117.42      | 123.70   |
| 1   | AA    | 159  | G    | C2-N3-C4    | 7.84  | 115.82      | 111.90   |
| 1   | AA    | 1343 | G    | O4'-C1'-N9  | 7.84  | 114.47      | 108.20   |
| 35  | BB    | 936  | A    | C4-C5-N7    | -7.84 | 106.78      | 110.70   |
| 35  | BB    | 1466 | U    | O4'-C1'-N1  | 7.84  | 114.47      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2129 | C    | C2-N3-C4    | 7.84  | 123.82      | 119.90   |
| 1   | AA    | 603  | U    | N1-C2-O2    | -7.84 | 117.31      | 122.80   |
| 22  | AV    | 71   | C    | O4'-C1'-N1  | 7.84  | 114.47      | 108.20   |
| 30  | B5    | 38   | PHE  | CB-CG-CD1   | 7.84  | 126.29      | 120.80   |
| 35  | BB    | 9    | G    | N1-C2-N3    | -7.84 | 119.19      | 123.90   |
| 35  | BB    | 79   | C    | C2-N3-C4    | 7.84  | 123.82      | 119.90   |
| 35  | BB    | 347  | A    | C5-C6-N1    | -7.84 | 113.78      | 117.70   |
| 35  | BB    | 1288 | G    | C6-C5-N7    | -7.84 | 125.69      | 130.40   |
| 35  | BB    | 1537 | G    | C6-N1-C2    | 7.84  | 129.81      | 125.10   |
| 35  | BB    | 2294 | G    | N1-C2-N3    | -7.84 | 119.19      | 123.90   |
| 35  | BB    | 2371 | G    | N7-C8-N9    | -7.84 | 109.18      | 113.10   |
| 35  | BB    | 2759 | G    | C5-C6-O6    | -7.84 | 123.89      | 128.60   |
| 35  | BB    | 2891 | U    | C5-C6-N1    | 7.84  | 126.62      | 122.70   |
| 35  | BB    | 1543 | G    | C4-C5-N7    | -7.84 | 107.66      | 110.80   |
| 35  | BB    | 1571 | A    | C4'-C3'-C2' | -7.84 | 94.76       | 102.60   |
| 35  | BB    | 2664 | G    | C6-N1-C2    | -7.84 | 120.40      | 125.10   |
| 1   | AA    | 1450 | U    | C6-N1-C2    | -7.84 | 116.30      | 121.00   |
| 35  | BB    | 1140 | C    | C3'-C2'-C1' | -7.84 | 95.23       | 101.50   |
| 1   | AA    | 737  | C    | O4'-C1'-N1  | 7.84  | 114.47      | 108.20   |
| 35  | BB    | 41   | C    | O4'-C1'-N1  | 7.84  | 114.47      | 108.20   |
| 35  | BB    | 100  | U    | C5-C4-O4    | -7.84 | 121.20      | 125.90   |
| 35  | BB    | 2337 | G    | N7-C8-N9    | 7.84  | 117.02      | 113.10   |
| 35  | BB    | 2398 | U    | O4'-C1'-N1  | 7.84  | 114.47      | 108.20   |
| 35  | BB    | 2621 | G    | O4'-C1'-N9  | 7.84  | 114.47      | 108.20   |
| 35  | BB    | 1903 | G    | C5-C6-N1    | 7.83  | 115.42      | 111.50   |
| 1   | AA    | 188  | C    | O4'-C1'-N1  | 7.83  | 114.47      | 108.20   |
| 1   | AA    | 319  | G    | C5-C6-O6    | -7.83 | 123.90      | 128.60   |
| 35  | BB    | 1354 | A    | C5-C6-N6    | -7.83 | 117.43      | 123.70   |
| 35  | BB    | 1463 | C    | C2-N3-C4    | 7.83  | 123.82      | 119.90   |
| 35  | BB    | 2321 | U    | O4'-C1'-N1  | 7.83  | 114.47      | 108.20   |
| 35  | BB    | 2620 | C    | N3-C4-N4    | 7.83  | 123.48      | 118.00   |
| 35  | BB    | 2682 | A    | O4'-C1'-N9  | 7.83  | 114.47      | 108.20   |
| 35  | BB    | 2776 | A    | C6-C5-N7    | -7.83 | 126.82      | 132.30   |
| 35  | BB    | 503  | A    | C5-C6-N6    | -7.83 | 117.44      | 123.70   |
| 35  | BB    | 877  | A    | N1-C6-N6    | 7.83  | 123.30      | 118.60   |
| 52  | BS    | 88   | ARG  | NE-CZ-NH2   | 7.83  | 124.22      | 120.30   |
| 1   | AA    | 60   | A    | C4'-C3'-C2' | -7.83 | 94.77       | 102.60   |
| 35  | BB    | 1481 | U    | N1-C2-O2    | -7.83 | 117.32      | 122.80   |
| 35  | BB    | 2632 | A    | C5-C6-N6    | -7.83 | 117.44      | 123.70   |
| 1   | AA    | 564  | C    | C5-C6-N1    | 7.83  | 124.91      | 121.00   |
| 35  | BB    | 391  | A    | C5-C6-N1    | -7.83 | 113.79      | 117.70   |
| 1   | AA    | 1309 | G    | N1-C6-O6    | 7.83  | 124.60      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1961 | C    | N3-C4-C5    | -7.83 | 118.77      | 121.90   |
| 35  | BB    | 2009 | A    | N7-C8-N9    | -7.83 | 109.89      | 113.80   |
| 1   | AA    | 115  | G    | N3-C4-C5    | -7.83 | 124.69      | 128.60   |
| 1   | AA    | 1522 | U    | C5-C6-N1    | 7.83  | 126.61      | 122.70   |
| 1   | AA    | 1524 | C    | N3-C4-C5    | -7.83 | 118.77      | 121.90   |
| 35  | BB    | 1551 | A    | C4'-C3'-C2' | -7.83 | 94.77       | 102.60   |
| 1   | AA    | 516  | U    | O4'-C1'-N1  | 7.82  | 114.46      | 108.20   |
| 1   | AA    | 1100 | C    | N3-C4-N4    | 7.82  | 123.48      | 118.00   |
| 1   | AA    | 1143 | G    | N3-C4-C5    | -7.82 | 124.69      | 128.60   |
| 28  | B3    | 28   | SER  | N-CA-CB     | 7.82  | 122.23      | 110.50   |
| 35  | BB    | 46   | G    | C5-C6-O6    | -7.82 | 123.91      | 128.60   |
| 1   | AA    | 1350 | A    | C5-C6-N6    | -7.82 | 117.44      | 123.70   |
| 35  | BB    | 1692 | U    | C6-N1-C2    | -7.82 | 116.31      | 121.00   |
| 1   | AA    | 177  | G    | C6-C5-N7    | -7.82 | 125.71      | 130.40   |
| 1   | AA    | 1347 | G    | C5-N7-C8    | 7.82  | 108.21      | 104.30   |
| 35  | BB    | 226  | A    | C8-N9-C4    | -7.82 | 102.67      | 105.80   |
| 35  | BB    | 382  | A    | N7-C8-N9    | -7.82 | 109.89      | 113.80   |
| 35  | BB    | 1007 | C    | O4'-C1'-N1  | 7.82  | 114.46      | 108.20   |
| 35  | BB    | 1186 | G    | N7-C8-N9    | 7.82  | 117.01      | 113.10   |
| 35  | BB    | 1252 | G    | C5-C6-N1    | -7.82 | 107.59      | 111.50   |
| 35  | BB    | 1755 | A    | C5-C6-N6    | -7.82 | 117.44      | 123.70   |
| 1   | AA    | 1295 | U    | C6-N1-C2    | -7.82 | 116.31      | 121.00   |
| 35  | BB    | 169  | G    | N1-C2-N3    | -7.82 | 119.21      | 123.90   |
| 35  | BB    | 1614 | A    | C4-C5-C6    | 7.82  | 120.91      | 117.00   |
| 35  | BB    | 1780 | A    | O4'-C1'-N9  | 7.82  | 114.46      | 108.20   |
| 35  | BB    | 2077 | A    | N9-C4-C5    | 7.82  | 108.93      | 105.80   |
| 1   | AA    | 27   | G    | C2-N3-C4    | 7.82  | 115.81      | 111.90   |
| 35  | BB    | 314  | C    | C5-C6-N1    | 7.82  | 124.91      | 121.00   |
| 35  | BB    | 2250 | G    | C5-C6-N1    | -7.82 | 107.59      | 111.50   |
| 35  | BB    | 2767 | C    | C4'-C3'-C2' | -7.82 | 94.78       | 102.60   |
| 1   | AA    | 313  | A    | C5-C6-N1    | -7.82 | 113.79      | 117.70   |
| 1   | AA    | 376  | G    | C6-C5-N7    | -7.82 | 125.71      | 130.40   |
| 1   | AA    | 600  | A    | C8-N9-C4    | 7.82  | 108.93      | 105.80   |
| 1   | AA    | 1434 | A    | C5-C6-N1    | -7.82 | 113.79      | 117.70   |
| 19  | AS    | 36   | ARG  | NE-CZ-NH1   | 7.81  | 124.21      | 120.30   |
| 35  | BB    | 1054 | A    | C5-C6-N6    | -7.81 | 117.45      | 123.70   |
| 35  | BB    | 1961 | C    | N3-C4-N4    | 7.81  | 123.47      | 118.00   |
| 1   | AA    | 591  | U    | C5-C6-N1    | 7.81  | 126.61      | 122.70   |
| 1   | AA    | 1530 | G    | C5-C6-O6    | -7.81 | 123.91      | 128.60   |
| 35  | BB    | 557  | C    | N3-C2-O2    | 7.81  | 127.37      | 121.90   |
| 35  | BB    | 704  | G    | N1-C2-N3    | -7.81 | 119.21      | 123.90   |
| 35  | BB    | 707  | G    | N1-C2-N2    | -7.81 | 109.17      | 116.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1737 | G    | N1-C6-O6    | 7.81  | 124.59      | 119.90   |
| 35  | BB    | 196  | A    | C5-C6-N6    | -7.81 | 117.45      | 123.70   |
| 35  | BB    | 1008 | A    | C4-C5-N7    | -7.81 | 106.80      | 110.70   |
| 35  | BB    | 1524 | G    | N3-C2-N2    | 7.81  | 125.37      | 119.90   |
| 35  | BB    | 2409 | G    | N7-C8-N9    | 7.81  | 117.00      | 113.10   |
| 35  | BB    | 2    | G    | O4'-C1'-N9  | 7.81  | 114.45      | 108.20   |
| 35  | BB    | 383  | C    | N3-C4-C5    | -7.81 | 118.78      | 121.90   |
| 35  | BB    | 1355 | G    | O4'-C1'-N9  | 7.81  | 114.45      | 108.20   |
| 1   | AA    | 1171 | A    | N1-C2-N3    | 7.81  | 133.20      | 129.30   |
| 35  | BB    | 180  | G    | C6-C5-N7    | -7.81 | 125.72      | 130.40   |
| 35  | BB    | 1164 | C    | O4'-C1'-N1  | 7.81  | 114.45      | 108.20   |
| 35  | BB    | 2063 | C    | N3-C2-O2    | 7.81  | 127.37      | 121.90   |
| 35  | BB    | 2567 | G    | C6-N1-C2    | -7.81 | 120.42      | 125.10   |
| 35  | BB    | 2798 | U    | N3-C4-C5    | -7.81 | 109.92      | 114.60   |
| 1   | AA    | 558  | G    | O4'-C1'-N9  | 7.81  | 114.44      | 108.20   |
| 35  | BB    | 909  | A    | C5-C6-N6    | -7.81 | 117.45      | 123.70   |
| 35  | BB    | 1617 | C    | C6-N1-C1'   | -7.81 | 111.43      | 120.80   |
| 35  | BB    | 2789 | C    | C5-C6-N1    | -7.81 | 117.10      | 121.00   |
| 1   | AA    | 384  | G    | N3-C4-C5    | -7.80 | 124.70      | 128.60   |
| 1   | AA    | 695  | A    | C2-N3-C4    | 7.80  | 114.50      | 110.60   |
| 1   | AA    | 710  | G    | O4'-C1'-N9  | 7.80  | 114.44      | 108.20   |
| 35  | BB    | 393  | C    | C6-N1-C2    | -7.80 | 117.18      | 120.30   |
| 35  | BB    | 796  | C    | C6-N1-C2    | 7.80  | 123.42      | 120.30   |
| 35  | BB    | 1089 | A    | P-O5'-C5'   | 7.80  | 133.39      | 120.90   |
| 35  | BB    | 2893 | A    | C4'-C3'-C2' | -7.80 | 94.80       | 102.60   |
| 1   | AA    | 423  | G    | C2-N3-C4    | 7.80  | 115.80      | 111.90   |
| 35  | BB    | 35   | G    | N3-C2-N2    | 7.80  | 125.36      | 119.90   |
| 35  | BB    | 305  | C    | N1-C2-O2    | 7.80  | 123.58      | 118.90   |
| 1   | AA    | 107  | G    | C6-C5-N7    | -7.80 | 125.72      | 130.40   |
| 1   | AA    | 374  | A    | C4-C5-C6    | 7.80  | 120.90      | 117.00   |
| 1   | AA    | 754  | C    | C6-N1-C2    | 7.80  | 123.42      | 120.30   |
| 1   | AA    | 966  | G    | C5-C6-N1    | -7.80 | 107.60      | 111.50   |
| 34  | BA    | 93   | C    | C2-N3-C4    | 7.80  | 123.80      | 119.90   |
| 35  | BB    | 887  | U    | N3-C2-O2    | -7.80 | 116.74      | 122.20   |
| 35  | BB    | 1248 | G    | C4-C5-N7    | 7.80  | 113.92      | 110.80   |
| 35  | BB    | 1334 | G    | N1-C2-N3    | -7.80 | 119.22      | 123.90   |
| 35  | BB    | 2406 | A    | N9-C4-C5    | 7.80  | 108.92      | 105.80   |
| 35  | BB    | 2761 | A    | O4'-C1'-N9  | 7.80  | 114.44      | 108.20   |
| 1   | AA    | 528  | C    | C4-C5-C6    | 7.80  | 121.30      | 117.40   |
| 35  | BB    | 1644 | C    | O4'-C1'-N1  | 7.80  | 114.44      | 108.20   |
| 1   | AA    | 250  | A    | C5-C6-N1    | -7.80 | 113.80      | 117.70   |
| 1   | AA    | 633  | G    | N9-C4-C5    | -7.80 | 102.28      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 475  | C    | N3-C4-N4    | 7.80  | 123.46      | 118.00   |
| 35  | BB    | 2036 | C    | C4-C5-C6    | 7.80  | 121.30      | 117.40   |
| 1   | AA    | 699  | C    | C5-C6-N1    | -7.79 | 117.10      | 121.00   |
| 34  | BA    | 34   | A    | O4'-C1'-N9  | 7.79  | 114.44      | 108.20   |
| 35  | BB    | 1052 | C    | C5-C6-N1    | 7.79  | 124.90      | 121.00   |
| 35  | BB    | 2063 | C    | N1-C2-N3    | -7.79 | 113.74      | 119.20   |
| 35  | BB    | 2369 | A    | C5-C6-N1    | -7.79 | 113.80      | 117.70   |
| 1   | AA    | 326  | G    | N3-C2-N2    | 7.79  | 125.36      | 119.90   |
| 1   | AA    | 700  | G    | N3-C2-N2    | 7.79  | 125.36      | 119.90   |
| 35  | BB    | 1560 | G    | O4'-C1'-N9  | 7.79  | 114.44      | 108.20   |
| 35  | BB    | 2685 | G    | O4'-C1'-N9  | 7.79  | 114.43      | 108.20   |
| 1   | AA    | 486  | U    | C5-C4-O4    | -7.79 | 121.22      | 125.90   |
| 1   | AA    | 925  | G    | N1-C2-N2    | -7.79 | 109.19      | 116.20   |
| 35  | BB    | 1976 | U    | P-O3'-C3'   | 7.79  | 129.05      | 119.70   |
| 1   | AA    | 1447 | A    | C5-C6-N1    | -7.79 | 113.81      | 117.70   |
| 35  | BB    | 44   | A    | O4'-C1'-N9  | 7.79  | 114.43      | 108.20   |
| 34  | BA    | 13   | G    | N3-C2-N2    | 7.79  | 125.35      | 119.90   |
| 35  | BB    | 237  | C    | C1'-O4'-C4' | 7.79  | 116.13      | 109.90   |
| 35  | BB    | 2442 | C    | N3-C4-N4    | 7.79  | 123.45      | 118.00   |
| 1   | AA    | 431  | A    | C5-N7-C8    | 7.79  | 107.79      | 103.90   |
| 1   | AA    | 1375 | A    | C8-N9-C4    | -7.79 | 102.69      | 105.80   |
| 34  | BA    | 75   | G    | O4'-C1'-N9  | 7.79  | 114.43      | 108.20   |
| 35  | BB    | 2274 | A    | C4-C5-C6    | 7.79  | 120.89      | 117.00   |
| 35  | BB    | 2571 | U    | C5-C4-O4    | -7.79 | 121.23      | 125.90   |
| 35  | BB    | 2585 | U    | C5-C6-N1    | 7.79  | 126.59      | 122.70   |
| 1   | AA    | 307  | C    | C5-C6-N1    | -7.79 | 117.11      | 121.00   |
| 1   | AA    | 800  | G    | N3-C2-N2    | 7.79  | 125.35      | 119.90   |
| 35  | BB    | 376  | G    | N1-C6-O6    | 7.79  | 124.57      | 119.90   |
| 35  | BB    | 750  | A    | N7-C8-N9    | 7.79  | 117.69      | 113.80   |
| 35  | BB    | 1706 | C    | N3-C4-C5    | -7.79 | 118.78      | 121.90   |
| 35  | BB    | 2012 | G    | C4'-C3'-C2' | -7.79 | 94.81       | 102.60   |
| 1   | AA    | 1214 | C    | C6-N1-C1'   | -7.78 | 111.46      | 120.80   |
| 1   | AA    | 1287 | A    | O4'-C1'-N9  | 7.78  | 114.43      | 108.20   |
| 1   | AA    | 1304 | G    | N3-C2-N2    | 7.78  | 125.35      | 119.90   |
| 35  | BB    | 930  | G    | N9-C4-C5    | 7.78  | 108.51      | 105.40   |
| 22  | AV    | 27   | C    | O4'-C1'-N1  | 7.78  | 114.43      | 108.20   |
| 35  | BB    | 373  | U    | O4'-C1'-N1  | 7.78  | 114.42      | 108.20   |
| 35  | BB    | 429  | A    | C5'-C4'-O4' | 7.78  | 118.44      | 109.10   |
| 35  | BB    | 793  | A    | O4'-C1'-N9  | 7.78  | 114.42      | 108.20   |
| 35  | BB    | 1516 | G    | N9-C4-C5    | -7.78 | 102.29      | 105.40   |
| 35  | BB    | 1682 | G    | C6-N1-C2    | 7.78  | 129.77      | 125.10   |
| 35  | BB    | 2224 | G    | N1-C2-N3    | -7.78 | 119.23      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36  | BC    | 166  | ARG  | NE-CZ-NH1   | 7.78  | 124.19      | 120.30   |
| 1   | AA    | 376  | G    | N1-C2-N2    | -7.78 | 109.20      | 116.20   |
| 35  | BB    | 626  | A    | N3-C4-C5    | -7.78 | 121.36      | 126.80   |
| 35  | BB    | 1738 | G    | C5-C6-O6    | -7.78 | 123.93      | 128.60   |
| 1   | AA    | 888  | G    | C5-C6-O6    | -7.78 | 123.93      | 128.60   |
| 1   | AA    | 1236 | A    | O4'-C1'-N9  | 7.78  | 114.42      | 108.20   |
| 1   | AA    | 1504 | G    | N3-C4-C5    | 7.78  | 132.49      | 128.60   |
| 1   | AA    | 1194 | U    | C5-C6-N1    | 7.78  | 126.59      | 122.70   |
| 34  | BA    | 4    | C    | C2-N3-C4    | -7.78 | 116.01      | 119.90   |
| 35  | BB    | 1023 | U    | O4'-C1'-N1  | 7.78  | 114.42      | 108.20   |
| 35  | BB    | 1408 | G    | C6-C5-N7    | -7.78 | 125.73      | 130.40   |
| 35  | BB    | 1990 | C    | C4-C5-C6    | 7.78  | 121.29      | 117.40   |
| 35  | BB    | 1059 | G    | C4-C5-N7    | 7.77  | 113.91      | 110.80   |
| 35  | BB    | 1923 | U    | N3-C4-C5    | -7.77 | 109.94      | 114.60   |
| 1   | AA    | 133  | U    | O4'-C1'-N1  | 7.77  | 114.42      | 108.20   |
| 1   | AA    | 394  | G    | C8-N9-C4    | -7.77 | 103.29      | 106.40   |
| 1   | AA    | 580  | C    | C4-C5-C6    | -7.77 | 113.51      | 117.40   |
| 1   | AA    | 988  | G    | C6-N1-C2    | -7.77 | 120.44      | 125.10   |
| 1   | AA    | 990  | C    | C5-C4-N4    | -7.77 | 114.76      | 120.20   |
| 1   | AA    | 1353 | G    | N1-C6-O6    | 7.77  | 124.56      | 119.90   |
| 35  | BB    | 290  | U    | N3-C4-C5    | 7.77  | 119.26      | 114.60   |
| 35  | BB    | 1491 | G    | N9-C4-C5    | -7.77 | 102.29      | 105.40   |
| 35  | BB    | 1919 | A    | O4'-C4'-C3' | -7.77 | 96.23       | 104.00   |
| 35  | BB    | 2144 | G    | C6-C5-N7    | -7.77 | 125.74      | 130.40   |
| 1   | AA    | 585  | G    | N9-C4-C5    | -7.77 | 102.29      | 105.40   |
| 35  | BB    | 670  | A    | C6-C5-N7    | -7.77 | 126.86      | 132.30   |
| 35  | BB    | 701  | G    | C4-C5-N7    | 7.77  | 113.91      | 110.80   |
| 1   | AA    | 270  | A    | C4-C5-N7    | -7.77 | 106.81      | 110.70   |
| 1   | AA    | 355  | C    | N1-C2-N3    | -7.77 | 113.76      | 119.20   |
| 1   | AA    | 366  | A    | C5-C6-N1    | -7.77 | 113.81      | 117.70   |
| 1   | AA    | 1237 | C    | C2-N3-C4    | 7.77  | 123.78      | 119.90   |
| 34  | BA    | 13   | G    | C8-N9-C4    | -7.77 | 103.29      | 106.40   |
| 35  | BB    | 915  | C    | O4'-C1'-N1  | 7.77  | 114.42      | 108.20   |
| 1   | AA    | 53   | A    | P-O3'-C3'   | 7.77  | 129.02      | 119.70   |
| 1   | AA    | 147  | G    | C1'-O4'-C4' | -7.77 | 103.69      | 109.90   |
| 1   | AA    | 310  | G    | C1'-O4'-C4' | 7.77  | 116.11      | 109.90   |
| 35  | BB    | 430  | A    | C6-C5-N7    | -7.77 | 126.86      | 132.30   |
| 35  | BB    | 535  | G    | C5-C6-O6    | -7.77 | 123.94      | 128.60   |
| 35  | BB    | 1140 | C    | N3-C4-C5    | -7.77 | 118.79      | 121.90   |
| 1   | AA    | 577  | G    | O4'-C1'-N9  | 7.76  | 114.41      | 108.20   |
| 1   | AA    | 1109 | C    | C5-C4-N4    | -7.76 | 114.77      | 120.20   |
| 35  | BB    | 52   | A    | C4-C5-C6    | 7.76  | 120.88      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1056 | G    | N3-C2-N2    | 7.76  | 125.33      | 119.90   |
| 35  | BB    | 1537 | G    | N1-C2-N3    | -7.76 | 119.24      | 123.90   |
| 35  | BB    | 2600 | A    | P-O3'-C3'   | -7.76 | 110.38      | 119.70   |
| 35  | BB    | 2748 | A    | C6-C5-N7    | -7.76 | 126.86      | 132.30   |
| 1   | AA    | 1304 | G    | C5-N7-C8    | -7.76 | 100.42      | 104.30   |
| 35  | BB    | 1171 | G    | C8-N9-C4    | -7.76 | 103.30      | 106.40   |
| 29  | B4    | 38   | PHE  | CB-CG-CD1   | 7.76  | 126.23      | 120.80   |
| 35  | BB    | 377  | G    | C5-C6-N1    | -7.76 | 107.62      | 111.50   |
| 35  | BB    | 538  | A    | C5-C6-N6    | -7.76 | 117.49      | 123.70   |
| 35  | BB    | 2004 | G    | O4'-C1'-N9  | 7.76  | 114.41      | 108.20   |
| 35  | BB    | 2602 | A    | C6-C5-N7    | -7.76 | 126.87      | 132.30   |
| 35  | BB    | 2611 | C    | O4'-C1'-N1  | 7.76  | 114.41      | 108.20   |
| 1   | AA    | 60   | A    | C4-C5-C6    | 7.76  | 120.88      | 117.00   |
| 1   | AA    | 198  | G    | O4'-C1'-N9  | 7.76  | 114.41      | 108.20   |
| 1   | AA    | 877  | G    | N3-C4-N9    | -7.76 | 121.34      | 126.00   |
| 2   | AB    | 138  | ARG  | NE-CZ-NH1   | -7.76 | 116.42      | 120.30   |
| 35  | BB    | 410  | G    | O4'-C1'-N9  | 7.76  | 114.41      | 108.20   |
| 35  | BB    | 491  | G    | N3-C4-N9    | 7.76  | 130.66      | 126.00   |
| 35  | BB    | 1093 | G    | C4-C5-N7    | -7.76 | 107.70      | 110.80   |
| 35  | BB    | 2869 | G    | C8-N9-C4    | -7.76 | 103.30      | 106.40   |
| 35  | BB    | 1272 | A    | C6-C5-N7    | -7.76 | 126.87      | 132.30   |
| 1   | AA    | 1164 | G    | C4-C5-C6    | 7.76  | 123.45      | 118.80   |
| 1   | AA    | 1184 | G    | C5-C6-N1    | -7.76 | 107.62      | 111.50   |
| 35  | BB    | 825  | A    | N3-C4-C5    | -7.76 | 121.37      | 126.80   |
| 35  | BB    | 1567 | G    | C5-N7-C8    | 7.76  | 108.18      | 104.30   |
| 35  | BB    | 2149 | U    | C5-C4-O4    | -7.76 | 121.25      | 125.90   |
| 35  | BB    | 2834 | G    | N3-C4-C5    | 7.76  | 132.48      | 128.60   |
| 1   | AA    | 509  | A    | C8-N9-C4    | -7.75 | 102.70      | 105.80   |
| 1   | AA    | 815  | A    | C6-C5-N7    | -7.75 | 126.87      | 132.30   |
| 35  | BB    | 558  | U    | C4'-C3'-C2' | -7.75 | 94.84       | 102.60   |
| 35  | BB    | 769  | U    | O4'-C1'-N1  | 7.75  | 114.40      | 108.20   |
| 35  | BB    | 1469 | A    | C4-C5-N7    | -7.75 | 106.82      | 110.70   |
| 35  | BB    | 1646 | C    | N3-C4-N4    | 7.75  | 123.43      | 118.00   |
| 1   | AA    | 649  | A    | O4'-C1'-N9  | 7.75  | 114.40      | 108.20   |
| 1   | AA    | 1288 | A    | C5-C6-N6    | -7.75 | 117.50      | 123.70   |
| 31  | B6    | 32   | ALA  | N-CA-CB     | 7.75  | 120.95      | 110.10   |
| 35  | BB    | 916  | G    | C6-C5-N7    | -7.75 | 125.75      | 130.40   |
| 35  | BB    | 1668 | A    | C4-C5-C6    | 7.75  | 120.88      | 117.00   |
| 35  | BB    | 1803 | A    | C8-N9-C4    | -7.75 | 102.70      | 105.80   |
| 35  | BB    | 2189 | U    | N1-C2-N3    | 7.75  | 119.55      | 114.90   |
| 35  | BB    | 2326 | C    | C5-C4-N4    | -7.75 | 114.77      | 120.20   |
| 1   | AA    | 32   | A    | C5-C6-N6    | -7.75 | 117.50      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 43   | C    | C4-C5-C6    | 7.75  | 121.28      | 117.40   |
| 1   | AA    | 528  | C    | C2-N3-C4    | 7.75  | 123.78      | 119.90   |
| 1   | AA    | 546  | A    | C4-C5-C6    | 7.75  | 120.88      | 117.00   |
| 35  | BB    | 423  | A    | C5-C6-N6    | -7.75 | 117.50      | 123.70   |
| 35  | BB    | 1427 | A    | O4'-C1'-N9  | 7.75  | 114.40      | 108.20   |
| 35  | BB    | 1496 | A    | N3-C4-C5    | -7.75 | 121.37      | 126.80   |
| 35  | BB    | 2351 | G    | N1-C2-N2    | -7.75 | 109.22      | 116.20   |
| 35  | BB    | 2516 | A    | N7-C8-N9    | 7.75  | 117.68      | 113.80   |
| 1   | AA    | 196  | A    | N1-C6-N6    | 7.75  | 123.25      | 118.60   |
| 1   | AA    | 214  | C    | N1-C2-N3    | -7.75 | 113.78      | 119.20   |
| 1   | AA    | 451  | A    | O4'-C1'-N9  | 7.75  | 114.40      | 108.20   |
| 1   | AA    | 1120 | C    | C5-C6-N1    | 7.75  | 124.88      | 121.00   |
| 1   | AA    | 1484 | C    | O4'-C1'-N1  | 7.75  | 114.40      | 108.20   |
| 35  | BB    | 1392 | A    | C5-C6-N6    | -7.75 | 117.50      | 123.70   |
| 35  | BB    | 2294 | G    | C4-C5-C6    | 7.75  | 123.45      | 118.80   |
| 1   | AA    | 277  | C    | N3-C4-C5    | -7.75 | 118.80      | 121.90   |
| 1   | AA    | 699  | C    | C4'-C3'-C2' | -7.75 | 94.85       | 102.60   |
| 1   | AA    | 1168 | U    | O4'-C1'-N1  | 7.75  | 114.40      | 108.20   |
| 1   | AA    | 1170 | A    | C5-C6-N1    | -7.75 | 113.83      | 117.70   |
| 1   | AA    | 1319 | A    | N1-C6-N6    | 7.75  | 123.25      | 118.60   |
| 35  | BB    | 920  | A    | C5-N7-C8    | 7.75  | 107.78      | 103.90   |
| 35  | BB    | 1483 | G    | N1-C2-N3    | -7.75 | 119.25      | 123.90   |
| 1   | AA    | 50   | A    | N9-C4-C5    | 7.75  | 108.90      | 105.80   |
| 1   | AA    | 951  | G    | N3-C2-N2    | 7.75  | 125.32      | 119.90   |
| 1   | AA    | 1206 | G    | C5-N7-C8    | -7.75 | 100.43      | 104.30   |
| 34  | BA    | 61   | G    | N1-C2-N3    | -7.75 | 119.25      | 123.90   |
| 35  | BB    | 1002 | G    | N1-C2-N3    | -7.75 | 119.25      | 123.90   |
| 35  | BB    | 1780 | A    | C5-C6-N6    | -7.75 | 117.50      | 123.70   |
| 35  | BB    | 199  | A    | C5-C6-N1    | -7.75 | 113.83      | 117.70   |
| 35  | BB    | 784  | G    | N3-C2-N2    | 7.75  | 125.32      | 119.90   |
| 56  | BY    | 76   | ARG  | NE-CZ-NH1   | 7.75  | 124.17      | 120.30   |
| 1   | AA    | 23   | C    | P-O5'-C5'   | 7.74  | 133.29      | 120.90   |
| 1   | AA    | 243  | A    | N1-C2-N3    | -7.74 | 125.43      | 129.30   |
| 1   | AA    | 1039 | G    | N7-C8-N9    | 7.74  | 116.97      | 113.10   |
| 1   | AA    | 1144 | G    | C2-N3-C4    | 7.74  | 115.77      | 111.90   |
| 35  | BB    | 537  | G    | O4'-C1'-N9  | 7.74  | 114.39      | 108.20   |
| 35  | BB    | 658  | U    | O4'-C1'-N1  | 7.74  | 114.39      | 108.20   |
| 35  | BB    | 937  | C    | P-O3'-C3'   | -7.74 | 110.41      | 119.70   |
| 35  | BB    | 1367 | A    | C5-N7-C8    | 7.74  | 107.77      | 103.90   |
| 35  | BB    | 2802 | G    | C8-N9-C4    | -7.74 | 103.30      | 106.40   |
| 35  | BB    | 2897 | U    | O4'-C1'-N1  | 7.74  | 114.39      | 108.20   |
| 1   | AA    | 166  | U    | C5'-C4'-O4' | 7.74  | 118.39      | 109.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1193 | G    | N1-C6-O6    | 7.74  | 124.55      | 119.90   |
| 41  | BH    | 25   | TYR  | CB-CG-CD1   | 7.74  | 125.64      | 121.00   |
| 1   | AA    | 1110 | A    | N1-C2-N3    | 7.74  | 133.17      | 129.30   |
| 7   | AG    | 90   | VAL  | CA-CB-CG2   | 7.74  | 122.51      | 110.90   |
| 35  | BB    | 64   | A    | N1-C2-N3    | 7.74  | 133.17      | 129.30   |
| 35  | BB    | 1431 | A    | N1-C6-N6    | 7.74  | 123.24      | 118.60   |
| 35  | BB    | 2037 | A    | O4'-C1'-N9  | 7.74  | 114.39      | 108.20   |
| 35  | BB    | 2571 | U    | N1-C2-N3    | -7.74 | 110.26      | 114.90   |
| 1   | AA    | 455  | G    | C8-N9-C4    | -7.74 | 103.30      | 106.40   |
| 1   | AA    | 640  | A    | C5-C6-N6    | -7.74 | 117.51      | 123.70   |
| 1   | AA    | 1037 | C    | C6-N1-C2    | -7.74 | 117.20      | 120.30   |
| 1   | AA    | 1221 | G    | C2-N3-C4    | 7.74  | 115.77      | 111.90   |
| 34  | BA    | 62   | C    | O4'-C1'-N1  | 7.74  | 114.39      | 108.20   |
| 35  | BB    | 2770 | G    | C5-C6-O6    | -7.74 | 123.96      | 128.60   |
| 1   | AA    | 201  | G    | C4-C5-N7    | -7.74 | 107.71      | 110.80   |
| 1   | AA    | 232  | G    | N1-C6-O6    | 7.74  | 124.54      | 119.90   |
| 1   | AA    | 270  | A    | C4-C5-C6    | 7.74  | 120.87      | 117.00   |
| 1   | AA    | 809  | G    | N3-C4-C5    | -7.74 | 124.73      | 128.60   |
| 1   | AA    | 1257 | A    | O4'-C1'-N9  | 7.74  | 114.39      | 108.20   |
| 35  | BB    | 857  | G    | N3-C2-N2    | 7.74  | 125.31      | 119.90   |
| 35  | BB    | 1376 | C    | C5-C6-N1    | 7.74  | 124.87      | 121.00   |
| 35  | BB    | 1432 | G    | C4-C5-N7    | 7.74  | 113.89      | 110.80   |
| 35  | BB    | 1526 | C    | O4'-C1'-N1  | 7.74  | 114.39      | 108.20   |
| 35  | BB    | 2476 | A    | C5'-C4'-C3' | -7.74 | 103.62      | 116.00   |
| 35  | BB    | 2699 | C    | N3-C4-N4    | 7.74  | 123.41      | 118.00   |
| 35  | BB    | 2826 | A    | C5-C6-N1    | -7.74 | 113.83      | 117.70   |
| 35  | BB    | 2828 | G    | N9-C4-C5    | -7.74 | 102.31      | 105.40   |
| 1   | AA    | 75   | G    | N9-C4-C5    | -7.73 | 102.31      | 105.40   |
| 1   | AA    | 798  | U    | C5-C6-N1    | -7.73 | 118.83      | 122.70   |
| 35  | BB    | 2547 | A    | O4'-C1'-N9  | 7.73  | 114.39      | 108.20   |
| 46  | BM    | 38   | ARG  | NE-CZ-NH2   | -7.73 | 116.43      | 120.30   |
| 1   | AA    | 76   | G    | C4-C5-N7    | 7.73  | 113.89      | 110.80   |
| 1   | AA    | 189  | A    | N1-C2-N3    | 7.73  | 133.17      | 129.30   |
| 1   | AA    | 311  | C    | C4-C5-C6    | -7.73 | 113.53      | 117.40   |
| 1   | AA    | 898  | G    | O4'-C1'-N9  | 7.73  | 114.39      | 108.20   |
| 35  | BB    | 822  | G    | C6-C5-N7    | -7.73 | 125.76      | 130.40   |
| 35  | BB    | 1680 | U    | C6-N1-C2    | -7.73 | 116.36      | 121.00   |
| 35  | BB    | 1890 | A    | C8-N9-C4    | -7.73 | 102.71      | 105.80   |
| 35  | BB    | 2250 | G    | C2-N3-C4    | 7.73  | 115.77      | 111.90   |
| 35  | BB    | 2410 | G    | N1-C2-N3    | -7.73 | 119.26      | 123.90   |
| 35  | BB    | 2564 | A    | P-O3'-C3'   | 7.73  | 128.98      | 119.70   |
| 1   | AA    | 737  | C    | N3-C4-N4    | 7.73  | 123.41      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1482 | G    | O4'-C1'-N9  | 7.73  | 114.38      | 108.20   |
| 35  | BB    | 2230 | G    | O4'-C1'-N9  | 7.73  | 114.39      | 108.20   |
| 1   | AA    | 819  | A    | O4'-C1'-N9  | 7.73  | 114.38      | 108.20   |
| 35  | BB    | 599  | A    | C2-N3-C4    | -7.73 | 106.74      | 110.60   |
| 35  | BB    | 939  | G    | N1-C6-O6    | 7.73  | 124.54      | 119.90   |
| 35  | BB    | 1359 | A    | C4-C5-C6    | 7.73  | 120.86      | 117.00   |
| 1   | AA    | 434  | U    | C5-C6-N1    | 7.73  | 126.56      | 122.70   |
| 1   | AA    | 1072 | G    | C5-C6-N1    | -7.73 | 107.64      | 111.50   |
| 1   | AA    | 1464 | U    | O4'-C1'-N1  | 7.73  | 114.38      | 108.20   |
| 35  | BB    | 1017 | G    | N3-C2-N2    | 7.73  | 125.31      | 119.90   |
| 35  | BB    | 1188 | U    | O4'-C1'-N1  | 7.73  | 114.38      | 108.20   |
| 35  | BB    | 1262 | A    | O4'-C1'-N9  | 7.73  | 114.38      | 108.20   |
| 35  | BB    | 1478 | G    | C5-C6-N1    | -7.73 | 107.64      | 111.50   |
| 35  | BB    | 2576 | G    | N1-C6-O6    | 7.73  | 124.54      | 119.90   |
| 1   | AA    | 310  | G    | O4'-C4'-C3' | -7.73 | 96.27       | 104.00   |
| 35  | BB    | 351  | C    | N3-C4-N4    | 7.73  | 123.41      | 118.00   |
| 35  | BB    | 1290 | C    | C5-C4-N4    | -7.73 | 114.79      | 120.20   |
| 35  | BB    | 2038 | G    | C5-C6-O6    | -7.73 | 123.96      | 128.60   |
| 1   | AA    | 26   | A    | N9-C4-C5    | 7.72  | 108.89      | 105.80   |
| 1   | AA    | 782  | A    | N1-C6-N6    | 7.72  | 123.23      | 118.60   |
| 35  | BB    | 515  | A    | C4-C5-C6    | 7.72  | 120.86      | 117.00   |
| 35  | BB    | 570  | G    | C8-N9-C4    | -7.72 | 103.31      | 106.40   |
| 35  | BB    | 1869 | G    | N1-C6-O6    | 7.72  | 124.53      | 119.90   |
| 35  | BB    | 2395 | C    | N3-C4-N4    | 7.72  | 123.41      | 118.00   |
| 35  | BB    | 2857 | G    | N1-C2-N2    | -7.72 | 109.25      | 116.20   |
| 1   | AA    | 189  | A    | O4'-C1'-N9  | 7.72  | 114.38      | 108.20   |
| 1   | AA    | 688  | G    | C5-N7-C8    | 7.72  | 108.16      | 104.30   |
| 9   | AI    | 37   | TYR  | CB-CG-CD2   | 7.72  | 125.63      | 121.00   |
| 35  | BB    | 2445 | G    | N1-C6-O6    | 7.72  | 124.53      | 119.90   |
| 35  | BB    | 2682 | A    | C5-N7-C8    | 7.72  | 107.76      | 103.90   |
| 35  | BB    | 2816 | G    | C4-C5-C6    | 7.72  | 123.43      | 118.80   |
| 1   | AA    | 78   | A    | C5-C6-N1    | -7.72 | 113.84      | 117.70   |
| 1   | AA    | 1133 | G    | N9-C4-C5    | 7.72  | 108.49      | 105.40   |
| 1   | AA    | 1239 | A    | C5-C6-N1    | -7.72 | 113.84      | 117.70   |
| 1   | AA    | 1517 | G    | C8-N9-C4    | -7.72 | 103.31      | 106.40   |
| 35  | BB    | 558  | U    | C5-C6-N1    | 7.72  | 126.56      | 122.70   |
| 35  | BB    | 1068 | G    | C6-N1-C2    | 7.72  | 129.73      | 125.10   |
| 35  | BB    | 1084 | A    | C5-C6-N6    | -7.72 | 117.52      | 123.70   |
| 35  | BB    | 1178 | C    | N3-C4-N4    | 7.72  | 123.41      | 118.00   |
| 1   | AA    | 1247 | U    | N1-C1'-C2'  | -7.72 | 103.51      | 112.00   |
| 1   | AA    | 1391 | U    | O4'-C1'-N1  | 7.72  | 114.38      | 108.20   |
| 34  | BA    | 10   | G    | C4-C5-N7    | 7.72  | 113.89      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 491  | G    | C6-C5-N7    | -7.72 | 125.77      | 130.40   |
| 35  | BB    | 1403 | A    | C1'-O4'-C4' | 7.72  | 116.08      | 109.90   |
| 35  | BB    | 1756 | G    | C8-N9-C4    | 7.72  | 109.49      | 106.40   |
| 35  | BB    | 2048 | G    | O4'-C1'-N9  | 7.72  | 114.38      | 108.20   |
| 35  | BB    | 2318 | G    | O4'-C1'-N9  | 7.72  | 114.38      | 108.20   |
| 1   | AA    | 446  | G    | P-O3'-C3'   | -7.72 | 110.44      | 119.70   |
| 35  | BB    | 738  | G    | O4'-C1'-N9  | 7.72  | 114.37      | 108.20   |
| 1   | AA    | 213  | G    | C4-C5-N7    | 7.72  | 113.89      | 110.80   |
| 35  | BB    | 684  | G    | N1-C2-N3    | -7.72 | 119.27      | 123.90   |
| 35  | BB    | 778  | G    | C4-C5-N7    | 7.72  | 113.89      | 110.80   |
| 35  | BB    | 855  | G    | C4-C5-N7    | 7.72  | 113.89      | 110.80   |
| 35  | BB    | 2365 | G    | C4-C5-C6    | 7.72  | 123.43      | 118.80   |
| 35  | BB    | 2689 | U    | N3-C4-C5    | -7.72 | 109.97      | 114.60   |
| 1   | AA    | 508  | U    | C5-C4-O4    | 7.71  | 130.53      | 125.90   |
| 1   | AA    | 852  | G    | N7-C8-N9    | -7.71 | 109.24      | 113.10   |
| 35  | BB    | 495  | G    | C5-C6-O6    | -7.71 | 123.97      | 128.60   |
| 35  | BB    | 2765 | A    | C5'-C4'-C3' | -7.71 | 103.66      | 116.00   |
| 35  | BB    | 2465 | C    | C5-C4-N4    | -7.71 | 114.80      | 120.20   |
| 35  | BB    | 2498 | C    | C6-N1-C2    | 7.71  | 123.39      | 120.30   |
| 1   | AA    | 330  | C    | C4'-C3'-C2' | -7.71 | 94.89       | 102.60   |
| 35  | BB    | 208  | C    | N3-C4-C5    | -7.71 | 118.82      | 121.90   |
| 35  | BB    | 243  | U    | N1-C2-O2    | 7.71  | 128.20      | 122.80   |
| 35  | BB    | 892  | A    | N1-C6-N6    | 7.71  | 123.23      | 118.60   |
| 35  | BB    | 2160 | C    | N3-C4-N4    | 7.71  | 123.40      | 118.00   |
| 35  | BB    | 2222 | C    | C5-C6-N1    | 7.71  | 124.86      | 121.00   |
| 35  | BB    | 2276 | G    | C5-C6-O6    | -7.71 | 123.97      | 128.60   |
| 35  | BB    | 1097 | U    | N3-C4-C5    | -7.71 | 109.97      | 114.60   |
| 35  | BB    | 1161 | C    | O4'-C1'-N1  | 7.71  | 114.37      | 108.20   |
| 35  | BB    | 2663 | G    | C4-C5-C6    | 7.71  | 123.43      | 118.80   |
| 35  | BB    | 953  | G    | O4'-C1'-N9  | 7.71  | 114.37      | 108.20   |
| 35  | BB    | 1733 | G    | N1-C2-N2    | -7.71 | 109.26      | 116.20   |
| 1   | AA    | 540  | G    | N7-C8-N9    | 7.71  | 116.95      | 113.10   |
| 1   | AA    | 739  | C    | C5-C4-N4    | -7.71 | 114.81      | 120.20   |
| 1   | AA    | 1032 | G    | C6-N1-C2    | 7.71  | 129.72      | 125.10   |
| 35  | BB    | 941  | A    | C4-C5-C6    | 7.71  | 120.85      | 117.00   |
| 35  | BB    | 2060 | A    | N9-C4-C5    | 7.71  | 108.88      | 105.80   |
| 35  | BB    | 2847 | U    | O4'-C1'-N1  | 7.71  | 114.36      | 108.20   |
| 1   | AA    | 59   | A    | N9-C4-C5    | 7.70  | 108.88      | 105.80   |
| 1   | AA    | 811  | C    | P-O3'-C3'   | 7.70  | 128.94      | 119.70   |
| 34  | BA    | 79   | G    | N1-C2-N3    | -7.70 | 119.28      | 123.90   |
| 35  | BB    | 188  | G    | C5-N7-C8    | 7.70  | 108.15      | 104.30   |
| 35  | BB    | 471  | A    | O4'-C1'-N9  | 7.70  | 114.36      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 708  | G    | N9-C4-C5   | -7.70 | 102.32      | 105.40   |
| 1   | AA    | 15   | G    | C4-C5-C6   | 7.70  | 123.42      | 118.80   |
| 1   | AA    | 703  | G    | N1-C6-O6   | 7.70  | 124.52      | 119.90   |
| 1   | AA    | 996  | A    | C5-N7-C8   | 7.70  | 107.75      | 103.90   |
| 35  | BB    | 302  | C    | C6-N1-C2   | -7.70 | 117.22      | 120.30   |
| 35  | BB    | 896  | A    | C6-C5-N7   | -7.70 | 126.91      | 132.30   |
| 35  | BB    | 1993 | U    | P-O5'-C5'  | -7.70 | 108.58      | 120.90   |
| 35  | BB    | 2014 | A    | N1-C6-N6   | 7.70  | 123.22      | 118.60   |
| 54  | BU    | 6    | ARG  | NE-CZ-NH1  | 7.70  | 124.15      | 120.30   |
| 1   | AA    | 589  | U    | C6-N1-C2   | -7.70 | 116.38      | 121.00   |
| 1   | AA    | 666  | G    | C4-C5-C6   | 7.70  | 123.42      | 118.80   |
| 31  | B6    | 35   | ARG  | NE-CZ-NH2  | -7.70 | 116.45      | 120.30   |
| 35  | BB    | 265  | A    | O4'-C1'-N9 | 7.70  | 114.36      | 108.20   |
| 35  | BB    | 1128 | G    | N3-C2-N2   | 7.70  | 125.29      | 119.90   |
| 35  | BB    | 1758 | U    | C5-C6-N1   | -7.70 | 118.85      | 122.70   |
| 35  | BB    | 1766 | G    | O4'-C1'-N9 | 7.70  | 114.36      | 108.20   |
| 35  | BB    | 2073 | C    | N1-C2-N3   | -7.70 | 113.81      | 119.20   |
| 35  | BB    | 2342 | C    | N1-C2-O2   | 7.70  | 123.52      | 118.90   |
| 35  | BB    | 20   | C    | N3-C4-C5   | -7.70 | 118.82      | 121.90   |
| 35  | BB    | 359  | G    | C5-C6-O6   | -7.70 | 123.98      | 128.60   |
| 35  | BB    | 579  | G    | O4'-C1'-N9 | 7.70  | 114.36      | 108.20   |
| 35  | BB    | 1140 | C    | C2-N3-C4   | 7.70  | 123.75      | 119.90   |
| 35  | BB    | 2201 | G    | O4'-C1'-N9 | 7.70  | 114.36      | 108.20   |
| 35  | BB    | 2264 | C    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 35  | BB    | 2616 | C    | C5-C6-N1   | 7.70  | 124.85      | 121.00   |
| 35  | BB    | 2890 | G    | N1-C6-O6   | 7.70  | 124.52      | 119.90   |
| 1   | AA    | 344  | A    | N1-C6-N6   | 7.70  | 123.22      | 118.60   |
| 1   | AA    | 1274 | A    | N1-C6-N6   | 7.70  | 123.22      | 118.60   |
| 1   | AA    | 269  | C    | C5-C4-N4   | -7.70 | 114.81      | 120.20   |
| 11  | AK    | 105  | ARG  | NE-CZ-NH1  | 7.70  | 124.15      | 120.30   |
| 34  | BA    | 84   | G    | C2-N3-C4   | -7.70 | 108.05      | 111.90   |
| 35  | BB    | 631  | A    | C5-C6-N6   | -7.70 | 117.54      | 123.70   |
| 35  | BB    | 875  | G    | C5-C6-O6   | -7.70 | 123.98      | 128.60   |
| 35  | BB    | 1038 | G    | C6-C5-N7   | -7.70 | 125.78      | 130.40   |
| 35  | BB    | 1684 | G    | O4'-C1'-N9 | 7.70  | 114.36      | 108.20   |
| 35  | BB    | 2178 | C    | N3-C4-C5   | -7.70 | 118.82      | 121.90   |
| 35  | BB    | 2191 | A    | C5-N7-C8   | 7.70  | 107.75      | 103.90   |
| 1   | AA    | 538  | G    | C4-C5-N7   | 7.69  | 113.88      | 110.80   |
| 35  | BB    | 2410 | G    | N9-C4-C5   | -7.69 | 102.32      | 105.40   |
| 35  | BB    | 2795 | C    | N3-C4-C5   | -7.69 | 118.82      | 121.90   |
| 1   | AA    | 58   | C    | C6-N1-C2   | 7.69  | 123.38      | 120.30   |
| 1   | AA    | 87   | C    | O4'-C1'-N1 | 7.69  | 114.35      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 241  | G    | C6-C5-N7    | -7.69 | 125.78      | 130.40   |
| 1   | AA    | 774  | G    | C5-C6-O6    | -7.69 | 123.98      | 128.60   |
| 1   | AA    | 1174 | G    | N7-C8-N9    | -7.69 | 109.25      | 113.10   |
| 1   | AA    | 1175 | G    | N3-C4-N9    | 7.69  | 130.62      | 126.00   |
| 34  | BA    | 23   | G    | O4'-C1'-N9  | 7.69  | 114.35      | 108.20   |
| 35  | BB    | 700  | G    | C5-C6-N1    | -7.69 | 107.65      | 111.50   |
| 35  | BB    | 1024 | G    | N3-C2-N2    | 7.69  | 125.28      | 119.90   |
| 35  | BB    | 2893 | A    | C5-N7-C8    | 7.69  | 107.75      | 103.90   |
| 44  | BK    | 108  | ARG  | NE-CZ-NH1   | 7.69  | 124.15      | 120.30   |
| 1   | AA    | 1047 | G    | N7-C8-N9    | 7.69  | 116.94      | 113.10   |
| 1   | AA    | 1502 | A    | C8-N9-C4    | -7.69 | 102.72      | 105.80   |
| 35  | BB    | 132  | G    | N1-C6-O6    | 7.69  | 124.52      | 119.90   |
| 35  | BB    | 217  | A    | N3-C4-C5    | -7.69 | 121.42      | 126.80   |
| 35  | BB    | 318  | C    | C5-C6-N1    | 7.69  | 124.84      | 121.00   |
| 35  | BB    | 2462 | C    | C4'-C3'-C2' | -7.69 | 94.91       | 102.60   |
| 35  | BB    | 507  | A    | C8-N9-C4    | -7.69 | 102.72      | 105.80   |
| 1   | AA    | 1138 | G    | N1-C2-N3    | -7.69 | 119.29      | 123.90   |
| 1   | AA    | 1185 | G    | O4'-C1'-N9  | 7.69  | 114.35      | 108.20   |
| 35  | BB    | 77   | G    | N9-C4-C5    | -7.69 | 102.33      | 105.40   |
| 35  | BB    | 313  | G    | N1-C6-O6    | 7.69  | 124.51      | 119.90   |
| 35  | BB    | 1505 | A    | N1-C2-N3    | -7.69 | 125.46      | 129.30   |
| 35  | BB    | 152  | A    | C5-C6-N1    | -7.69 | 113.86      | 117.70   |
| 35  | BB    | 167  | A    | O4'-C1'-N9  | 7.69  | 114.35      | 108.20   |
| 35  | BB    | 1325 | U    | C6-N1-C2    | -7.69 | 116.39      | 121.00   |
| 1   | AA    | 496  | A    | N7-C8-N9    | 7.68  | 117.64      | 113.80   |
| 1   | AA    | 595  | A    | C5-C6-N6    | -7.68 | 117.55      | 123.70   |
| 1   | AA    | 1392 | G    | C4-C5-N7    | -7.68 | 107.73      | 110.80   |
| 35  | BB    | 50   | U    | C2-N1-C1'   | 7.68  | 126.92      | 117.70   |
| 35  | BB    | 178  | G    | C6-C5-N7    | -7.68 | 125.79      | 130.40   |
| 35  | BB    | 708  | G    | O4'-C1'-N9  | 7.68  | 114.35      | 108.20   |
| 35  | BB    | 1136 | G    | C6-N1-C2    | -7.68 | 120.49      | 125.10   |
| 35  | BB    | 1405 | U    | N3-C2-O2    | 7.68  | 127.58      | 122.20   |
| 35  | BB    | 2154 | A    | C5-N7-C8    | 7.68  | 107.74      | 103.90   |
| 35  | BB    | 2362 | C    | O4'-C1'-N1  | 7.68  | 114.35      | 108.20   |
| 1   | AA    | 201  | G    | O4'-C1'-N9  | 7.68  | 114.34      | 108.20   |
| 1   | AA    | 402  | G    | C4-C5-C6    | 7.68  | 123.41      | 118.80   |
| 35  | BB    | 477  | A    | N7-C8-N9    | -7.68 | 109.96      | 113.80   |
| 35  | BB    | 648  | G    | N7-C8-N9    | 7.68  | 116.94      | 113.10   |
| 35  | BB    | 886  | A    | N3-C4-C5    | -7.68 | 121.42      | 126.80   |
| 35  | BB    | 1162 | G    | C8-N9-C4    | -7.68 | 103.33      | 106.40   |
| 44  | BK    | 31   | ARG  | NE-CZ-NH2   | 7.68  | 124.14      | 120.30   |
| 1   | AA    | 1458 | G    | C5-C6-O6    | -7.68 | 123.99      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1284 | A    | C4-C5-N7    | -7.68 | 106.86      | 110.70   |
| 35  | BB    | 2060 | A    | P-O5'-C5'   | -7.68 | 108.61      | 120.90   |
| 1   | AA    | 192  | A    | C4-C5-C6    | 7.68  | 120.84      | 117.00   |
| 1   | AA    | 858  | G    | C4-C5-C6    | 7.68  | 123.41      | 118.80   |
| 1   | AA    | 953  | G    | N9-C4-C5    | -7.68 | 102.33      | 105.40   |
| 1   | AA    | 978  | A    | N1-C6-N6    | 7.68  | 123.21      | 118.60   |
| 22  | AV    | 46   | G    | C5-C6-O6    | -7.68 | 123.99      | 128.60   |
| 35  | BB    | 57   | C    | C6-N1-C2    | -7.68 | 117.23      | 120.30   |
| 35  | BB    | 893  | C    | N3-C4-N4    | 7.68  | 123.38      | 118.00   |
| 35  | BB    | 2137 | U    | C5'-C4'-O4' | 7.68  | 118.31      | 109.10   |
| 35  | BB    | 2374 | C    | O4'-C1'-N1  | 7.68  | 114.34      | 108.20   |
| 35  | BB    | 2735 | G    | C5-C6-N1    | -7.68 | 107.66      | 111.50   |
| 35  | BB    | 2809 | A    | C4-C5-C6    | 7.68  | 120.84      | 117.00   |
| 1   | AA    | 110  | C    | N3-C4-C5    | -7.68 | 118.83      | 121.90   |
| 35  | BB    | 212  | G    | C4-C5-N7    | -7.68 | 107.73      | 110.80   |
| 35  | BB    | 627  | A    | C4-C5-C6    | 7.68  | 120.84      | 117.00   |
| 35  | BB    | 1691 | C    | C6-N1-C2    | -7.68 | 117.23      | 120.30   |
| 1   | AA    | 439  | U    | C5-C4-O4    | 7.68  | 130.51      | 125.90   |
| 1   | AA    | 532  | A    | C8-N9-C4    | -7.68 | 102.73      | 105.80   |
| 1   | AA    | 623  | C    | C3'-C2'-C1' | 7.68  | 107.64      | 101.50   |
| 35  | BB    | 1038 | G    | N9-C4-C5    | -7.68 | 102.33      | 105.40   |
| 35  | BB    | 1213 | A    | N1-C2-N3    | 7.68  | 133.14      | 129.30   |
| 35  | BB    | 1294 | U    | C2-N3-C4    | -7.68 | 122.39      | 127.00   |
| 35  | BB    | 1773 | A    | N7-C8-N9    | -7.68 | 109.96      | 113.80   |
| 35  | BB    | 2153 | C    | N3-C4-C5    | -7.68 | 118.83      | 121.90   |
| 35  | BB    | 2509 | G    | C6-C5-N7    | -7.68 | 125.79      | 130.40   |
| 35  | BB    | 2566 | A    | O4'-C1'-N9  | 7.68  | 114.34      | 108.20   |
| 35  | BB    | 2692 | G    | C5-C6-N1    | -7.68 | 107.66      | 111.50   |
| 35  | BB    | 2827 | C    | N3-C4-N4    | 7.68  | 123.37      | 118.00   |
| 1   | AA    | 698  | G    | C5-C6-N1    | -7.67 | 107.66      | 111.50   |
| 35  | BB    | 1735 | A    | C5-C6-N6    | -7.67 | 117.56      | 123.70   |
| 35  | BB    | 2723 | C    | N3-C4-C5    | -7.67 | 118.83      | 121.90   |
| 34  | BA    | 28   | C    | C5-C4-N4    | -7.67 | 114.83      | 120.20   |
| 35  | BB    | 305  | C    | C5-C4-N4    | -7.67 | 114.83      | 120.20   |
| 35  | BB    | 947  | A    | C5-C6-N1    | -7.67 | 113.86      | 117.70   |
| 35  | BB    | 1235 | G    | C5-C6-O6    | -7.67 | 124.00      | 128.60   |
| 35  | BB    | 1664 | A    | C4-N9-C1'   | 7.67  | 140.11      | 126.30   |
| 1   | AA    | 106  | C    | N3-C4-C5    | -7.67 | 118.83      | 121.90   |
| 1   | AA    | 510  | A    | N1-C2-N3    | 7.67  | 133.14      | 129.30   |
| 1   | AA    | 759  | A    | C5-N7-C8    | -7.67 | 100.06      | 103.90   |
| 1   | AA    | 783  | C    | P-O3'-C3'   | -7.67 | 110.49      | 119.70   |
| 1   | AA    | 1043 | G    | C6-C5-N7    | -7.67 | 125.80      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1364 | U    | N3-C2-O2    | 7.67  | 127.57      | 122.20   |
| 35  | BB    | 291  | G    | C5-C6-N1    | -7.67 | 107.66      | 111.50   |
| 35  | BB    | 301  | G    | C5-C6-O6    | -7.67 | 124.00      | 128.60   |
| 35  | BB    | 1032 | A    | C5-C6-N6    | -7.67 | 117.56      | 123.70   |
| 1   | AA    | 1192 | C    | C4-C5-C6    | 7.67  | 121.23      | 117.40   |
| 35  | BB    | 1330 | C    | P-O5'-C5'   | -7.67 | 108.63      | 120.90   |
| 35  | BB    | 1751 | U    | N3-C4-O4    | 7.67  | 124.77      | 119.40   |
| 35  | BB    | 2216 | G    | C4-C5-N7    | 7.67  | 113.87      | 110.80   |
| 35  | BB    | 2286 | G    | C5-C6-N1    | -7.67 | 107.67      | 111.50   |
| 1   | AA    | 187  | G    | N1-C6-O6    | 7.67  | 124.50      | 119.90   |
| 1   | AA    | 318  | G    | O4'-C4'-C3' | -7.67 | 96.33       | 104.00   |
| 1   | AA    | 380  | G    | O4'-C1'-N9  | 7.67  | 114.33      | 108.20   |
| 1   | AA    | 629  | A    | C5-C6-N6    | -7.67 | 117.56      | 123.70   |
| 1   | AA    | 1026 | G    | C5-C6-O6    | -7.67 | 124.00      | 128.60   |
| 1   | AA    | 1027 | C    | C6-N1-C2    | -7.67 | 117.23      | 120.30   |
| 1   | AA    | 1399 | C    | N1-C2-O2    | -7.67 | 114.30      | 118.90   |
| 35  | BB    | 1715 | G    | C4'-C3'-C2' | -7.67 | 94.93       | 102.60   |
| 35  | BB    | 1823 | G    | N9-C4-C5    | -7.67 | 102.33      | 105.40   |
| 35  | BB    | 2226 | C    | C5-C6-N1    | 7.67  | 124.83      | 121.00   |
| 35  | BB    | 2764 | A    | N3-C4-C5    | -7.67 | 121.43      | 126.80   |
| 1   | AA    | 164  | G    | C5-N7-C8    | -7.67 | 100.47      | 104.30   |
| 1   | AA    | 394  | G    | C2-N3-C4    | 7.67  | 115.73      | 111.90   |
| 35  | BB    | 13   | A    | C5-C6-N1    | -7.67 | 113.87      | 117.70   |
| 35  | BB    | 437  | U    | O4'-C1'-N1  | 7.67  | 114.33      | 108.20   |
| 35  | BB    | 553  | G    | N1-C6-O6    | 7.67  | 124.50      | 119.90   |
| 35  | BB    | 971  | G    | C5-C6-O6    | -7.67 | 124.00      | 128.60   |
| 35  | BB    | 1168 | G    | C8-N9-C1'   | 7.67  | 136.97      | 127.00   |
| 35  | BB    | 1337 | G    | C2-N3-C4    | 7.67  | 115.73      | 111.90   |
| 1   | AA    | 306  | A    | P-O5'-C5'   | 7.67  | 133.16      | 120.90   |
| 1   | AA    | 414  | A    | C2-N3-C4    | 7.67  | 114.43      | 110.60   |
| 1   | AA    | 863  | U    | N3-C2-O2    | -7.67 | 116.83      | 122.20   |
| 35  | BB    | 1362 | C    | C4-C5-C6    | -7.67 | 113.57      | 117.40   |
| 35  | BB    | 2319 | G    | C5-N7-C8    | 7.67  | 108.13      | 104.30   |
| 35  | BB    | 2863 | C    | N3-C4-N4    | 7.67  | 123.37      | 118.00   |
| 1   | AA    | 774  | G    | C8-N9-C4    | -7.66 | 103.33      | 106.40   |
| 1   | AA    | 935  | A    | C5-C6-N1    | -7.66 | 113.87      | 117.70   |
| 35  | BB    | 413  | C    | C5-C4-N4    | -7.66 | 114.83      | 120.20   |
| 35  | BB    | 673  | C    | P-O3'-C3'   | -7.66 | 110.50      | 119.70   |
| 35  | BB    | 793  | A    | C5-C6-N6    | -7.66 | 117.57      | 123.70   |
| 35  | BB    | 972  | A    | C6-C5-N7    | -7.66 | 126.94      | 132.30   |
| 35  | BB    | 1425 | G    | N1-C2-N3    | -7.66 | 119.30      | 123.90   |
| 1   | AA    | 771  | G    | O4'-C1'-N9  | 7.66  | 114.33      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 277  | G    | N3-C4-N9    | 7.66  | 130.60      | 126.00   |
| 35  | BB    | 830  | G    | C5-C6-N1    | -7.66 | 107.67      | 111.50   |
| 35  | BB    | 2377 | A    | C5-C6-N6    | -7.66 | 117.57      | 123.70   |
| 1   | AA    | 195  | A    | C1'-O4'-C4' | 7.66  | 116.03      | 109.90   |
| 1   | AA    | 250  | A    | C5-N7-C8    | 7.66  | 107.73      | 103.90   |
| 35  | BB    | 1391 | U    | N1-C2-N3    | 7.66  | 119.50      | 114.90   |
| 35  | BB    | 1699 | G    | O4'-C1'-N9  | 7.66  | 114.33      | 108.20   |
| 35  | BB    | 2434 | A    | C6-C5-N7    | -7.66 | 126.94      | 132.30   |
| 1   | AA    | 506  | G    | N3-C2-N2    | 7.66  | 125.26      | 119.90   |
| 1   | AA    | 806  | C    | N3-C4-N4    | 7.66  | 123.36      | 118.00   |
| 1   | AA    | 1050 | G    | N9-C4-C5    | -7.66 | 102.34      | 105.40   |
| 35  | BB    | 681  | G    | C5-C6-N1    | -7.66 | 107.67      | 111.50   |
| 35  | BB    | 1453 | A    | N9-C4-C5    | -7.66 | 102.74      | 105.80   |
| 35  | BB    | 1665 | A    | C4-C5-C6    | 7.66  | 120.83      | 117.00   |
| 35  | BB    | 501  | A    | C2-N3-C4    | -7.66 | 106.77      | 110.60   |
| 55  | BW    | 82   | TYR  | CB-CG-CD1   | -7.66 | 116.41      | 121.00   |
| 1   | AA    | 592  | G    | C2-N3-C4    | 7.66  | 115.73      | 111.90   |
| 1   | AA    | 786  | G    | C8-N9-C4    | -7.66 | 103.34      | 106.40   |
| 1   | AA    | 1379 | G    | C5-C6-N1    | -7.66 | 107.67      | 111.50   |
| 35  | BB    | 1999 | C    | O4'-C1'-N1  | 7.66  | 114.33      | 108.20   |
| 35  | BB    | 2154 | A    | O4'-C1'-N9  | 7.66  | 114.33      | 108.20   |
| 1   | AA    | 449  | G    | C4-C5-C6    | 7.65  | 123.39      | 118.80   |
| 1   | AA    | 923  | A    | C4-C5-C6    | 7.65  | 120.83      | 117.00   |
| 35  | BB    | 2749 | A    | N1-C2-N3    | -7.65 | 125.47      | 129.30   |
| 37  | BD    | 13   | ARG  | NE-CZ-NH1   | 7.65  | 124.13      | 120.30   |
| 1   | AA    | 59   | A    | N1-C6-N6    | 7.65  | 123.19      | 118.60   |
| 1   | AA    | 149  | A    | C6-N1-C2    | -7.65 | 114.01      | 118.60   |
| 1   | AA    | 1065 | U    | C5-C6-N1    | 7.65  | 126.53      | 122.70   |
| 35  | BB    | 1420 | A    | N9-C4-C5    | -7.65 | 102.74      | 105.80   |
| 35  | BB    | 1739 | A    | O4'-C1'-N9  | 7.65  | 114.32      | 108.20   |
| 35  | BB    | 1832 | C    | N3-C4-C5    | -7.65 | 118.84      | 121.90   |
| 35  | BB    | 2181 | U    | N3-C4-O4    | 7.65  | 124.76      | 119.40   |
| 35  | BB    | 2322 | A    | N1-C6-N6    | 7.65  | 123.19      | 118.60   |
| 35  | BB    | 2451 | A    | C6-N1-C2    | 7.65  | 123.19      | 118.60   |
| 1   | AA    | 263  | A    | C5-C6-N6    | -7.65 | 117.58      | 123.70   |
| 35  | BB    | 963  | U    | N1-C2-O2    | -7.65 | 117.44      | 122.80   |
| 46  | BM    | 18   | ARG  | NE-CZ-NH2   | 7.65  | 124.13      | 120.30   |
| 1   | AA    | 277  | C    | C6-N1-C2    | -7.65 | 117.24      | 120.30   |
| 1   | AA    | 1255 | G    | C5-N7-C8    | 7.65  | 108.12      | 104.30   |
| 34  | BA    | 73   | A    | C1'-O4'-C4' | 7.65  | 116.02      | 109.90   |
| 35  | BB    | 69   | C    | C5-C6-N1    | 7.65  | 124.82      | 121.00   |
| 35  | BB    | 560  | C    | N3-C4-N4    | 7.65  | 123.35      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1719 | G    | C5-N7-C8   | -7.65 | 100.47      | 104.30   |
| 1   | AA    | 858  | G    | N1-C2-N3   | -7.65 | 119.31      | 123.90   |
| 1   | AA    | 1496 | C    | C5-C4-N4   | -7.65 | 114.85      | 120.20   |
| 35  | BB    | 1227 | G    | C4-C5-C6   | 7.65  | 123.39      | 118.80   |
| 35  | BB    | 1293 | C    | O4'-C1'-N1 | 7.65  | 114.32      | 108.20   |
| 35  | BB    | 1574 | C    | C2-N1-C1'  | 7.65  | 127.21      | 118.80   |
| 35  | BB    | 1724 | G    | N1-C6-O6   | 7.65  | 124.49      | 119.90   |
| 35  | BB    | 311  | A    | C5-N7-C8   | 7.65  | 107.72      | 103.90   |
| 1   | AA    | 656  | G    | O4'-C1'-N9 | 7.64  | 114.32      | 108.20   |
| 1   | AA    | 717  | U    | C5-C6-N1   | 7.64  | 126.52      | 122.70   |
| 1   | AA    | 1325 | C    | N3-C4-N4   | 7.64  | 123.35      | 118.00   |
| 35  | BB    | 366  | C    | O4'-C1'-N1 | 7.64  | 114.32      | 108.20   |
| 35  | BB    | 845  | A    | C4-C5-C6   | 7.64  | 120.82      | 117.00   |
| 35  | BB    | 1922 | G    | N7-C8-N9   | 7.64  | 116.92      | 113.10   |
| 35  | BB    | 1984 | G    | N7-C8-N9   | -7.64 | 109.28      | 113.10   |
| 35  | BB    | 2078 | C    | C4-C5-C6   | 7.64  | 121.22      | 117.40   |
| 35  | BB    | 2092 | U    | C5-C6-N1   | 7.64  | 126.52      | 122.70   |
| 1   | AA    | 685  | G    | N9-C4-C5   | -7.64 | 102.34      | 105.40   |
| 1   | AA    | 1263 | C    | N3-C4-N4   | 7.64  | 123.35      | 118.00   |
| 35  | BB    | 1392 | A    | C5-N7-C8   | 7.64  | 107.72      | 103.90   |
| 35  | BB    | 1439 | A    | C4-C5-C6   | 7.64  | 120.82      | 117.00   |
| 35  | BB    | 1539 | U    | N3-C4-O4   | 7.64  | 124.75      | 119.40   |
| 35  | BB    | 1767 | G    | N1-C2-N3   | -7.64 | 119.31      | 123.90   |
| 35  | BB    | 2031 | A    | C5-N7-C8   | 7.64  | 107.72      | 103.90   |
| 35  | BB    | 2722 | G    | N1-C2-N3   | -7.64 | 119.31      | 123.90   |
| 1   | AA    | 232  | G    | C5-N7-C8   | -7.64 | 100.48      | 104.30   |
| 1   | AA    | 825  | A    | N1-C6-N6   | 7.64  | 123.19      | 118.60   |
| 35  | BB    | 1605 | C    | N3-C4-C5   | -7.64 | 118.84      | 121.90   |
| 1   | AA    | 446  | G    | N1-C2-N3   | -7.64 | 119.32      | 123.90   |
| 1   | AA    | 793  | U    | C5-C6-N1   | 7.64  | 126.52      | 122.70   |
| 1   | AA    | 974  | A    | O4'-C1'-N9 | 7.64  | 114.31      | 108.20   |
| 18  | AR    | 27   | THR  | CA-CB-CG2  | -7.64 | 101.70      | 112.40   |
| 35  | BB    | 220  | G    | N3-C2-N2   | 7.64  | 125.25      | 119.90   |
| 35  | BB    | 2657 | A    | C4-C5-C6   | 7.64  | 120.82      | 117.00   |
| 35  | BB    | 2867 | G    | P-O3'-C3'  | -7.64 | 110.53      | 119.70   |
| 1   | AA    | 1019 | A    | C2-N3-C4   | 7.64  | 114.42      | 110.60   |
| 1   | AA    | 1295 | U    | N1-C2-N3   | 7.64  | 119.48      | 114.90   |
| 25  | B0    | 10   | ARG  | NE-CZ-NH2  | 7.64  | 124.12      | 120.30   |
| 33  | B8    | 12   | ARG  | NE-CZ-NH2  | -7.64 | 116.48      | 120.30   |
| 35  | BB    | 36   | G    | C4-C5-N7   | -7.64 | 107.75      | 110.80   |
| 35  | BB    | 506  | G    | C6-C5-N7   | -7.64 | 125.82      | 130.40   |
| 35  | BB    | 1212 | G    | C5-C6-N1   | -7.64 | 107.68      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1573 | G    | C5-C6-N1    | -7.64 | 107.68      | 111.50   |
| 35  | BB    | 1618 | A    | O4'-C1'-N9  | 7.64  | 114.31      | 108.20   |
| 35  | BB    | 1715 | G    | N1-C2-N3    | -7.64 | 119.32      | 123.90   |
| 35  | BB    | 2071 | A    | C5-C6-N1    | -7.64 | 113.88      | 117.70   |
| 35  | BB    | 2273 | A    | C5-N7-C8    | 7.64  | 107.72      | 103.90   |
| 35  | BB    | 2391 | G    | C6-N1-C2    | -7.64 | 120.52      | 125.10   |
| 1   | AA    | 1339 | A    | C4-C5-C6    | 7.63  | 120.82      | 117.00   |
| 2   | AB    | 209  | VAL  | CA-CB-CG2   | -7.63 | 99.45       | 110.90   |
| 22  | AV    | 20   | U    | O4'-C1'-N1  | 7.63  | 114.31      | 108.20   |
| 34  | BA    | 58   | A    | C5-C6-N6    | -7.63 | 117.59      | 123.70   |
| 35  | BB    | 13   | A    | C5-C6-N6    | -7.63 | 117.59      | 123.70   |
| 35  | BB    | 2109 | U    | C2-N3-C4    | -7.63 | 122.42      | 127.00   |
| 35  | BB    | 2655 | G    | C4'-C3'-C2' | -7.63 | 94.97       | 102.60   |
| 1   | AA    | 587  | G    | N9-C4-C5    | -7.63 | 102.35      | 105.40   |
| 22  | AV    | 70   | C    | N1-C2-O2    | 7.63  | 123.48      | 118.90   |
| 35  | BB    | 2223 | G    | C5-C6-N1    | -7.63 | 107.68      | 111.50   |
| 35  | BB    | 2526 | G    | N9-C4-C5    | -7.63 | 102.35      | 105.40   |
| 35  | BB    | 2606 | C    | O4'-C1'-N1  | 7.63  | 114.31      | 108.20   |
| 1   | AA    | 163  | C    | O4'-C1'-N1  | 7.63  | 114.31      | 108.20   |
| 1   | AA    | 895  | G    | C5-C6-O6    | -7.63 | 124.02      | 128.60   |
| 35  | BB    | 277  | G    | N1-C6-O6    | 7.63  | 124.48      | 119.90   |
| 35  | BB    | 503  | A    | C6-C5-N7    | -7.63 | 126.96      | 132.30   |
| 35  | BB    | 525  | U    | N1-C2-O2    | -7.63 | 117.46      | 122.80   |
| 35  | BB    | 536  | G    | N1-C6-O6    | 7.63  | 124.48      | 119.90   |
| 35  | BB    | 585  | G    | C5-C6-O6    | -7.63 | 124.02      | 128.60   |
| 35  | BB    | 2418 | A    | C5-C6-N6    | -7.63 | 117.59      | 123.70   |
| 34  | BA    | 45   | A    | N9-C4-C5    | 7.63  | 108.85      | 105.80   |
| 35  | BB    | 1276 | A    | C5-C6-N1    | -7.63 | 113.89      | 117.70   |
| 35  | BB    | 1869 | G    | N3-C2-N2    | 7.63  | 125.24      | 119.90   |
| 1   | AA    | 451  | A    | N3-C4-C5    | -7.63 | 121.46      | 126.80   |
| 1   | AA    | 1238 | A    | C4-C5-C6    | 7.63  | 120.81      | 117.00   |
| 35  | BB    | 187  | G    | C8-N9-C4    | 7.63  | 109.45      | 106.40   |
| 35  | BB    | 330  | A    | C4-C5-N7    | 7.63  | 114.51      | 110.70   |
| 35  | BB    | 1798 | U    | O4'-C1'-N1  | 7.63  | 114.30      | 108.20   |
| 35  | BB    | 2241 | A    | O4'-C1'-N9  | 7.63  | 114.30      | 108.20   |
| 35  | BB    | 2639 | A    | C4-C5-C6    | 7.63  | 120.81      | 117.00   |
| 1   | AA    | 155  | A    | O4'-C1'-N9  | 7.63  | 114.30      | 108.20   |
| 1   | AA    | 331  | G    | C5-N7-C8    | 7.63  | 108.11      | 104.30   |
| 1   | AA    | 548  | G    | C4-C5-N7    | 7.63  | 113.85      | 110.80   |
| 35  | BB    | 410  | G    | N3-C2-N2    | 7.63  | 125.24      | 119.90   |
| 35  | BB    | 549  | G    | C5-C6-O6    | -7.63 | 124.03      | 128.60   |
| 35  | BB    | 1004 | U    | O4'-C1'-N1  | 7.63  | 114.30      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1893 | C    | C5-C4-N4    | -7.63 | 114.86      | 120.20   |
| 35  | BB    | 2859 | G    | N3-C2-N2    | 7.63  | 125.24      | 119.90   |
| 35  | BB    | 31   | C    | C6-N1-C2    | -7.62 | 117.25      | 120.30   |
| 35  | BB    | 1664 | A    | C8-N9-C4    | -7.62 | 102.75      | 105.80   |
| 35  | BB    | 2664 | G    | N1-C2-N2    | -7.62 | 109.34      | 116.20   |
| 1   | AA    | 353  | A    | P-O3'-C3'   | 7.62  | 128.85      | 119.70   |
| 1   | AA    | 402  | G    | N1-C6-O6    | 7.62  | 124.47      | 119.90   |
| 1   | AA    | 1242 | G    | C4-C5-N7    | -7.62 | 107.75      | 110.80   |
| 35  | BB    | 350  | G    | N3-C2-N2    | 7.62  | 125.24      | 119.90   |
| 35  | BB    | 1042 | G    | C5-N7-C8    | 7.62  | 108.11      | 104.30   |
| 35  | BB    | 2860 | A    | O4'-C1'-N9  | 7.62  | 114.30      | 108.20   |
| 37  | BD    | 33   | ARG  | NE-CZ-NH1   | -7.62 | 116.49      | 120.30   |
| 54  | BU    | 85   | ARG  | NE-CZ-NH1   | -7.62 | 116.49      | 120.30   |
| 1   | AA    | 189  | A    | C4-C5-C6    | 7.62  | 120.81      | 117.00   |
| 1   | AA    | 490  | C    | N3-C4-C5    | -7.62 | 118.85      | 121.90   |
| 1   | AA    | 1076 | U    | C6-N1-C2    | -7.62 | 116.43      | 121.00   |
| 35  | BB    | 75   | G    | N1-C2-N3    | -7.62 | 119.33      | 123.90   |
| 35  | BB    | 753  | A    | N1-C2-N3    | 7.62  | 133.11      | 129.30   |
| 35  | BB    | 739  | A    | C5-C6-N6    | -7.62 | 117.60      | 123.70   |
| 35  | BB    | 1155 | A    | N7-C8-N9    | -7.62 | 109.99      | 113.80   |
| 35  | BB    | 1551 | A    | C5-C6-N6    | -7.62 | 117.60      | 123.70   |
| 35  | BB    | 2036 | C    | C5'-C4'-O4' | 7.62  | 118.24      | 109.10   |
| 35  | BB    | 2268 | A    | C5-C6-N1    | -7.62 | 113.89      | 117.70   |
| 1   | AA    | 294  | U    | O4'-C1'-N1  | 7.62  | 114.30      | 108.20   |
| 2   | AB    | 193  | ASP  | CB-CG-OD2   | -7.62 | 111.44      | 118.30   |
| 35  | BB    | 85   | G    | N3-C4-C5    | -7.62 | 124.79      | 128.60   |
| 35  | BB    | 2095 | A    | C1'-O4'-C4' | 7.62  | 116.00      | 109.90   |
| 1   | AA    | 320  | A    | C4-C5-C6    | 7.62  | 120.81      | 117.00   |
| 1   | AA    | 1358 | U    | O4'-C1'-N1  | 7.62  | 114.29      | 108.20   |
| 35  | BB    | 322  | A    | C5-C6-N1    | -7.62 | 113.89      | 117.70   |
| 35  | BB    | 2663 | G    | C5-C6-N1    | -7.62 | 107.69      | 111.50   |
| 1   | AA    | 1150 | A    | C2-N3-C4    | -7.62 | 106.79      | 110.60   |
| 1   | AA    | 1408 | A    | C3'-C2'-C1' | 7.62  | 107.59      | 101.50   |
| 35  | BB    | 182  | A    | N3-C4-C5    | -7.62 | 121.47      | 126.80   |
| 35  | BB    | 1451 | C    | O4'-C1'-N1  | 7.62  | 114.29      | 108.20   |
| 1   | AA    | 109  | A    | N1-C2-N3    | -7.61 | 125.49      | 129.30   |
| 1   | AA    | 550  | G    | N1-C6-O6    | 7.61  | 124.47      | 119.90   |
| 35  | BB    | 304  | U    | C3'-C2'-C1' | 7.61  | 107.59      | 101.50   |
| 35  | BB    | 768  | G    | N9-C4-C5    | -7.61 | 102.36      | 105.40   |
| 35  | BB    | 1889 | A    | C8-N9-C4    | -7.61 | 102.75      | 105.80   |
| 35  | BB    | 2868 | A    | C4-C5-N7    | -7.61 | 106.89      | 110.70   |
| 1   | AA    | 1015 | G    | C6-C5-N7    | -7.61 | 125.83      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 28   | A    | C6-N1-C2    | -7.61 | 114.03      | 118.60   |
| 35  | BB    | 163  | C    | C5-C6-N1    | -7.61 | 117.19      | 121.00   |
| 35  | BB    | 669  | G    | P-O5'-C5'   | -7.61 | 108.72      | 120.90   |
| 35  | BB    | 892  | A    | P-O3'-C3'   | -7.61 | 110.57      | 119.70   |
| 54  | BU    | 6    | ARG  | NE-CZ-NH2   | -7.61 | 116.49      | 120.30   |
| 1   | AA    | 424  | G    | C4-C5-C6    | 7.61  | 123.37      | 118.80   |
| 1   | AA    | 700  | G    | C5-C6-N1    | -7.61 | 107.69      | 111.50   |
| 18  | AR    | 47   | ARG  | NE-CZ-NH2   | -7.61 | 116.50      | 120.30   |
| 35  | BB    | 930  | G    | C8-N9-C4    | -7.61 | 103.36      | 106.40   |
| 35  | BB    | 2668 | G    | C5-C6-N1    | -7.61 | 107.69      | 111.50   |
| 1   | AA    | 127  | G    | C5-C6-O6    | -7.61 | 124.03      | 128.60   |
| 35  | BB    | 605  | G    | N1-C2-N3    | -7.61 | 119.33      | 123.90   |
| 35  | BB    | 2554 | U    | C5-C6-N1    | 7.61  | 126.50      | 122.70   |
| 1   | AA    | 207  | C    | N1-C2-N3    | 7.61  | 124.53      | 119.20   |
| 1   | AA    | 448  | A    | C4-C5-C6    | 7.61  | 120.80      | 117.00   |
| 1   | AA    | 548  | G    | C5-C6-O6    | -7.61 | 124.03      | 128.60   |
| 1   | AA    | 596  | A    | N3-C4-N9    | 7.61  | 133.49      | 127.40   |
| 1   | AA    | 991  | U    | O4'-C1'-N1  | 7.61  | 114.28      | 108.20   |
| 22  | AV    | 23   | C    | O4'-C1'-N1  | 7.61  | 114.28      | 108.20   |
| 35  | BB    | 1403 | A    | C5-C6-N6    | -7.61 | 117.61      | 123.70   |
| 35  | BB    | 1537 | G    | C4-C5-C6    | 7.61  | 123.36      | 118.80   |
| 35  | BB    | 1677 | A    | N1-C6-N6    | 7.61  | 123.16      | 118.60   |
| 35  | BB    | 2229 | U    | N3-C4-O4    | 7.61  | 124.73      | 119.40   |
| 1   | AA    | 684  | U    | C4-C5-C6    | -7.61 | 115.14      | 119.70   |
| 1   | AA    | 973  | G    | C5-C6-O6    | -7.61 | 124.04      | 128.60   |
| 1   | AA    | 1300 | G    | O4'-C1'-N9  | 7.61  | 114.28      | 108.20   |
| 35  | BB    | 2705 | A    | C5-C6-N6    | -7.61 | 117.62      | 123.70   |
| 1   | AA    | 90   | C    | N3-C4-C5    | -7.60 | 118.86      | 121.90   |
| 1   | AA    | 919  | A    | N3-C4-N9    | 7.60  | 133.48      | 127.40   |
| 1   | AA    | 1028 | C    | N3-C4-C5    | -7.60 | 118.86      | 121.90   |
| 34  | BA    | 87   | U    | O4'-C1'-N1  | 7.60  | 114.28      | 108.20   |
| 35  | BB    | 1218 | G    | N7-C8-N9    | -7.60 | 109.30      | 113.10   |
| 35  | BB    | 1847 | A    | C5-C6-N1    | -7.60 | 113.90      | 117.70   |
| 35  | BB    | 2608 | G    | N1-C6-O6    | 7.60  | 124.46      | 119.90   |
| 35  | BB    | 2863 | C    | N3-C4-C5    | -7.60 | 118.86      | 121.90   |
| 36  | BC    | 95   | TYR  | CB-CG-CD1   | -7.60 | 116.44      | 121.00   |
| 1   | AA    | 29   | U    | N1-C2-N3    | -7.60 | 110.34      | 114.90   |
| 1   | AA    | 160  | A    | C2-N3-C4    | -7.60 | 106.80      | 110.60   |
| 1   | AA    | 1212 | U    | C1'-O4'-C4' | -7.60 | 103.82      | 109.90   |
| 35  | BB    | 1380 | G    | N9-C4-C5    | -7.60 | 102.36      | 105.40   |
| 35  | BB    | 1947 | C    | N3-C4-N4    | 7.60  | 123.32      | 118.00   |
| 1   | AA    | 250  | A    | C5-C6-N6    | -7.60 | 117.62      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1093 | A    | P-O3'-C3'   | 7.60  | 128.82      | 119.70   |
| 1   | AA    | 1282 | C    | N3-C2-O2    | 7.60  | 127.22      | 121.90   |
| 1   | AA    | 1373 | G    | C8-N9-C4    | -7.60 | 103.36      | 106.40   |
| 35  | BB    | 7    | G    | N3-C4-C5    | 7.60  | 132.40      | 128.60   |
| 35  | BB    | 93   | G    | O4'-C1'-N9  | 7.60  | 114.28      | 108.20   |
| 35  | BB    | 984  | A    | N1-C6-N6    | 7.60  | 123.16      | 118.60   |
| 35  | BB    | 1228 | G    | C5-C6-O6    | -7.60 | 124.04      | 128.60   |
| 35  | BB    | 1639 | C    | C4-C5-C6    | 7.60  | 121.20      | 117.40   |
| 35  | BB    | 2030 | A    | C5-C6-N6    | -7.60 | 117.62      | 123.70   |
| 35  | BB    | 2743 | U    | O4'-C1'-N1  | 7.60  | 114.28      | 108.20   |
| 35  | BB    | 2875 | C    | N3-C4-N4    | 7.60  | 123.32      | 118.00   |
| 1   | AA    | 552  | U    | C6-N1-C2    | -7.60 | 116.44      | 121.00   |
| 1   | AA    | 1454 | G    | C8-N9-C4    | -7.60 | 103.36      | 106.40   |
| 15  | AO    | 88   | ARG  | NE-CZ-NH2   | -7.60 | 116.50      | 120.30   |
| 35  | BB    | 843  | G    | N3-C2-N2    | 7.60  | 125.22      | 119.90   |
| 35  | BB    | 1163 | G    | N1-C6-O6    | 7.60  | 124.46      | 119.90   |
| 35  | BB    | 1527 | G    | C8-N9-C4    | -7.60 | 103.36      | 106.40   |
| 35  | BB    | 2331 | G    | C8-N9-C4    | -7.60 | 103.36      | 106.40   |
| 1   | AA    | 483  | C    | N3-C4-N4    | 7.60  | 123.32      | 118.00   |
| 1   | AA    | 923  | A    | O4'-C1'-N9  | 7.60  | 114.28      | 108.20   |
| 35  | BB    | 115  | C    | N3-C4-N4    | 7.60  | 123.32      | 118.00   |
| 35  | BB    | 161  | A    | C5-N7-C8    | 7.60  | 107.70      | 103.90   |
| 35  | BB    | 246  | C    | N1-C2-O2    | 7.60  | 123.46      | 118.90   |
| 35  | BB    | 1758 | U    | C4-C5-C6    | 7.59  | 124.26      | 119.70   |
| 35  | BB    | 2742 | G    | C6-C5-N7    | -7.59 | 125.84      | 130.40   |
| 35  | BB    | 1410 | G    | C5-N7-C8    | 7.59  | 108.10      | 104.30   |
| 35  | BB    | 1750 | G    | C8-N9-C1'   | 7.59  | 136.87      | 127.00   |
| 35  | BB    | 1903 | G    | N1-C6-O6    | 7.59  | 124.46      | 119.90   |
| 35  | BB    | 2569 | G    | C2-N3-C4    | 7.59  | 115.70      | 111.90   |
| 1   | AA    | 229  | U    | C2-N3-C4    | 7.59  | 131.56      | 127.00   |
| 34  | BA    | 106  | G    | C8-N9-C4    | 7.59  | 109.44      | 106.40   |
| 35  | BB    | 645  | C    | O4'-C1'-N1  | 7.59  | 114.27      | 108.20   |
| 35  | BB    | 2052 | A    | N1-C6-N6    | 7.59  | 123.16      | 118.60   |
| 35  | BB    | 2159 | G    | O4'-C1'-C2' | -7.59 | 98.21       | 105.80   |
| 35  | BB    | 2284 | A    | C8-N9-C4    | -7.59 | 102.76      | 105.80   |
| 35  | BB    | 2394 | C    | O4'-C1'-N1  | 7.59  | 114.27      | 108.20   |
| 35  | BB    | 2488 | G    | N3-C2-N2    | 7.59  | 125.21      | 119.90   |
| 1   | AA    | 778  | G    | O4'-C1'-N9  | 7.59  | 114.27      | 108.20   |
| 1   | AA    | 1362 | A    | N1-C6-N6    | 7.59  | 123.15      | 118.60   |
| 35  | BB    | 1581 | G    | N3-C2-N2    | 7.59  | 125.21      | 119.90   |
| 35  | BB    | 1741 | C    | O4'-C1'-N1  | 7.59  | 114.27      | 108.20   |
| 35  | BB    | 1930 | G    | C3'-C2'-C1' | 7.59  | 107.57      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2116 | G    | C6-C5-N7    | -7.59 | 125.85      | 130.40   |
| 1   | AA    | 519  | C    | C2-N3-C4    | 7.59  | 123.69      | 119.90   |
| 1   | AA    | 771  | G    | N1-C6-O6    | 7.59  | 124.45      | 119.90   |
| 1   | AA    | 860  | A    | N1-C2-N3    | 7.59  | 133.09      | 129.30   |
| 35  | BB    | 660  | C    | N3-C4-C5    | -7.59 | 118.86      | 121.90   |
| 35  | BB    | 1521 | G    | N1-C2-N3    | -7.59 | 119.35      | 123.90   |
| 35  | BB    | 2498 | C    | P-O3'-C3'   | -7.59 | 110.59      | 119.70   |
| 35  | BB    | 1030 | C    | N1-C2-O2    | 7.59  | 123.45      | 118.90   |
| 35  | BB    | 1062 | G    | N7-C8-N9    | -7.59 | 109.31      | 113.10   |
| 35  | BB    | 1101 | U    | N3-C2-O2    | 7.59  | 127.51      | 122.20   |
| 35  | BB    | 2280 | G    | N3-C2-N2    | 7.59  | 125.21      | 119.90   |
| 1   | AA    | 36   | C    | C6-N1-C2    | -7.58 | 117.27      | 120.30   |
| 1   | AA    | 333  | U    | O4'-C1'-N1  | 7.58  | 114.27      | 108.20   |
| 22  | AV    | 10   | G    | C5-C6-O6    | -7.58 | 124.05      | 128.60   |
| 35  | BB    | 256  | A    | C5-C6-N1    | -7.58 | 113.91      | 117.70   |
| 1   | AA    | 595  | A    | O4'-C1'-N9  | 7.58  | 114.27      | 108.20   |
| 1   | AA    | 1367 | C    | O4'-C1'-N1  | 7.58  | 114.27      | 108.20   |
| 35  | BB    | 383  | C    | C2-N3-C4    | 7.58  | 123.69      | 119.90   |
| 35  | BB    | 514  | A    | C6-C5-N7    | -7.58 | 126.99      | 132.30   |
| 35  | BB    | 722  | A    | N1-C2-N3    | 7.58  | 133.09      | 129.30   |
| 35  | BB    | 957  | C    | C6-N1-C2    | -7.58 | 117.27      | 120.30   |
| 35  | BB    | 1029 | A    | C5-C6-N1    | -7.58 | 113.91      | 117.70   |
| 35  | BB    | 2115 | G    | O4'-C1'-N9  | 7.58  | 114.27      | 108.20   |
| 1   | AA    | 409  | U    | N3-C2-O2    | 7.58  | 127.51      | 122.20   |
| 1   | AA    | 966  | G    | C1'-O4'-C4' | 7.58  | 115.97      | 109.90   |
| 2   | AB    | 183  | PHE  | CB-CG-CD2   | -7.58 | 115.49      | 120.80   |
| 35  | BB    | 1185 | G    | C5-N7-C8    | 7.58  | 108.09      | 104.30   |
| 35  | BB    | 1784 | A    | N1-C6-N6    | 7.58  | 123.15      | 118.60   |
| 35  | BB    | 2000 | C    | C5-C4-N4    | -7.58 | 114.89      | 120.20   |
| 35  | BB    | 2542 | A    | C5-C6-N6    | -7.58 | 117.63      | 123.70   |
| 1   | AA    | 158  | G    | C8-N9-C4    | -7.58 | 103.37      | 106.40   |
| 1   | AA    | 830  | G    | N3-C2-N2    | 7.58  | 125.21      | 119.90   |
| 1   | AA    | 1203 | C    | C6-N1-C2    | -7.58 | 117.27      | 120.30   |
| 1   | AA    | 1329 | A    | C4-C5-N7    | -7.58 | 106.91      | 110.70   |
| 35  | BB    | 313  | G    | C4-C5-C6    | 7.58  | 123.35      | 118.80   |
| 35  | BB    | 536  | G    | C8-N9-C4    | 7.58  | 109.43      | 106.40   |
| 36  | BC    | 19   | VAL  | CA-CB-CG2   | 7.58  | 122.27      | 110.90   |
| 1   | AA    | 94   | G    | N1-C6-O6    | 7.58  | 124.45      | 119.90   |
| 1   | AA    | 411  | A    | O4'-C1'-N9  | 7.58  | 114.26      | 108.20   |
| 1   | AA    | 453  | G    | C5-C6-O6    | -7.58 | 124.05      | 128.60   |
| 1   | AA    | 852  | G    | C5-C6-O6    | -7.58 | 124.05      | 128.60   |
| 1   | AA    | 1138 | G    | C5-N7-C8    | -7.58 | 100.51      | 104.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1331 | G    | N1-C2-N3    | -7.58 | 119.35      | 123.90   |
| 35  | BB    | 406  | G    | C5-N7-C8    | 7.58  | 108.09      | 104.30   |
| 35  | BB    | 718  | A    | C5-C6-N6    | -7.58 | 117.64      | 123.70   |
| 35  | BB    | 1569 | A    | O4'-C1'-N9  | 7.58  | 114.26      | 108.20   |
| 35  | BB    | 2821 | A    | O4'-C1'-N9  | 7.58  | 114.26      | 108.20   |
| 35  | BB    | 180  | G    | C5-C6-N1    | -7.58 | 107.71      | 111.50   |
| 35  | BB    | 687  | C    | O4'-C1'-N1  | 7.58  | 114.26      | 108.20   |
| 35  | BB    | 707  | G    | N9-C4-C5    | -7.58 | 102.37      | 105.40   |
| 35  | BB    | 1685 | C    | N3-C4-N4    | 7.58  | 123.30      | 118.00   |
| 35  | BB    | 2793 | C    | N3-C4-N4    | 7.58  | 123.30      | 118.00   |
| 1   | AA    | 1300 | G    | C5-C6-O6    | -7.58 | 124.05      | 128.60   |
| 1   | AA    | 1416 | G    | C4-C5-C6    | 7.58  | 123.34      | 118.80   |
| 34  | BA    | 59   | A    | C5-N7-C8    | 7.58  | 107.69      | 103.90   |
| 35  | BB    | 161  | A    | C4-C5-N7    | -7.58 | 106.91      | 110.70   |
| 35  | BB    | 517  | C    | C4-C5-C6    | 7.58  | 121.19      | 117.40   |
| 35  | BB    | 528  | A    | C5-N7-C8    | 7.58  | 107.69      | 103.90   |
| 35  | BB    | 766  | U    | O4'-C1'-N1  | 7.58  | 114.26      | 108.20   |
| 35  | BB    | 1194 | A    | O4'-C1'-N9  | 7.58  | 114.26      | 108.20   |
| 35  | BB    | 1563 | U    | N3-C4-O4    | 7.58  | 124.70      | 119.40   |
| 35  | BB    | 1685 | C    | O4'-C1'-N1  | 7.58  | 114.26      | 108.20   |
| 35  | BB    | 1745 | A    | N1-C6-N6    | 7.58  | 123.15      | 118.60   |
| 35  | BB    | 2224 | G    | C5-C6-O6    | -7.58 | 124.05      | 128.60   |
| 1   | AA    | 1148 | U    | N1-C2-O2    | -7.57 | 117.50      | 122.80   |
| 1   | AA    | 1336 | C    | C3'-C2'-C1' | -7.57 | 95.44       | 101.50   |
| 22  | AV    | 28   | C    | O4'-C1'-N1  | 7.57  | 114.26      | 108.20   |
| 35  | BB    | 681  | G    | C4-C5-C6    | 7.57  | 123.34      | 118.80   |
| 35  | BB    | 1566 | A    | C4-C5-C6    | 7.57  | 120.79      | 117.00   |
| 35  | BB    | 2778 | A    | C5-C6-N1    | -7.57 | 113.91      | 117.70   |
| 1   | AA    | 1308 | U    | N1-C2-N3    | 7.57  | 119.44      | 114.90   |
| 35  | BB    | 487  | C    | O4'-C1'-N1  | 7.57  | 114.26      | 108.20   |
| 35  | BB    | 930  | G    | C2-N3-C4    | 7.57  | 115.69      | 111.90   |
| 1   | AA    | 24   | U    | N3-C4-C5    | 7.57  | 119.14      | 114.60   |
| 1   | AA    | 1005 | A    | C5-C6-N6    | -7.57 | 117.64      | 123.70   |
| 35  | BB    | 781  | A    | C4-C5-N7    | -7.57 | 106.92      | 110.70   |
| 35  | BB    | 1009 | A    | C5-C6-N1    | -7.57 | 113.92      | 117.70   |
| 35  | BB    | 1278 | C    | O4'-C1'-N1  | 7.57  | 114.26      | 108.20   |
| 35  | BB    | 1574 | C    | C6-N1-C2    | -7.57 | 117.27      | 120.30   |
| 1   | AA    | 275  | G    | N3-C2-N2    | 7.57  | 125.20      | 119.90   |
| 1   | AA    | 679  | C    | O4'-C1'-N1  | 7.57  | 114.25      | 108.20   |
| 35  | BB    | 361  | G    | N3-C4-C5    | -7.57 | 124.81      | 128.60   |
| 35  | BB    | 995  | C    | C1'-O4'-C4' | -7.57 | 103.84      | 109.90   |
| 1   | AA    | 6    | G    | N3-C4-N9    | -7.57 | 121.46      | 126.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1331 | G    | C2-N3-C4    | 7.57  | 115.68      | 111.90   |
| 35  | BB    | 48   | G    | C5'-C4'-O4' | 7.57  | 118.18      | 109.10   |
| 35  | BB    | 201  | C    | N3-C4-C5    | -7.57 | 118.87      | 121.90   |
| 35  | BB    | 310  | A    | C4-C5-C6    | 7.57  | 120.78      | 117.00   |
| 35  | BB    | 1215 | G    | N1-C2-N3    | -7.57 | 119.36      | 123.90   |
| 35  | BB    | 1531 | C    | N3-C4-C5    | -7.57 | 118.87      | 121.90   |
| 35  | BB    | 1740 | G    | N1-C2-N2    | -7.57 | 109.39      | 116.20   |
| 35  | BB    | 1849 | G    | N3-C2-N2    | 7.57  | 125.20      | 119.90   |
| 35  | BB    | 2041 | U    | N1-C2-O2    | -7.57 | 117.50      | 122.80   |
| 35  | BB    | 2087 | G    | C6-C5-N7    | -7.57 | 125.86      | 130.40   |
| 1   | AA    | 462  | G    | N3-C4-C5    | -7.57 | 124.82      | 128.60   |
| 1   | AA    | 780  | A    | C6-C5-N7    | -7.57 | 127.00      | 132.30   |
| 35  | BB    | 1608 | A    | C4-C5-N7    | 7.57  | 114.48      | 110.70   |
| 35  | BB    | 2659 | G    | O4'-C1'-N9  | 7.57  | 114.25      | 108.20   |
| 1   | AA    | 90   | C    | O4'-C1'-N1  | 7.56  | 114.25      | 108.20   |
| 35  | BB    | 954  | G    | C5-C6-N1    | -7.56 | 107.72      | 111.50   |
| 35  | BB    | 2403 | C    | O4'-C1'-N1  | 7.56  | 114.25      | 108.20   |
| 35  | BB    | 2838 | G    | N1-C6-O6    | 7.56  | 124.44      | 119.90   |
| 34  | BA    | 47   | C    | N3-C4-N4    | 7.56  | 123.29      | 118.00   |
| 35  | BB    | 1157 | G    | C5-N7-C8    | 7.56  | 108.08      | 104.30   |
| 35  | BB    | 1206 | G    | O4'-C4'-C3' | -7.56 | 96.44       | 104.00   |
| 35  | BB    | 2209 | G    | C2-N3-C4    | 7.56  | 115.68      | 111.90   |
| 1   | AA    | 1405 | G    | C2-N3-C4    | 7.56  | 115.68      | 111.90   |
| 35  | BB    | 1553 | A    | C4-C5-C6    | 7.56  | 120.78      | 117.00   |
| 35  | BB    | 1826 | G    | C6-C5-N7    | -7.56 | 125.86      | 130.40   |
| 1   | AA    | 62   | U    | N3-C4-O4    | 7.56  | 124.69      | 119.40   |
| 1   | AA    | 1099 | G    | N1-C6-O6    | 7.56  | 124.44      | 119.90   |
| 35  | BB    | 63   | A    | C8-N9-C4    | -7.56 | 102.78      | 105.80   |
| 35  | BB    | 535  | G    | C4-C5-C6    | 7.56  | 123.34      | 118.80   |
| 35  | BB    | 924  | G    | C2-N3-C4    | 7.56  | 115.68      | 111.90   |
| 35  | BB    | 1535 | A    | N7-C8-N9    | 7.56  | 117.58      | 113.80   |
| 35  | BB    | 2399 | G    | C4-C5-C6    | 7.56  | 123.33      | 118.80   |
| 35  | BB    | 2399 | G    | N1-C6-O6    | 7.56  | 124.44      | 119.90   |
| 35  | BB    | 2587 | A    | N1-C6-N6    | 7.56  | 123.14      | 118.60   |
| 35  | BB    | 2899 | A    | N1-C2-N3    | 7.56  | 133.08      | 129.30   |
| 1   | AA    | 166  | U    | N3-C4-O4    | 7.56  | 124.69      | 119.40   |
| 1   | AA    | 449  | G    | C5-N7-C8    | -7.56 | 100.52      | 104.30   |
| 1   | AA    | 759  | A    | P-O3'-C3'   | -7.56 | 110.63      | 119.70   |
| 1   | AA    | 1022 | A    | N1-C2-N3    | 7.56  | 133.08      | 129.30   |
| 35  | BB    | 424  | G    | O4'-C1'-N9  | 7.56  | 114.25      | 108.20   |
| 35  | BB    | 624  | C    | N3-C4-N4    | 7.56  | 123.29      | 118.00   |
| 35  | BB    | 795  | C    | N3-C4-C5    | -7.56 | 118.88      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 837  | C    | C4-C5-C6    | 7.56  | 121.18      | 117.40   |
| 35  | BB    | 1848 | A    | N9-C4-C5    | -7.56 | 102.78      | 105.80   |
| 35  | BB    | 2061 | G    | N1-C2-N3    | -7.56 | 119.37      | 123.90   |
| 35  | BB    | 2862 | G    | N1-C2-N2    | 7.56  | 123.00      | 116.20   |
| 34  | BA    | 4    | C    | O4'-C1'-N1  | 7.56  | 114.25      | 108.20   |
| 1   | AA    | 122  | G    | C5-C6-O6    | -7.55 | 124.07      | 128.60   |
| 1   | AA    | 1061 | G    | N3-C4-C5    | -7.55 | 124.82      | 128.60   |
| 35  | BB    | 1601 | G    | C4-C5-N7    | 7.55  | 113.82      | 110.80   |
| 35  | BB    | 1767 | G    | N3-C2-N2    | 7.55  | 125.19      | 119.90   |
| 35  | BB    | 2378 | A    | N1-C2-N3    | 7.55  | 133.08      | 129.30   |
| 1   | AA    | 1390 | U    | C6-N1-C2    | -7.55 | 116.47      | 121.00   |
| 35  | BB    | 80   | G    | N3-C4-C5    | -7.55 | 124.82      | 128.60   |
| 35  | BB    | 928  | A    | C6-N1-C2    | -7.55 | 114.07      | 118.60   |
| 35  | BB    | 2549 | G    | N3-C2-N2    | 7.55  | 125.19      | 119.90   |
| 1   | AA    | 574  | A    | P-O5'-C5'   | 7.55  | 132.98      | 120.90   |
| 35  | BB    | 239  | C    | C6-N1-C2    | -7.55 | 117.28      | 120.30   |
| 35  | BB    | 1368 | G    | C4-C5-C6    | 7.55  | 123.33      | 118.80   |
| 35  | BB    | 1760 | C    | C4-C5-C6    | 7.55  | 121.18      | 117.40   |
| 35  | BB    | 2134 | A    | C2-N3-C4    | 7.55  | 114.38      | 110.60   |
| 1   | AA    | 81   | A    | C5'-C4'-O4' | 7.55  | 118.16      | 109.10   |
| 1   | AA    | 96   | U    | O4'-C1'-N1  | 7.55  | 114.24      | 108.20   |
| 1   | AA    | 115  | G    | P-O3'-C3'   | 7.55  | 128.76      | 119.70   |
| 1   | AA    | 336  | A    | N7-C8-N9    | -7.55 | 110.03      | 113.80   |
| 1   | AA    | 506  | G    | C5-C6-O6    | -7.55 | 124.07      | 128.60   |
| 1   | AA    | 814  | A    | C6-C5-N7    | -7.55 | 127.02      | 132.30   |
| 1   | AA    | 1350 | A    | C4-C5-C6    | 7.55  | 120.78      | 117.00   |
| 35  | BB    | 440  | C    | N1-C2-N3    | -7.55 | 113.92      | 119.20   |
| 35  | BB    | 671  | C    | C3'-C2'-C1' | -7.55 | 95.46       | 101.50   |
| 1   | AA    | 1475 | G    | C5-N7-C8    | 7.55  | 108.07      | 104.30   |
| 35  | BB    | 1488 | C    | C5'-C4'-C3' | 7.55  | 128.08      | 116.00   |
| 35  | BB    | 2841 | C    | N3-C4-N4    | 7.55  | 123.28      | 118.00   |
| 1   | AA    | 93   | U    | C5-C4-O4    | -7.55 | 121.37      | 125.90   |
| 1   | AA    | 415  | A    | C5'-C4'-C3' | -7.55 | 103.93      | 116.00   |
| 1   | AA    | 483  | C    | C5-C4-N4    | -7.55 | 114.92      | 120.20   |
| 22  | AV    | 30   | U    | O4'-C1'-N1  | 7.55  | 114.24      | 108.20   |
| 34  | BA    | 4    | C    | N3-C4-C5    | -7.55 | 118.88      | 121.90   |
| 35  | BB    | 1862 | G    | N3-C4-C5    | -7.55 | 124.83      | 128.60   |
| 35  | BB    | 2005 | A    | C5-C6-N6    | -7.55 | 117.66      | 123.70   |
| 1   | AA    | 1214 | C    | N1-C2-N3    | -7.54 | 113.92      | 119.20   |
| 35  | BB    | 130  | C    | N3-C4-N4    | 7.54  | 123.28      | 118.00   |
| 35  | BB    | 1681 | G    | C6-C5-N7    | -7.54 | 125.87      | 130.40   |
| 1   | AA    | 9    | G    | N1-C6-O6    | 7.54  | 124.43      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 803  | G    | O4'-C1'-N9  | 7.54  | 114.23      | 108.20   |
| 1   | AA    | 1166 | G    | C6-C5-N7    | -7.54 | 125.87      | 130.40   |
| 1   | AA    | 1499 | A    | C4-C5-N7    | -7.54 | 106.93      | 110.70   |
| 1   | AA    | 1499 | A    | N7-C8-N9    | -7.54 | 110.03      | 113.80   |
| 35  | BB    | 715  | A    | C5-N7-C8    | 7.54  | 107.67      | 103.90   |
| 35  | BB    | 885  | C    | N3-C4-C5    | -7.54 | 118.88      | 121.90   |
| 35  | BB    | 1223 | G    | C5-N7-C8    | 7.54  | 108.07      | 104.30   |
| 35  | BB    | 2147 | A    | C5-C6-N1    | -7.54 | 113.93      | 117.70   |
| 1   | AA    | 428  | G    | N1-C6-O6    | 7.54  | 124.42      | 119.90   |
| 1   | AA    | 1353 | G    | N3-C4-N9    | 7.54  | 130.53      | 126.00   |
| 35  | BB    | 568  | U    | O4'-C1'-N1  | 7.54  | 114.23      | 108.20   |
| 35  | BB    | 1717 | A    | C5-C6-N1    | -7.54 | 113.93      | 117.70   |
| 35  | BB    | 2702 | G    | C5-N7-C8    | 7.54  | 108.07      | 104.30   |
| 1   | AA    | 259  | G    | N1-C6-O6    | 7.54  | 124.42      | 119.90   |
| 35  | BB    | 54   | G    | C6-C5-N7    | -7.54 | 125.88      | 130.40   |
| 35  | BB    | 274  | C    | C1'-O4'-C4' | -7.54 | 103.87      | 109.90   |
| 1   | AA    | 1146 | A    | N1-C2-N3    | 7.54  | 133.07      | 129.30   |
| 35  | BB    | 2044 | C    | N3-C4-N4    | 7.54  | 123.28      | 118.00   |
| 1   | AA    | 1521 | C    | C5-C6-N1    | 7.54  | 124.77      | 121.00   |
| 35  | BB    | 340  | A    | N1-C6-N6    | 7.54  | 123.12      | 118.60   |
| 35  | BB    | 821  | A    | C5-C6-N1    | -7.54 | 113.93      | 117.70   |
| 35  | BB    | 1495 | A    | C4-C5-C6    | 7.54  | 120.77      | 117.00   |
| 1   | AA    | 77   | A    | N1-C2-N3    | -7.54 | 125.53      | 129.30   |
| 35  | BB    | 275  | C    | C2-N3-C4    | 7.54  | 123.67      | 119.90   |
| 35  | BB    | 307  | G    | N1-C6-O6    | 7.54  | 124.42      | 119.90   |
| 35  | BB    | 456  | C    | N3-C2-O2    | -7.54 | 116.62      | 121.90   |
| 35  | BB    | 600  | G    | C5-C6-N1    | 7.54  | 115.27      | 111.50   |
| 35  | BB    | 620  | G    | N1-C6-O6    | 7.54  | 124.42      | 119.90   |
| 35  | BB    | 1491 | G    | C5-C6-O6    | -7.54 | 124.08      | 128.60   |
| 35  | BB    | 1862 | G    | C6-C5-N7    | -7.54 | 125.88      | 130.40   |
| 35  | BB    | 2120 | G    | C8-N9-C4    | 7.54  | 109.42      | 106.40   |
| 35  | BB    | 2232 | C    | N3-C4-N4    | 7.54  | 123.28      | 118.00   |
| 35  | BB    | 2754 | U    | N1-C2-O2    | -7.54 | 117.53      | 122.80   |
| 1   | AA    | 605  | U    | C5-C6-N1    | 7.53  | 126.47      | 122.70   |
| 1   | AA    | 909  | A    | C5-C6-N6    | -7.53 | 117.67      | 123.70   |
| 16  | AP    | 69   | ASP  | CB-CG-OD2   | -7.53 | 111.52      | 118.30   |
| 35  | BB    | 83   | A    | C4-C5-C6    | 7.53  | 120.77      | 117.00   |
| 35  | BB    | 1091 | G    | O4'-C1'-N9  | 7.53  | 114.23      | 108.20   |
| 35  | BB    | 1471 | G    | N3-C4-N9    | 7.53  | 130.52      | 126.00   |
| 35  | BB    | 1904 | G    | N3-C4-N9    | 7.53  | 130.52      | 126.00   |
| 1   | AA    | 665  | A    | C4-C5-N7    | -7.53 | 106.93      | 110.70   |
| 1   | AA    | 1453 | G    | C5-C6-O6    | -7.53 | 124.08      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1300 | G    | C5-C6-N1    | -7.53 | 107.73      | 111.50   |
| 35  | BB    | 1852 | U    | C2-N3-C4    | -7.53 | 122.48      | 127.00   |
| 35  | BB    | 2283 | C    | O5'-P-OP2   | -7.53 | 98.92       | 105.70   |
| 35  | BB    | 2405 | G    | N1-C2-N3    | -7.53 | 119.38      | 123.90   |
| 35  | BB    | 2665 | A    | C6-C5-N7    | -7.53 | 127.03      | 132.30   |
| 1   | AA    | 69   | G    | C8-N9-C4    | -7.53 | 103.39      | 106.40   |
| 1   | AA    | 139  | A    | N1-C6-N6    | 7.53  | 123.12      | 118.60   |
| 1   | AA    | 200  | G    | O4'-C1'-N9  | 7.53  | 114.22      | 108.20   |
| 1   | AA    | 367  | U    | C5-C6-N1    | 7.53  | 126.47      | 122.70   |
| 1   | AA    | 687  | A    | O4'-C1'-N9  | 7.53  | 114.22      | 108.20   |
| 35  | BB    | 260  | G    | C8-N9-C4    | -7.53 | 103.39      | 106.40   |
| 35  | BB    | 801  | G    | N1-C6-O6    | 7.53  | 124.42      | 119.90   |
| 35  | BB    | 815  | C    | C5-C4-N4    | -7.53 | 114.93      | 120.20   |
| 35  | BB    | 1132 | U    | N3-C4-O4    | 7.53  | 124.67      | 119.40   |
| 35  | BB    | 2098 | U    | C4-C5-C6    | -7.53 | 115.18      | 119.70   |
| 40  | BG    | 118  | ALA  | N-CA-CB     | 7.53  | 120.64      | 110.10   |
| 1   | AA    | 722  | G    | C8-N9-C4    | -7.53 | 103.39      | 106.40   |
| 1   | AA    | 826  | C    | O4'-C1'-N1  | 7.53  | 114.22      | 108.20   |
| 1   | AA    | 1150 | A    | N1-C2-N3    | 7.53  | 133.06      | 129.30   |
| 35  | BB    | 252  | G    | C5-C6-O6    | -7.53 | 124.08      | 128.60   |
| 1   | AA    | 168  | G    | N1-C2-N2    | -7.53 | 109.42      | 116.20   |
| 1   | AA    | 1106 | G    | N1-C2-N2    | -7.53 | 109.42      | 116.20   |
| 5   | AE    | 28   | ARG  | NE-CZ-NH2   | -7.53 | 116.54      | 120.30   |
| 35  | BB    | 1132 | U    | N3-C4-C5    | -7.53 | 110.08      | 114.60   |
| 1   | AA    | 113  | G    | C1'-O4'-C4' | 7.53  | 115.92      | 109.90   |
| 1   | AA    | 155  | A    | C6-C5-N7    | -7.53 | 127.03      | 132.30   |
| 1   | AA    | 1043 | G    | C4-C5-C6    | 7.53  | 123.31      | 118.80   |
| 1   | AA    | 1486 | G    | N3-C2-N2    | 7.53  | 125.17      | 119.90   |
| 35  | BB    | 484  | C    | N3-C4-N4    | 7.53  | 123.27      | 118.00   |
| 35  | BB    | 1891 | G    | C4-C5-C6    | 7.53  | 123.31      | 118.80   |
| 35  | BB    | 2604 | U    | P-O3'-C3'   | -7.53 | 110.67      | 119.70   |
| 37  | BD    | 35   | THR  | CA-CB-CG2   | -7.53 | 101.86      | 112.40   |
| 35  | BB    | 117  | G    | C5-C6-O6    | -7.52 | 124.09      | 128.60   |
| 35  | BB    | 2357 | G    | C5-C6-N1    | -7.52 | 107.74      | 111.50   |
| 1   | AA    | 39   | G    | C6-C5-N7    | -7.52 | 125.89      | 130.40   |
| 1   | AA    | 324  | G    | C6-C5-N7    | -7.52 | 125.89      | 130.40   |
| 1   | AA    | 829  | G    | C8-N9-C4    | -7.52 | 103.39      | 106.40   |
| 1   | AA    | 1144 | G    | C5-C6-N1    | -7.52 | 107.74      | 111.50   |
| 1   | AA    | 1237 | C    | N3-C4-C5    | -7.52 | 118.89      | 121.90   |
| 35  | BB    | 82   | U    | C5-C6-N1    | 7.52  | 126.46      | 122.70   |
| 35  | BB    | 1014 | A    | N3-C4-C5    | -7.52 | 121.53      | 126.80   |
| 35  | BB    | 1775 | U    | C4-C5-C6    | 7.52  | 124.21      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2266 | A    | O4'-C1'-N9  | 7.52  | 114.22      | 108.20   |
| 1   | AA    | 427  | U    | O4'-C1'-N1  | 7.52  | 114.22      | 108.20   |
| 1   | AA    | 454  | G    | C5-C6-O6    | -7.52 | 124.09      | 128.60   |
| 1   | AA    | 459  | A    | N1-C2-N3    | 7.52  | 133.06      | 129.30   |
| 1   | AA    | 559  | A    | N9-C4-C5    | 7.52  | 108.81      | 105.80   |
| 1   | AA    | 1016 | A    | C1'-O4'-C4' | 7.52  | 115.92      | 109.90   |
| 35  | BB    | 792  | A    | N1-C6-N6    | 7.52  | 123.11      | 118.60   |
| 35  | BB    | 1109 | C    | P-O3'-C3'   | 7.52  | 128.73      | 119.70   |
| 35  | BB    | 1569 | A    | C6-C5-N7    | -7.52 | 127.04      | 132.30   |
| 35  | BB    | 2518 | A    | C4-C5-C6    | 7.52  | 120.76      | 117.00   |
| 1   | AA    | 148  | G    | O4'-C1'-N9  | 7.52  | 114.22      | 108.20   |
| 1   | AA    | 172  | A    | N3-C4-C5    | -7.52 | 121.54      | 126.80   |
| 1   | AA    | 179  | A    | O4'-C1'-N9  | 7.52  | 114.22      | 108.20   |
| 1   | AA    | 438  | U    | C5-C6-N1    | 7.52  | 126.46      | 122.70   |
| 1   | AA    | 638  | U    | C4-C5-C6    | 7.52  | 124.21      | 119.70   |
| 1   | AA    | 987  | G    | C4-C5-N7    | -7.52 | 107.79      | 110.80   |
| 1   | AA    | 1020 | G    | C5-C6-O6    | -7.52 | 124.09      | 128.60   |
| 1   | AA    | 1034 | G    | C5-C6-O6    | -7.52 | 124.09      | 128.60   |
| 1   | AA    | 1331 | G    | C4-C5-C6    | 7.52  | 123.31      | 118.80   |
| 35  | BB    | 358  | U    | N3-C4-O4    | 7.52  | 124.66      | 119.40   |
| 35  | BB    | 1887 | C    | P-O3'-C3'   | -7.52 | 110.68      | 119.70   |
| 35  | BB    | 1938 | A    | C1'-O4'-C4' | -7.52 | 103.88      | 109.90   |
| 35  | BB    | 2019 | A    | C5-C6-N1    | -7.52 | 113.94      | 117.70   |
| 1   | AA    | 165  | G    | O4'-C1'-N9  | 7.52  | 114.21      | 108.20   |
| 1   | AA    | 421  | U    | O4'-C1'-N1  | 7.52  | 114.21      | 108.20   |
| 1   | AA    | 1076 | U    | N1-C2-O2    | -7.52 | 117.54      | 122.80   |
| 1   | AA    | 1204 | A    | O4'-C1'-N9  | 7.52  | 114.21      | 108.20   |
| 22  | AV    | 17   | C    | O4'-C1'-N1  | 7.52  | 114.21      | 108.20   |
| 35  | BB    | 61   | C    | C4-C5-C6    | 7.52  | 121.16      | 117.40   |
| 35  | BB    | 127  | A    | N1-C2-N3    | 7.52  | 133.06      | 129.30   |
| 35  | BB    | 1362 | C    | C5-C6-N1    | 7.52  | 124.76      | 121.00   |
| 35  | BB    | 1382 | G    | C1'-O4'-C4' | -7.52 | 103.89      | 109.90   |
| 35  | BB    | 2347 | C    | C6-N1-C2    | -7.52 | 117.29      | 120.30   |
| 35  | BB    | 2399 | G    | N1-C2-N3    | -7.52 | 119.39      | 123.90   |
| 35  | BB    | 2560 | A    | N1-C2-N3    | 7.52  | 133.06      | 129.30   |
| 35  | BB    | 254  | G    | N1-C2-N2    | -7.52 | 109.44      | 116.20   |
| 35  | BB    | 627  | A    | C5-C6-N1    | -7.52 | 113.94      | 117.70   |
| 35  | BB    | 912  | C    | N1-C2-O2    | -7.52 | 114.39      | 118.90   |
| 35  | BB    | 1567 | G    | C4-C5-N7    | -7.52 | 107.79      | 110.80   |
| 35  | BB    | 2847 | U    | N3-C4-C5    | -7.52 | 110.09      | 114.60   |
| 1   | AA    | 36   | C    | N3-C4-C5    | -7.51 | 118.89      | 121.90   |
| 1   | AA    | 642  | A    | C5-C6-N1    | -7.51 | 113.94      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 760  | G    | N9-C4-C5    | 7.51  | 108.41      | 105.40   |
| 35  | BB    | 228  | C    | O4'-C1'-N1  | 7.51  | 114.21      | 108.20   |
| 35  | BB    | 903  | C    | C5-C6-N1    | 7.51  | 124.76      | 121.00   |
| 1   | AA    | 20   | U    | N3-C4-O4    | 7.51  | 124.66      | 119.40   |
| 35  | BB    | 1537 | G    | P-O3'-C3'   | 7.51  | 128.72      | 119.70   |
| 35  | BB    | 2066 | C    | C6-N1-C2    | -7.51 | 117.30      | 120.30   |
| 35  | BB    | 2867 | G    | C5-C6-O6    | -7.51 | 124.09      | 128.60   |
| 35  | BB    | 2893 | A    | C2-N3-C4    | -7.51 | 106.84      | 110.60   |
| 1   | AA    | 576  | C    | O4'-C1'-N1  | 7.51  | 114.21      | 108.20   |
| 1   | AA    | 1334 | G    | C5-C6-O6    | -7.51 | 124.09      | 128.60   |
| 35  | BB    | 1083 | U    | P-O5'-C5'   | -7.51 | 108.88      | 120.90   |
| 35  | BB    | 1094 | U    | N3-C4-O4    | -7.51 | 114.14      | 119.40   |
| 35  | BB    | 2394 | C    | C2-N3-C4    | 7.51  | 123.66      | 119.90   |
| 52  | BS    | 25   | ARG  | NE-CZ-NH1   | 7.51  | 124.06      | 120.30   |
| 1   | AA    | 428  | G    | C5-C6-O6    | -7.51 | 124.09      | 128.60   |
| 1   | AA    | 1519 | A    | C8-N9-C4    | -7.51 | 102.80      | 105.80   |
| 35  | BB    | 104  | A    | C1'-O4'-C4' | -7.51 | 103.89      | 109.90   |
| 35  | BB    | 1011 | G    | C8-N9-C1'   | 7.51  | 136.76      | 127.00   |
| 35  | BB    | 1216 | G    | N1-C6-O6    | 7.51  | 124.41      | 119.90   |
| 35  | BB    | 1492 | G    | N3-C4-C5    | 7.51  | 132.35      | 128.60   |
| 35  | BB    | 1688 | U    | N3-C4-O4    | 7.51  | 124.66      | 119.40   |
| 35  | BB    | 1871 | A    | N1-C2-N3    | 7.51  | 133.06      | 129.30   |
| 35  | BB    | 2006 | C    | N1-C2-N3    | -7.51 | 113.94      | 119.20   |
| 35  | BB    | 382  | A    | C5-N7-C8    | 7.51  | 107.65      | 103.90   |
| 35  | BB    | 1233 | C    | O4'-C1'-N1  | 7.51  | 114.21      | 108.20   |
| 1   | AA    | 845  | A    | C8-N9-C4    | -7.51 | 102.80      | 105.80   |
| 1   | AA    | 949  | A    | C6-N1-C2    | 7.51  | 123.10      | 118.60   |
| 1   | AA    | 995  | C    | C6-N1-C2    | -7.51 | 117.30      | 120.30   |
| 16  | AP    | 1    | MET  | CG-SD-CE    | -7.51 | 88.19       | 100.20   |
| 35  | BB    | 437  | U    | C3'-C2'-C1' | -7.51 | 95.50       | 101.50   |
| 35  | BB    | 1261 | C    | N3-C4-N4    | 7.51  | 123.25      | 118.00   |
| 35  | BB    | 2283 | C    | P-O3'-C3'   | -7.51 | 110.69      | 119.70   |
| 35  | BB    | 2421 | G    | N7-C8-N9    | -7.51 | 109.35      | 113.10   |
| 1   | AA    | 366  | A    | C8-N9-C4    | -7.50 | 102.80      | 105.80   |
| 1   | AA    | 446  | G    | C5-C6-O6    | -7.50 | 124.10      | 128.60   |
| 35  | BB    | 843  | G    | N3-C4-N9    | 7.50  | 130.50      | 126.00   |
| 1   | AA    | 367  | U    | C4-C5-C6    | -7.50 | 115.20      | 119.70   |
| 1   | AA    | 613  | C    | N3-C4-N4    | 7.50  | 123.25      | 118.00   |
| 1   | AA    | 808  | C    | N1-C2-N3    | -7.50 | 113.95      | 119.20   |
| 1   | AA    | 885  | G    | N9-C4-C5    | 7.50  | 108.40      | 105.40   |
| 35  | BB    | 49   | A    | C8-N9-C4    | -7.50 | 102.80      | 105.80   |
| 35  | BB    | 153  | U    | O4'-C1'-C2' | -7.50 | 98.30       | 105.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1578 | U    | C4'-C3'-C2' | -7.50 | 95.10       | 102.60   |
| 35  | BB    | 1645 | G    | O4'-C1'-N9  | 7.50  | 114.20      | 108.20   |
| 35  | BB    | 1717 | A    | C4-C5-C6    | 7.50  | 120.75      | 117.00   |
| 35  | BB    | 1885 | A    | C4-C5-C6    | 7.50  | 120.75      | 117.00   |
| 35  | BB    | 2654 | A    | C5-C6-N6    | -7.50 | 117.70      | 123.70   |
| 1   | AA    | 902  | G    | C6-C5-N7    | -7.50 | 125.90      | 130.40   |
| 9   | AI    | 19   | PHE  | CB-CG-CD1   | -7.50 | 115.55      | 120.80   |
| 15  | AO    | 67   | ASP  | CB-CG-OD2   | -7.50 | 111.55      | 118.30   |
| 35  | BB    | 250  | G    | N1-C2-N2    | -7.50 | 109.45      | 116.20   |
| 35  | BB    | 271  | G    | C3'-C2'-C1' | -7.50 | 95.50       | 101.50   |
| 35  | BB    | 319  | G    | N1-C6-O6    | 7.50  | 124.40      | 119.90   |
| 35  | BB    | 763  | G    | C5-C6-O6    | -7.50 | 124.10      | 128.60   |
| 35  | BB    | 1314 | C    | N3-C4-N4    | 7.50  | 123.25      | 118.00   |
| 1   | AA    | 588  | G    | N1-C2-N3    | -7.50 | 119.40      | 123.90   |
| 1   | AA    | 830  | G    | C8-N9-C4    | -7.50 | 103.40      | 106.40   |
| 35  | BB    | 206  | U    | N3-C2-O2    | 7.50  | 127.45      | 122.20   |
| 35  | BB    | 750  | A    | O4'-C1'-N9  | 7.50  | 114.20      | 108.20   |
| 35  | BB    | 781  | A    | C5-N7-C8    | 7.50  | 107.65      | 103.90   |
| 35  | BB    | 926  | G    | P-O3'-C3'   | -7.50 | 110.70      | 119.70   |
| 35  | BB    | 1179 | G    | C6-N1-C2    | 7.50  | 129.60      | 125.10   |
| 35  | BB    | 2283 | C    | N1-C2-O2    | -7.50 | 114.40      | 118.90   |
| 35  | BB    | 2896 | C    | C5-C6-N1    | 7.50  | 124.75      | 121.00   |
| 41  | BH    | 27   | ARG  | NE-CZ-NH1   | 7.50  | 124.05      | 120.30   |
| 1   | AA    | 64   | G    | C4-C5-N7    | 7.50  | 113.80      | 110.80   |
| 1   | AA    | 221  | C    | N3-C2-O2    | 7.50  | 127.15      | 121.90   |
| 1   | AA    | 821  | G    | C4-C5-N7    | -7.50 | 107.80      | 110.80   |
| 35  | BB    | 235  | U    | O4'-C1'-N1  | 7.50  | 114.20      | 108.20   |
| 35  | BB    | 1856 | U    | C5-C4-O4    | 7.50  | 130.40      | 125.90   |
| 1   | AA    | 558  | G    | C6-C5-N7    | -7.50 | 125.90      | 130.40   |
| 1   | AA    | 1353 | G    | C6-N1-C2    | 7.50  | 129.60      | 125.10   |
| 18  | AR    | 31   | TYR  | CB-CG-CD1   | 7.50  | 125.50      | 121.00   |
| 35  | BB    | 265  | A    | C6-N1-C2    | 7.50  | 123.10      | 118.60   |
| 35  | BB    | 1533 | C    | C2-N3-C4    | 7.50  | 123.65      | 119.90   |
| 35  | BB    | 2743 | U    | C6-N1-C2    | -7.50 | 116.50      | 121.00   |
| 1   | AA    | 113  | G    | N9-C4-C5    | -7.49 | 102.40      | 105.40   |
| 1   | AA    | 912  | C    | O4'-C1'-N1  | 7.49  | 114.19      | 108.20   |
| 1   | AA    | 1220 | G    | N1-C6-O6    | 7.49  | 124.40      | 119.90   |
| 1   | AA    | 1459 | G    | C4-C5-N7    | 7.49  | 113.80      | 110.80   |
| 34  | BA    | 64   | G    | N1-C6-O6    | 7.49  | 124.40      | 119.90   |
| 35  | BB    | 137  | U    | O4'-C1'-N1  | 7.49  | 114.19      | 108.20   |
| 35  | BB    | 278  | A    | C2-N3-C4    | 7.49  | 114.35      | 110.60   |
| 35  | BB    | 1028 | A    | C8-N9-C4    | -7.49 | 102.80      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2295 | C    | O4'-C1'-N1  | 7.49  | 114.19      | 108.20   |
| 35  | BB    | 2430 | A    | C2-N3-C4    | -7.49 | 106.85      | 110.60   |
| 35  | BB    | 2557 | G    | C4-C5-C6    | 7.49  | 123.30      | 118.80   |
| 35  | BB    | 2771 | C    | C4-C5-C6    | 7.49  | 121.15      | 117.40   |
| 1   | AA    | 285  | C    | N3-C4-N4    | 7.49  | 123.24      | 118.00   |
| 1   | AA    | 945  | G    | P-O5'-C5'   | 7.49  | 132.89      | 120.90   |
| 35  | BB    | 45   | G    | P-O3'-C3'   | 7.49  | 128.69      | 119.70   |
| 35  | BB    | 882  | G    | N1-C6-O6    | 7.49  | 124.39      | 119.90   |
| 35  | BB    | 1989 | G    | C5-C6-O6    | -7.49 | 124.11      | 128.60   |
| 35  | BB    | 2119 | A    | C2-N3-C4    | -7.49 | 106.85      | 110.60   |
| 35  | BB    | 2338 | C    | N3-C2-O2    | 7.49  | 127.14      | 121.90   |
| 35  | BB    | 2866 | U    | N3-C4-C5    | -7.49 | 110.11      | 114.60   |
| 1   | AA    | 895  | G    | N1-C6-O6    | 7.49  | 124.39      | 119.90   |
| 1   | AA    | 1038 | C    | C5-C6-N1    | 7.49  | 124.75      | 121.00   |
| 35  | BB    | 19   | A    | C8-N9-C4    | -7.49 | 102.80      | 105.80   |
| 35  | BB    | 615  | U    | C5-C4-O4    | -7.49 | 121.41      | 125.90   |
| 35  | BB    | 1276 | A    | C4-C5-C6    | 7.49  | 120.75      | 117.00   |
| 35  | BB    | 1657 | U    | O4'-C1'-N1  | 7.49  | 114.19      | 108.20   |
| 13  | AM    | 34   | ALA  | N-CA-CB     | 7.49  | 120.58      | 110.10   |
| 35  | BB    | 103  | A    | N1-C2-N3    | -7.49 | 125.56      | 129.30   |
| 35  | BB    | 973  | A    | N7-C8-N9    | 7.49  | 117.54      | 113.80   |
| 35  | BB    | 1026 | G    | C6-C5-N7    | -7.49 | 125.91      | 130.40   |
| 35  | BB    | 1324 | G    | N1-C6-O6    | 7.49  | 124.39      | 119.90   |
| 35  | BB    | 1652 | A    | C5-C6-N1    | -7.49 | 113.96      | 117.70   |
| 1   | AA    | 917  | G    | C6-C5-N7    | -7.49 | 125.91      | 130.40   |
| 35  | BB    | 374  | A    | C5-C6-N6    | -7.49 | 117.71      | 123.70   |
| 35  | BB    | 1699 | G    | N9-C4-C5    | 7.49  | 108.39      | 105.40   |
| 1   | AA    | 1117 | A    | C5-C6-N6    | -7.49 | 117.71      | 123.70   |
| 1   | AA    | 1419 | G    | C2-N3-C4    | -7.49 | 108.16      | 111.90   |
| 1   | AA    | 1503 | A    | C5-C6-N6    | -7.49 | 117.71      | 123.70   |
| 35  | BB    | 1692 | U    | O4'-C1'-N1  | 7.49  | 114.19      | 108.20   |
| 35  | BB    | 2829 | A    | C5-C6-N6    | -7.49 | 117.71      | 123.70   |
| 35  | BB    | 2900 | A    | P-O3'-C3'   | -7.49 | 110.72      | 119.70   |
| 1   | AA    | 646  | G    | C4'-C3'-C2' | -7.48 | 95.12       | 102.60   |
| 1   | AA    | 709  | U    | O4'-C1'-N1  | 7.48  | 114.19      | 108.20   |
| 1   | AA    | 729  | A    | C8-N9-C4    | -7.48 | 102.81      | 105.80   |
| 1   | AA    | 748  | G    | C5-C6-O6    | -7.48 | 124.11      | 128.60   |
| 1   | AA    | 1374 | A    | N1-C2-N3    | 7.48  | 133.04      | 129.30   |
| 35  | BB    | 718  | A    | O4'-C1'-N9  | 7.48  | 114.19      | 108.20   |
| 35  | BB    | 1126 | A    | C4-C5-C6    | 7.48  | 120.74      | 117.00   |
| 35  | BB    | 1642 | G    | C6-C5-N7    | -7.48 | 125.91      | 130.40   |
| 1   | AA    | 514  | C    | C6-N1-C2    | -7.48 | 117.31      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 809  | G    | C6-C5-N7    | -7.48 | 125.91      | 130.40   |
| 25  | B0    | 45   | PHE  | CB-CG-CD2   | -7.48 | 115.56      | 120.80   |
| 35  | BB    | 513  | A    | N1-C2-N3    | 7.48  | 133.04      | 129.30   |
| 35  | BB    | 1856 | U    | N1-C2-N3    | -7.48 | 110.41      | 114.90   |
| 1   | AA    | 1328 | C    | C6-N1-C2    | -7.48 | 117.31      | 120.30   |
| 35  | BB    | 1874 | C    | C5-C4-N4    | -7.48 | 114.97      | 120.20   |
| 35  | BB    | 2064 | C    | O4'-C1'-N1  | 7.48  | 114.18      | 108.20   |
| 1   | AA    | 32   | A    | C8-N9-C4    | -7.48 | 102.81      | 105.80   |
| 1   | AA    | 749  | A    | C6-C5-N7    | -7.48 | 127.07      | 132.30   |
| 5   | AE    | 156  | ARG  | NE-CZ-NH2   | -7.48 | 116.56      | 120.30   |
| 35  | BB    | 759  | G    | O4'-C1'-N9  | 7.48  | 114.18      | 108.20   |
| 35  | BB    | 831  | G    | N1-C6-O6    | 7.48  | 124.39      | 119.90   |
| 35  | BB    | 2443 | C    | C4-C5-C6    | -7.48 | 113.66      | 117.40   |
| 35  | BB    | 2678 | C    | C4'-C3'-C2' | -7.48 | 95.12       | 102.60   |
| 1   | AA    | 247  | G    | N1-C6-O6    | 7.48  | 124.39      | 119.90   |
| 1   | AA    | 324  | G    | C5-C6-N1    | -7.48 | 107.76      | 111.50   |
| 34  | BA    | 58   | A    | C5-C6-N1    | -7.48 | 113.96      | 117.70   |
| 35  | BB    | 373  | U    | C5-C4-O4    | -7.48 | 121.41      | 125.90   |
| 35  | BB    | 580  | U    | C5-C4-O4    | -7.48 | 121.41      | 125.90   |
| 35  | BB    | 1202 | G    | C4-C5-C6    | 7.48  | 123.29      | 118.80   |
| 35  | BB    | 1204 | A    | C5-N7-C8    | 7.48  | 107.64      | 103.90   |
| 35  | BB    | 1240 | U    | N3-C2-O2    | 7.48  | 127.43      | 122.20   |
| 35  | BB    | 1968 | G    | C6-C5-N7    | -7.48 | 125.91      | 130.40   |
| 1   | AA    | 1510 | C    | N3-C2-O2    | -7.47 | 116.67      | 121.90   |
| 35  | BB    | 959  | A    | O4'-C1'-N9  | 7.47  | 114.18      | 108.20   |
| 35  | BB    | 1040 | A    | C1'-O4'-C4' | 7.47  | 115.88      | 109.90   |
| 35  | BB    | 1768 | C    | N3-C4-N4    | 7.47  | 123.23      | 118.00   |
| 35  | BB    | 2362 | C    | O4'-C4'-C3' | -7.47 | 96.53       | 104.00   |
| 37  | BD    | 43   | ASP  | CB-CG-OD2   | 7.47  | 125.03      | 118.30   |
| 1   | AA    | 250  | A    | C6-N1-C2    | 7.47  | 123.08      | 118.60   |
| 1   | AA    | 715  | A    | C5-C6-N1    | -7.47 | 113.96      | 117.70   |
| 1   | AA    | 1153 | G    | C8-N9-C4    | -7.47 | 103.41      | 106.40   |
| 1   | AA    | 1444 | U    | C5-C4-O4    | -7.47 | 121.42      | 125.90   |
| 35  | BB    | 241  | A    | O4'-C1'-N9  | 7.47  | 114.18      | 108.20   |
| 35  | BB    | 2017 | U    | N3-C4-O4    | 7.47  | 124.63      | 119.40   |
| 1   | AA    | 604  | G    | N3-C2-N2    | 7.47  | 125.13      | 119.90   |
| 1   | AA    | 1061 | G    | N7-C8-N9    | 7.47  | 116.84      | 113.10   |
| 1   | AA    | 1493 | A    | O4'-C1'-N9  | 7.47  | 114.18      | 108.20   |
| 1   | AA    | 816  | A    | C1'-O4'-C4' | -7.47 | 103.92      | 109.90   |
| 35  | BB    | 673  | C    | C6-N1-C1'   | -7.47 | 111.84      | 120.80   |
| 35  | BB    | 1374 | G    | C6-C5-N7    | -7.47 | 125.92      | 130.40   |
| 35  | BB    | 1430 | G    | N9-C4-C5    | -7.47 | 102.41      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1891 | G    | N3-C4-C5    | -7.47 | 124.86      | 128.60   |
| 35  | BB    | 2535 | G    | N1-C6-O6    | 7.47  | 124.38      | 119.90   |
| 35  | BB    | 146  | A    | C8-N9-C4    | -7.47 | 102.81      | 105.80   |
| 35  | BB    | 2178 | C    | C2-N3-C4    | 7.47  | 123.63      | 119.90   |
| 1   | AA    | 647  | C    | N3-C4-N4    | 7.47  | 123.23      | 118.00   |
| 1   | AA    | 1032 | G    | C4-C5-C6    | 7.47  | 123.28      | 118.80   |
| 1   | AA    | 1172 | C    | C6-N1-C2    | -7.47 | 117.31      | 120.30   |
| 35  | BB    | 1058 | U    | N3-C4-O4    | 7.47  | 124.63      | 119.40   |
| 35  | BB    | 2158 | A    | N7-C8-N9    | 7.47  | 117.53      | 113.80   |
| 1   | AA    | 9    | G    | N9-C4-C5    | -7.46 | 102.41      | 105.40   |
| 1   | AA    | 99   | C    | N1-C2-O2    | 7.46  | 123.38      | 118.90   |
| 1   | AA    | 722  | G    | C5-C6-N1    | -7.46 | 107.77      | 111.50   |
| 1   | AA    | 1009 | U    | P-O3'-C3'   | 7.46  | 128.66      | 119.70   |
| 1   | AA    | 1344 | C    | C4'-C3'-C2' | -7.46 | 95.14       | 102.60   |
| 35  | BB    | 108  | G    | C2-N3-C4    | 7.46  | 115.63      | 111.90   |
| 35  | BB    | 182  | A    | N1-C2-N3    | 7.46  | 133.03      | 129.30   |
| 35  | BB    | 495  | G    | N1-C2-N3    | -7.46 | 119.42      | 123.90   |
| 35  | BB    | 618  | G    | C4-C5-C6    | 7.46  | 123.28      | 118.80   |
| 1   | AA    | 319  | G    | C6-N1-C2    | 7.46  | 129.58      | 125.10   |
| 1   | AA    | 1222 | G    | N1-C2-N3    | -7.46 | 119.42      | 123.90   |
| 35  | BB    | 1722 | A    | O4'-C1'-N9  | 7.46  | 114.17      | 108.20   |
| 35  | BB    | 2053 | G    | N3-C2-N2    | 7.46  | 125.12      | 119.90   |
| 35  | BB    | 2780 | G    | N3-C2-N2    | 7.46  | 125.12      | 119.90   |
| 1   | AA    | 676  | A    | C5-C6-N6    | -7.46 | 117.73      | 123.70   |
| 1   | AA    | 1497 | G    | N7-C8-N9    | -7.46 | 109.37      | 113.10   |
| 1   | AA    | 1524 | C    | O4'-C1'-N1  | 7.46  | 114.17      | 108.20   |
| 22  | AV    | 41   | C    | O4'-C1'-N1  | 7.46  | 114.17      | 108.20   |
| 35  | BB    | 249  | C    | P-O3'-C3'   | 7.46  | 128.65      | 119.70   |
| 35  | BB    | 459  | U    | N3-C4-O4    | 7.46  | 124.62      | 119.40   |
| 35  | BB    | 564  | C    | O4'-C1'-N1  | 7.46  | 114.17      | 108.20   |
| 35  | BB    | 608  | A    | C4-C5-C6    | 7.46  | 120.73      | 117.00   |
| 35  | BB    | 938  | G    | C4-C5-N7    | 7.46  | 113.78      | 110.80   |
| 35  | BB    | 1085 | A    | N9-C4-C5    | 7.46  | 108.78      | 105.80   |
| 35  | BB    | 1099 | G    | N1-C2-N3    | -7.46 | 119.42      | 123.90   |
| 35  | BB    | 1678 | A    | C6-N1-C2    | -7.46 | 114.12      | 118.60   |
| 35  | BB    | 2322 | A    | O4'-C1'-N9  | 7.46  | 114.17      | 108.20   |
| 35  | BB    | 2531 | A    | N7-C8-N9    | -7.46 | 110.07      | 113.80   |
| 35  | BB    | 2876 | G    | O4'-C1'-N9  | 7.46  | 114.17      | 108.20   |
| 35  | BB    | 303  | G    | N1-C6-O6    | 7.46  | 124.38      | 119.90   |
| 35  | BB    | 614  | A    | C1'-O4'-C4' | -7.46 | 103.93      | 109.90   |
| 1   | AA    | 604  | G    | C6-C5-N7    | -7.46 | 125.92      | 130.40   |
| 1   | AA    | 711  | G    | C4-C5-N7    | 7.46  | 113.78      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 825  | A    | C5-N7-C8    | -7.46 | 100.17      | 103.90   |
| 34  | BA    | 50   | A    | O4'-C4'-C3' | -7.46 | 96.54       | 104.00   |
| 35  | BB    | 21   | A    | C6-C5-N7    | -7.46 | 127.08      | 132.30   |
| 35  | BB    | 711  | G    | C2-N3-C4    | 7.46  | 115.63      | 111.90   |
| 35  | BB    | 1206 | G    | N3-C4-C5    | 7.46  | 132.33      | 128.60   |
| 35  | BB    | 1277 | G    | N9-C4-C5    | 7.46  | 108.38      | 105.40   |
| 35  | BB    | 2006 | C    | C5-C6-N1    | -7.46 | 117.27      | 121.00   |
| 35  | BB    | 2477 | U    | N3-C4-C5    | -7.46 | 110.12      | 114.60   |
| 35  | BB    | 2744 | G    | C5-C6-O6    | -7.46 | 124.12      | 128.60   |
| 1   | AA    | 47   | C    | O4'-C1'-N1  | 7.46  | 114.17      | 108.20   |
| 1   | AA    | 1287 | A    | C5-N7-C8    | 7.46  | 107.63      | 103.90   |
| 35  | BB    | 760  | G    | N3-C2-N2    | 7.46  | 125.12      | 119.90   |
| 35  | BB    | 1102 | C    | O4'-C1'-N1  | 7.46  | 114.17      | 108.20   |
| 35  | BB    | 1261 | C    | C4'-C3'-C2' | -7.46 | 95.14       | 102.60   |
| 35  | BB    | 1565 | C    | C5-C4-N4    | -7.46 | 114.98      | 120.20   |
| 35  | BB    | 1689 | A    | C5-N7-C8    | 7.46  | 107.63      | 103.90   |
| 35  | BB    | 1902 | C    | C5-C4-N4    | -7.46 | 114.98      | 120.20   |
| 35  | BB    | 2047 | C    | C6-N1-C2    | -7.46 | 117.32      | 120.30   |
| 35  | BB    | 2468 | A    | N7-C8-N9    | -7.46 | 110.07      | 113.80   |
| 1   | AA    | 503  | C    | C5-C6-N1    | 7.46  | 124.73      | 121.00   |
| 35  | BB    | 154  | U    | C5-C6-N1    | 7.46  | 126.43      | 122.70   |
| 35  | BB    | 418  | C    | N3-C4-C5    | -7.46 | 118.92      | 121.90   |
| 35  | BB    | 1616 | A    | C5-C6-N1    | 7.46  | 121.43      | 117.70   |
| 35  | BB    | 1818 | U    | N1-C2-N3    | -7.46 | 110.43      | 114.90   |
| 35  | BB    | 2051 | A    | N1-C6-N6    | 7.46  | 123.07      | 118.60   |
| 36  | BC    | 261  | ARG  | NE-CZ-NH1   | 7.46  | 124.03      | 120.30   |
| 1   | AA    | 402  | G    | C5-N7-C8    | 7.45  | 108.03      | 104.30   |
| 22  | AV    | 2    | G    | C6-N1-C2    | 7.45  | 129.57      | 125.10   |
| 35  | BB    | 432  | A    | C5-N7-C8    | 7.45  | 107.63      | 103.90   |
| 35  | BB    | 1121 | C    | N3-C4-C5    | -7.45 | 118.92      | 121.90   |
| 35  | BB    | 1475 | G    | C4-C5-C6    | 7.45  | 123.27      | 118.80   |
| 35  | BB    | 2145 | C    | C5-C6-N1    | 7.45  | 124.73      | 121.00   |
| 35  | BB    | 2485 | G    | O4'-C1'-N9  | 7.45  | 114.16      | 108.20   |
| 35  | BB    | 2536 | G    | C8-N9-C4    | -7.45 | 103.42      | 106.40   |
| 1   | AA    | 198  | G    | C4-C5-N7    | 7.45  | 113.78      | 110.80   |
| 1   | AA    | 1153 | G    | C5-C6-O6    | -7.45 | 124.13      | 128.60   |
| 8   | AH    | 83   | ARG  | NH1-CZ-NH2  | 7.45  | 127.60      | 119.40   |
| 35  | BB    | 483  | A    | C5-N7-C8    | 7.45  | 107.63      | 103.90   |
| 35  | BB    | 824  | U    | N3-C4-O4    | -7.45 | 114.18      | 119.40   |
| 35  | BB    | 1100 | C    | C5-C4-N4    | -7.45 | 114.98      | 120.20   |
| 35  | BB    | 1196 | C    | N1-C2-N3    | -7.45 | 113.98      | 119.20   |
| 35  | BB    | 1623 | G    | O4'-C1'-N9  | 7.45  | 114.16      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 682  | G    | N7-C8-N9    | -7.45 | 109.38      | 113.10   |
| 34  | BA    | 87   | U    | N1-C2-N3    | -7.45 | 110.43      | 114.90   |
| 35  | BB    | 143  | C    | C2-N3-C4    | 7.45  | 123.63      | 119.90   |
| 35  | BB    | 1028 | A    | O4'-C1'-N9  | 7.45  | 114.16      | 108.20   |
| 1   | AA    | 167  | A    | C4-C5-C6    | 7.45  | 120.72      | 117.00   |
| 1   | AA    | 507  | C    | C5-C4-N4    | -7.45 | 114.99      | 120.20   |
| 1   | AA    | 988  | G    | C3'-C2'-C1' | -7.45 | 95.54       | 101.50   |
| 1   | AA    | 1075 | U    | N3-C4-O4    | 7.45  | 124.61      | 119.40   |
| 1   | AA    | 1282 | C    | N1-C2-O2    | -7.45 | 114.43      | 118.90   |
| 35  | BB    | 221  | A    | N3-C4-N9    | 7.45  | 133.36      | 127.40   |
| 35  | BB    | 698  | C    | N3-C4-N4    | 7.45  | 123.21      | 118.00   |
| 35  | BB    | 952  | G    | C8-N9-C1'   | 7.45  | 136.68      | 127.00   |
| 35  | BB    | 1338 | G    | C6-C5-N7    | -7.45 | 125.93      | 130.40   |
| 35  | BB    | 2190 | G    | N9-C4-C5    | -7.45 | 102.42      | 105.40   |
| 35  | BB    | 2426 | A    | P-O3'-C3'   | 7.45  | 128.64      | 119.70   |
| 1   | AA    | 542  | G    | C5-C6-O6    | -7.45 | 124.13      | 128.60   |
| 1   | AA    | 749  | A    | N1-C6-N6    | 7.45  | 123.07      | 118.60   |
| 35  | BB    | 1123 | C    | C5-C4-N4    | -7.45 | 114.99      | 120.20   |
| 35  | BB    | 1622 | G    | N1-C2-N3    | -7.45 | 119.43      | 123.90   |
| 35  | BB    | 1767 | G    | C4-C5-C6    | 7.45  | 123.27      | 118.80   |
| 50  | BQ    | 52   | ARG  | NE-CZ-NH1   | 7.45  | 124.02      | 120.30   |
| 1   | AA    | 735  | C    | N1-C2-O2    | -7.45 | 114.43      | 118.90   |
| 15  | AO    | 68   | TYR  | CG-CD2-CE2  | -7.45 | 115.34      | 121.30   |
| 35  | BB    | 538  | A    | C5-C6-N1    | -7.45 | 113.98      | 117.70   |
| 35  | BB    | 752  | A    | P-O3'-C3'   | 7.45  | 128.63      | 119.70   |
| 35  | BB    | 1025 | G    | N3-C4-N9    | 7.45  | 130.47      | 126.00   |
| 35  | BB    | 1032 | A    | O4'-C1'-N9  | 7.45  | 114.16      | 108.20   |
| 35  | BB    | 1697 | G    | C5-C6-N1    | -7.45 | 107.78      | 111.50   |
| 1   | AA    | 798  | U    | C6-N1-C2    | 7.44  | 125.47      | 121.00   |
| 1   | AA    | 1284 | C    | C6-N1-C1'   | -7.44 | 111.87      | 120.80   |
| 35  | BB    | 1629 | U    | O4'-C1'-N1  | 7.44  | 114.16      | 108.20   |
| 1   | AA    | 780  | A    | N1-C6-N6    | 7.44  | 123.06      | 118.60   |
| 1   | AA    | 918  | A    | C5-C6-N6    | -7.44 | 117.75      | 123.70   |
| 35  | BB    | 10   | A    | O4'-C1'-N9  | 7.44  | 114.15      | 108.20   |
| 35  | BB    | 140  | C    | O4'-C1'-N1  | 7.44  | 114.15      | 108.20   |
| 35  | BB    | 1555 | G    | C5-C6-N1    | -7.44 | 107.78      | 111.50   |
| 35  | BB    | 2132 | U    | N3-C4-O4    | 7.44  | 124.61      | 119.40   |
| 35  | BB    | 2779 | U    | C3'-C2'-C1' | -7.44 | 95.55       | 101.50   |
| 49  | BP    | 108  | ARG  | NE-CZ-NH1   | -7.44 | 116.58      | 120.30   |
| 1   | AA    | 530  | G    | C6-C5-N7    | -7.44 | 125.94      | 130.40   |
| 1   | AA    | 602  | A    | C4-C5-C6    | 7.44  | 120.72      | 117.00   |
| 1   | AA    | 770  | C    | C4-C5-C6    | 7.44  | 121.12      | 117.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 35   | G    | C6-C5-N7    | -7.44 | 125.94      | 130.40   |
| 35  | BB    | 285  | G    | N3-C4-C5    | -7.44 | 124.88      | 128.60   |
| 35  | BB    | 1086 | A    | O4'-C1'-N9  | 7.44  | 114.15      | 108.20   |
| 35  | BB    | 1136 | G    | N3-C4-N9    | 7.44  | 130.47      | 126.00   |
| 35  | BB    | 2787 | C    | N1-C2-N3    | -7.44 | 113.99      | 119.20   |
| 1   | AA    | 1051 | C    | C5-C6-N1    | 7.44  | 124.72      | 121.00   |
| 1   | AA    | 1054 | C    | C6-N1-C1'   | -7.44 | 111.87      | 120.80   |
| 1   | AA    | 1409 | C    | C5-C6-N1    | 7.44  | 124.72      | 121.00   |
| 35  | BB    | 552  | U    | C5-C6-N1    | 7.44  | 126.42      | 122.70   |
| 1   | AA    | 1248 | A    | C5-C6-N6    | -7.44 | 117.75      | 123.70   |
| 1   | AA    | 1415 | G    | C8-N9-C4    | -7.44 | 103.42      | 106.40   |
| 35  | BB    | 226  | A    | N1-C6-N6    | 7.44  | 123.06      | 118.60   |
| 35  | BB    | 413  | C    | O4'-C1'-N1  | 7.44  | 114.15      | 108.20   |
| 35  | BB    | 2070 | A    | N9-C4-C5    | -7.44 | 102.83      | 105.80   |
| 1   | AA    | 322  | C    | O4'-C1'-N1  | 7.44  | 114.15      | 108.20   |
| 1   | AA    | 1046 | A    | C4'-C3'-C2' | -7.44 | 95.16       | 102.60   |
| 35  | BB    | 73   | A    | N9-C4-C5    | 7.44  | 108.77      | 105.80   |
| 35  | BB    | 1883 | U    | O4'-C1'-N1  | 7.44  | 114.15      | 108.20   |
| 35  | BB    | 2148 | G    | C2-N3-C4    | 7.44  | 115.62      | 111.90   |
| 35  | BB    | 2369 | A    | C1'-O4'-C4' | 7.44  | 115.85      | 109.90   |
| 1   | AA    | 31   | G    | C4-C5-N7    | 7.43  | 113.77      | 110.80   |
| 34  | BA    | 28   | C    | N3-C4-N4    | 7.43  | 123.20      | 118.00   |
| 35  | BB    | 446  | G    | C5-C6-O6    | -7.43 | 124.14      | 128.60   |
| 35  | BB    | 1201 | U    | N1-C2-O2    | -7.43 | 117.60      | 122.80   |
| 35  | BB    | 1910 | G    | C4-C5-N7    | 7.43  | 113.77      | 110.80   |
| 1   | AA    | 360  | G    | C6-C5-N7    | -7.43 | 125.94      | 130.40   |
| 1   | AA    | 724  | G    | O4'-C1'-N9  | 7.43  | 114.15      | 108.20   |
| 35  | BB    | 68   | G    | C4'-C3'-C2' | -7.43 | 95.17       | 102.60   |
| 35  | BB    | 317  | G    | N3-C4-C5    | 7.43  | 132.32      | 128.60   |
| 35  | BB    | 1911 | U    | C5-C6-N1    | 7.43  | 126.42      | 122.70   |
| 35  | BB    | 2176 | A    | C4-C5-C6    | 7.43  | 120.72      | 117.00   |
| 35  | BB    | 2489 | U    | O4'-C1'-N1  | 7.43  | 114.15      | 108.20   |
| 1   | AA    | 384  | G    | N3-C4-N9    | 7.43  | 130.46      | 126.00   |
| 35  | BB    | 63   | A    | C5-N7-C8    | 7.43  | 107.61      | 103.90   |
| 35  | BB    | 2588 | G    | P-O3'-C3'   | -7.43 | 110.78      | 119.70   |
| 35  | BB    | 2862 | G    | N3-C4-C5    | -7.43 | 124.88      | 128.60   |
| 1   | AA    | 193  | C    | C5-C6-N1    | 7.43  | 124.72      | 121.00   |
| 1   | AA    | 626  | G    | N1-C2-N3    | -7.43 | 119.44      | 123.90   |
| 35  | BB    | 402  | A    | O4'-C1'-N9  | 7.43  | 114.14      | 108.20   |
| 35  | BB    | 627  | A    | O4'-C1'-N9  | 7.43  | 114.14      | 108.20   |
| 35  | BB    | 992  | C    | C5-C4-N4    | 7.43  | 125.40      | 120.20   |
| 35  | BB    | 1489 | C    | O4'-C1'-N1  | 7.43  | 114.14      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1715 | G    | N1-C6-O6    | 7.43  | 124.36      | 119.90   |
| 35  | BB    | 2561 | U    | C6-N1-C2    | -7.43 | 116.54      | 121.00   |
| 1   | AA    | 493  | A    | N7-C8-N9    | 7.43  | 117.51      | 113.80   |
| 1   | AA    | 957  | U    | C5-C6-N1    | 7.43  | 126.41      | 122.70   |
| 35  | BB    | 1608 | A    | C4-C5-C6    | 7.43  | 120.71      | 117.00   |
| 1   | AA    | 77   | A    | C6-C5-N7    | -7.43 | 127.10      | 132.30   |
| 1   | AA    | 455  | G    | N1-C6-O6    | 7.43  | 124.36      | 119.90   |
| 1   | AA    | 818  | G    | C5-N7-C8    | -7.43 | 100.59      | 104.30   |
| 1   | AA    | 841  | C    | N3-C4-N4    | 7.43  | 123.20      | 118.00   |
| 35  | BB    | 770  | G    | N9-C4-C5    | -7.43 | 102.43      | 105.40   |
| 35  | BB    | 1107 | G    | C1'-O4'-C4' | 7.43  | 115.84      | 109.90   |
| 35  | BB    | 1441 | G    | O4'-C1'-N9  | 7.43  | 114.14      | 108.20   |
| 35  | BB    | 1585 | C    | N3-C4-N4    | 7.43  | 123.20      | 118.00   |
| 35  | BB    | 1638 | C    | C5-C4-N4    | -7.43 | 115.00      | 120.20   |
| 35  | BB    | 1813 | G    | C4-C5-C6    | 7.43  | 123.26      | 118.80   |
| 35  | BB    | 2152 | G    | N3-C2-N2    | 7.43  | 125.10      | 119.90   |
| 35  | BB    | 2187 | U    | O4'-C1'-N1  | 7.43  | 114.14      | 108.20   |
| 35  | BB    | 2739 | U    | N3-C2-O2    | -7.43 | 117.00      | 122.20   |
| 1   | AA    | 198  | G    | N9-C4-C5    | -7.42 | 102.43      | 105.40   |
| 1   | AA    | 774  | G    | C4-C5-C6    | 7.42  | 123.25      | 118.80   |
| 1   | AA    | 1173 | U    | N1-C2-O2    | 7.42  | 128.00      | 122.80   |
| 35  | BB    | 128  | C    | N3-C2-O2    | -7.42 | 116.70      | 121.90   |
| 35  | BB    | 2776 | A    | C4-C5-N7    | -7.42 | 106.99      | 110.70   |
| 35  | BB    | 1478 | G    | C6-N1-C2    | 7.42  | 129.55      | 125.10   |
| 35  | BB    | 1583 | A    | O4'-C1'-N9  | 7.42  | 114.14      | 108.20   |
| 35  | BB    | 2411 | A    | C6-C5-N7    | -7.42 | 127.10      | 132.30   |
| 35  | BB    | 487  | C    | N1-C2-N3    | -7.42 | 114.00      | 119.20   |
| 35  | BB    | 1306 | C    | N1-C2-O2    | 7.42  | 123.35      | 118.90   |
| 35  | BB    | 1905 | C    | N3-C4-N4    | 7.42  | 123.19      | 118.00   |
| 1   | AA    | 122  | G    | C4-C5-N7    | -7.42 | 107.83      | 110.80   |
| 1   | AA    | 1210 | C    | C4-C5-C6    | 7.42  | 121.11      | 117.40   |
| 35  | BB    | 429  | A    | C5-C6-N1    | -7.42 | 113.99      | 117.70   |
| 35  | BB    | 431  | U    | N3-C4-C5    | -7.42 | 110.15      | 114.60   |
| 35  | BB    | 2667 | C    | O4'-C1'-N1  | 7.42  | 114.14      | 108.20   |
| 1   | AA    | 104  | G    | N3-C2-N2    | 7.42  | 125.09      | 119.90   |
| 1   | AA    | 347  | G    | C4'-C3'-C2' | -7.42 | 95.18       | 102.60   |
| 1   | AA    | 1016 | A    | C2-N3-C4    | -7.42 | 106.89      | 110.60   |
| 35  | BB    | 67   | U    | N1-C2-N3    | -7.42 | 110.45      | 114.90   |
| 35  | BB    | 213  | A    | O4'-C1'-N9  | 7.42  | 114.13      | 108.20   |
| 35  | BB    | 668  | A    | C4-C5-N7    | -7.42 | 106.99      | 110.70   |
| 35  | BB    | 1576 | U    | C4-C5-C6    | -7.42 | 115.25      | 119.70   |
| 35  | BB    | 1699 | G    | C5'-C4'-O4' | 7.42  | 118.00      | 109.10   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1797 | G    | C6-N1-C2   | 7.42  | 129.55      | 125.10   |
| 35  | BB    | 1861 | G    | N3-C2-N2   | 7.42  | 125.09      | 119.90   |
| 35  | BB    | 2332 | C    | C5-C6-N1   | 7.42  | 124.71      | 121.00   |
| 1   | AA    | 93   | U    | O4'-C1'-N1 | 7.42  | 114.13      | 108.20   |
| 1   | AA    | 557  | G    | C4-C5-C6   | 7.42  | 123.25      | 118.80   |
| 1   | AA    | 1345 | U    | O4'-C1'-N1 | 7.42  | 114.13      | 108.20   |
| 35  | BB    | 355  | U    | C2-N3-C4   | 7.42  | 131.45      | 127.00   |
| 35  | BB    | 1021 | A    | C5-C6-N1   | -7.42 | 113.99      | 117.70   |
| 35  | BB    | 1187 | G    | N7-C8-N9   | 7.42  | 116.81      | 113.10   |
| 35  | BB    | 1498 | C    | C4-C5-C6   | 7.42  | 121.11      | 117.40   |
| 35  | BB    | 1785 | A    | N7-C8-N9   | -7.42 | 110.09      | 113.80   |
| 35  | BB    | 2674 | G    | N3-C4-C5   | -7.42 | 124.89      | 128.60   |
| 35  | BB    | 2735 | G    | C4-C5-C6   | 7.42  | 123.25      | 118.80   |
| 1   | AA    | 887  | G    | O4'-C1'-N9 | 7.41  | 114.13      | 108.20   |
| 34  | BA    | 105  | G    | N7-C8-N9   | -7.41 | 109.39      | 113.10   |
| 35  | BB    | 185  | G    | C8-N9-C4   | -7.41 | 103.44      | 106.40   |
| 35  | BB    | 217  | A    | C2-N3-C4   | 7.41  | 114.31      | 110.60   |
| 35  | BB    | 294  | A    | C5-N7-C8   | 7.41  | 107.61      | 103.90   |
| 35  | BB    | 1291 | C    | C6-N1-C2   | -7.41 | 117.33      | 120.30   |
| 35  | BB    | 2024 | G    | C2-N3-C4   | 7.41  | 115.61      | 111.90   |
| 35  | BB    | 2224 | G    | N3-C4-C5   | -7.41 | 124.89      | 128.60   |
| 1   | AA    | 294  | U    | C5-C4-O4   | -7.41 | 121.45      | 125.90   |
| 35  | BB    | 348  | A    | C5-C6-N6   | -7.41 | 117.77      | 123.70   |
| 35  | BB    | 1090 | A    | C5-C6-N1   | -7.41 | 113.99      | 117.70   |
| 35  | BB    | 1842 | G    | C5-C6-N1   | -7.41 | 107.79      | 111.50   |
| 35  | BB    | 2320 | U    | C4-C5-C6   | -7.41 | 115.25      | 119.70   |
| 1   | AA    | 160  | A    | C5-C6-N1   | -7.41 | 114.00      | 117.70   |
| 1   | AA    | 524  | G    | C6-C5-N7   | -7.41 | 125.95      | 130.40   |
| 1   | AA    | 831  | A    | C5-N7-C8   | 7.41  | 107.61      | 103.90   |
| 35  | BB    | 661  | A    | O4'-C1'-N9 | 7.41  | 114.13      | 108.20   |
| 35  | BB    | 955  | U    | C4-C5-C6   | -7.41 | 115.25      | 119.70   |
| 35  | BB    | 1133 | A    | N1-C6-N6   | 7.41  | 123.05      | 118.60   |
| 35  | BB    | 1512 | C    | C5-C4-N4   | -7.41 | 115.01      | 120.20   |
| 35  | BB    | 2275 | C    | N1-C2-O2   | 7.41  | 123.35      | 118.90   |
| 35  | BB    | 2385 | C    | C5-C6-N1   | 7.41  | 124.70      | 121.00   |
| 1   | AA    | 286  | C    | C6-N1-C1'  | -7.41 | 111.91      | 120.80   |
| 35  | BB    | 167  | A    | N1-C6-N6   | 7.41  | 123.05      | 118.60   |
| 35  | BB    | 363  | G    | N9-C4-C5   | -7.41 | 102.44      | 105.40   |
| 35  | BB    | 864  | G    | N3-C2-N2   | 7.41  | 125.09      | 119.90   |
| 35  | BB    | 1160 | G    | C8-N9-C4   | -7.41 | 103.44      | 106.40   |
| 35  | BB    | 1232 | G    | C8-N9-C4   | -7.41 | 103.44      | 106.40   |
| 35  | BB    | 1473 | G    | N9-C4-C5   | 7.41  | 108.36      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2269 | G    | O4'-C1'-N9  | 7.41  | 114.13      | 108.20   |
| 35  | BB    | 2885 | G    | N3-C4-C5    | 7.41  | 132.30      | 128.60   |
| 1   | AA    | 504  | C    | C6-N1-C2    | -7.41 | 117.34      | 120.30   |
| 1   | AA    | 842  | U    | N1-C2-N3    | -7.41 | 110.46      | 114.90   |
| 1   | AA    | 1420 | U    | C4'-C3'-C2' | -7.41 | 95.19       | 102.60   |
| 35  | BB    | 68   | G    | C2-N3-C4    | 7.41  | 115.60      | 111.90   |
| 35  | BB    | 485  | C    | C5-C4-N4    | -7.41 | 115.02      | 120.20   |
| 35  | BB    | 496  | G    | C6-C5-N7    | -7.41 | 125.96      | 130.40   |
| 35  | BB    | 2700 | A    | N3-C4-C5    | -7.41 | 121.61      | 126.80   |
| 1   | AA    | 908  | A    | N9-C4-C5    | 7.41  | 108.76      | 105.80   |
| 35  | BB    | 479  | A    | N1-C6-N6    | 7.41  | 123.04      | 118.60   |
| 35  | BB    | 817  | C    | N3-C4-N4    | 7.41  | 123.18      | 118.00   |
| 35  | BB    | 1350 | C    | N3-C4-C5    | -7.41 | 118.94      | 121.90   |
| 35  | BB    | 1352 | U    | N3-C4-O4    | 7.41  | 124.58      | 119.40   |
| 35  | BB    | 2303 | G    | N1-C6-O6    | 7.41  | 124.34      | 119.90   |
| 35  | BB    | 2352 | A    | N9-C4-C5    | -7.41 | 102.84      | 105.80   |
| 35  | BB    | 2778 | A    | N7-C8-N9    | -7.41 | 110.10      | 113.80   |
| 35  | BB    | 1506 | U    | P-O5'-C5'   | 7.40  | 132.75      | 120.90   |
| 1   | AA    | 380  | G    | N3-C2-N2    | 7.40  | 125.08      | 119.90   |
| 1   | AA    | 927  | G    | C6-N1-C2    | 7.40  | 129.54      | 125.10   |
| 35  | BB    | 388  | G    | O4'-C1'-N9  | 7.40  | 114.12      | 108.20   |
| 35  | BB    | 1153 | C    | N3-C4-C5    | 7.40  | 124.86      | 121.90   |
| 35  | BB    | 2346 | A    | C8-N9-C4    | -7.40 | 102.84      | 105.80   |
| 35  | BB    | 2355 | G    | N1-C6-O6    | 7.40  | 124.34      | 119.90   |
| 35  | BB    | 2423 | U    | N3-C4-C5    | -7.40 | 110.16      | 114.60   |
| 35  | BB    | 2565 | A    | C2-N3-C4    | 7.40  | 114.30      | 110.60   |
| 35  | BB    | 2648 | G    | N9-C4-C5    | -7.40 | 102.44      | 105.40   |
| 1   | AA    | 484  | G    | C8-N9-C4    | 7.40  | 109.36      | 106.40   |
| 1   | AA    | 837  | U    | N3-C4-O4    | 7.40  | 124.58      | 119.40   |
| 1   | AA    | 1032 | G    | C6-C5-N7    | -7.40 | 125.96      | 130.40   |
| 1   | AA    | 1067 | A    | C5'-C4'-C3' | -7.40 | 104.16      | 116.00   |
| 1   | AA    | 1175 | G    | C8-N9-C4    | 7.40  | 109.36      | 106.40   |
| 35  | BB    | 1104 | C    | O4'-C1'-N1  | 7.40  | 114.12      | 108.20   |
| 1   | AA    | 76   | G    | C4'-C3'-C2' | -7.40 | 95.20       | 102.60   |
| 1   | AA    | 523  | A    | C6-N1-C2    | -7.40 | 114.16      | 118.60   |
| 1   | AA    | 1279 | G    | C2-N3-C4    | 7.40  | 115.60      | 111.90   |
| 1   | AA    | 305  | G    | C4-C5-N7    | -7.40 | 107.84      | 110.80   |
| 35  | BB    | 196  | A    | O4'-C1'-N9  | 7.40  | 114.12      | 108.20   |
| 35  | BB    | 266  | G    | C8-N9-C4    | 7.40  | 109.36      | 106.40   |
| 35  | BB    | 406  | G    | P-O5'-C5'   | -7.40 | 109.06      | 120.90   |
| 35  | BB    | 604  | G    | N1-C2-N3    | -7.40 | 119.46      | 123.90   |
| 35  | BB    | 649  | G    | N7-C8-N9    | 7.40  | 116.80      | 113.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 753  | A    | C2-N3-C4    | -7.40 | 106.90      | 110.60   |
| 35  | BB    | 1178 | C    | C5-C6-N1    | 7.40  | 124.70      | 121.00   |
| 35  | BB    | 1587 | G    | O4'-C1'-N9  | 7.40  | 114.12      | 108.20   |
| 35  | BB    | 1907 | G    | C6-N1-C2    | 7.40  | 129.54      | 125.10   |
| 35  | BB    | 2276 | G    | C4-C5-N7    | 7.40  | 113.76      | 110.80   |
| 35  | BB    | 2788 | C    | C5-C4-N4    | -7.40 | 115.02      | 120.20   |
| 35  | BB    | 2789 | C    | C5-C4-N4    | -7.40 | 115.02      | 120.20   |
| 1   | AA    | 253  | A    | N3-C4-N9    | 7.40  | 133.32      | 127.40   |
| 1   | AA    | 847  | G    | C4-N9-C1'   | -7.40 | 116.89      | 126.50   |
| 35  | BB    | 848  | C    | O4'-C1'-N1  | 7.40  | 114.12      | 108.20   |
| 35  | BB    | 1836 | C    | C5-C6-N1    | 7.40  | 124.70      | 121.00   |
| 1   | AA    | 801  | U    | O4'-C1'-N1  | 7.39  | 114.11      | 108.20   |
| 1   | AA    | 864  | A    | O4'-C1'-N9  | 7.39  | 114.12      | 108.20   |
| 1   | AA    | 1309 | G    | O4'-C1'-N9  | 7.39  | 114.11      | 108.20   |
| 14  | AN    | 64   | ARG  | NE-CZ-NH2   | 7.39  | 124.00      | 120.30   |
| 35  | BB    | 643  | A    | C5-C6-N1    | -7.39 | 114.00      | 117.70   |
| 35  | BB    | 705  | A    | C4-C5-C6    | 7.39  | 120.70      | 117.00   |
| 35  | BB    | 728  | G    | N9-C4-C5    | -7.39 | 102.44      | 105.40   |
| 35  | BB    | 1168 | G    | O5'-P-OP2   | -7.39 | 99.05       | 105.70   |
| 35  | BB    | 2037 | A    | C4-C5-C6    | 7.39  | 120.70      | 117.00   |
| 1   | AA    | 310  | G    | C5-N7-C8    | 7.39  | 108.00      | 104.30   |
| 1   | AA    | 1382 | C    | O4'-C1'-N1  | 7.39  | 114.11      | 108.20   |
| 35  | BB    | 142  | A    | N1-C2-N3    | 7.39  | 133.00      | 129.30   |
| 35  | BB    | 529  | A    | C5-N7-C8    | 7.39  | 107.60      | 103.90   |
| 35  | BB    | 559  | G    | C8-N9-C4    | -7.39 | 103.44      | 106.40   |
| 35  | BB    | 1832 | C    | C5-C4-N4    | -7.39 | 115.03      | 120.20   |
| 35  | BB    | 2134 | A    | C4-C5-C6    | 7.39  | 120.70      | 117.00   |
| 35  | BB    | 2225 | A    | O4'-C1'-N9  | 7.39  | 114.11      | 108.20   |
| 35  | BB    | 2281 | A    | C4-C5-C6    | 7.39  | 120.70      | 117.00   |
| 35  | BB    | 2433 | A    | C5-C6-N1    | -7.39 | 114.00      | 117.70   |
| 1   | AA    | 913  | A    | N3-C4-C5    | -7.39 | 121.63      | 126.80   |
| 35  | BB    | 530  | G    | C6-C5-N7    | -7.39 | 125.97      | 130.40   |
| 35  | BB    | 598  | U    | C2-N3-C4    | -7.39 | 122.56      | 127.00   |
| 35  | BB    | 1598 | A    | C5-C6-N6    | -7.39 | 117.79      | 123.70   |
| 35  | BB    | 1745 | A    | O4'-C1'-N9  | 7.39  | 114.11      | 108.20   |
| 35  | BB    | 1970 | A    | N1-C2-N3    | -7.39 | 125.61      | 129.30   |
| 1   | AA    | 85   | U    | C6-N1-C1'   | -7.39 | 110.85      | 121.20   |
| 1   | AA    | 1025 | U    | C6-N1-C2    | 7.39  | 125.43      | 121.00   |
| 1   | AA    | 1085 | U    | N1-C2-N3    | -7.39 | 110.47      | 114.90   |
| 1   | AA    | 1229 | A    | C4-C5-C6    | 7.39  | 120.69      | 117.00   |
| 1   | AA    | 1416 | G    | P-O5'-C5'   | 7.39  | 132.72      | 120.90   |
| 1   | AA    | 1493 | A    | C4'-C3'-C2' | -7.39 | 95.21       | 102.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 975  | A    | N1-C6-N6    | 7.39  | 123.03      | 118.60   |
| 35  | BB    | 2159 | G    | C5-N7-C8    | 7.39  | 107.99      | 104.30   |
| 35  | BB    | 2612 | C    | C1'-O4'-C4' | 7.39  | 115.81      | 109.90   |
| 9   | AI    | 105  | ARG  | NE-CZ-NH1   | 7.39  | 123.99      | 120.30   |
| 35  | BB    | 847  | U    | C5-C4-O4    | -7.39 | 121.47      | 125.90   |
| 35  | BB    | 2321 | U    | P-O3'-C3'   | -7.39 | 110.83      | 119.70   |
| 35  | BB    | 2406 | A    | C1'-O4'-C4' | -7.39 | 103.99      | 109.90   |
| 1   | AA    | 944  | G    | C5-C6-O6    | -7.39 | 124.17      | 128.60   |
| 34  | BA    | 88   | C    | N3-C4-C5    | -7.39 | 118.95      | 121.90   |
| 35  | BB    | 3    | U    | O4'-C1'-N1  | 7.39  | 114.11      | 108.20   |
| 35  | BB    | 257  | C    | C6-N1-C2    | -7.39 | 117.34      | 120.30   |
| 35  | BB    | 752  | A    | C1'-O4'-C4' | -7.39 | 103.99      | 109.90   |
| 35  | BB    | 768  | G    | C4-C5-N7    | 7.39  | 113.75      | 110.80   |
| 35  | BB    | 853  | C    | C5-C6-N1    | 7.39  | 124.69      | 121.00   |
| 35  | BB    | 871  | U    | O4'-C1'-N1  | 7.39  | 114.11      | 108.20   |
| 35  | BB    | 1420 | A    | C5-C6-N1    | -7.39 | 114.01      | 117.70   |
| 35  | BB    | 1630 | A    | C5-C6-N6    | -7.39 | 117.79      | 123.70   |
| 35  | BB    | 2131 | U    | O4'-C1'-N1  | 7.39  | 114.11      | 108.20   |
| 35  | BB    | 2782 | G    | C5-C6-O6    | -7.39 | 124.17      | 128.60   |
| 1   | AA    | 178  | C    | C6-N1-C2    | 7.38  | 123.25      | 120.30   |
| 1   | AA    | 182  | A    | C5-C6-N1    | -7.38 | 114.01      | 117.70   |
| 1   | AA    | 300  | A    | C5-C6-N6    | -7.38 | 117.79      | 123.70   |
| 35  | BB    | 163  | C    | C2-N3-C4    | -7.38 | 116.21      | 119.90   |
| 35  | BB    | 286  | U    | O4'-C1'-N1  | 7.38  | 114.11      | 108.20   |
| 35  | BB    | 530  | G    | C5-C6-O6    | -7.38 | 124.17      | 128.60   |
| 35  | BB    | 764  | A    | C6-N1-C2    | 7.38  | 123.03      | 118.60   |
| 35  | BB    | 1205 | A    | C6-N1-C2    | -7.38 | 114.17      | 118.60   |
| 35  | BB    | 1302 | A    | C5-N7-C8    | 7.38  | 107.59      | 103.90   |
| 35  | BB    | 1533 | C    | P-O5'-C5'   | 7.38  | 132.71      | 120.90   |
| 35  | BB    | 2520 | C    | C4-C5-C6    | 7.38  | 121.09      | 117.40   |
| 1   | AA    | 328  | C    | N1-C2-N3    | -7.38 | 114.03      | 119.20   |
| 1   | AA    | 1223 | C    | N3-C4-N4    | 7.38  | 123.17      | 118.00   |
| 14  | AN    | 41   | TRP  | CB-CG-CD1   | 7.38  | 136.60      | 127.00   |
| 35  | BB    | 758  | C    | C5-C6-N1    | 7.38  | 124.69      | 121.00   |
| 35  | BB    | 1393 | A    | O4'-C4'-C3' | 7.38  | 112.01      | 106.10   |
| 1   | AA    | 1041 | G    | C5-C6-O6    | -7.38 | 124.17      | 128.60   |
| 1   | AA    | 1172 | C    | N3-C2-O2    | 7.38  | 127.07      | 121.90   |
| 35  | BB    | 184  | C    | O4'-C1'-N1  | 7.38  | 114.11      | 108.20   |
| 35  | BB    | 1240 | U    | O4'-C1'-N1  | 7.38  | 114.11      | 108.20   |
| 35  | BB    | 1361 | G    | C4-C5-C6    | 7.38  | 123.23      | 118.80   |
| 35  | BB    | 1912 | A    | C4-C5-C6    | 7.38  | 120.69      | 117.00   |
| 35  | BB    | 2779 | U    | C1'-O4'-C4' | -7.38 | 104.00      | 109.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 289  | G    | C6-N1-C2    | -7.38 | 120.67      | 125.10   |
| 1   | AA    | 732  | C    | C6-N1-C2    | -7.38 | 117.35      | 120.30   |
| 35  | BB    | 318  | C    | C6-N1-C2    | -7.38 | 117.35      | 120.30   |
| 35  | BB    | 1027 | A    | C4-C5-C6    | 7.38  | 120.69      | 117.00   |
| 35  | BB    | 1059 | G    | N1-C2-N3    | -7.38 | 119.47      | 123.90   |
| 35  | BB    | 1220 | G    | O4'-C1'-N9  | 7.38  | 114.10      | 108.20   |
| 35  | BB    | 1329 | U    | C2-N3-C4    | 7.38  | 131.43      | 127.00   |
| 1   | AA    | 90   | C    | N3-C4-N4    | 7.38  | 123.17      | 118.00   |
| 1   | AA    | 340  | U    | O4'-C1'-N1  | 7.38  | 114.10      | 108.20   |
| 1   | AA    | 426  | U    | O4'-C1'-N1  | 7.38  | 114.10      | 108.20   |
| 1   | AA    | 1310 | G    | C6-N1-C2    | -7.38 | 120.67      | 125.10   |
| 1   | AA    | 1416 | G    | C6-C5-N7    | -7.38 | 125.97      | 130.40   |
| 2   | AB    | 125  | PHE  | CB-CG-CD1   | 7.38  | 125.97      | 120.80   |
| 23  | AX    | 19   | A    | N1-C2-N3    | 7.38  | 132.99      | 129.30   |
| 34  | BA    | 18   | G    | N1-C6-O6    | 7.38  | 124.33      | 119.90   |
| 35  | BB    | 387  | U    | N3-C4-C5    | -7.38 | 110.17      | 114.60   |
| 35  | BB    | 602  | A    | C6-N1-C2    | 7.38  | 123.03      | 118.60   |
| 35  | BB    | 2746 | U    | C5-C6-N1    | 7.38  | 126.39      | 122.70   |
| 1   | AA    | 125  | U    | N3-C4-O4    | 7.38  | 124.56      | 119.40   |
| 1   | AA    | 327  | A    | N3-C4-C5    | -7.38 | 121.64      | 126.80   |
| 1   | AA    | 742  | G    | C5-C6-O6    | -7.38 | 124.17      | 128.60   |
| 1   | AA    | 1150 | A    | O4'-C1'-N9  | 7.38  | 114.10      | 108.20   |
| 34  | BA    | 4    | C    | C1'-O4'-C4' | 7.38  | 115.80      | 109.90   |
| 35  | BB    | 466  | A    | C5-C6-N6    | -7.38 | 117.80      | 123.70   |
| 1   | AA    | 55   | A    | O4'-C1'-N9  | 7.38  | 114.10      | 108.20   |
| 1   | AA    | 362  | G    | C6-C5-N7    | -7.37 | 125.98      | 130.40   |
| 1   | AA    | 781  | A    | C4-C5-N7    | -7.37 | 107.01      | 110.70   |
| 1   | AA    | 809  | G    | N1-C6-O6    | 7.37  | 124.32      | 119.90   |
| 1   | AA    | 1465 | A    | C4-C5-C6    | 7.37  | 120.69      | 117.00   |
| 1   | AA    | 1529 | G    | C5-C6-O6    | -7.37 | 124.18      | 128.60   |
| 35  | BB    | 54   | G    | N3-C4-N9    | 7.37  | 130.43      | 126.00   |
| 35  | BB    | 450  | G    | C5-C6-O6    | -7.37 | 124.17      | 128.60   |
| 35  | BB    | 940  | G    | C2-N3-C4    | -7.37 | 108.21      | 111.90   |
| 35  | BB    | 1073 | A    | C5-C6-N1    | -7.37 | 114.01      | 117.70   |
| 35  | BB    | 1447 | C    | N3-C4-N4    | 7.37  | 123.16      | 118.00   |
| 35  | BB    | 1544 | A    | C4'-C3'-C2' | -7.37 | 95.23       | 102.60   |
| 35  | BB    | 2594 | C    | C5-C6-N1    | 7.37  | 124.69      | 121.00   |
| 35  | BB    | 2851 | A    | C5-C6-N6    | -7.37 | 117.80      | 123.70   |
| 1   | AA    | 784  | A    | C5-C6-N1    | -7.37 | 114.01      | 117.70   |
| 1   | AA    | 803  | G    | C5-C6-O6    | -7.37 | 124.18      | 128.60   |
| 1   | AA    | 831  | A    | O4'-C1'-N9  | 7.37  | 114.10      | 108.20   |
| 1   | AA    | 1011 | C    | O4'-C1'-N1  | 7.37  | 114.10      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1416 | G    | C6-N1-C2    | 7.37  | 129.52      | 125.10   |
| 35  | BB    | 239  | C    | C2-N1-C1'   | 7.37  | 126.91      | 118.80   |
| 35  | BB    | 324  | A    | N1-C2-N3    | -7.37 | 125.61      | 129.30   |
| 35  | BB    | 332  | A    | P-O3'-C3'   | 7.37  | 128.54      | 119.70   |
| 35  | BB    | 439  | A    | C6-C5-N7    | -7.37 | 127.14      | 132.30   |
| 35  | BB    | 467  | G    | N1-C2-N3    | -7.37 | 119.48      | 123.90   |
| 35  | BB    | 1013 | C    | O4'-C1'-N1  | 7.37  | 114.10      | 108.20   |
| 35  | BB    | 1111 | A    | N1-C2-N3    | 7.37  | 132.99      | 129.30   |
| 35  | BB    | 1622 | G    | C6-C5-N7    | -7.37 | 125.98      | 130.40   |
| 1   | AA    | 179  | A    | C2-N3-C4    | 7.37  | 114.28      | 110.60   |
| 1   | AA    | 403  | C    | N3-C4-C5    | -7.37 | 118.95      | 121.90   |
| 1   | AA    | 1220 | G    | C6-N1-C2    | -7.37 | 120.68      | 125.10   |
| 15  | AO    | 52   | ARG  | NE-CZ-NH1   | -7.37 | 116.61      | 120.30   |
| 27  | B2    | 52   | PHE  | CB-CG-CD2   | -7.37 | 115.64      | 120.80   |
| 35  | BB    | 143  | C    | N3-C4-C5    | -7.37 | 118.95      | 121.90   |
| 35  | BB    | 1204 | A    | N7-C8-N9    | -7.37 | 110.11      | 113.80   |
| 35  | BB    | 1583 | A    | C6-N1-C2    | -7.37 | 114.18      | 118.60   |
| 1   | AA    | 811  | C    | C1'-O4'-C4' | 7.37  | 115.80      | 109.90   |
| 18  | AR    | 63   | TYR  | CB-CG-CD1   | 7.37  | 125.42      | 121.00   |
| 34  | BA    | 53   | A    | C2-N3-C4    | 7.37  | 114.28      | 110.60   |
| 1   | AA    | 75   | G    | C2-N3-C4    | -7.37 | 108.22      | 111.90   |
| 1   | AA    | 451  | A    | C6-C5-N7    | -7.37 | 127.14      | 132.30   |
| 6   | AF    | 44   | ARG  | NE-CZ-NH1   | 7.37  | 123.98      | 120.30   |
| 35  | BB    | 75   | G    | C4-C5-C6    | 7.37  | 123.22      | 118.80   |
| 35  | BB    | 777  | G    | O4'-C1'-N9  | 7.37  | 114.09      | 108.20   |
| 35  | BB    | 2347 | C    | O4'-C1'-N1  | 7.37  | 114.09      | 108.20   |
| 1   | AA    | 474  | G    | N7-C8-N9    | -7.36 | 109.42      | 113.10   |
| 1   | AA    | 1195 | C    | N1-C2-O2    | 7.36  | 123.32      | 118.90   |
| 35  | BB    | 673  | C    | C6-N1-C2    | -7.36 | 117.36      | 120.30   |
| 35  | BB    | 1464 | G    | N1-C2-N3    | -7.36 | 119.48      | 123.90   |
| 35  | BB    | 1941 | C    | N1-C2-O2    | -7.36 | 114.48      | 118.90   |
| 50  | BQ    | 24   | TYR  | CB-CG-CD1   | -7.36 | 116.58      | 121.00   |
| 55  | BW    | 26   | PHE  | CB-CG-CD1   | -7.36 | 115.64      | 120.80   |
| 1   | AA    | 506  | G    | C5-N7-C8    | 7.36  | 107.98      | 104.30   |
| 22  | AV    | 3    | G    | N3-C2-N2    | 7.36  | 125.05      | 119.90   |
| 35  | BB    | 2168 | G    | O4'-C1'-N9  | 7.36  | 114.09      | 108.20   |
| 1   | AA    | 171  | A    | C5-C6-N1    | -7.36 | 114.02      | 117.70   |
| 1   | AA    | 331  | G    | C5-C6-N1    | 7.36  | 115.18      | 111.50   |
| 1   | AA    | 665  | A    | C5-C6-N6    | -7.36 | 117.81      | 123.70   |
| 1   | AA    | 773  | G    | C4-C5-C6    | 7.36  | 123.22      | 118.80   |
| 34  | BA    | 92   | C    | O4'-C1'-N1  | 7.36  | 114.09      | 108.20   |
| 34  | BA    | 109  | A    | O4'-C1'-N9  | 7.36  | 114.09      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 789  | A    | C6-N1-C2    | -7.36 | 114.18      | 118.60   |
| 35  | BB    | 792  | A    | C2-N3-C4    | -7.36 | 106.92      | 110.60   |
| 35  | BB    | 794  | A    | C4-C5-C6    | 7.36  | 120.68      | 117.00   |
| 35  | BB    | 1265 | A    | C4-C5-C6    | 7.36  | 120.68      | 117.00   |
| 35  | BB    | 2216 | G    | N1-C2-N3    | -7.36 | 119.48      | 123.90   |
| 35  | BB    | 2250 | G    | N1-C2-N2    | 7.36  | 122.83      | 116.20   |
| 35  | BB    | 2879 | A    | N1-C6-N6    | 7.36  | 123.02      | 118.60   |
| 35  | BB    | 2820 | A    | C6-C5-N7    | -7.36 | 127.15      | 132.30   |
| 1   | AA    | 1353 | G    | C5-C6-O6    | -7.36 | 124.19      | 128.60   |
| 1   | AA    | 1481 | U    | C5-C6-N1    | 7.36  | 126.38      | 122.70   |
| 22  | AV    | 22   | G    | C5-C6-O6    | -7.36 | 124.19      | 128.60   |
| 35  | BB    | 1660 | G    | O4'-C1'-N9  | 7.36  | 114.09      | 108.20   |
| 35  | BB    | 2049 | G    | C8-N9-C4    | -7.36 | 103.46      | 106.40   |
| 35  | BB    | 240  | C    | O4'-C1'-N1  | 7.36  | 114.08      | 108.20   |
| 35  | BB    | 290  | U    | C2-N3-C4    | -7.36 | 122.59      | 127.00   |
| 35  | BB    | 309  | A    | C5-C6-N6    | -7.36 | 117.82      | 123.70   |
| 35  | BB    | 1540 | G    | C5-C6-N1    | -7.36 | 107.82      | 111.50   |
| 35  | BB    | 1664 | A    | C5'-C4'-O4' | 7.36  | 117.93      | 109.10   |
| 35  | BB    | 1775 | U    | N3-C4-O4    | 7.36  | 124.55      | 119.40   |
| 35  | BB    | 2670 | A    | C2-N3-C4    | -7.36 | 106.92      | 110.60   |
| 35  | BB    | 2873 | A    | N1-C6-N6    | 7.36  | 123.01      | 118.60   |
| 34  | BA    | 81   | G    | C5-C6-O6    | -7.35 | 124.19      | 128.60   |
| 35  | BB    | 633  | A    | O4'-C1'-N9  | 7.35  | 114.08      | 108.20   |
| 35  | BB    | 2335 | A    | O4'-C1'-N9  | 7.35  | 114.08      | 108.20   |
| 1   | AA    | 279  | A    | C5-C6-N6    | -7.35 | 117.82      | 123.70   |
| 35  | BB    | 392  | U    | O4'-C1'-N1  | 7.35  | 114.08      | 108.20   |
| 35  | BB    | 627  | A    | C3'-C2'-C1' | -7.35 | 95.62       | 101.50   |
| 35  | BB    | 1002 | G    | N1-C6-O6    | 7.35  | 124.31      | 119.90   |
| 35  | BB    | 1176 | U    | C5-C6-N1    | 7.35  | 126.38      | 122.70   |
| 35  | BB    | 1186 | G    | N9-C4-C5    | -7.35 | 102.46      | 105.40   |
| 35  | BB    | 1606 | C    | C1'-O4'-C4' | -7.35 | 104.02      | 109.90   |
| 1   | AA    | 1492 | A    | C5-C6-N6    | -7.35 | 117.82      | 123.70   |
| 35  | BB    | 205  | G    | C5'-C4'-O4' | 7.35  | 117.92      | 109.10   |
| 35  | BB    | 469  | G    | O4'-C1'-N9  | 7.35  | 114.08      | 108.20   |
| 35  | BB    | 808  | G    | C5-C6-O6    | -7.35 | 124.19      | 128.60   |
| 35  | BB    | 1134 | A    | N9-C4-C5    | 7.35  | 108.74      | 105.80   |
| 35  | BB    | 2642 | G    | C4'-C3'-C2' | -7.35 | 95.25       | 102.60   |
| 35  | BB    | 2796 | U    | N3-C4-O4    | 7.35  | 124.54      | 119.40   |
| 35  | BB    | 20   | C    | C6-N1-C2    | -7.35 | 117.36      | 120.30   |
| 35  | BB    | 1183 | U    | C1'-O4'-C4' | 7.35  | 115.78      | 109.90   |
| 35  | BB    | 1479 | G    | O4'-C1'-N9  | 7.35  | 114.08      | 108.20   |
| 35  | BB    | 1922 | G    | C5-N7-C8    | -7.35 | 100.63      | 104.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2753 | A    | C4-C5-N7    | -7.35 | 107.03      | 110.70   |
| 1   | AA    | 176  | C    | N3-C4-N4    | 7.35  | 123.14      | 118.00   |
| 1   | AA    | 1334 | G    | C3'-C2'-C1' | 7.35  | 107.38      | 101.50   |
| 35  | BB    | 128  | C    | N1-C2-O2    | 7.35  | 123.31      | 118.90   |
| 35  | BB    | 2273 | A    | C5-C6-N6    | -7.35 | 117.82      | 123.70   |
| 1   | AA    | 312  | C    | O4'-C1'-N1  | 7.34  | 114.08      | 108.20   |
| 1   | AA    | 1145 | A    | C4-C5-C6    | 7.34  | 120.67      | 117.00   |
| 1   | AA    | 1146 | A    | C2-N3-C4    | -7.34 | 106.93      | 110.60   |
| 35  | BB    | 504  | A    | C4-C5-C6    | 7.34  | 120.67      | 117.00   |
| 35  | BB    | 520  | G    | P-O5'-C5'   | -7.34 | 109.15      | 120.90   |
| 35  | BB    | 592  | A    | N9-C4-C5    | -7.34 | 102.86      | 105.80   |
| 35  | BB    | 2036 | C    | N3-C4-C5    | -7.34 | 118.96      | 121.90   |
| 35  | BB    | 2604 | U    | N3-C4-C5    | -7.34 | 110.19      | 114.60   |
| 35  | BB    | 1484 | U    | N1-C2-O2    | -7.34 | 117.66      | 122.80   |
| 50  | BQ    | 27   | ARG  | NE-CZ-NH1   | 7.34  | 123.97      | 120.30   |
| 1   | AA    | 108  | G    | C5-C6-O6    | -7.34 | 124.19      | 128.60   |
| 35  | BB    | 1344 | U    | P-O5'-C5'   | 7.34  | 132.65      | 120.90   |
| 35  | BB    | 1431 | A    | C6-N1-C2    | -7.34 | 114.19      | 118.60   |
| 35  | BB    | 1514 | G    | N3-C4-N9    | 7.34  | 130.41      | 126.00   |
| 35  | BB    | 2109 | U    | P-O3'-C3'   | 7.34  | 128.51      | 119.70   |
| 1   | AA    | 38   | G    | N7-C8-N9    | 7.34  | 116.77      | 113.10   |
| 1   | AA    | 593  | U    | N3-C4-O4    | 7.34  | 124.54      | 119.40   |
| 1   | AA    | 881  | G    | C4-C5-N7    | -7.34 | 107.86      | 110.80   |
| 35  | BB    | 60   | G    | P-O3'-C3'   | 7.34  | 128.51      | 119.70   |
| 35  | BB    | 113  | U    | O4'-C1'-N1  | 7.34  | 114.07      | 108.20   |
| 35  | BB    | 549  | G    | N1-C2-N3    | -7.34 | 119.50      | 123.90   |
| 35  | BB    | 703  | U    | N3-C4-O4    | 7.34  | 124.54      | 119.40   |
| 35  | BB    | 741  | U    | O4'-C4'-C3' | -7.34 | 96.66       | 104.00   |
| 35  | BB    | 1747 | U    | O4'-C1'-N1  | 7.34  | 114.07      | 108.20   |
| 35  | BB    | 1816 | C    | C6-N1-C1'   | -7.34 | 111.99      | 120.80   |
| 35  | BB    | 2330 | G    | C4-C5-C6    | 7.34  | 123.20      | 118.80   |
| 35  | BB    | 664  | G    | O4'-C1'-N9  | 7.34  | 114.07      | 108.20   |
| 35  | BB    | 2610 | C    | C2-N3-C4    | 7.34  | 123.57      | 119.90   |
| 35  | BB    | 2812 | G    | N1-C2-N3    | -7.34 | 119.50      | 123.90   |
| 1   | AA    | 77   | A    | O4'-C1'-N9  | 7.34  | 114.07      | 108.20   |
| 1   | AA    | 129  | A    | O4'-C1'-N9  | 7.34  | 114.07      | 108.20   |
| 1   | AA    | 174  | A    | C6-C5-N7    | -7.34 | 127.17      | 132.30   |
| 1   | AA    | 521  | G    | C8-N9-C4    | -7.34 | 103.47      | 106.40   |
| 1   | AA    | 577  | G    | N7-C8-N9    | -7.34 | 109.43      | 113.10   |
| 1   | AA    | 1358 | U    | C5'-C4'-C3' | -7.34 | 104.26      | 116.00   |
| 35  | BB    | 277  | G    | C5-C6-O6    | -7.34 | 124.20      | 128.60   |
| 35  | BB    | 924  | G    | N1-C6-O6    | 7.34  | 124.30      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1878 | G    | N1-C6-O6    | 7.34  | 124.30      | 119.90   |
| 35  | BB    | 2531 | A    | C5-C6-N1    | -7.34 | 114.03      | 117.70   |
| 35  | BB    | 2763 | G    | N9-C4-C5    | 7.34  | 108.33      | 105.40   |
| 1   | AA    | 510  | A    | C4'-C3'-C2' | -7.33 | 95.27       | 102.60   |
| 1   | AA    | 590  | U    | O4'-C1'-N1  | 7.33  | 114.07      | 108.20   |
| 1   | AA    | 686  | U    | C3'-C2'-C1' | -7.33 | 95.63       | 101.50   |
| 35  | BB    | 952  | G    | N1-C6-O6    | 7.33  | 124.30      | 119.90   |
| 35  | BB    | 1835 | G    | P-O3'-C3'   | -7.33 | 110.90      | 119.70   |
| 35  | BB    | 2177 | C    | N3-C4-N4    | 7.33  | 123.14      | 118.00   |
| 1   | AA    | 760  | G    | C4-C5-C6    | 7.33  | 123.20      | 118.80   |
| 35  | BB    | 1471 | G    | C8-N9-C1'   | 7.33  | 136.53      | 127.00   |
| 35  | BB    | 1899 | A    | C4-C5-C6    | 7.33  | 120.67      | 117.00   |
| 35  | BB    | 2503 | A    | O4'-C1'-N9  | 7.33  | 114.07      | 108.20   |
| 1   | AA    | 66   | A    | C6-N1-C2    | 7.33  | 123.00      | 118.60   |
| 1   | AA    | 198  | G    | O4'-C4'-C3' | -7.33 | 96.67       | 104.00   |
| 1   | AA    | 356  | A    | C4-C5-C6    | 7.33  | 120.67      | 117.00   |
| 1   | AA    | 835  | U    | C5'-C4'-C3' | -7.33 | 104.27      | 116.00   |
| 1   | AA    | 1355 | G    | O4'-C1'-N9  | 7.33  | 114.06      | 108.20   |
| 21  | AU    | 32   | ARG  | NE-CZ-NH1   | 7.33  | 123.97      | 120.30   |
| 33  | B8    | 19   | ARG  | NE-CZ-NH2   | -7.33 | 116.63      | 120.30   |
| 35  | BB    | 12   | U    | P-O3'-C3'   | 7.33  | 128.50      | 119.70   |
| 35  | BB    | 1555 | G    | C5-C6-O6    | -7.33 | 124.20      | 128.60   |
| 35  | BB    | 2205 | A    | N1-C6-N6    | 7.33  | 123.00      | 118.60   |
| 35  | BB    | 2313 | C    | C2-N3-C4    | -7.33 | 116.23      | 119.90   |
| 1   | AA    | 544  | G    | N1-C2-N2    | -7.33 | 109.60      | 116.20   |
| 14  | AN    | 84   | ARG  | NE-CZ-NH1   | -7.33 | 116.64      | 120.30   |
| 26  | B1    | 7    | ARG  | NE-CZ-NH1   | 7.33  | 123.97      | 120.30   |
| 35  | BB    | 1221 | C    | N3-C4-N4    | 7.33  | 123.13      | 118.00   |
| 35  | BB    | 1696 | G    | N3-C2-N2    | 7.33  | 125.03      | 119.90   |
| 35  | BB    | 2009 | A    | O4'-C1'-N9  | 7.33  | 114.06      | 108.20   |
| 35  | BB    | 2114 | A    | N9-C4-C5    | 7.33  | 108.73      | 105.80   |
| 1   | AA    | 44   | A    | N1-C6-N6    | 7.33  | 123.00      | 118.60   |
| 1   | AA    | 370  | C    | N3-C4-N4    | 7.33  | 123.13      | 118.00   |
| 35  | BB    | 753  | A    | C5-C6-N6    | -7.33 | 117.84      | 123.70   |
| 35  | BB    | 1591 | A    | C6-C5-N7    | -7.33 | 127.17      | 132.30   |
| 35  | BB    | 2092 | U    | C5-C4-O4    | -7.33 | 121.50      | 125.90   |
| 1   | AA    | 691  | G    | O4'-C1'-N9  | 7.33  | 114.06      | 108.20   |
| 1   | AA    | 744  | C    | N1-C2-N3    | -7.33 | 114.07      | 119.20   |
| 1   | AA    | 901  | A    | P-O3'-C3'   | 7.33  | 128.49      | 119.70   |
| 35  | BB    | 799  | G    | C6-C5-N7    | -7.33 | 126.00      | 130.40   |
| 35  | BB    | 2175 | C    | N1-C2-N3    | -7.33 | 114.07      | 119.20   |
| 1   | AA    | 331  | G    | C1'-O4'-C4' | -7.33 | 104.04      | 109.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 432  | A    | C4-C5-C6    | 7.33  | 120.66      | 117.00   |
| 1   | AA    | 768  | A    | C6-N1-C2    | -7.33 | 114.20      | 118.60   |
| 35  | BB    | 701  | G    | O4'-C1'-N9  | 7.33  | 114.06      | 108.20   |
| 35  | BB    | 1305 | C    | O4'-C1'-N1  | 7.33  | 114.06      | 108.20   |
| 35  | BB    | 1682 | G    | N3-C2-N2    | 7.33  | 125.03      | 119.90   |
| 35  | BB    | 2132 | U    | O4'-C4'-C3' | -7.33 | 96.67       | 104.00   |
| 40  | BG    | 156  | TYR  | CG-CD2-CE2  | -7.33 | 115.44      | 121.30   |
| 1   | AA    | 9    | G    | C4-N9-C1'   | -7.32 | 116.98      | 126.50   |
| 1   | AA    | 51   | A    | O4'-C1'-C2' | 7.32  | 114.19      | 107.60   |
| 1   | AA    | 155  | A    | N9-C4-C5    | -7.32 | 102.87      | 105.80   |
| 1   | AA    | 818  | G    | O4'-C1'-N9  | 7.32  | 114.06      | 108.20   |
| 1   | AA    | 982  | U    | P-O3'-C3'   | 7.32  | 128.49      | 119.70   |
| 1   | AA    | 1164 | G    | N3-C4-C5    | -7.32 | 124.94      | 128.60   |
| 35  | BB    | 1000 | A    | C5-C6-N1    | -7.32 | 114.04      | 117.70   |
| 35  | BB    | 1743 | G    | C5-N7-C8    | -7.32 | 100.64      | 104.30   |
| 1   | AA    | 1158 | C    | N3-C4-C5    | -7.32 | 118.97      | 121.90   |
| 35  | BB    | 1522 | A    | N1-C2-N3    | -7.32 | 125.64      | 129.30   |
| 35  | BB    | 2046 | G    | C5-C6-N1    | -7.32 | 107.84      | 111.50   |
| 1   | AA    | 472  | U    | C6-N1-C2    | -7.32 | 116.61      | 121.00   |
| 1   | AA    | 718  | A    | C4-C5-C6    | 7.32  | 120.66      | 117.00   |
| 35  | BB    | 2406 | A    | C5-C6-N6    | -7.32 | 117.84      | 123.70   |
| 35  | BB    | 2692 | G    | P-O3'-C3'   | -7.32 | 110.92      | 119.70   |
| 35  | BB    | 2815 | C    | N3-C4-N4    | 7.32  | 123.12      | 118.00   |
| 1   | AA    | 1252 | A    | O4'-C1'-N9  | 7.32  | 114.06      | 108.20   |
| 34  | BA    | 115  | A    | O4'-C1'-N9  | 7.32  | 114.06      | 108.20   |
| 35  | BB    | 1345 | C    | O4'-C1'-N1  | 7.32  | 114.06      | 108.20   |
| 1   | AA    | 415  | A    | C5-C6-N6    | -7.32 | 117.85      | 123.70   |
| 1   | AA    | 528  | C    | O4'-C1'-N1  | 7.32  | 114.05      | 108.20   |
| 1   | AA    | 1220 | G    | C6-C5-N7    | -7.32 | 126.01      | 130.40   |
| 34  | BA    | 72   | G    | N1-C2-N3    | -7.32 | 119.51      | 123.90   |
| 35  | BB    | 67   | U    | N3-C2-O2    | 7.32  | 127.32      | 122.20   |
| 35  | BB    | 449  | A    | N1-C2-N3    | -7.32 | 125.64      | 129.30   |
| 35  | BB    | 482  | A    | C5-C6-N1    | -7.32 | 114.04      | 117.70   |
| 35  | BB    | 1134 | A    | C8-N9-C4    | -7.32 | 102.87      | 105.80   |
| 35  | BB    | 1828 | G    | N9-C4-C5    | -7.32 | 102.47      | 105.40   |
| 35  | BB    | 2172 | U    | N3-C2-O2    | 7.32  | 127.32      | 122.20   |
| 35  | BB    | 2662 | A    | C5-C6-N1    | -7.32 | 114.04      | 117.70   |
| 1   | AA    | 1220 | G    | N3-C4-C5    | -7.32 | 124.94      | 128.60   |
| 1   | AA    | 1269 | A    | C5-C6-N6    | -7.32 | 117.85      | 123.70   |
| 1   | AA    | 1271 | A    | C8-N9-C4    | -7.32 | 102.87      | 105.80   |
| 35  | BB    | 459  | U    | C4'-C3'-C2' | -7.32 | 95.28       | 102.60   |
| 35  | BB    | 819  | A    | C4-C5-C6    | 7.32  | 120.66      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1189 | A    | N7-C8-N9    | -7.32 | 110.14      | 113.80   |
| 35  | BB    | 1373 | A    | O4'-C1'-N9  | 7.32  | 114.05      | 108.20   |
| 1   | AA    | 270  | A    | N1-C6-N6    | 7.31  | 122.99      | 118.60   |
| 1   | AA    | 404  | G    | C4-C5-C6    | 7.31  | 123.19      | 118.80   |
| 1   | AA    | 475  | C    | C6-N1-C2    | -7.31 | 117.37      | 120.30   |
| 1   | AA    | 1438 | G    | N1-C6-O6    | 7.31  | 124.29      | 119.90   |
| 22  | AV    | 43   | G    | C5-C6-O6    | -7.31 | 124.21      | 128.60   |
| 35  | BB    | 1446 | C    | C3'-C2'-C1' | 7.31  | 107.35      | 101.50   |
| 1   | AA    | 681  | A    | C4-C5-N7    | 7.31  | 114.36      | 110.70   |
| 35  | BB    | 829  | A    | C5-C6-N6    | -7.31 | 117.85      | 123.70   |
| 35  | BB    | 1778 | U    | N1-C2-N3    | 7.31  | 119.29      | 114.90   |
| 35  | BB    | 2278 | A    | O4'-C1'-N9  | 7.31  | 114.05      | 108.20   |
| 35  | BB    | 2646 | C    | O4'-C1'-N1  | 7.31  | 114.05      | 108.20   |
| 35  | BB    | 2777 | G    | N1-C6-O6    | 7.31  | 124.29      | 119.90   |
| 1   | AA    | 408  | A    | C2-N3-C4    | -7.31 | 106.94      | 110.60   |
| 1   | AA    | 1272 | G    | N3-C2-N2    | 7.31  | 125.02      | 119.90   |
| 35  | BB    | 3    | U    | C1'-O4'-C4' | 7.31  | 115.75      | 109.90   |
| 35  | BB    | 636  | G    | O4'-C1'-N9  | 7.31  | 114.05      | 108.20   |
| 1   | AA    | 388  | G    | C6-C5-N7    | -7.31 | 126.02      | 130.40   |
| 1   | AA    | 407  | U    | C2-N3-C4    | -7.31 | 122.61      | 127.00   |
| 35  | BB    | 1697 | G    | N7-C8-N9    | 7.31  | 116.75      | 113.10   |
| 1   | AA    | 46   | G    | N1-C2-N3    | -7.31 | 119.52      | 123.90   |
| 35  | BB    | 1071 | G    | N3-C4-C5    | -7.31 | 124.95      | 128.60   |
| 35  | BB    | 2207 | C    | C6-N1-C2    | -7.31 | 117.38      | 120.30   |
| 1   | AA    | 601  | G    | C3'-C2'-C1' | -7.31 | 95.66       | 101.50   |
| 35  | BB    | 834  | G    | C6-C5-N7    | -7.31 | 126.02      | 130.40   |
| 35  | BB    | 2229 | U    | O4'-C1'-N1  | 7.31  | 114.04      | 108.20   |
| 1   | AA    | 222  | C    | C4-C5-C6    | 7.30  | 121.05      | 117.40   |
| 1   | AA    | 1296 | C    | O4'-C1'-N1  | 7.30  | 114.04      | 108.20   |
| 1   | AA    | 1415 | G    | N1-C6-O6    | 7.30  | 124.28      | 119.90   |
| 30  | B5    | 137  | MET  | CG-SD-CE    | -7.30 | 88.51       | 100.20   |
| 35  | BB    | 271  | G    | C4-C5-C6    | -7.30 | 114.42      | 118.80   |
| 35  | BB    | 624  | C    | C4-C5-C6    | 7.30  | 121.05      | 117.40   |
| 35  | BB    | 1064 | C    | C2-N3-C4    | -7.30 | 116.25      | 119.90   |
| 35  | BB    | 1495 | A    | C5-C6-N1    | -7.30 | 114.05      | 117.70   |
| 35  | BB    | 2367 | G    | P-O5'-C5'   | 7.30  | 132.59      | 120.90   |
| 1   | AA    | 95   | C    | N3-C4-C5    | -7.30 | 118.98      | 121.90   |
| 1   | AA    | 1091 | U    | N3-C4-O4    | 7.30  | 124.51      | 119.40   |
| 1   | AA    | 1141 | C    | C6-N1-C2    | -7.30 | 117.38      | 120.30   |
| 35  | BB    | 600  | G    | C4-C5-N7    | 7.30  | 113.72      | 110.80   |
| 35  | BB    | 1907 | G    | N3-C2-N2    | 7.30  | 125.01      | 119.90   |
| 35  | BB    | 2148 | G    | N9-C4-C5    | 7.30  | 108.32      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 143  | A    | C4-C5-C6    | 7.30  | 120.65      | 117.00   |
| 1   | AA    | 506  | G    | N7-C8-N9    | -7.30 | 109.45      | 113.10   |
| 1   | AA    | 655  | A    | O4'-C1'-N9  | 7.30  | 114.04      | 108.20   |
| 1   | AA    | 814  | A    | N1-C2-N3    | 7.30  | 132.95      | 129.30   |
| 1   | AA    | 964  | A    | C5-C6-N1    | -7.30 | 114.05      | 117.70   |
| 1   | AA    | 1208 | C    | N3-C4-N4    | 7.30  | 123.11      | 118.00   |
| 35  | BB    | 1037 | G    | C5-C6-N1    | -7.30 | 107.85      | 111.50   |
| 35  | BB    | 1218 | G    | C5-C6-O6    | -7.30 | 124.22      | 128.60   |
| 35  | BB    | 1333 | G    | C4-C5-N7    | -7.30 | 107.88      | 110.80   |
| 35  | BB    | 1391 | U    | N3-C4-O4    | 7.30  | 124.51      | 119.40   |
| 35  | BB    | 1707 | G    | O4'-C1'-N9  | 7.30  | 114.04      | 108.20   |
| 1   | AA    | 244  | U    | N3-C2-O2    | 7.30  | 127.31      | 122.20   |
| 22  | AV    | 76   | A    | C8-N9-C4    | -7.30 | 102.88      | 105.80   |
| 35  | BB    | 449  | A    | C5-C6-N1    | -7.30 | 114.05      | 117.70   |
| 35  | BB    | 697  | G    | C5-C6-N1    | 7.30  | 115.15      | 111.50   |
| 35  | BB    | 1000 | A    | O4'-C4'-C3' | -7.30 | 96.70       | 104.00   |
| 35  | BB    | 1459 | G    | N1-C6-O6    | 7.30  | 124.28      | 119.90   |
| 35  | BB    | 1471 | G    | C4-C5-C6    | 7.30  | 123.18      | 118.80   |
| 35  | BB    | 1576 | U    | C5-C6-N1    | 7.30  | 126.35      | 122.70   |
| 35  | BB    | 2299 | U    | N3-C4-C5    | -7.30 | 110.22      | 114.60   |
| 35  | BB    | 2351 | G    | O4'-C1'-N9  | 7.30  | 114.04      | 108.20   |
| 1   | AA    | 46   | G    | C2-N3-C4    | 7.30  | 115.55      | 111.90   |
| 1   | AA    | 986  | U    | C5-C4-O4    | -7.30 | 121.52      | 125.90   |
| 35  | BB    | 24   | G    | N1-C6-O6    | 7.30  | 124.28      | 119.90   |
| 35  | BB    | 736  | C    | N3-C4-N4    | 7.30  | 123.11      | 118.00   |
| 1   | AA    | 319  | G    | C5-C6-N1    | -7.30 | 107.85      | 111.50   |
| 1   | AA    | 352  | C    | C4-C5-C6    | -7.30 | 113.75      | 117.40   |
| 1   | AA    | 1309 | G    | C1'-O4'-C4' | -7.30 | 104.06      | 109.90   |
| 35  | BB    | 512  | G    | C2-N3-C4    | -7.30 | 108.25      | 111.90   |
| 35  | BB    | 546  | U    | P-O3'-C3'   | 7.30  | 128.46      | 119.70   |
| 35  | BB    | 1122 | G    | C5-C6-N1    | -7.30 | 107.85      | 111.50   |
| 35  | BB    | 2066 | C    | N3-C4-N4    | 7.30  | 123.11      | 118.00   |
| 1   | AA    | 126  | G    | N1-C2-N3    | -7.29 | 119.52      | 123.90   |
| 1   | AA    | 775  | G    | N1-C6-O6    | 7.29  | 124.28      | 119.90   |
| 35  | BB    | 2145 | C    | N3-C4-N4    | 7.29  | 123.11      | 118.00   |
| 1   | AA    | 537  | G    | C6-C5-N7    | -7.29 | 126.02      | 130.40   |
| 1   | AA    | 1294 | G    | N3-C2-N2    | 7.29  | 125.00      | 119.90   |
| 1   | AA    | 1367 | C    | C1'-O4'-C4' | -7.29 | 104.07      | 109.90   |
| 1   | AA    | 1531 | A    | C4-C5-C6    | 7.29  | 120.65      | 117.00   |
| 22  | AV    | 3    | G    | C2-N3-C4    | 7.29  | 115.55      | 111.90   |
| 35  | BB    | 725  | G    | N1-C6-O6    | 7.29  | 124.28      | 119.90   |
| 35  | BB    | 777  | G    | C5-N7-C8    | 7.29  | 107.95      | 104.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1689 | A    | N9-C4-C5    | -7.29 | 102.88      | 105.80   |
| 35  | BB    | 1719 | G    | C4-C5-N7    | 7.29  | 113.72      | 110.80   |
| 35  | BB    | 2544 | G    | N9-C4-C5    | -7.29 | 102.48      | 105.40   |
| 1   | AA    | 472  | U    | C5-C4-O4    | 7.29  | 130.28      | 125.90   |
| 1   | AA    | 856  | C    | N3-C4-C5    | -7.29 | 118.98      | 121.90   |
| 34  | BA    | 29   | A    | C5-C6-N1    | -7.29 | 114.05      | 117.70   |
| 35  | BB    | 182  | A    | P-O3'-C3'   | -7.29 | 110.95      | 119.70   |
| 35  | BB    | 2763 | G    | N3-C2-N2    | 7.29  | 125.00      | 119.90   |
| 1   | AA    | 6    | G    | C8-N9-C4    | -7.29 | 103.48      | 106.40   |
| 1   | AA    | 71   | A    | C5-C6-N1    | -7.29 | 114.06      | 117.70   |
| 1   | AA    | 945  | G    | C8-N9-C4    | -7.29 | 103.48      | 106.40   |
| 1   | AA    | 1515 | G    | O4'-C1'-N9  | 7.29  | 114.03      | 108.20   |
| 35  | BB    | 2481 | G    | N1-C2-N3    | -7.29 | 119.53      | 123.90   |
| 35  | BB    | 2494 | G    | N1-C6-O6    | 7.29  | 124.27      | 119.90   |
| 1   | AA    | 297  | G    | C4-C5-N7    | 7.29  | 113.72      | 110.80   |
| 1   | AA    | 716  | A    | N9-C4-C5    | 7.29  | 108.72      | 105.80   |
| 1   | AA    | 1016 | A    | O4'-C1'-N9  | 7.29  | 114.03      | 108.20   |
| 1   | AA    | 1043 | G    | P-O3'-C3'   | 7.29  | 128.45      | 119.70   |
| 1   | AA    | 1162 | C    | C4'-C3'-C2' | -7.29 | 95.31       | 102.60   |
| 35  | BB    | 459  | U    | O4'-C1'-N1  | 7.29  | 114.03      | 108.20   |
| 35  | BB    | 707  | G    | N7-C8-N9    | -7.29 | 109.45      | 113.10   |
| 35  | BB    | 1339 | G    | C6-N1-C2    | -7.29 | 120.73      | 125.10   |
| 35  | BB    | 1341 | G    | C5-C6-N1    | -7.29 | 107.86      | 111.50   |
| 35  | BB    | 1724 | G    | C2-N3-C4    | -7.29 | 108.26      | 111.90   |
| 1   | AA    | 1121 | U    | O4'-C1'-N1  | 7.29  | 114.03      | 108.20   |
| 1   | AA    | 1350 | A    | N3-C4-N9    | 7.29  | 133.23      | 127.40   |
| 35  | BB    | 469  | G    | C5'-C4'-O4' | 7.29  | 117.84      | 109.10   |
| 1   | AA    | 380  | G    | C5-C6-O6    | -7.29 | 124.23      | 128.60   |
| 35  | BB    | 197  | A    | C4-C5-C6    | 7.29  | 120.64      | 117.00   |
| 35  | BB    | 382  | A    | N1-C6-N6    | 7.29  | 122.97      | 118.60   |
| 35  | BB    | 2749 | A    | C6-C5-N7    | -7.29 | 127.20      | 132.30   |
| 53  | BT    | 10   | VAL  | CA-CB-CG2   | 7.29  | 121.83      | 110.90   |
| 1   | AA    | 64   | G    | C5-C6-O6    | -7.28 | 124.23      | 128.60   |
| 1   | AA    | 487  | A    | C5-N7-C8    | 7.28  | 107.54      | 103.90   |
| 1   | AA    | 1164 | G    | C6-N1-C2    | 7.28  | 129.47      | 125.10   |
| 8   | AH    | 76   | ARG  | NE-CZ-NH1   | 7.28  | 123.94      | 120.30   |
| 35  | BB    | 1650 | A    | N1-C6-N6    | 7.28  | 122.97      | 118.60   |
| 1   | AA    | 9    | G    | N3-C4-N9    | 7.28  | 130.37      | 126.00   |
| 35  | BB    | 809  | G    | O4'-C1'-N9  | 7.28  | 114.03      | 108.20   |
| 35  | BB    | 2154 | A    | C4-C5-N7    | -7.28 | 107.06      | 110.70   |
| 35  | BB    | 2412 | A    | C5-C6-N1    | -7.28 | 114.06      | 117.70   |
| 1   | AA    | 43   | C    | O4'-C1'-N1  | 7.28  | 114.02      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 254  | G    | N3-C2-N2    | 7.28  | 125.00      | 119.90   |
| 1   | AA    | 674  | G    | O4'-C1'-N9  | 7.28  | 114.02      | 108.20   |
| 1   | AA    | 964  | A    | C4-C5-C6    | 7.28  | 120.64      | 117.00   |
| 1   | AA    | 1029 | U    | C6-N1-C2    | -7.28 | 116.63      | 121.00   |
| 1   | AA    | 1204 | A    | C5-C6-N6    | -7.28 | 117.88      | 123.70   |
| 35  | BB    | 845  | A    | P-O3'-C3'   | -7.28 | 110.96      | 119.70   |
| 35  | BB    | 1828 | G    | C5'-C4'-O4' | 7.28  | 117.84      | 109.10   |
| 35  | BB    | 2177 | C    | C5-C6-N1    | 7.28  | 124.64      | 121.00   |
| 1   | AA    | 104  | G    | N1-C6-O6    | 7.28  | 124.27      | 119.90   |
| 1   | AA    | 378  | G    | O4'-C1'-N9  | 7.28  | 114.02      | 108.20   |
| 1   | AA    | 760  | G    | N7-C8-N9    | -7.28 | 109.46      | 113.10   |
| 1   | AA    | 1402 | C    | N3-C4-C5    | -7.28 | 118.99      | 121.90   |
| 35  | BB    | 1797 | G    | N9-C4-C5    | 7.28  | 108.31      | 105.40   |
| 1   | AA    | 1273 | C    | N3-C4-C5    | -7.28 | 118.99      | 121.90   |
| 35  | BB    | 1627 | G    | O4'-C1'-N9  | 7.28  | 114.02      | 108.20   |
| 35  | BB    | 1932 | A    | C5-C6-N1    | -7.28 | 114.06      | 117.70   |
| 35  | BB    | 2158 | A    | C8-N9-C4    | -7.28 | 102.89      | 105.80   |
| 1   | AA    | 705  | G    | C6-N1-C2    | -7.28 | 120.73      | 125.10   |
| 1   | AA    | 812  | G    | C2-N3-C4    | 7.28  | 115.54      | 111.90   |
| 10  | AJ    | 86   | ALA  | O-C-N       | -7.28 | 111.06      | 122.70   |
| 13  | AM    | 22   | TYR  | CB-CG-CD2   | 7.28  | 125.36      | 121.00   |
| 35  | BB    | 104  | A    | N1-C2-N3    | 7.28  | 132.94      | 129.30   |
| 35  | BB    | 181  | A    | C6-C5-N7    | -7.28 | 127.21      | 132.30   |
| 35  | BB    | 689  | A    | N7-C8-N9    | -7.28 | 110.16      | 113.80   |
| 35  | BB    | 1277 | G    | P-O3'-C3'   | -7.28 | 110.97      | 119.70   |
| 35  | BB    | 1600 | C    | C5-C4-N4    | -7.28 | 115.11      | 120.20   |
| 35  | BB    | 1742 | U    | N1-C2-N3    | -7.28 | 110.53      | 114.90   |
| 35  | BB    | 1790 | C    | C6-N1-C2    | -7.28 | 117.39      | 120.30   |
| 35  | BB    | 1975 | G    | C5-N7-C8    | -7.28 | 100.66      | 104.30   |
| 35  | BB    | 1996 | C    | N3-C4-C5    | -7.28 | 118.99      | 121.90   |
| 35  | BB    | 2062 | A    | C6-N1-C2    | -7.28 | 114.23      | 118.60   |
| 1   | AA    | 232  | G    | C6-N1-C2    | 7.27  | 129.47      | 125.10   |
| 1   | AA    | 536  | C    | C2-N3-C4    | 7.27  | 123.54      | 119.90   |
| 1   | AA    | 906  | A    | C6-C5-N7    | -7.27 | 127.21      | 132.30   |
| 16  | AP    | 65   | ALA  | N-CA-CB     | 7.27  | 120.28      | 110.10   |
| 35  | BB    | 68   | G    | O4'-C1'-C2' | -7.27 | 98.53       | 105.80   |
| 35  | BB    | 717  | C    | N1-C2-O2    | 7.27  | 123.26      | 118.90   |
| 35  | BB    | 756  | A    | C8-N9-C4    | -7.27 | 102.89      | 105.80   |
| 35  | BB    | 983  | A    | N9-C4-C5    | 7.27  | 108.71      | 105.80   |
| 35  | BB    | 1824 | G    | N1-C2-N2    | 7.27  | 122.75      | 116.20   |
| 35  | BB    | 2004 | G    | C8-N9-C4    | -7.27 | 103.49      | 106.40   |
| 1   | AA    | 491  | G    | N1-C2-N3    | -7.27 | 119.54      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1319 | A    | C5-C6-N1    | -7.27 | 114.06      | 117.70   |
| 1   | AA    | 1380 | U    | C3'-C2'-C1' | 7.27  | 107.32      | 101.50   |
| 1   | AA    | 1530 | G    | N1-C6-O6    | 7.27  | 124.26      | 119.90   |
| 35  | BB    | 370  | G    | N3-C2-N2    | 7.27  | 124.99      | 119.90   |
| 35  | BB    | 1164 | C    | N3-C4-C5    | -7.27 | 118.99      | 121.90   |
| 35  | BB    | 1439 | A    | C5-C6-N1    | -7.27 | 114.06      | 117.70   |
| 35  | BB    | 1465 | G    | C8-N9-C4    | -7.27 | 103.49      | 106.40   |
| 35  | BB    | 1948 | G    | C8-N9-C4    | -7.27 | 103.49      | 106.40   |
| 35  | BB    | 2159 | G    | N3-C2-N2    | 7.27  | 124.99      | 119.90   |
| 36  | BC    | 101  | ARG  | NE-CZ-NH1   | 7.27  | 123.94      | 120.30   |
| 1   | AA    | 789  | U    | C2-N3-C4    | -7.27 | 122.64      | 127.00   |
| 1   | AA    | 1435 | G    | C5-C6-O6    | -7.27 | 124.24      | 128.60   |
| 34  | BA    | 96   | G    | C2-N3-C4    | -7.27 | 108.27      | 111.90   |
| 35  | BB    | 798  | G    | N9-C4-C5    | 7.27  | 108.31      | 105.40   |
| 35  | BB    | 1576 | U    | C5-C4-O4    | -7.27 | 121.54      | 125.90   |
| 1   | AA    | 712  | A    | C5-N7-C8    | 7.27  | 107.53      | 103.90   |
| 1   | AA    | 935  | A    | N7-C8-N9    | 7.27  | 117.43      | 113.80   |
| 1   | AA    | 1223 | C    | C5'-C4'-O4' | 7.27  | 117.82      | 109.10   |
| 35  | BB    | 36   | G    | C5-C6-O6    | -7.27 | 124.24      | 128.60   |
| 35  | BB    | 422  | A    | N7-C8-N9    | -7.27 | 110.17      | 113.80   |
| 35  | BB    | 483  | A    | C4-C5-N7    | -7.27 | 107.06      | 110.70   |
| 35  | BB    | 1638 | C    | N3-C2-O2    | 7.27  | 126.99      | 121.90   |
| 35  | BB    | 1918 | A    | N1-C6-N6    | 7.27  | 122.96      | 118.60   |
| 35  | BB    | 2311 | A    | O4'-C1'-N9  | 7.27  | 114.02      | 108.20   |
| 35  | BB    | 2733 | A    | C4-C5-C6    | 7.27  | 120.64      | 117.00   |
| 1   | AA    | 50   | A    | C2-N3-C4    | 7.27  | 114.23      | 110.60   |
| 1   | AA    | 577  | G    | N3-C2-N2    | 7.27  | 124.99      | 119.90   |
| 1   | AA    | 847  | G    | C8-N9-C1'   | 7.27  | 136.45      | 127.00   |
| 1   | AA    | 1045 | C    | C5-C6-N1    | 7.27  | 124.63      | 121.00   |
| 1   | AA    | 1271 | A    | C4-C5-C6    | 7.27  | 120.63      | 117.00   |
| 1   | AA    | 1438 | G    | N1-C2-N3    | -7.27 | 119.54      | 123.90   |
| 7   | AG    | 110  | ARG  | NE-CZ-NH1   | 7.27  | 123.93      | 120.30   |
| 35  | BB    | 58   | G    | N3-C4-C5    | -7.27 | 124.97      | 128.60   |
| 35  | BB    | 963  | U    | O4'-C4'-C3' | -7.27 | 96.73       | 104.00   |
| 35  | BB    | 1236 | G    | C2-N3-C4    | 7.27  | 115.53      | 111.90   |
| 35  | BB    | 1317 | G    | C6-C5-N7    | -7.27 | 126.04      | 130.40   |
| 35  | BB    | 1473 | G    | C8-N9-C4    | -7.27 | 103.49      | 106.40   |
| 35  | BB    | 2780 | G    | C5-C6-O6    | -7.27 | 124.24      | 128.60   |
| 35  | BB    | 2893 | A    | C4-C5-N7    | -7.27 | 107.07      | 110.70   |
| 1   | AA    | 224  | U    | N3-C4-O4    | 7.27  | 124.49      | 119.40   |
| 1   | AA    | 898  | G    | C5-C6-O6    | -7.27 | 124.24      | 128.60   |
| 35  | BB    | 412  | A    | C5-N7-C8    | 7.27  | 107.53      | 103.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 748  | G    | O4'-C1'-N9 | 7.27  | 114.01      | 108.20   |
| 35  | BB    | 948  | C    | N3-C4-C5   | -7.27 | 118.99      | 121.90   |
| 35  | BB    | 1506 | U    | O4'-C1'-N1 | 7.27  | 114.01      | 108.20   |
| 35  | BB    | 1672 | A    | N1-C2-N3   | 7.27  | 132.93      | 129.30   |
| 1   | AA    | 271  | C    | C5-C4-N4   | -7.26 | 115.11      | 120.20   |
| 1   | AA    | 706  | A    | C5-C6-N1   | -7.26 | 114.07      | 117.70   |
| 1   | AA    | 714  | G    | N3-C2-N2   | 7.26  | 124.98      | 119.90   |
| 35  | BB    | 463  | G    | O4'-C1'-N9 | 7.26  | 114.01      | 108.20   |
| 35  | BB    | 718  | A    | C5-N7-C8   | 7.26  | 107.53      | 103.90   |
| 35  | BB    | 1589 | U    | N3-C4-C5   | 7.26  | 118.96      | 114.60   |
| 35  | BB    | 2192 | U    | C5-C4-O4   | -7.26 | 121.54      | 125.90   |
| 35  | BB    | 2311 | A    | C5-N7-C8   | 7.26  | 107.53      | 103.90   |
| 35  | BB    | 2341 | G    | O4'-C1'-N9 | 7.26  | 114.01      | 108.20   |
| 35  | BB    | 2713 | U    | P-O5'-C5'  | -7.26 | 109.28      | 120.90   |
| 1   | AA    | 337  | G    | C6-C5-N7   | -7.26 | 126.04      | 130.40   |
| 35  | BB    | 2839 | G    | C2-N3-C4   | 7.26  | 115.53      | 111.90   |
| 35  | BB    | 585  | G    | C6-C5-N7   | -7.26 | 126.04      | 130.40   |
| 35  | BB    | 2346 | A    | N1-C6-N6   | 7.26  | 122.96      | 118.60   |
| 35  | BB    | 538  | A    | C2-N3-C4   | -7.26 | 106.97      | 110.60   |
| 35  | BB    | 562  | U    | C5-C4-O4   | -7.26 | 121.54      | 125.90   |
| 35  | BB    | 577  | G    | N9-C4-C5   | -7.26 | 102.50      | 105.40   |
| 35  | BB    | 941  | A    | O4'-C1'-N9 | 7.26  | 114.01      | 108.20   |
| 35  | BB    | 1540 | G    | C2-N3-C4   | 7.26  | 115.53      | 111.90   |
| 35  | BB    | 2057 | G    | C4-C5-N7   | 7.26  | 113.70      | 110.80   |
| 35  | BB    | 370  | G    | C5-C6-O6   | -7.26 | 124.25      | 128.60   |
| 35  | BB    | 601  | C    | N3-C4-C5   | -7.26 | 119.00      | 121.90   |
| 35  | BB    | 900  | A    | C4-C5-N7   | -7.26 | 107.07      | 110.70   |
| 1   | AA    | 252  | U    | O4'-C1'-N1 | 7.26  | 114.00      | 108.20   |
| 1   | AA    | 313  | A    | O4'-C1'-N9 | 7.26  | 114.00      | 108.20   |
| 1   | AA    | 321  | A    | C8-N9-C4   | -7.26 | 102.90      | 105.80   |
| 1   | AA    | 507  | C    | C6-N1-C2   | -7.26 | 117.40      | 120.30   |
| 35  | BB    | 916  | G    | C5-C6-O6   | -7.26 | 124.25      | 128.60   |
| 35  | BB    | 1005 | C    | C6-N1-C2   | -7.26 | 117.40      | 120.30   |
| 35  | BB    | 2108 | A    | C6-C5-N7   | -7.26 | 127.22      | 132.30   |
| 35  | BB    | 2218 | G    | O4'-C1'-N9 | 7.26  | 114.00      | 108.20   |
| 1   | AA    | 1214 | C    | C2-N1-C1'  | 7.25  | 126.78      | 118.80   |
| 1   | AA    | 1339 | A    | C6-N1-C2   | 7.25  | 122.95      | 118.60   |
| 35  | BB    | 11   | C    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 35  | BB    | 142  | A    | O4'-C1'-N9 | 7.25  | 114.00      | 108.20   |
| 35  | BB    | 526  | A    | N9-C4-C5   | -7.25 | 102.90      | 105.80   |
| 35  | BB    | 1617 | C    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 35  | BB    | 2883 | A    | C4-C5-N7   | -7.25 | 107.07      | 110.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 912  | C    | N3-C4-N4    | 7.25  | 123.08      | 118.00   |
| 1   | AA    | 1241 | G    | C4'-C3'-C2' | -7.25 | 95.35       | 102.60   |
| 1   | AA    | 1260 | G    | N7-C8-N9    | 7.25  | 116.73      | 113.10   |
| 1   | AA    | 1386 | G    | C4-C5-C6    | 7.25  | 123.15      | 118.80   |
| 35  | BB    | 579  | G    | N3-C2-N2    | 7.25  | 124.98      | 119.90   |
| 35  | BB    | 838  | C    | C5-C4-N4    | -7.25 | 115.12      | 120.20   |
| 35  | BB    | 965  | C    | C5'-C4'-C3' | -7.25 | 104.39      | 116.00   |
| 35  | BB    | 1549 | A    | C6-N1-C2    | 7.25  | 122.95      | 118.60   |
| 54  | BU    | 84   | PHE  | CB-CG-CD1   | 7.25  | 125.88      | 120.80   |
| 1   | AA    | 7    | A    | N1-C6-N6    | 7.25  | 122.95      | 118.60   |
| 1   | AA    | 110  | C    | C5-C6-N1    | 7.25  | 124.63      | 121.00   |
| 1   | AA    | 236  | A    | C5-N7-C8    | 7.25  | 107.53      | 103.90   |
| 35  | BB    | 579  | G    | N9-C4-C5    | 7.25  | 108.30      | 105.40   |
| 35  | BB    | 1363 | C    | N3-C4-N4    | 7.25  | 123.08      | 118.00   |
| 35  | BB    | 1500 | G    | N1-C6-O6    | 7.25  | 124.25      | 119.90   |
| 35  | BB    | 1987 | A    | C5-C6-N1    | -7.25 | 114.07      | 117.70   |
| 35  | BB    | 2057 | G    | O4'-C1'-N9  | 7.25  | 114.00      | 108.20   |
| 35  | BB    | 2214 | C    | C5-C4-N4    | -7.25 | 115.12      | 120.20   |
| 35  | BB    | 2330 | G    | N3-C4-C5    | -7.25 | 124.97      | 128.60   |
| 35  | BB    | 2400 | G    | C5-C6-N1    | -7.25 | 107.88      | 111.50   |
| 1   | AA    | 192  | A    | N1-C2-N3    | 7.25  | 132.93      | 129.30   |
| 1   | AA    | 623  | C    | N3-C4-N4    | 7.25  | 123.08      | 118.00   |
| 35  | BB    | 1100 | C    | N3-C2-O2    | 7.25  | 126.97      | 121.90   |
| 35  | BB    | 1197 | G    | C5-N7-C8    | -7.25 | 100.67      | 104.30   |
| 35  | BB    | 1596 | A    | C6-C5-N7    | -7.25 | 127.23      | 132.30   |
| 35  | BB    | 1800 | C    | C5-C6-N1    | -7.25 | 117.38      | 121.00   |
| 35  | BB    | 1981 | A    | C4-C5-C6    | 7.25  | 120.62      | 117.00   |
| 35  | BB    | 2308 | G    | C5-C6-O6    | -7.25 | 124.25      | 128.60   |
| 1   | AA    | 504  | C    | N3-C4-N4    | 7.25  | 123.07      | 118.00   |
| 1   | AA    | 919  | A    | N1-C6-N6    | 7.25  | 122.95      | 118.60   |
| 1   | AA    | 947  | G    | N7-C8-N9    | 7.25  | 116.72      | 113.10   |
| 1   | AA    | 1042 | A    | C5-N7-C8    | 7.25  | 107.52      | 103.90   |
| 1   | AA    | 1312 | G    | C5-C6-O6    | -7.25 | 124.25      | 128.60   |
| 1   | AA    | 1529 | G    | N1-C6-O6    | 7.25  | 124.25      | 119.90   |
| 35  | BB    | 41   | C    | C4'-C3'-C2' | -7.25 | 95.35       | 102.60   |
| 35  | BB    | 361  | G    | C5-C6-O6    | -7.25 | 124.25      | 128.60   |
| 35  | BB    | 418  | C    | O4'-C1'-N1  | 7.25  | 114.00      | 108.20   |
| 35  | BB    | 650  | C    | N3-C4-N4    | 7.25  | 123.07      | 118.00   |
| 35  | BB    | 1030 | C    | P-O3'-C3'   | -7.25 | 111.00      | 119.70   |
| 35  | BB    | 1475 | G    | N3-C4-N9    | 7.25  | 130.35      | 126.00   |
| 35  | BB    | 1591 | A    | O4'-C1'-N9  | 7.25  | 114.00      | 108.20   |
| 35  | BB    | 1872 | A    | C4-C5-C6    | 7.25  | 120.62      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 969  | A    | C5-C6-N6    | -7.25 | 117.90      | 123.70   |
| 35  | BB    | 2192 | U    | C5'-C4'-C3' | -7.25 | 104.41      | 116.00   |
| 1   | AA    | 326  | G    | N1-C2-N3    | -7.24 | 119.55      | 123.90   |
| 4   | AD    | 13   | ARG  | NE-CZ-NH2   | -7.24 | 116.68      | 120.30   |
| 35  | BB    | 1420 | A    | P-O3'-C3'   | 7.24  | 128.39      | 119.70   |
| 35  | BB    | 1812 | U    | O4'-C1'-N1  | 7.24  | 114.00      | 108.20   |
| 35  | BB    | 2069 | G    | N3-C4-N9    | 7.24  | 130.35      | 126.00   |
| 35  | BB    | 2294 | G    | N3-C4-N9    | -7.24 | 121.65      | 126.00   |
| 35  | BB    | 2418 | A    | C8-N9-C4    | -7.24 | 102.90      | 105.80   |
| 35  | BB    | 1861 | G    | N1-C6-O6    | 7.24  | 124.25      | 119.90   |
| 1   | AA    | 747  | A    | P-O3'-C3'   | 7.24  | 128.39      | 119.70   |
| 1   | AA    | 1118 | U    | C5-C4-O4    | 7.24  | 130.24      | 125.90   |
| 1   | AA    | 1157 | A    | C5-C6-N1    | -7.24 | 114.08      | 117.70   |
| 1   | AA    | 1446 | A    | C4-C5-C6    | 7.24  | 120.62      | 117.00   |
| 34  | BA    | 86   | G    | N3-C4-C5    | 7.24  | 132.22      | 128.60   |
| 34  | BA    | 101  | A    | C6-C5-N7    | -7.24 | 127.23      | 132.30   |
| 35  | BB    | 1169 | A    | C4-C5-N7    | -7.24 | 107.08      | 110.70   |
| 35  | BB    | 2567 | G    | C6-C5-N7    | -7.24 | 126.06      | 130.40   |
| 1   | AA    | 8    | A    | C5-C6-N6    | -7.24 | 117.91      | 123.70   |
| 1   | AA    | 1070 | U    | N3-C2-O2    | 7.24  | 127.27      | 122.20   |
| 34  | BA    | 76   | G    | N3-C2-N2    | 7.24  | 124.97      | 119.90   |
| 35  | BB    | 83   | A    | P-O5'-C5'   | 7.24  | 132.48      | 120.90   |
| 35  | BB    | 381  | G    | C2-N3-C4    | -7.24 | 108.28      | 111.90   |
| 35  | BB    | 470  | A    | N9-C4-C5    | -7.24 | 102.90      | 105.80   |
| 35  | BB    | 1283 | G    | C5-C6-O6    | -7.24 | 124.26      | 128.60   |
| 35  | BB    | 1516 | G    | N7-C8-N9    | 7.24  | 116.72      | 113.10   |
| 1   | AA    | 8    | A    | C6-N1-C2    | -7.24 | 114.26      | 118.60   |
| 1   | AA    | 51   | A    | P-O3'-C3'   | 7.24  | 128.38      | 119.70   |
| 1   | AA    | 602  | A    | N1-C2-N3    | 7.24  | 132.92      | 129.30   |
| 1   | AA    | 1321 | U    | P-O5'-C5'   | 7.24  | 132.48      | 120.90   |
| 1   | AA    | 1515 | G    | C8-N9-C4    | -7.24 | 103.51      | 106.40   |
| 35  | BB    | 185  | G    | C6-C5-N7    | -7.24 | 126.06      | 130.40   |
| 35  | BB    | 303  | G    | C5-C6-O6    | -7.24 | 124.26      | 128.60   |
| 35  | BB    | 745  | G    | C4'-C3'-C2' | 7.24  | 109.83      | 102.60   |
| 35  | BB    | 1224 | U    | C2-N3-C4    | -7.24 | 122.66      | 127.00   |
| 35  | BB    | 1456 | G    | N3-C2-N2    | 7.24  | 124.97      | 119.90   |
| 35  | BB    | 1584 | U    | C1'-O4'-C4' | 7.24  | 115.69      | 109.90   |
| 35  | BB    | 1900 | A    | C2-N3-C4    | 7.24  | 114.22      | 110.60   |
| 35  | BB    | 2000 | C    | N3-C4-N4    | 7.24  | 123.06      | 118.00   |
| 35  | BB    | 2213 | U    | P-O3'-C3'   | 7.24  | 128.38      | 119.70   |
| 1   | AA    | 168  | G    | O4'-C1'-N9  | 7.23  | 113.99      | 108.20   |
| 35  | BB    | 580  | U    | C6-N1-C2    | -7.23 | 116.66      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2489 | U    | C5-C4-O4    | -7.23 | 121.56      | 125.90   |
| 1   | AA    | 364  | A    | C8-N9-C4    | -7.23 | 102.91      | 105.80   |
| 18  | AR    | 42   | ARG  | NE-CZ-NH1   | 7.23  | 123.92      | 120.30   |
| 35  | BB    | 480  | A    | C8-N9-C4    | -7.23 | 102.91      | 105.80   |
| 35  | BB    | 650  | C    | C2-N3-C4    | -7.23 | 116.28      | 119.90   |
| 35  | BB    | 1067 | A    | C4-C5-N7    | -7.23 | 107.08      | 110.70   |
| 35  | BB    | 1512 | C    | N3-C4-N4    | 7.23  | 123.06      | 118.00   |
| 35  | BB    | 2251 | G    | N3-C4-N9    | -7.23 | 121.66      | 126.00   |
| 35  | BB    | 2536 | G    | C2-N3-C4    | 7.23  | 115.52      | 111.90   |
| 35  | BB    | 2686 | G    | O4'-C1'-N9  | 7.23  | 113.99      | 108.20   |
| 43  | BJ    | 42   | ALA  | N-CA-CB     | 7.23  | 120.22      | 110.10   |
| 1   | AA    | 201  | G    | N3-C2-N2    | 7.23  | 124.96      | 119.90   |
| 1   | AA    | 928  | G    | C6-N1-C2    | -7.23 | 120.76      | 125.10   |
| 1   | AA    | 1501 | C    | C5-C4-N4    | -7.23 | 115.14      | 120.20   |
| 22  | AV    | 75   | C    | N3-C4-C5    | -7.23 | 119.01      | 121.90   |
| 35  | BB    | 1219 | U    | O4'-C1'-N1  | 7.23  | 113.98      | 108.20   |
| 35  | BB    | 1843 | C    | C4-C5-C6    | 7.23  | 121.02      | 117.40   |
| 35  | BB    | 1852 | U    | N3-C4-O4    | 7.23  | 124.46      | 119.40   |
| 35  | BB    | 1976 | U    | N3-C4-C5    | -7.23 | 110.26      | 114.60   |
| 1   | AA    | 860  | A    | C6-N1-C2    | -7.23 | 114.26      | 118.60   |
| 35  | BB    | 91   | A    | C4-C5-C6    | 7.23  | 120.61      | 117.00   |
| 35  | BB    | 1650 | A    | C4-C5-C6    | 7.23  | 120.61      | 117.00   |
| 35  | BB    | 2759 | G    | O4'-C1'-N9  | 7.23  | 113.98      | 108.20   |
| 1   | AA    | 482  | A    | O4'-C1'-N9  | 7.23  | 113.98      | 108.20   |
| 27  | B2    | 52   | PHE  | CB-CG-CD1   | 7.23  | 125.86      | 120.80   |
| 35  | BB    | 616  | A    | C2-N3-C4    | -7.23 | 106.99      | 110.60   |
| 35  | BB    | 1284 | A    | C4-C5-C6    | 7.23  | 120.61      | 117.00   |
| 35  | BB    | 1926 | U    | O4'-C1'-N1  | 7.23  | 113.98      | 108.20   |
| 35  | BB    | 2341 | G    | N7-C8-N9    | 7.23  | 116.71      | 113.10   |
| 35  | BB    | 2464 | G    | N1-C6-O6    | 7.23  | 124.24      | 119.90   |
| 35  | BB    | 2877 | G    | C2-N3-C4    | 7.23  | 115.51      | 111.90   |
| 1   | AA    | 498  | A    | C5-C6-N6    | -7.23 | 117.92      | 123.70   |
| 1   | AA    | 765  | G    | P-O3'-C3'   | -7.23 | 111.03      | 119.70   |
| 1   | AA    | 1207 | G    | C8-N9-C4    | 7.23  | 109.29      | 106.40   |
| 35  | BB    | 1288 | G    | N9-C4-C5    | -7.23 | 102.51      | 105.40   |
| 1   | AA    | 117  | G    | C3'-C2'-C1' | -7.22 | 95.72       | 101.50   |
| 34  | BA    | 114  | C    | C5-C4-N4    | -7.22 | 115.14      | 120.20   |
| 35  | BB    | 191  | A    | N1-C6-N6    | 7.22  | 122.94      | 118.60   |
| 35  | BB    | 1878 | G    | C5-C6-O6    | -7.22 | 124.27      | 128.60   |
| 38  | BE    | 140  | ASP  | CB-CG-OD2   | -7.22 | 111.80      | 118.30   |
| 1   | AA    | 286  | C    | N3-C4-C5    | -7.22 | 119.01      | 121.90   |
| 35  | BB    | 514  | A    | N1-C6-N6    | 7.22  | 122.93      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 818  | G    | N1-C2-N2    | -7.22 | 109.70      | 116.20   |
| 35  | BB    | 909  | A    | O4'-C1'-N9  | 7.22  | 113.98      | 108.20   |
| 35  | BB    | 1331 | G    | N9-C4-C5    | -7.22 | 102.51      | 105.40   |
| 35  | BB    | 1702 | G    | N1-C6-O6    | 7.22  | 124.23      | 119.90   |
| 35  | BB    | 2015 | A    | C8-N9-C4    | -7.22 | 102.91      | 105.80   |
| 35  | BB    | 2211 | A    | C6-C5-N7    | -7.22 | 127.24      | 132.30   |
| 35  | BB    | 2651 | C    | O4'-C1'-N1  | 7.22  | 113.98      | 108.20   |
| 1   | AA    | 246  | A    | C5-C6-N1    | -7.22 | 114.09      | 117.70   |
| 1   | AA    | 760  | G    | N3-C2-N2    | 7.22  | 124.95      | 119.90   |
| 1   | AA    | 1101 | A    | C4-C5-C6    | 7.22  | 120.61      | 117.00   |
| 35  | BB    | 735  | A    | N1-C2-N3    | 7.22  | 132.91      | 129.30   |
| 35  | BB    | 2583 | G    | C5-C6-O6    | -7.22 | 124.27      | 128.60   |
| 1   | AA    | 533  | A    | C3'-C2'-C1' | -7.22 | 95.72       | 101.50   |
| 1   | AA    | 676  | A    | N3-C4-C5    | -7.22 | 121.75      | 126.80   |
| 1   | AA    | 938  | A    | C4'-C3'-C2' | -7.22 | 95.38       | 102.60   |
| 1   | AA    | 1180 | A    | P-O3'-C3'   | 7.22  | 128.36      | 119.70   |
| 2   | AB    | 68   | PHE  | CB-CG-CD1   | 7.22  | 125.85      | 120.80   |
| 35  | BB    | 34   | U    | O4'-C1'-N1  | 7.22  | 113.97      | 108.20   |
| 35  | BB    | 662  | G    | O4'-C1'-N9  | 7.22  | 113.97      | 108.20   |
| 35  | BB    | 850  | U    | C6-N1-C2    | -7.22 | 116.67      | 121.00   |
| 35  | BB    | 1021 | A    | P-O3'-C3'   | 7.22  | 128.36      | 119.70   |
| 35  | BB    | 1455 | G    | C8-N9-C4    | -7.22 | 103.51      | 106.40   |
| 35  | BB    | 1552 | A    | C5-C6-N6    | -7.22 | 117.92      | 123.70   |
| 35  | BB    | 1857 | G    | N9-C4-C5    | -7.22 | 102.51      | 105.40   |
| 1   | AA    | 181  | A    | C6-C5-N7    | -7.22 | 127.25      | 132.30   |
| 1   | AA    | 622  | A    | C4-C5-C6    | 7.22  | 120.61      | 117.00   |
| 1   | AA    | 835  | U    | P-O3'-C3'   | -7.22 | 111.04      | 119.70   |
| 35  | BB    | 1923 | U    | N3-C4-O4    | 7.22  | 124.45      | 119.40   |
| 35  | BB    | 1958 | C    | N3-C4-C5    | -7.22 | 119.01      | 121.90   |
| 35  | BB    | 54   | G    | C2-N3-C4    | 7.22  | 115.51      | 111.90   |
| 35  | BB    | 568  | U    | P-O5'-C5'   | 7.22  | 132.45      | 120.90   |
| 35  | BB    | 1968 | G    | N3-C4-N9    | 7.22  | 130.33      | 126.00   |
| 35  | BB    | 2443 | C    | N1-C2-O2    | 7.22  | 123.23      | 118.90   |
| 35  | BB    | 2891 | U    | N1-C2-O2    | -7.22 | 117.75      | 122.80   |
| 1   | AA    | 306  | A    | N9-C4-C5    | 7.21  | 108.69      | 105.80   |
| 1   | AA    | 992  | U    | C6-N1-C2    | -7.21 | 116.67      | 121.00   |
| 35  | BB    | 81   | G    | N3-C4-C5    | 7.21  | 132.21      | 128.60   |
| 35  | BB    | 1044 | C    | N1-C2-O2    | -7.21 | 114.57      | 118.90   |
| 35  | BB    | 1248 | G    | C5'-C4'-O4' | 7.21  | 117.76      | 109.10   |
| 1   | AA    | 446  | G    | C6-N1-C2    | 7.21  | 129.43      | 125.10   |
| 1   | AA    | 750  | C    | O4'-C4'-C3' | -7.21 | 96.79       | 104.00   |
| 35  | BB    | 351  | C    | C6-N1-C2    | -7.21 | 117.42      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 563  | A    | O4'-C1'-N9  | 7.21  | 113.97      | 108.20   |
| 35  | BB    | 1064 | C    | C5-C4-N4    | -7.21 | 115.15      | 120.20   |
| 35  | BB    | 2035 | G    | N1-C2-N3    | -7.21 | 119.57      | 123.90   |
| 1   | AA    | 280  | C    | C1'-O4'-C4' | 7.21  | 115.67      | 109.90   |
| 1   | AA    | 475  | C    | O4'-C1'-N1  | 7.21  | 113.97      | 108.20   |
| 1   | AA    | 1201 | A    | C4-C5-N7    | -7.21 | 107.09      | 110.70   |
| 1   | AA    | 1427 | C    | O4'-C1'-N1  | 7.21  | 113.97      | 108.20   |
| 35  | BB    | 340  | A    | N9-C4-C5    | -7.21 | 102.92      | 105.80   |
| 35  | BB    | 407  | G    | P-O3'-C3'   | -7.21 | 111.05      | 119.70   |
| 35  | BB    | 1029 | A    | C4-C5-C6    | 7.21  | 120.61      | 117.00   |
| 35  | BB    | 1201 | U    | O4'-C1'-N1  | 7.21  | 113.97      | 108.20   |
| 35  | BB    | 1309 | G    | N9-C4-C5    | 7.21  | 108.28      | 105.40   |
| 35  | BB    | 1381 | G    | O4'-C1'-N9  | 7.21  | 113.97      | 108.20   |
| 35  | BB    | 1710 | G    | N1-C6-O6    | 7.21  | 124.23      | 119.90   |
| 35  | BB    | 2714 | G    | N3-C4-C5    | -7.21 | 125.00      | 128.60   |
| 1   | AA    | 998  | C    | O4'-C1'-N1  | 7.21  | 113.97      | 108.20   |
| 1   | AA    | 1125 | U    | C5'-C4'-O4' | 7.21  | 117.75      | 109.10   |
| 35  | BB    | 53   | A    | O4'-C1'-N9  | 7.21  | 113.97      | 108.20   |
| 35  | BB    | 527  | C    | O4'-C1'-N1  | 7.21  | 113.97      | 108.20   |
| 35  | BB    | 2046 | G    | O4'-C1'-N9  | 7.21  | 113.97      | 108.20   |
| 1   | AA    | 521  | G    | O4'-C1'-N9  | 7.21  | 113.97      | 108.20   |
| 1   | AA    | 771  | G    | C5-C6-N1    | 7.21  | 115.10      | 111.50   |
| 28  | B3    | 48   | TYR  | CG-CD1-CE1  | -7.21 | 115.53      | 121.30   |
| 35  | BB    | 7    | G    | O4'-C1'-N9  | 7.21  | 113.97      | 108.20   |
| 35  | BB    | 2633 | G    | O4'-C1'-N9  | 7.21  | 113.97      | 108.20   |
| 1   | AA    | 449  | G    | N7-C8-N9    | 7.21  | 116.70      | 113.10   |
| 1   | AA    | 1140 | C    | C6-N1-C2    | -7.21 | 117.42      | 120.30   |
| 16  | AP    | 56   | ARG  | NE-CZ-NH2   | -7.21 | 116.70      | 120.30   |
| 35  | BB    | 67   | U    | C5-C4-O4    | -7.21 | 121.58      | 125.90   |
| 35  | BB    | 104  | A    | N1-C6-N6    | 7.21  | 122.92      | 118.60   |
| 35  | BB    | 706  | A    | O4'-C1'-N9  | 7.21  | 113.97      | 108.20   |
| 35  | BB    | 1726 | C    | O4'-C1'-N1  | 7.21  | 113.97      | 108.20   |
| 35  | BB    | 1913 | A    | C5-C6-N1    | -7.21 | 114.10      | 117.70   |
| 35  | BB    | 2225 | A    | N9-C4-C5    | 7.21  | 108.68      | 105.80   |
| 35  | BB    | 2892 | G    | O4'-C1'-N9  | 7.21  | 113.97      | 108.20   |
| 35  | BB    | 345  | A    | N3-C4-C5    | -7.21 | 121.76      | 126.80   |
| 35  | BB    | 1656 | C    | C4-C5-C6    | -7.21 | 113.80      | 117.40   |
| 30  | B5    | 43   | ASP  | CB-CG-OD2   | -7.20 | 111.82      | 118.30   |
| 34  | BA    | 27   | C    | C5-C6-N1    | 7.20  | 124.60      | 121.00   |
| 34  | BA    | 29   | A    | C4-C5-C6    | 7.20  | 120.60      | 117.00   |
| 35  | BB    | 989  | G    | N3-C4-N9    | -7.20 | 121.68      | 126.00   |
| 35  | BB    | 2087 | G    | C5-C6-O6    | -7.20 | 124.28      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2208 | C    | P-O3'-C3'   | -7.20 | 111.06      | 119.70   |
| 1   | AA    | 1222 | G    | N1-C6-O6    | 7.20  | 124.22      | 119.90   |
| 35  | BB    | 2254 | C    | N3-C4-C5    | -7.20 | 119.02      | 121.90   |
| 35  | BB    | 2330 | G    | C5-C6-N1    | -7.20 | 107.90      | 111.50   |
| 1   | AA    | 526  | C    | C6-N1-C2    | -7.20 | 117.42      | 120.30   |
| 1   | AA    | 1164 | G    | N3-C4-N9    | 7.20  | 130.32      | 126.00   |
| 13  | AM    | 86   | ARG  | NE-CZ-NH1   | 7.20  | 123.90      | 120.30   |
| 35  | BB    | 327  | G    | C5-C6-N1    | -7.20 | 107.90      | 111.50   |
| 35  | BB    | 643  | A    | O4'-C1'-N9  | 7.20  | 113.96      | 108.20   |
| 35  | BB    | 1266 | G    | C4-C5-C6    | 7.20  | 123.12      | 118.80   |
| 35  | BB    | 1661 | G    | N1-C2-N3    | -7.20 | 119.58      | 123.90   |
| 1   | AA    | 567  | G    | C6-C5-N7    | -7.20 | 126.08      | 130.40   |
| 35  | BB    | 211  | C    | C6-N1-C2    | -7.20 | 117.42      | 120.30   |
| 35  | BB    | 522  | A    | C4-C5-N7    | -7.20 | 107.10      | 110.70   |
| 35  | BB    | 914  | G    | C6-C5-N7    | -7.20 | 126.08      | 130.40   |
| 35  | BB    | 1983 | G    | C4'-C3'-C2' | -7.20 | 95.40       | 102.60   |
| 35  | BB    | 2448 | A    | O4'-C1'-N9  | 7.20  | 113.96      | 108.20   |
| 1   | AA    | 432  | A    | N1-C2-N3    | 7.20  | 132.90      | 129.30   |
| 35  | BB    | 37   | C    | C6-N1-C2    | -7.20 | 117.42      | 120.30   |
| 35  | BB    | 163  | C    | C2-N1-C1'   | 7.20  | 126.72      | 118.80   |
| 35  | BB    | 759  | G    | C5-C6-N1    | -7.20 | 107.90      | 111.50   |
| 1   | AA    | 1198 | G    | N3-C4-N9    | 7.20  | 130.32      | 126.00   |
| 19  | AS    | 33   | TRP  | CE2-CD2-CG  | -7.20 | 101.54      | 107.30   |
| 35  | BB    | 48   | G    | N3-C2-N2    | 7.20  | 124.94      | 119.90   |
| 35  | BB    | 539  | G    | C4-C5-N7    | 7.20  | 113.68      | 110.80   |
| 35  | BB    | 1565 | C    | C5-C6-N1    | 7.20  | 124.60      | 121.00   |
| 35  | BB    | 2248 | C    | N3-C4-C5    | -7.20 | 119.02      | 121.90   |
| 35  | BB    | 2306 | C    | C6-N1-C2    | -7.20 | 117.42      | 120.30   |
| 35  | BB    | 2755 | C    | N3-C4-C5    | 7.20  | 124.78      | 121.90   |
| 1   | AA    | 357  | G    | N7-C8-N9    | -7.19 | 109.50      | 113.10   |
| 35  | BB    | 699  | A    | C1'-O4'-C4' | 7.19  | 115.66      | 109.90   |
| 35  | BB    | 756  | A    | N9-C4-C5    | 7.19  | 108.68      | 105.80   |
| 35  | BB    | 2435 | A    | C6-C5-N7    | -7.19 | 127.26      | 132.30   |
| 35  | BB    | 2484 | G    | C4'-C3'-C2' | -7.19 | 95.41       | 102.60   |
| 1   | AA    | 69   | G    | C4-C5-N7    | 7.19  | 113.68      | 110.80   |
| 1   | AA    | 630  | A    | P-O3'-C3'   | 7.19  | 128.33      | 119.70   |
| 1   | AA    | 874  | G    | C6-C5-N7    | -7.19 | 126.08      | 130.40   |
| 1   | AA    | 934  | C    | O4'-C1'-N1  | 7.19  | 113.95      | 108.20   |
| 35  | BB    | 590  | A    | C5-C6-N6    | -7.19 | 117.95      | 123.70   |
| 35  | BB    | 1119 | U    | C5-C4-O4    | 7.19  | 130.22      | 125.90   |
| 35  | BB    | 1580 | A    | C4-C5-C6    | 7.19  | 120.60      | 117.00   |
| 35  | BB    | 1615 | C    | C4-C5-C6    | -7.19 | 113.80      | 117.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1799 | G    | C5-N7-C8    | -7.19 | 100.70      | 104.30   |
| 35  | BB    | 2049 | G    | C2-N3-C4    | 7.19  | 115.50      | 111.90   |
| 41  | BH    | 17   | ASP  | CB-CG-OD2   | -7.19 | 111.83      | 118.30   |
| 1   | AA    | 1375 | A    | C5-N7-C8    | 7.19  | 107.50      | 103.90   |
| 6   | AF    | 99   | ALA  | N-CA-CB     | 7.19  | 120.17      | 110.10   |
| 26  | B1    | 29   | ARG  | NE-CZ-NH1   | -7.19 | 116.70      | 120.30   |
| 34  | BA    | 101  | A    | C5-N7-C8    | -7.19 | 100.31      | 103.90   |
| 35  | BB    | 651  | G    | C5-C6-O6    | -7.19 | 124.28      | 128.60   |
| 35  | BB    | 1017 | G    | C2-N3-C4    | 7.19  | 115.50      | 111.90   |
| 35  | BB    | 1940 | U    | C4-C5-C6    | -7.19 | 115.39      | 119.70   |
| 35  | BB    | 2111 | U    | C5-C4-O4    | -7.19 | 121.58      | 125.90   |
| 35  | BB    | 2135 | A    | P-O3'-C3'   | 7.19  | 128.33      | 119.70   |
| 35  | BB    | 2143 | C    | N1-C2-O2    | -7.19 | 114.59      | 118.90   |
| 35  | BB    | 2575 | C    | N3-C4-C5    | -7.19 | 119.02      | 121.90   |
| 35  | BB    | 2621 | G    | C2-N3-C4    | -7.19 | 108.31      | 111.90   |
| 35  | BB    | 2842 | G    | C2-N3-C4    | 7.19  | 115.50      | 111.90   |
| 1   | AA    | 686  | U    | P-O3'-C3'   | 7.19  | 128.33      | 119.70   |
| 1   | AA    | 1324 | A    | C2-N3-C4    | 7.19  | 114.19      | 110.60   |
| 34  | BA    | 86   | G    | C5-C6-O6    | -7.19 | 124.29      | 128.60   |
| 35  | BB    | 298  | G    | N3-C4-C5    | -7.19 | 125.01      | 128.60   |
| 35  | BB    | 604  | G    | C6-N1-C2    | 7.19  | 129.41      | 125.10   |
| 35  | BB    | 820  | A    | C4-C5-C6    | 7.19  | 120.59      | 117.00   |
| 35  | BB    | 971  | G    | O5'-P-OP1   | -7.19 | 99.23       | 105.70   |
| 1   | AA    | 698  | G    | C6-C5-N7    | -7.19 | 126.09      | 130.40   |
| 1   | AA    | 738  | C    | N3-C4-C5    | -7.19 | 119.03      | 121.90   |
| 1   | AA    | 769  | G    | C5-C6-O6    | -7.19 | 124.29      | 128.60   |
| 35  | BB    | 688  | U    | N1-C2-N3    | -7.19 | 110.59      | 114.90   |
| 35  | BB    | 984  | A    | C5-C6-N1    | -7.19 | 114.11      | 117.70   |
| 35  | BB    | 1912 | A    | C6-C5-N7    | -7.19 | 127.27      | 132.30   |
| 35  | BB    | 1954 | G    | C5-C6-O6    | -7.19 | 124.29      | 128.60   |
| 35  | BB    | 1050 | A    | C8-N9-C4    | -7.19 | 102.93      | 105.80   |
| 35  | BB    | 2300 | C    | N3-C2-O2    | 7.19  | 126.93      | 121.90   |
| 1   | AA    | 418  | C    | C6-N1-C1'   | -7.18 | 112.18      | 120.80   |
| 1   | AA    | 687  | A    | N1-C6-N6    | 7.18  | 122.91      | 118.60   |
| 35  | BB    | 1020 | A    | N1-C2-N3    | 7.18  | 132.89      | 129.30   |
| 35  | BB    | 2125 | G    | N7-C8-N9    | -7.18 | 109.51      | 113.10   |
| 35  | BB    | 2882 | A    | C4'-C3'-C2' | -7.18 | 95.42       | 102.60   |
| 1   | AA    | 32   | A    | C4-C5-C6    | 7.18  | 120.59      | 117.00   |
| 1   | AA    | 567  | G    | C5-C6-O6    | -7.18 | 124.29      | 128.60   |
| 1   | AA    | 589  | U    | O4'-C1'-N1  | 7.18  | 113.95      | 108.20   |
| 1   | AA    | 688  | G    | N3-C4-N9    | -7.18 | 121.69      | 126.00   |
| 35  | BB    | 182  | A    | O4'-C1'-N9  | 7.18  | 113.95      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 757  | G    | N1-C6-O6    | 7.18  | 124.21      | 119.90   |
| 35  | BB    | 1074 | G    | C8-N9-C4    | -7.18 | 103.53      | 106.40   |
| 35  | BB    | 1715 | G    | N3-C2-N2    | 7.18  | 124.93      | 119.90   |
| 35  | BB    | 2208 | C    | C2-N3-C4    | 7.18  | 123.49      | 119.90   |
| 35  | BB    | 2364 | C    | C4-C5-C6    | 7.18  | 120.99      | 117.40   |
| 1   | AA    | 55   | A    | N1-C6-N6    | 7.18  | 122.91      | 118.60   |
| 23  | AX    | 16   | C    | C2-N1-C1'   | 7.18  | 126.70      | 118.80   |
| 1   | AA    | 156  | C    | C4-C5-C6    | 7.18  | 120.99      | 117.40   |
| 35  | BB    | 539  | G    | C5-C6-N1    | -7.18 | 107.91      | 111.50   |
| 35  | BB    | 936  | A    | N1-C2-N3    | 7.18  | 132.89      | 129.30   |
| 35  | BB    | 1045 | C    | P-O3'-C3'   | 7.18  | 128.31      | 119.70   |
| 35  | BB    | 1870 | C    | C2-N3-C4    | 7.18  | 123.49      | 119.90   |
| 35  | BB    | 2000 | C    | C6-N1-C2    | -7.18 | 117.43      | 120.30   |
| 41  | BH    | 50   | ARG  | NE-CZ-NH1   | 7.18  | 123.89      | 120.30   |
| 1   | AA    | 592  | G    | C5-C6-O6    | -7.18 | 124.29      | 128.60   |
| 35  | BB    | 49   | A    | C5-C6-N1    | -7.18 | 114.11      | 117.70   |
| 35  | BB    | 880  | G    | N1-C6-O6    | 7.18  | 124.21      | 119.90   |
| 35  | BB    | 1147 | A    | O4'-C1'-N9  | 7.18  | 113.94      | 108.20   |
| 35  | BB    | 1385 | A    | O4'-C1'-N9  | 7.18  | 113.94      | 108.20   |
| 35  | BB    | 2219 | U    | O4'-C1'-N1  | 7.18  | 113.94      | 108.20   |
| 35  | BB    | 2572 | A    | C4-C5-N7    | -7.18 | 107.11      | 110.70   |
| 35  | BB    | 2631 | G    | C5-N7-C8    | -7.18 | 100.71      | 104.30   |
| 1   | AA    | 220  | G    | C6-N1-C2    | -7.17 | 120.80      | 125.10   |
| 1   | AA    | 333  | U    | N3-C2-O2    | -7.17 | 117.18      | 122.20   |
| 1   | AA    | 418  | C    | C5-C4-N4    | -7.17 | 115.18      | 120.20   |
| 1   | AA    | 558  | G    | N1-C2-N3    | -7.17 | 119.59      | 123.90   |
| 1   | AA    | 573  | A    | N9-C4-C5    | 7.17  | 108.67      | 105.80   |
| 8   | AH    | 76   | ARG  | NH1-CZ-NH2  | -7.17 | 111.51      | 119.40   |
| 35  | BB    | 112  | U    | C6-N1-C2    | -7.17 | 116.70      | 121.00   |
| 35  | BB    | 402  | A    | C4-C5-C6    | 7.17  | 120.59      | 117.00   |
| 35  | BB    | 644  | A    | O4'-C1'-N9  | 7.17  | 113.94      | 108.20   |
| 35  | BB    | 1431 | A    | C5-C6-N6    | -7.17 | 117.96      | 123.70   |
| 35  | BB    | 1702 | G    | C4-C5-C6    | 7.17  | 123.11      | 118.80   |
| 35  | BB    | 1906 | G    | N9-C4-C5    | -7.17 | 102.53      | 105.40   |
| 37  | BD    | 13   | ARG  | NE-CZ-NH2   | -7.17 | 116.71      | 120.30   |
| 1   | AA    | 933  | G    | C5-C6-N1    | -7.17 | 107.91      | 111.50   |
| 1   | AA    | 342  | C    | C2-N3-C4    | 7.17  | 123.49      | 119.90   |
| 1   | AA    | 1404 | C    | C6-N1-C1'   | -7.17 | 112.19      | 120.80   |
| 34  | BA    | 60   | C    | C6-N1-C2    | -7.17 | 117.43      | 120.30   |
| 35  | BB    | 140  | C    | C3'-C2'-C1' | -7.17 | 95.76       | 101.50   |
| 35  | BB    | 1068 | G    | N3-C2-N2    | 7.17  | 124.92      | 119.90   |
| 35  | BB    | 2793 | C    | C4-C5-C6    | 7.17  | 120.99      | 117.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 430  | A    | N9-C4-C5    | 7.17  | 108.67      | 105.80   |
| 35  | BB    | 569  | U    | O4'-C1'-N1  | 7.17  | 113.94      | 108.20   |
| 35  | BB    | 829  | A    | C5-C6-N1    | -7.17 | 114.11      | 117.70   |
| 35  | BB    | 950  | G    | C5-C6-O6    | -7.17 | 124.30      | 128.60   |
| 35  | BB    | 1090 | A    | C5-N7-C8    | 7.17  | 107.48      | 103.90   |
| 1   | AA    | 701  | U    | C4'-C3'-C2' | -7.17 | 95.43       | 102.60   |
| 1   | AA    | 978  | A    | C4-C5-C6    | 7.17  | 120.58      | 117.00   |
| 1   | AA    | 1047 | G    | N1-C6-O6    | 7.17  | 124.20      | 119.90   |
| 1   | AA    | 1162 | C    | N3-C4-C5    | -7.17 | 119.03      | 121.90   |
| 1   | AA    | 1322 | C    | C6-N1-C1'   | -7.17 | 112.20      | 120.80   |
| 1   | AA    | 1381 | U    | C1'-O4'-C4' | -7.17 | 104.17      | 109.90   |
| 2   | AB    | 49   | PHE  | CB-CG-CD1   | -7.17 | 115.78      | 120.80   |
| 35  | BB    | 53   | A    | C5-C6-N6    | -7.17 | 117.97      | 123.70   |
| 35  | BB    | 71   | A    | C5-C6-N6    | -7.17 | 117.97      | 123.70   |
| 35  | BB    | 1246 | A    | C8-N9-C4    | -7.17 | 102.93      | 105.80   |
| 35  | BB    | 1419 | A    | C8-N9-C4    | -7.17 | 102.93      | 105.80   |
| 35  | BB    | 2093 | G    | N3-C4-N9    | -7.17 | 121.70      | 126.00   |
| 36  | BC    | 62   | ARG  | NE-CZ-NH1   | 7.17  | 123.89      | 120.30   |
| 1   | AA    | 188  | C    | C5-C6-N1    | 7.17  | 124.58      | 121.00   |
| 1   | AA    | 435  | A    | N9-C4-C5    | 7.17  | 108.67      | 105.80   |
| 1   | AA    | 577  | G    | C8-N9-C4    | 7.17  | 109.27      | 106.40   |
| 35  | BB    | 602  | A    | C2-N3-C4    | -7.17 | 107.02      | 110.60   |
| 35  | BB    | 2502 | G    | O4'-C1'-N9  | 7.17  | 113.93      | 108.20   |
| 1   | AA    | 1227 | A    | N9-C4-C5    | -7.17 | 102.93      | 105.80   |
| 35  | BB    | 228  | C    | O4'-C4'-C3' | -7.17 | 96.83       | 104.00   |
| 35  | BB    | 1599 | U    | C5-C4-O4    | 7.17  | 130.20      | 125.90   |
| 35  | BB    | 2398 | U    | C5-C4-O4    | -7.17 | 121.60      | 125.90   |
| 1   | AA    | 16   | A    | N3-C4-C5    | -7.16 | 121.79      | 126.80   |
| 1   | AA    | 569  | C    | C4-C5-C6    | -7.16 | 113.82      | 117.40   |
| 1   | AA    | 694  | A    | C4-C5-C6    | 7.16  | 120.58      | 117.00   |
| 34  | BA    | 37   | C    | N3-C4-C5    | -7.16 | 119.03      | 121.90   |
| 35  | BB    | 585  | G    | N1-C6-O6    | 7.16  | 124.20      | 119.90   |
| 35  | BB    | 1036 | G    | N1-C2-N3    | -7.16 | 119.60      | 123.90   |
| 35  | BB    | 1245 | G    | C8-N9-C4    | -7.16 | 103.53      | 106.40   |
| 35  | BB    | 1333 | G    | N7-C8-N9    | -7.16 | 109.52      | 113.10   |
| 35  | BB    | 2088 | A    | C5-N7-C8    | 7.16  | 107.48      | 103.90   |
| 35  | BB    | 2115 | G    | C4'-C3'-C2' | -7.16 | 95.44       | 102.60   |
| 35  | BB    | 2157 | G    | N1-C6-O6    | 7.16  | 124.20      | 119.90   |
| 35  | BB    | 2193 | G    | C4-C5-C6    | 7.16  | 123.10      | 118.80   |
| 35  | BB    | 2228 | G    | C2-N3-C4    | 7.16  | 115.48      | 111.90   |
| 35  | BB    | 2693 | G    | C4-C5-C6    | 7.16  | 123.10      | 118.80   |
| 1   | AA    | 301  | G    | O4'-C1'-N9  | 7.16  | 113.93      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 482  | A    | N1-C2-N3    | 7.16  | 132.88      | 129.30   |
| 35  | BB    | 608  | A    | C2-N3-C4    | -7.16 | 107.02      | 110.60   |
| 35  | BB    | 712  | G    | O4'-C1'-N9  | 7.16  | 113.93      | 108.20   |
| 35  | BB    | 1011 | G    | O4'-C1'-N9  | 7.16  | 113.93      | 108.20   |
| 35  | BB    | 1676 | A    | C5-C6-N6    | -7.16 | 117.97      | 123.70   |
| 35  | BB    | 1760 | C    | O4'-C1'-N1  | 7.16  | 113.93      | 108.20   |
| 1   | AA    | 981  | U    | O4'-C1'-N1  | 7.16  | 113.93      | 108.20   |
| 1   | AA    | 1036 | A    | C6-C5-N7    | -7.16 | 127.29      | 132.30   |
| 1   | AA    | 1302 | C    | N3-C4-N4    | 7.16  | 123.01      | 118.00   |
| 35  | BB    | 15   | G    | C6-C5-N7    | -7.16 | 126.10      | 130.40   |
| 35  | BB    | 1897 | G    | N1-C2-N2    | -7.16 | 109.76      | 116.20   |
| 35  | BB    | 2048 | G    | C2-N3-C4    | 7.16  | 115.48      | 111.90   |
| 35  | BB    | 2847 | U    | OP1-P-OP2   | -7.16 | 108.86      | 119.60   |
| 1   | AA    | 75   | G    | C6-C5-N7    | -7.16 | 126.11      | 130.40   |
| 1   | AA    | 135  | C    | O4'-C1'-N1  | 7.16  | 113.92      | 108.20   |
| 1   | AA    | 349  | A    | C6-N1-C2    | -7.16 | 114.31      | 118.60   |
| 1   | AA    | 1395 | C    | C1'-O4'-C4' | 7.16  | 115.62      | 109.90   |
| 14  | AN    | 98   | ALA  | N-CA-CB     | 7.16  | 120.12      | 110.10   |
| 34  | BA    | 101  | A    | O4'-C1'-N9  | 7.16  | 113.92      | 108.20   |
| 35  | BB    | 470  | A    | C5-C6-N1    | 7.16  | 121.28      | 117.70   |
| 35  | BB    | 686  | U    | O4'-C1'-C2' | -7.16 | 98.64       | 105.80   |
| 35  | BB    | 1824 | G    | N1-C6-O6    | 7.16  | 124.19      | 119.90   |
| 35  | BB    | 1826 | G    | N1-C2-N2    | -7.16 | 109.76      | 116.20   |
| 35  | BB    | 2801 | G    | O4'-C4'-C3' | -7.16 | 96.84       | 104.00   |
| 53  | BT    | 60   | THR  | CA-CB-CG2   | -7.16 | 102.38      | 112.40   |
| 1   | AA    | 153  | C    | C2-N3-C4    | 7.15  | 123.48      | 119.90   |
| 35  | BB    | 1642 | G    | O4'-C1'-N9  | 7.15  | 113.92      | 108.20   |
| 1   | AA    | 22   | G    | C6-N1-C2    | 7.15  | 129.39      | 125.10   |
| 1   | AA    | 647  | C    | P-O5'-C5'   | -7.15 | 109.46      | 120.90   |
| 1   | AA    | 1106 | G    | C1'-O4'-C4' | -7.15 | 104.18      | 109.90   |
| 35  | BB    | 569  | U    | P-O3'-C3'   | -7.15 | 111.12      | 119.70   |
| 35  | BB    | 936  | A    | N9-C4-C5    | 7.15  | 108.66      | 105.80   |
| 35  | BB    | 1271 | G    | O5'-P-OP1   | 7.15  | 119.28      | 110.70   |
| 35  | BB    | 1979 | U    | C5-C4-O4    | -7.15 | 121.61      | 125.90   |
| 35  | BB    | 2903 | U    | C5'-C4'-O4' | 7.15  | 117.68      | 109.10   |
| 1   | AA    | 222  | C    | C2-N3-C4    | 7.15  | 123.48      | 119.90   |
| 1   | AA    | 360  | G    | C4-C5-C6    | 7.15  | 123.09      | 118.80   |
| 1   | AA    | 920  | U    | O4'-C1'-N1  | 7.15  | 113.92      | 108.20   |
| 1   | AA    | 1153 | G    | C5-N7-C8    | -7.15 | 100.72      | 104.30   |
| 35  | BB    | 1874 | C    | C5-C6-N1    | 7.15  | 124.58      | 121.00   |
| 35  | BB    | 2781 | A    | O4'-C1'-N9  | 7.15  | 113.92      | 108.20   |
| 1   | AA    | 861  | G    | C4-C5-C6    | 7.15  | 123.09      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 955  | U    | P-O3'-C3'  | -7.15 | 111.12      | 119.70   |
| 34  | BA    | 43   | C    | P-O5'-C5'  | -7.15 | 109.46      | 120.90   |
| 35  | BB    | 1266 | G    | N1-C6-O6   | 7.15  | 124.19      | 119.90   |
| 35  | BB    | 2193 | G    | O4'-C1'-N9 | 7.15  | 113.92      | 108.20   |
| 35  | BB    | 2475 | C    | N3-C4-N4   | 7.15  | 123.00      | 118.00   |
| 1   | AA    | 1455 | G    | C6-C5-N7   | -7.15 | 126.11      | 130.40   |
| 32  | B7    | 21   | PHE  | CB-CG-CD1  | -7.15 | 115.80      | 120.80   |
| 35  | BB    | 1207 | C    | N3-C2-O2   | -7.15 | 116.90      | 121.90   |
| 35  | BB    | 2256 | G    | O4'-C1'-N9 | 7.15  | 113.92      | 108.20   |
| 35  | BB    | 2773 | C    | N1-C2-O2   | -7.15 | 114.61      | 118.90   |
| 41  | BH    | 68   | ARG  | NE-CZ-NH2  | -7.15 | 116.73      | 120.30   |
| 53  | BT    | 73   | ARG  | NE-CZ-NH2  | -7.15 | 116.73      | 120.30   |
| 1   | AA    | 722  | G    | O5'-P-OP1  | -7.15 | 99.27       | 105.70   |
| 35  | BB    | 796  | C    | O4'-C1'-N1 | 7.15  | 113.92      | 108.20   |
| 35  | BB    | 1469 | A    | N1-C6-N6   | 7.15  | 122.89      | 118.60   |
| 1   | AA    | 486  | U    | P-O3'-C3'  | -7.14 | 111.13      | 119.70   |
| 1   | AA    | 730  | G    | N1-C2-N3   | -7.14 | 119.61      | 123.90   |
| 1   | AA    | 1166 | G    | C5-C6-N1   | -7.14 | 107.93      | 111.50   |
| 1   | AA    | 1404 | C    | O4'-C1'-N1 | 7.14  | 113.92      | 108.20   |
| 35  | BB    | 646  | U    | C5-C6-N1   | 7.14  | 126.27      | 122.70   |
| 35  | BB    | 985  | C    | C6-N1-C2   | -7.14 | 117.44      | 120.30   |
| 35  | BB    | 1573 | G    | C6-N1-C2   | 7.14  | 129.39      | 125.10   |
| 35  | BB    | 1842 | G    | N9-C4-C5   | 7.14  | 108.26      | 105.40   |
| 35  | BB    | 1890 | A    | N1-C6-N6   | 7.14  | 122.89      | 118.60   |
| 35  | BB    | 2497 | A    | C4-C5-C6   | 7.14  | 120.57      | 117.00   |
| 1   | AA    | 420  | U    | P-O3'-C3'  | 7.14  | 128.27      | 119.70   |
| 1   | AA    | 687  | A    | C5-C6-N6   | -7.14 | 117.99      | 123.70   |
| 1   | AA    | 849  | G    | C6-N1-C2   | 7.14  | 129.38      | 125.10   |
| 35  | BB    | 331  | C    | O4'-C1'-N1 | 7.14  | 113.91      | 108.20   |
| 35  | BB    | 438  | G    | N3-C4-C5   | -7.14 | 125.03      | 128.60   |
| 35  | BB    | 1090 | A    | C4-C5-N7   | -7.14 | 107.13      | 110.70   |
| 1   | AA    | 567  | G    | N7-C8-N9   | 7.14  | 116.67      | 113.10   |
| 35  | BB    | 2564 | A    | N7-C8-N9   | 7.14  | 117.37      | 113.80   |
| 1   | AA    | 404  | G    | C5-C6-N1   | -7.14 | 107.93      | 111.50   |
| 1   | AA    | 801  | U    | N3-C4-O4   | -7.14 | 114.40      | 119.40   |
| 1   | AA    | 905  | U    | C5-C4-O4   | -7.14 | 121.62      | 125.90   |
| 35  | BB    | 117  | G    | C6-C5-N7   | -7.14 | 126.12      | 130.40   |
| 35  | BB    | 739  | A    | N7-C8-N9   | 7.14  | 117.37      | 113.80   |
| 35  | BB    | 777  | G    | N1-C6-O6   | 7.14  | 124.18      | 119.90   |
| 35  | BB    | 1378 | A    | C5-C6-N1   | -7.14 | 114.13      | 117.70   |
| 35  | BB    | 1638 | C    | O4'-C1'-N1 | 7.14  | 113.91      | 108.20   |
| 1   | AA    | 275  | G    | P-O5'-C5'  | 7.14  | 132.32      | 120.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1016 | A    | C4-C5-C6    | 7.14  | 120.57      | 117.00   |
| 1   | AA    | 1145 | A    | N9-C4-C5    | 7.14  | 108.66      | 105.80   |
| 35  | BB    | 1294 | U    | N3-C4-C5    | 7.14  | 118.88      | 114.60   |
| 35  | BB    | 1570 | A    | C8-N9-C4    | 7.14  | 108.66      | 105.80   |
| 1   | AA    | 767  | A    | C5-C6-N6    | -7.14 | 117.99      | 123.70   |
| 1   | AA    | 1047 | G    | C8-N9-C4    | -7.14 | 103.55      | 106.40   |
| 35  | BB    | 1036 | G    | C2-N3-C4    | 7.14  | 115.47      | 111.90   |
| 35  | BB    | 1596 | A    | C4-C5-C6    | 7.14  | 120.57      | 117.00   |
| 35  | BB    | 1674 | G    | C4-C5-N7    | -7.14 | 107.95      | 110.80   |
| 35  | BB    | 2350 | C    | O4'-C1'-N1  | 7.14  | 113.91      | 108.20   |
| 1   | AA    | 245  | U    | P-O5'-C5'   | -7.13 | 109.48      | 120.90   |
| 1   | AA    | 395  | C    | O4'-C1'-N1  | 7.13  | 113.91      | 108.20   |
| 1   | AA    | 1429 | A    | C8-N9-C4    | -7.13 | 102.95      | 105.80   |
| 34  | BA    | 72   | G    | N3-C4-N9    | 7.13  | 130.28      | 126.00   |
| 35  | BB    | 25   | U    | C6-N1-C2    | -7.13 | 116.72      | 121.00   |
| 35  | BB    | 243  | U    | P-O5'-C5'   | 7.13  | 132.32      | 120.90   |
| 35  | BB    | 561  | G    | O4'-C1'-N9  | 7.13  | 113.91      | 108.20   |
| 35  | BB    | 925  | A    | C3'-C2'-C1' | -7.13 | 95.79       | 101.50   |
| 35  | BB    | 2179 | C    | C5'-C4'-O4' | 7.13  | 117.66      | 109.10   |
| 35  | BB    | 2508 | G    | C8-N9-C4    | -7.13 | 103.55      | 106.40   |
| 1   | AA    | 445  | G    | C4-C5-C6    | 7.13  | 123.08      | 118.80   |
| 1   | AA    | 1497 | G    | N3-C2-N2    | 7.13  | 124.89      | 119.90   |
| 35  | BB    | 1498 | C    | N3-C4-C5    | -7.13 | 119.05      | 121.90   |
| 35  | BB    | 2353 | G    | O4'-C4'-C3' | -7.13 | 96.87       | 104.00   |
| 1   | AA    | 675  | A    | C4-C5-N7    | -7.13 | 107.14      | 110.70   |
| 35  | BB    | 311  | A    | C4-C5-C6    | 7.13  | 120.57      | 117.00   |
| 35  | BB    | 532  | A    | P-O3'-C3'   | 7.13  | 128.26      | 119.70   |
| 35  | BB    | 1515 | A    | C4-C5-N7    | -7.13 | 107.14      | 110.70   |
| 35  | BB    | 1759 | A    | C1'-O4'-C4' | -7.13 | 104.19      | 109.90   |
| 35  | BB    | 2227 | A    | C5-N7-C8    | 7.13  | 107.47      | 103.90   |
| 35  | BB    | 2300 | C    | C2-N3-C4    | 7.13  | 123.47      | 119.90   |
| 35  | BB    | 2674 | G    | N3-C4-N9    | 7.13  | 130.28      | 126.00   |
| 1   | AA    | 784  | A    | C5-C6-N6    | -7.13 | 118.00      | 123.70   |
| 34  | BA    | 101  | A    | C4-C5-N7    | 7.13  | 114.27      | 110.70   |
| 35  | BB    | 479  | A    | C8-N9-C4    | 7.13  | 108.65      | 105.80   |
| 35  | BB    | 870  | U    | C6-N1-C2    | 7.13  | 125.28      | 121.00   |
| 35  | BB    | 1561 | C    | O4'-C4'-C3' | -7.13 | 96.87       | 104.00   |
| 35  | BB    | 1972 | G    | C4-C5-C6    | 7.13  | 123.08      | 118.80   |
| 35  | BB    | 2277 | G    | C8-N9-C4    | 7.13  | 109.25      | 106.40   |
| 46  | BM    | 55   | ARG  | NE-CZ-NH2   | 7.13  | 123.86      | 120.30   |
| 1   | AA    | 172  | A    | C2-N3-C4    | 7.13  | 114.17      | 110.60   |
| 35  | BB    | 3    | U    | N3-C4-O4    | 7.13  | 124.39      | 119.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 745  | G    | N3-C2-N2    | 7.13  | 124.89      | 119.90   |
| 35  | BB    | 989  | G    | C4-C5-N7    | -7.13 | 107.95      | 110.80   |
| 35  | BB    | 1016 | G    | C4-C5-C6    | 7.13  | 123.08      | 118.80   |
| 35  | BB    | 1491 | G    | C6-C5-N7    | -7.13 | 126.12      | 130.40   |
| 35  | BB    | 1593 | A    | C4-C5-N7    | -7.13 | 107.14      | 110.70   |
| 35  | BB    | 1984 | G    | N3-C4-C5    | 7.13  | 132.16      | 128.60   |
| 35  | BB    | 2042 | A    | C8-N9-C4    | 7.13  | 108.65      | 105.80   |
| 35  | BB    | 2121 | G    | N3-C2-N2    | 7.13  | 124.89      | 119.90   |
| 1   | AA    | 177  | G    | P-O5'-C5'   | 7.13  | 132.30      | 120.90   |
| 1   | AA    | 682  | G    | C4'-C3'-C2' | -7.13 | 95.47       | 102.60   |
| 35  | BB    | 350  | G    | C5-C6-N1    | -7.13 | 107.94      | 111.50   |
| 35  | BB    | 980  | A    | N1-C2-N3    | 7.13  | 132.86      | 129.30   |
| 35  | BB    | 1422 | G    | N1-C2-N3    | -7.13 | 119.62      | 123.90   |
| 35  | BB    | 1881 | C    | N3-C4-N4    | 7.13  | 122.99      | 118.00   |
| 35  | BB    | 1894 | C    | C5-C4-N4    | -7.13 | 115.21      | 120.20   |
| 35  | BB    | 2778 | A    | C6-C5-N7    | -7.13 | 127.31      | 132.30   |
| 34  | BA    | 46   | A    | C8-N9-C4    | 7.12  | 108.65      | 105.80   |
| 35  | BB    | 1298 | C    | O4'-C1'-N1  | 7.12  | 113.90      | 108.20   |
| 1   | AA    | 565  | U    | N3-C2-O2    | 7.12  | 127.19      | 122.20   |
| 34  | BA    | 38   | C    | C5-C4-N4    | -7.12 | 115.21      | 120.20   |
| 34  | BA    | 95   | U    | O4'-C1'-N1  | 7.12  | 113.90      | 108.20   |
| 35  | BB    | 438  | G    | C5-C6-O6    | -7.12 | 124.33      | 128.60   |
| 35  | BB    | 1169 | A    | C5-N7-C8    | 7.12  | 107.46      | 103.90   |
| 35  | BB    | 2324 | U    | P-O3'-C3'   | 7.12  | 128.25      | 119.70   |
| 1   | AA    | 79   | G    | N9-C4-C5    | 7.12  | 108.25      | 105.40   |
| 1   | AA    | 203  | G    | C3'-C2'-C1' | -7.12 | 95.80       | 101.50   |
| 1   | AA    | 929  | G    | O4'-C1'-N9  | 7.12  | 113.90      | 108.20   |
| 35  | BB    | 117  | G    | N9-C4-C5    | -7.12 | 102.55      | 105.40   |
| 35  | BB    | 233  | A    | C2-N3-C4    | -7.12 | 107.04      | 110.60   |
| 35  | BB    | 261  | G    | C5-N7-C8    | -7.12 | 100.74      | 104.30   |
| 35  | BB    | 430  | A    | C5-C6-N6    | -7.12 | 118.00      | 123.70   |
| 35  | BB    | 1238 | G    | O4'-C4'-C3' | -7.12 | 96.88       | 104.00   |
| 35  | BB    | 1291 | C    | P-O3'-C3'   | -7.12 | 111.15      | 119.70   |
| 35  | BB    | 2147 | A    | C5-C6-N6    | -7.12 | 118.00      | 123.70   |
| 35  | BB    | 2284 | A    | N1-C2-N3    | 7.12  | 132.86      | 129.30   |
| 1   | AA    | 392  | C    | C5-C6-N1    | -7.12 | 117.44      | 121.00   |
| 1   | AA    | 768  | A    | C5-N7-C8    | 7.12  | 107.46      | 103.90   |
| 1   | AA    | 1229 | A    | N1-C6-N6    | 7.12  | 122.87      | 118.60   |
| 1   | AA    | 1455 | G    | C5-C6-N1    | -7.12 | 107.94      | 111.50   |
| 34  | BA    | 43   | C    | C5-C4-N4    | -7.12 | 115.22      | 120.20   |
| 35  | BB    | 1267 | U    | C6-N1-C2    | -7.12 | 116.73      | 121.00   |
| 35  | BB    | 1516 | G    | C4-C5-N7    | 7.12  | 113.65      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1694 | C    | C4-C5-C6    | 7.12  | 120.96      | 117.40   |
| 1   | AA    | 52   | C    | N3-C4-N4    | 7.12  | 122.98      | 118.00   |
| 1   | AA    | 100  | G    | C6-N1-C2    | 7.12  | 129.37      | 125.10   |
| 1   | AA    | 527  | G    | C6-C5-N7    | -7.12 | 126.13      | 130.40   |
| 1   | AA    | 666  | G    | C5-C6-N1    | -7.12 | 107.94      | 111.50   |
| 1   | AA    | 866  | C    | N3-C4-N4    | 7.12  | 122.98      | 118.00   |
| 35  | BB    | 106  | C    | C5-C4-N4    | -7.12 | 115.22      | 120.20   |
| 35  | BB    | 580  | U    | C5-C6-N1    | 7.12  | 126.26      | 122.70   |
| 35  | BB    | 690  | G    | C5-C6-O6    | -7.12 | 124.33      | 128.60   |
| 35  | BB    | 1029 | A    | C5-C6-N6    | -7.12 | 118.01      | 123.70   |
| 35  | BB    | 1173 | U    | C3'-C2'-C1' | 7.12  | 107.19      | 101.50   |
| 35  | BB    | 1492 | G    | C5-C6-O6    | -7.12 | 124.33      | 128.60   |
| 35  | BB    | 1877 | A    | C4-C5-C6    | 7.12  | 120.56      | 117.00   |
| 1   | AA    | 1465 | A    | C2-N3-C4    | -7.12 | 107.04      | 110.60   |
| 34  | BA    | 82   | U    | C5-C6-N1    | 7.12  | 126.26      | 122.70   |
| 35  | BB    | 439  | A    | C8-N9-C4    | -7.12 | 102.95      | 105.80   |
| 43  | BJ    | 89   | PHE  | CB-CG-CD2   | 7.12  | 125.78      | 120.80   |
| 45  | BL    | 136  | GLU  | N-CA-CB     | 7.12  | 123.41      | 110.60   |
| 1   | AA    | 1031 | C    | P-O3'-C3'   | 7.11  | 128.24      | 119.70   |
| 27  | B2    | 9    | THR  | CA-CB-CG2   | -7.11 | 102.44      | 112.40   |
| 35  | BB    | 938  | G    | N3-C4-C5    | 7.11  | 132.16      | 128.60   |
| 35  | BB    | 1162 | G    | C5-C6-O6    | -7.11 | 124.33      | 128.60   |
| 35  | BB    | 1410 | G    | C4-C5-N7    | -7.11 | 107.95      | 110.80   |
| 35  | BB    | 1756 | G    | C5-C6-O6    | -7.11 | 124.33      | 128.60   |
| 35  | BB    | 1807 | G    | O4'-C1'-N9  | 7.11  | 113.89      | 108.20   |
| 35  | BB    | 2059 | A    | C5-C6-N1    | -7.11 | 114.14      | 117.70   |
| 35  | BB    | 2810 | A    | C8-N9-C4    | -7.11 | 102.95      | 105.80   |
| 35  | BB    | 1167 | C    | C6-N1-C2    | -7.11 | 117.45      | 120.30   |
| 35  | BB    | 2250 | G    | C6-C5-N7    | -7.11 | 126.13      | 130.40   |
| 35  | BB    | 2269 | G    | C5-C6-N1    | -7.11 | 107.94      | 111.50   |
| 1   | AA    | 882  | C    | N3-C4-C5    | -7.11 | 119.06      | 121.90   |
| 1   | AA    | 1236 | A    | C2-N3-C4    | -7.11 | 107.05      | 110.60   |
| 1   | AA    | 1428 | A    | C2-N3-C4    | -7.11 | 107.05      | 110.60   |
| 22  | AV    | 37   | G    | C4-C5-C6    | 7.11  | 123.07      | 118.80   |
| 35  | BB    | 159  | G    | C4-C5-N7    | -7.11 | 107.96      | 110.80   |
| 35  | BB    | 283  | G    | OP1-P-OP2   | -7.11 | 108.93      | 119.60   |
| 35  | BB    | 973  | A    | C5-C6-N1    | -7.11 | 114.14      | 117.70   |
| 35  | BB    | 975  | A    | C8-N9-C4    | -7.11 | 102.96      | 105.80   |
| 35  | BB    | 1702 | G    | N7-C8-N9    | 7.11  | 116.66      | 113.10   |
| 1   | AA    | 80   | A    | P-O3'-C3'   | 7.11  | 128.23      | 119.70   |
| 1   | AA    | 834  | U    | N1-C2-N3    | 7.11  | 119.17      | 114.90   |
| 34  | BA    | 9    | G    | C5'-C4'-O4' | 7.11  | 117.63      | 109.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | BA    | 60   | C    | C2-N1-C1'   | 7.11  | 126.62      | 118.80   |
| 35  | BB    | 779  | U    | C5-C6-N1    | 7.11  | 126.25      | 122.70   |
| 1   | AA    | 412  | A    | N1-C6-N6    | 7.11  | 122.86      | 118.60   |
| 1   | AA    | 678  | U    | O4'-C1'-N1  | 7.11  | 113.89      | 108.20   |
| 9   | AI    | 19   | PHE  | CB-CG-CD2   | 7.11  | 125.78      | 120.80   |
| 34  | BA    | 18   | G    | C6-C5-N7    | -7.11 | 126.14      | 130.40   |
| 35  | BB    | 576  | U    | O4'-C1'-N1  | 7.11  | 113.89      | 108.20   |
| 35  | BB    | 1699 | G    | N7-C8-N9    | 7.11  | 116.65      | 113.10   |
| 35  | BB    | 2621 | G    | N3-C4-C5    | 7.11  | 132.15      | 128.60   |
| 1   | AA    | 1071 | C    | N3-C4-C5    | -7.11 | 119.06      | 121.90   |
| 1   | AA    | 1308 | U    | O4'-C4'-C3' | -7.11 | 96.89       | 104.00   |
| 35  | BB    | 91   | A    | C5-C6-N1    | -7.11 | 114.15      | 117.70   |
| 35  | BB    | 285  | G    | O4'-C1'-N9  | 7.11  | 113.88      | 108.20   |
| 35  | BB    | 819  | A    | N1-C2-N3    | 7.11  | 132.85      | 129.30   |
| 35  | BB    | 1538 | G    | C6-C5-N7    | -7.11 | 126.14      | 130.40   |
| 35  | BB    | 1888 | G    | N7-C8-N9    | -7.11 | 109.55      | 113.10   |
| 35  | BB    | 2552 | U    | O4'-C1'-N1  | 7.11  | 113.89      | 108.20   |
| 1   | AA    | 280  | C    | O4'-C1'-N1  | 7.10  | 113.88      | 108.20   |
| 1   | AA    | 744  | C    | C2-N3-C4    | 7.10  | 123.45      | 119.90   |
| 4   | AD    | 103  | ARG  | NE-CZ-NH1   | 7.10  | 123.85      | 120.30   |
| 35  | BB    | 16   | C    | N3-C4-C5    | -7.10 | 119.06      | 121.90   |
| 35  | BB    | 1057 | A    | N1-C6-N6    | 7.10  | 122.86      | 118.60   |
| 35  | BB    | 1473 | G    | C4-C5-N7    | -7.10 | 107.96      | 110.80   |
| 1   | AA    | 640  | A    | C8-N9-C4    | -7.10 | 102.96      | 105.80   |
| 1   | AA    | 1162 | C    | P-O3'-C3'   | -7.10 | 111.18      | 119.70   |
| 1   | AA    | 1351 | U    | C5-C4-O4    | 7.10  | 130.16      | 125.90   |
| 35  | BB    | 2689 | U    | C5-C4-O4    | 7.10  | 130.16      | 125.90   |
| 35  | BB    | 2854 | G    | C5-C6-O6    | -7.10 | 124.34      | 128.60   |
| 22  | AV    | 15   | G    | C5-C6-O6    | -7.10 | 124.34      | 128.60   |
| 22  | AV    | 63   | U    | O4'-C1'-N1  | 7.10  | 113.88      | 108.20   |
| 35  | BB    | 220  | G    | C6-C5-N7    | -7.10 | 126.14      | 130.40   |
| 35  | BB    | 1099 | G    | C5-C6-N1    | 7.10  | 115.05      | 111.50   |
| 35  | BB    | 1103 | A    | O4'-C1'-N9  | 7.10  | 113.88      | 108.20   |
| 35  | BB    | 1811 | G    | C5-C6-O6    | -7.10 | 124.34      | 128.60   |
| 35  | BB    | 2103 | C    | C6-N1-C2    | 7.10  | 123.14      | 120.30   |
| 35  | BB    | 2291 | U    | N3-C4-C5    | -7.10 | 110.34      | 114.60   |
| 1   | AA    | 879  | C    | C5-C4-N4    | -7.10 | 115.23      | 120.20   |
| 35  | BB    | 288  | U    | N3-C4-O4    | 7.10  | 124.37      | 119.40   |
| 35  | BB    | 605  | G    | N1-C6-O6    | 7.10  | 124.16      | 119.90   |
| 35  | BB    | 979  | A    | C5-C6-N1    | -7.10 | 114.15      | 117.70   |
| 35  | BB    | 1328 | A    | C1'-O4'-C4' | 7.10  | 115.58      | 109.90   |
| 35  | BB    | 1691 | C    | N3-C4-N4    | 7.10  | 122.97      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1710 | G    | C5-N7-C8    | 7.10  | 107.85      | 104.30   |
| 35  | BB    | 195  | A    | C5-C6-N6    | -7.10 | 118.02      | 123.70   |
| 35  | BB    | 886  | A    | C5-N7-C8    | 7.10  | 107.45      | 103.90   |
| 35  | BB    | 1030 | C    | N3-C4-N4    | 7.10  | 122.97      | 118.00   |
| 35  | BB    | 1058 | U    | C5'-C4'-C3' | -7.10 | 104.65      | 116.00   |
| 35  | BB    | 1947 | C    | O4'-C1'-N1  | 7.10  | 113.88      | 108.20   |
| 1   | AA    | 491  | G    | C5-C6-O6    | -7.09 | 124.34      | 128.60   |
| 1   | AA    | 1022 | A    | N7-C8-N9    | 7.09  | 117.35      | 113.80   |
| 1   | AA    | 1072 | G    | C6-N1-C2    | 7.09  | 129.36      | 125.10   |
| 35  | BB    | 86   | G    | N1-C6-O6    | 7.09  | 124.16      | 119.90   |
| 35  | BB    | 364  | C    | N3-C2-O2    | -7.09 | 116.93      | 121.90   |
| 35  | BB    | 874  | G    | O4'-C1'-N9  | 7.09  | 113.88      | 108.20   |
| 35  | BB    | 1983 | G    | N1-C6-O6    | 7.09  | 124.16      | 119.90   |
| 35  | BB    | 2515 | C    | N3-C4-N4    | 7.09  | 122.97      | 118.00   |
| 35  | BB    | 2898 | U    | N1-C1'-C2'  | -7.09 | 104.19      | 112.00   |
| 1   | AA    | 614  | C    | N3-C4-C5    | -7.09 | 119.06      | 121.90   |
| 35  | BB    | 903  | C    | C4'-C3'-C2' | -7.09 | 95.51       | 102.60   |
| 35  | BB    | 1234 | U    | N3-C4-O4    | 7.09  | 124.36      | 119.40   |
| 1   | AA    | 249  | U    | N1-C2-N3    | -7.09 | 110.64      | 114.90   |
| 1   | AA    | 280  | C    | C6-N1-C2    | 7.09  | 123.14      | 120.30   |
| 1   | AA    | 359  | G    | N9-C4-C5    | -7.09 | 102.56      | 105.40   |
| 1   | AA    | 411  | A    | C8-N9-C4    | 7.09  | 108.64      | 105.80   |
| 1   | AA    | 430  | A    | N1-C6-N6    | 7.09  | 122.85      | 118.60   |
| 1   | AA    | 1370 | G    | O4'-C4'-C3' | -7.09 | 96.91       | 104.00   |
| 1   | AA    | 1413 | A    | C6-N1-C2    | -7.09 | 114.34      | 118.60   |
| 34  | BA    | 13   | G    | N3-C4-C5    | -7.09 | 125.05      | 128.60   |
| 34  | BA    | 57   | A    | N1-C2-N3    | 7.09  | 132.85      | 129.30   |
| 35  | BB    | 231  | A    | N7-C8-N9    | -7.09 | 110.25      | 113.80   |
| 35  | BB    | 1103 | A    | C4-C5-C6    | 7.09  | 120.55      | 117.00   |
| 35  | BB    | 2145 | C    | C4-C5-C6    | -7.09 | 113.85      | 117.40   |
| 1   | AA    | 462  | G    | N1-C2-N3    | -7.09 | 119.65      | 123.90   |
| 1   | AA    | 819  | A    | C5-C6-N6    | -7.09 | 118.03      | 123.70   |
| 34  | BA    | 18   | G    | C5-C6-N1    | -7.09 | 107.95      | 111.50   |
| 35  | BB    | 524  | G    | C6-C5-N7    | -7.09 | 126.15      | 130.40   |
| 35  | BB    | 602  | A    | N7-C8-N9    | -7.09 | 110.25      | 113.80   |
| 35  | BB    | 1303 | G    | C4-C5-N7    | -7.09 | 107.97      | 110.80   |
| 39  | BF    | 91   | ARG  | NE-CZ-NH1   | 7.09  | 123.84      | 120.30   |
| 35  | BB    | 1157 | G    | N1-C6-O6    | 7.09  | 124.15      | 119.90   |
| 1   | AA    | 275  | G    | N3-C4-N9    | 7.09  | 130.25      | 126.00   |
| 1   | AA    | 1502 | A    | C5-N7-C8    | 7.09  | 107.44      | 103.90   |
| 35  | BB    | 125  | A    | O4'-C1'-N9  | 7.09  | 113.87      | 108.20   |
| 35  | BB    | 487  | C    | C5-C4-N4    | -7.09 | 115.24      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 492  | A    | N3-C4-C5    | -7.09 | 121.84      | 126.80   |
| 35  | BB    | 907  | G    | C5-C6-N1    | -7.09 | 107.96      | 111.50   |
| 35  | BB    | 1080 | A    | C8-N9-C4    | -7.09 | 102.97      | 105.80   |
| 35  | BB    | 492  | A    | N1-C2-N3    | 7.08  | 132.84      | 129.30   |
| 35  | BB    | 1256 | G    | C4-C5-C6    | 7.08  | 123.05      | 118.80   |
| 1   | AA    | 893  | C    | C6-N1-C2    | 7.08  | 123.13      | 120.30   |
| 1   | AA    | 1031 | C    | C5-C4-N4    | -7.08 | 115.24      | 120.20   |
| 1   | AA    | 1163 | A    | N7-C8-N9    | 7.08  | 117.34      | 113.80   |
| 1   | AA    | 1249 | C    | O4'-C1'-N1  | 7.08  | 113.87      | 108.20   |
| 1   | AA    | 1258 | G    | C5-C6-O6    | -7.08 | 124.35      | 128.60   |
| 2   | AB    | 70   | GLY  | N-CA-C      | -7.08 | 95.39       | 113.10   |
| 35  | BB    | 488  | G    | C6-N1-C2    | 7.08  | 129.35      | 125.10   |
| 35  | BB    | 1140 | C    | N3-C4-N4    | 7.08  | 122.96      | 118.00   |
| 35  | BB    | 2156 | G    | N7-C8-N9    | -7.08 | 109.56      | 113.10   |
| 35  | BB    | 2610 | C    | N3-C2-O2    | 7.08  | 126.86      | 121.90   |
| 1   | AA    | 1447 | A    | C5-N7-C8    | 7.08  | 107.44      | 103.90   |
| 34  | BA    | 73   | A    | N9-C4-C5    | 7.08  | 108.63      | 105.80   |
| 35  | BB    | 346  | A    | C4'-C3'-C2' | -7.08 | 95.52       | 102.60   |
| 35  | BB    | 681  | G    | C4-C5-N7    | -7.08 | 107.97      | 110.80   |
| 35  | BB    | 946  | C    | N3-C4-N4    | 7.08  | 122.96      | 118.00   |
| 35  | BB    | 1435 | G    | C4-C5-N7    | -7.08 | 107.97      | 110.80   |
| 35  | BB    | 1719 | G    | C6-C5-N7    | -7.08 | 126.15      | 130.40   |
| 35  | BB    | 1999 | C    | N1-C2-O2    | 7.08  | 123.15      | 118.90   |
| 35  | BB    | 2053 | G    | N9-C4-C5    | -7.08 | 102.57      | 105.40   |
| 35  | BB    | 2532 | G    | C5-C6-O6    | -7.08 | 124.35      | 128.60   |
| 35  | BB    | 2718 | G    | C5-C6-O6    | -7.08 | 124.35      | 128.60   |
| 1   | AA    | 756  | C    | N3-C4-C5    | -7.08 | 119.07      | 121.90   |
| 34  | BA    | 34   | A    | C8-N9-C4    | -7.08 | 102.97      | 105.80   |
| 35  | BB    | 8    | C    | O4'-C1'-N1  | 7.08  | 113.86      | 108.20   |
| 35  | BB    | 2700 | A    | C5-C6-N1    | -7.08 | 114.16      | 117.70   |
| 1   | AA    | 336  | A    | C6-N1-C2    | 7.08  | 122.85      | 118.60   |
| 1   | AA    | 846  | G    | N3-C2-N2    | 7.08  | 124.86      | 119.90   |
| 1   | AA    | 889  | A    | C5-N7-C8    | 7.08  | 107.44      | 103.90   |
| 35  | BB    | 128  | C    | C6-N1-C2    | -7.08 | 117.47      | 120.30   |
| 35  | BB    | 295  | G    | C6-C5-N7    | -7.08 | 126.15      | 130.40   |
| 35  | BB    | 1350 | C    | N3-C4-N4    | 7.08  | 122.95      | 118.00   |
| 35  | BB    | 1753 | G    | N3-C4-N9    | -7.08 | 121.75      | 126.00   |
| 35  | BB    | 1864 | U    | P-O5'-C5'   | -7.08 | 109.58      | 120.90   |
| 35  | BB    | 2088 | A    | C4'-C3'-C2' | -7.08 | 95.52       | 102.60   |
| 44  | BK    | 112  | PHE  | CB-CG-CD1   | -7.08 | 115.84      | 120.80   |
| 1   | AA    | 201  | G    | C2-N3-C4    | 7.08  | 115.44      | 111.90   |
| 1   | AA    | 451  | A    | C5-C6-N1    | -7.08 | 114.16      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 977  | A    | C5'-C4'-O4' | 7.08  | 117.59      | 109.10   |
| 35  | BB    | 145  | C    | O4'-C1'-N1  | 7.08  | 113.86      | 108.20   |
| 35  | BB    | 807  | U    | N3-C4-C5    | -7.08 | 110.35      | 114.60   |
| 35  | BB    | 1554 | U    | O4'-C1'-N1  | 7.08  | 113.86      | 108.20   |
| 35  | BB    | 2446 | G    | N3-C4-C5    | 7.08  | 132.14      | 128.60   |
| 1   | AA    | 618  | C    | O4'-C1'-N1  | 7.08  | 113.86      | 108.20   |
| 1   | AA    | 1504 | G    | O4'-C1'-N9  | 7.08  | 113.86      | 108.20   |
| 35  | BB    | 200  | U    | N3-C4-C5    | -7.08 | 110.36      | 114.60   |
| 35  | BB    | 364  | C    | P-O5'-C5'   | -7.08 | 109.58      | 120.90   |
| 35  | BB    | 521  | U    | N3-C4-C5    | -7.08 | 110.35      | 114.60   |
| 35  | BB    | 1705 | A    | N7-C8-N9    | -7.08 | 110.26      | 113.80   |
| 35  | BB    | 2104 | C    | C1'-O4'-C4' | -7.08 | 104.24      | 109.90   |
| 35  | BB    | 2126 | A    | N9-C4-C5    | 7.08  | 108.63      | 105.80   |
| 35  | BB    | 2412 | A    | C4-C5-N7    | -7.08 | 107.16      | 110.70   |
| 35  | BB    | 2767 | C    | N1-C2-O2    | -7.08 | 114.66      | 118.90   |
| 35  | BB    | 2882 | A    | N9-C4-C5    | 7.08  | 108.63      | 105.80   |
| 47  | BN    | 90   | ARG  | NE-CZ-NH2   | -7.08 | 116.76      | 120.30   |
| 1   | AA    | 1415 | G    | C4-C5-N7    | -7.07 | 107.97      | 110.80   |
| 1   | AA    | 1436 | U    | C6-N1-C2    | -7.07 | 116.76      | 121.00   |
| 35  | BB    | 699  | A    | N3-C4-N9    | 7.07  | 133.06      | 127.40   |
| 35  | BB    | 1229 | C    | N3-C4-N4    | 7.07  | 122.95      | 118.00   |
| 35  | BB    | 1857 | G    | N3-C4-N9    | 7.07  | 130.24      | 126.00   |
| 35  | BB    | 2575 | C    | O4'-C1'-N1  | 7.07  | 113.86      | 108.20   |
| 35  | BB    | 46   | G    | C2-N3-C4    | 7.07  | 115.44      | 111.90   |
| 35  | BB    | 533  | G    | C5-C6-N1    | -7.07 | 107.96      | 111.50   |
| 35  | BB    | 2376 | A    | C8-N9-C4    | -7.07 | 102.97      | 105.80   |
| 35  | BB    | 2490 | G    | O4'-C1'-N9  | 7.07  | 113.86      | 108.20   |
| 35  | BB    | 2814 | A    | C4-C5-C6    | 7.07  | 120.54      | 117.00   |
| 1   | AA    | 602  | A    | N1-C6-N6    | 7.07  | 122.84      | 118.60   |
| 1   | AA    | 711  | G    | N9-C4-C5    | -7.07 | 102.57      | 105.40   |
| 1   | AA    | 1319 | A    | O4'-C1'-N9  | 7.07  | 113.86      | 108.20   |
| 22  | AV    | 37   | G    | N1-C2-N3    | -7.07 | 119.66      | 123.90   |
| 34  | BA    | 47   | C    | N1-C2-O2    | 7.07  | 123.14      | 118.90   |
| 35  | BB    | 477  | A    | C6-N1-C2    | 7.07  | 122.84      | 118.60   |
| 35  | BB    | 800  | A    | C6-C5-N7    | -7.07 | 127.35      | 132.30   |
| 35  | BB    | 1687 | G    | O4'-C1'-N9  | 7.07  | 113.86      | 108.20   |
| 1   | AA    | 25   | C    | C5-C6-N1    | 7.07  | 124.53      | 121.00   |
| 1   | AA    | 282  | A    | N9-C4-C5    | -7.07 | 102.97      | 105.80   |
| 35  | BB    | 530  | G    | O5'-P-OP2   | -7.07 | 99.34       | 105.70   |
| 35  | BB    | 1253 | A    | C4-C5-C6    | 7.07  | 120.53      | 117.00   |
| 35  | BB    | 2762 | C    | C2-N3-C4    | 7.07  | 123.44      | 119.90   |
| 35  | BB    | 2864 | G    | N1-C2-N2    | -7.07 | 109.84      | 116.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 879  | C    | C6-N1-C2    | -7.07 | 117.47      | 120.30   |
| 35  | BB    | 943  | A    | N1-C2-N3    | 7.07  | 132.83      | 129.30   |
| 35  | BB    | 967  | U    | C5-C4-O4    | -7.07 | 121.66      | 125.90   |
| 35  | BB    | 1045 | C    | N3-C4-C5    | -7.07 | 119.07      | 121.90   |
| 35  | BB    | 1643 | G    | N7-C8-N9    | 7.07  | 116.63      | 113.10   |
| 35  | BB    | 2842 | G    | N1-C2-N3    | -7.07 | 119.66      | 123.90   |
| 1   | AA    | 275  | G    | N9-C4-C5    | -7.07 | 102.57      | 105.40   |
| 1   | AA    | 550  | G    | C8-N9-C4    | -7.07 | 103.57      | 106.40   |
| 1   | AA    | 789  | U    | O4'-C1'-N1  | 7.07  | 113.85      | 108.20   |
| 1   | AA    | 1154 | G    | C8-N9-C4    | -7.07 | 103.57      | 106.40   |
| 1   | AA    | 1220 | G    | N3-C4-N9    | 7.07  | 130.24      | 126.00   |
| 1   | AA    | 1365 | G    | O4'-C1'-N9  | 7.07  | 113.85      | 108.20   |
| 19  | AS    | 60   | PHE  | CB-CG-CD1   | 7.07  | 125.75      | 120.80   |
| 35  | BB    | 40   | U    | N3-C2-O2    | -7.07 | 117.25      | 122.20   |
| 35  | BB    | 108  | G    | O4'-C1'-N9  | 7.07  | 113.85      | 108.20   |
| 35  | BB    | 798  | G    | O4'-C1'-N9  | 7.07  | 113.85      | 108.20   |
| 35  | BB    | 1246 | A    | C5-N7-C8    | 7.07  | 107.43      | 103.90   |
| 35  | BB    | 1300 | G    | C4-C5-C6    | 7.07  | 123.04      | 118.80   |
| 35  | BB    | 1538 | G    | N3-C2-N2    | 7.07  | 124.85      | 119.90   |
| 35  | BB    | 2402 | U    | N1-C2-N3    | -7.07 | 110.66      | 114.90   |
| 35  | BB    | 2556 | C    | N3-C4-C5    | -7.07 | 119.07      | 121.90   |
| 1   | AA    | 1043 | G    | O4'-C4'-C3' | -7.06 | 96.94       | 104.00   |
| 1   | AA    | 1224 | U    | C2-N3-C4    | -7.06 | 122.76      | 127.00   |
| 35  | BB    | 1222 | U    | C5-C4-O4    | -7.06 | 121.66      | 125.90   |
| 35  | BB    | 1567 | G    | C4'-C3'-C2' | 7.06  | 109.66      | 102.60   |
| 35  | BB    | 1577 | C    | N3-C4-C5    | -7.06 | 119.08      | 121.90   |
| 35  | BB    | 1663 | G    | O4'-C1'-N9  | 7.06  | 113.85      | 108.20   |
| 35  | BB    | 2647 | U    | N3-C2-O2    | -7.06 | 117.25      | 122.20   |
| 1   | AA    | 597  | G    | C6-C5-N7    | -7.06 | 126.16      | 130.40   |
| 1   | AA    | 717  | U    | C5-C4-O4    | 7.06  | 130.14      | 125.90   |
| 1   | AA    | 1190 | G    | N1-C2-N3    | -7.06 | 119.66      | 123.90   |
| 35  | BB    | 323  | C    | N1-C2-O2    | 7.06  | 123.14      | 118.90   |
| 35  | BB    | 1002 | G    | C5-C6-O6    | -7.06 | 124.36      | 128.60   |
| 35  | BB    | 1041 | G    | N1-C6-O6    | 7.06  | 124.14      | 119.90   |
| 35  | BB    | 1884 | G    | C2-N3-C4    | 7.06  | 115.43      | 111.90   |
| 35  | BB    | 2734 | A    | C4-C5-C6    | 7.06  | 120.53      | 117.00   |
| 1   | AA    | 437  | U    | C5-C6-N1    | 7.06  | 126.23      | 122.70   |
| 1   | AA    | 47   | C    | C6-N1-C2    | -7.06 | 117.48      | 120.30   |
| 1   | AA    | 782  | A    | C5-C6-N6    | -7.06 | 118.05      | 123.70   |
| 30  | B5    | 144  | THR  | N-CA-CB     | 7.06  | 123.71      | 110.30   |
| 35  | BB    | 367  | G    | C8-N9-C4    | -7.06 | 103.58      | 106.40   |
| 35  | BB    | 519  | U    | N3-C4-O4    | 7.06  | 124.34      | 119.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 837  | C    | N3-C4-N4    | 7.06  | 122.94      | 118.00   |
| 35  | BB    | 977  | G    | N9-C4-C5    | 7.06  | 108.22      | 105.40   |
| 35  | BB    | 1399 | C    | O4'-C1'-N1  | 7.06  | 113.85      | 108.20   |
| 35  | BB    | 1422 | G    | O4'-C1'-N9  | 7.06  | 113.85      | 108.20   |
| 35  | BB    | 2014 | A    | C6-N1-C2    | 7.06  | 122.83      | 118.60   |
| 35  | BB    | 2572 | A    | C5-C6-N6    | -7.06 | 118.05      | 123.70   |
| 1   | AA    | 899  | C    | O4'-C1'-N1  | 7.06  | 113.85      | 108.20   |
| 1   | AA    | 1119 | C    | N3-C4-C5    | -7.06 | 119.08      | 121.90   |
| 35  | BB    | 432  | A    | N1-C2-N3    | 7.06  | 132.83      | 129.30   |
| 35  | BB    | 1094 | U    | N1-C2-O2    | -7.06 | 117.86      | 122.80   |
| 35  | BB    | 2668 | G    | N9-C4-C5    | 7.06  | 108.22      | 105.40   |
| 1   | AA    | 332  | G    | N9-C4-C5    | -7.06 | 102.58      | 105.40   |
| 1   | AA    | 451  | A    | C5-C6-N6    | -7.06 | 118.06      | 123.70   |
| 1   | AA    | 1359 | C    | C1'-O4'-C4' | -7.06 | 104.25      | 109.90   |
| 1   | AA    | 1468 | A    | C6-C5-N7    | -7.06 | 127.36      | 132.30   |
| 35  | BB    | 306  | U    | C5-C4-O4    | -7.06 | 121.67      | 125.90   |
| 35  | BB    | 1769 | U    | O4'-C1'-N1  | 7.06  | 113.84      | 108.20   |
| 1   | AA    | 587  | G    | N3-C2-N2    | 7.05  | 124.84      | 119.90   |
| 1   | AA    | 1418 | A    | C5-C6-N6    | -7.05 | 118.06      | 123.70   |
| 1   | AA    | 1473 | G    | C5-N7-C8    | -7.05 | 100.77      | 104.30   |
| 35  | BB    | 300  | A    | C5-C6-N1    | -7.05 | 114.17      | 117.70   |
| 35  | BB    | 919  | U    | N3-C2-O2    | 7.05  | 127.14      | 122.20   |
| 35  | BB    | 995  | C    | C5-C6-N1    | 7.05  | 124.53      | 121.00   |
| 35  | BB    | 1002 | G    | C4-C5-N7    | 7.05  | 113.62      | 110.80   |
| 35  | BB    | 1264 | A    | O4'-C1'-N9  | 7.05  | 113.84      | 108.20   |
| 41  | BH    | 51   | ARG  | NE-CZ-NH2   | -7.05 | 116.77      | 120.30   |
| 1   | AA    | 963  | G    | N1-C6-O6    | 7.05  | 124.13      | 119.90   |
| 1   | AA    | 1296 | C    | P-O3'-C3'   | 7.05  | 128.16      | 119.70   |
| 35  | BB    | 682  | G    | C5-N7-C8    | -7.05 | 100.77      | 104.30   |
| 35  | BB    | 1417 | C    | C5-C4-N4    | -7.05 | 115.26      | 120.20   |
| 1   | AA    | 207  | C    | C5-C4-N4    | -7.05 | 115.26      | 120.20   |
| 1   | AA    | 559  | A    | P-O3'-C3'   | 7.05  | 128.16      | 119.70   |
| 1   | AA    | 909  | A    | C5-C6-N1    | -7.05 | 114.17      | 117.70   |
| 8   | AH    | 42   | GLU  | C-N-CA      | 7.05  | 137.11      | 122.30   |
| 39  | BF    | 142  | TYR  | CB-CG-CD2   | -7.05 | 116.77      | 121.00   |
| 1   | AA    | 210  | C    | O4'-C1'-N1  | 7.05  | 113.84      | 108.20   |
| 1   | AA    | 1419 | G    | C5-N7-C8    | 7.05  | 107.83      | 104.30   |
| 35  | BB    | 543  | G    | C4-C5-N7    | -7.05 | 107.98      | 110.80   |
| 35  | BB    | 1865 | U    | N3-C4-O4    | 7.05  | 124.33      | 119.40   |
| 35  | BB    | 2238 | G    | C2-N3-C4    | 7.05  | 115.42      | 111.90   |
| 35  | BB    | 2250 | G    | C6-N1-C2    | 7.05  | 129.33      | 125.10   |
| 35  | BB    | 2316 | G    | N9-C4-C5    | -7.05 | 102.58      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 436  | C    | C5-C4-N4    | -7.05 | 115.27      | 120.20   |
| 1   | AA    | 516  | U    | N1-C2-O2    | -7.05 | 117.87      | 122.80   |
| 1   | AA    | 1518 | A    | N7-C8-N9    | 7.05  | 117.32      | 113.80   |
| 35  | BB    | 30   | G    | O4'-C1'-N9  | 7.05  | 113.84      | 108.20   |
| 35  | BB    | 1919 | A    | C4-C5-C6    | 7.05  | 120.52      | 117.00   |
| 35  | BB    | 2148 | G    | C8-N9-C4    | -7.05 | 103.58      | 106.40   |
| 1   | AA    | 608  | A    | N9-C4-C5    | -7.05 | 102.98      | 105.80   |
| 1   | AA    | 994  | A    | C4-C5-C6    | 7.05  | 120.52      | 117.00   |
| 30  | B5    | 162  | ARG  | NE-CZ-NH2   | -7.05 | 116.78      | 120.30   |
| 35  | BB    | 80   | G    | C4-C5-N7    | -7.05 | 107.98      | 110.80   |
| 35  | BB    | 879  | G    | C8-N9-C4    | -7.05 | 103.58      | 106.40   |
| 35  | BB    | 1973 | G    | C5-C6-N1    | -7.05 | 107.98      | 111.50   |
| 1   | AA    | 118  | U    | N1-C2-O2    | -7.04 | 117.87      | 122.80   |
| 1   | AA    | 246  | A    | C8-N9-C4    | 7.04  | 108.62      | 105.80   |
| 1   | AA    | 549  | C    | N3-C4-C5    | -7.04 | 119.08      | 121.90   |
| 1   | AA    | 1259 | C    | O4'-C1'-N1  | 7.04  | 113.84      | 108.20   |
| 1   | AA    | 1426 | G    | N3-C2-N2    | 7.04  | 124.83      | 119.90   |
| 35  | BB    | 1557 | C    | C5-C4-N4    | -7.04 | 115.27      | 120.20   |
| 1   | AA    | 307  | C    | O4'-C1'-N1  | 7.04  | 113.83      | 108.20   |
| 35  | BB    | 1077 | A    | N3-C4-C5    | -7.04 | 121.87      | 126.80   |
| 35  | BB    | 1140 | C    | C6-N1-C2    | -7.04 | 117.48      | 120.30   |
| 35  | BB    | 1292 | G    | O4'-C1'-N9  | 7.04  | 113.83      | 108.20   |
| 35  | BB    | 2405 | G    | O4'-C1'-N9  | 7.04  | 113.83      | 108.20   |
| 35  | BB    | 2548 | U    | O4'-C1'-N1  | 7.04  | 113.83      | 108.20   |
| 1   | AA    | 510  | A    | C5-C6-N1    | -7.04 | 114.18      | 117.70   |
| 1   | AA    | 1468 | A    | C5-N7-C8    | 7.04  | 107.42      | 103.90   |
| 34  | BA    | 98   | G    | N9-C4-C5    | -7.04 | 102.58      | 105.40   |
| 35  | BB    | 245  | G    | N1-C2-N3    | -7.04 | 119.67      | 123.90   |
| 35  | BB    | 446  | G    | N1-C2-N2    | -7.04 | 109.86      | 116.20   |
| 35  | BB    | 1236 | G    | O4'-C1'-N9  | 7.04  | 113.83      | 108.20   |
| 35  | BB    | 1475 | G    | N3-C2-N2    | 7.04  | 124.83      | 119.90   |
| 35  | BB    | 1938 | A    | C4'-C3'-C2' | 7.04  | 109.64      | 102.60   |
| 35  | BB    | 2136 | G    | N3-C2-N2    | 7.04  | 124.83      | 119.90   |
| 45  | BL    | 12   | SER  | N-CA-CB     | 7.04  | 121.06      | 110.50   |
| 1   | AA    | 974  | A    | N3-C4-C5    | -7.04 | 121.87      | 126.80   |
| 35  | BB    | 21   | A    | C4-C5-N7    | 7.04  | 114.22      | 110.70   |
| 35  | BB    | 697  | G    | N1-C2-N3    | -7.04 | 119.68      | 123.90   |
| 35  | BB    | 1509 | A    | C8-N9-C4    | -7.04 | 102.98      | 105.80   |
| 1   | AA    | 357  | G    | C4-C5-C6    | 7.04  | 123.02      | 118.80   |
| 1   | AA    | 1327 | C    | C6-N1-C2    | -7.04 | 117.48      | 120.30   |
| 1   | AA    | 1359 | C    | C2-N1-C1'   | 7.04  | 126.54      | 118.80   |
| 1   | AA    | 1461 | G    | C6-C5-N7    | -7.04 | 126.18      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | AE    | 67   | ARG  | NE-CZ-NH1   | 7.04  | 123.82      | 120.30   |
| 35  | BB    | 50   | U    | P-O3'-C3'   | 7.04  | 128.15      | 119.70   |
| 35  | BB    | 69   | C    | C4'-C3'-C2' | -7.04 | 95.56       | 102.60   |
| 35  | BB    | 262  | A    | C8-N9-C4    | -7.04 | 102.98      | 105.80   |
| 35  | BB    | 359  | G    | N1-C6-O6    | 7.04  | 124.12      | 119.90   |
| 35  | BB    | 1697 | G    | C5-N7-C8    | -7.04 | 100.78      | 104.30   |
| 35  | BB    | 1880 | U    | C5-C4-O4    | -7.04 | 121.68      | 125.90   |
| 35  | BB    | 2507 | C    | O4'-C1'-N1  | 7.04  | 113.83      | 108.20   |
| 1   | AA    | 139  | A    | C5-C6-N1    | -7.04 | 114.18      | 117.70   |
| 1   | AA    | 1217 | C    | C1'-O4'-C4' | -7.04 | 104.27      | 109.90   |
| 35  | BB    | 402  | A    | N9-C4-C5    | 7.04  | 108.61      | 105.80   |
| 35  | BB    | 597  | G    | C5-C6-O6    | -7.04 | 124.38      | 128.60   |
| 35  | BB    | 1212 | G    | O4'-C1'-N9  | 7.04  | 113.83      | 108.20   |
| 1   | AA    | 122  | G    | C8-N9-C4    | -7.04 | 103.59      | 106.40   |
| 1   | AA    | 1211 | U    | N1-C2-N3    | -7.04 | 110.68      | 114.90   |
| 1   | AA    | 1211 | U    | C6-N1-C2    | 7.04  | 125.22      | 121.00   |
| 35  | BB    | 341  | C    | C5-C6-N1    | 7.04  | 124.52      | 121.00   |
| 35  | BB    | 510  | C    | C2-N1-C1'   | 7.04  | 126.54      | 118.80   |
| 35  | BB    | 1200 | C    | N3-C4-N4    | 7.04  | 122.92      | 118.00   |
| 35  | BB    | 1826 | G    | N1-C6-O6    | 7.04  | 124.12      | 119.90   |
| 35  | BB    | 2750 | A    | C4-C5-N7    | -7.04 | 107.18      | 110.70   |
| 35  | BB    | 2803 | G    | N1-C6-O6    | 7.04  | 124.12      | 119.90   |
| 1   | AA    | 183  | C    | O4'-C1'-N1  | 7.03  | 113.83      | 108.20   |
| 1   | AA    | 1035 | A    | C5-C6-N1    | -7.03 | 114.18      | 117.70   |
| 34  | BA    | 64   | G    | C5-C6-O6    | -7.03 | 124.38      | 128.60   |
| 35  | BB    | 575  | A    | N1-C2-N3    | -7.03 | 125.78      | 129.30   |
| 35  | BB    | 785  | G    | C4-C5-N7    | -7.03 | 107.99      | 110.80   |
| 35  | BB    | 956  | G    | C5-C6-O6    | -7.03 | 124.38      | 128.60   |
| 35  | BB    | 1342 | A    | C5-C6-N1    | -7.03 | 114.18      | 117.70   |
| 35  | BB    | 1343 | G    | C6-C5-N7    | -7.03 | 126.18      | 130.40   |
| 35  | BB    | 1569 | A    | N1-C6-N6    | 7.03  | 122.82      | 118.60   |
| 35  | BB    | 1733 | G    | N7-C8-N9    | 7.03  | 116.62      | 113.10   |
| 35  | BB    | 2893 | A    | N9-C4-C5    | 7.03  | 108.61      | 105.80   |
| 38  | BE    | 102  | ARG  | NE-CZ-NH1   | -7.03 | 116.78      | 120.30   |
| 1   | AA    | 47   | C    | N3-C2-O2    | 7.03  | 126.82      | 121.90   |
| 35  | BB    | 2882 | A    | C2-N3-C4    | -7.03 | 107.08      | 110.60   |
| 1   | AA    | 975  | A    | C4-C5-C6    | 7.03  | 120.52      | 117.00   |
| 1   | AA    | 1144 | G    | C8-N9-C4    | -7.03 | 103.59      | 106.40   |
| 1   | AA    | 1255 | G    | C5-C6-O6    | -7.03 | 124.38      | 128.60   |
| 1   | AA    | 1331 | G    | C5-C6-N1    | -7.03 | 107.98      | 111.50   |
| 35  | BB    | 1201 | U    | C3'-C2'-C1' | -7.03 | 95.88       | 101.50   |
| 35  | BB    | 1841 | U    | O4'-C1'-N1  | 7.03  | 113.82      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2365 | G    | C6-C5-N7    | -7.03 | 126.18      | 130.40   |
| 35  | BB    | 2547 | A    | C4'-C3'-C2' | -7.03 | 95.57       | 102.60   |
| 1   | AA    | 604  | G    | C5-N7-C8    | -7.03 | 100.78      | 104.30   |
| 1   | AA    | 942  | G    | C5-N7-C8    | 7.03  | 107.81      | 104.30   |
| 22  | AV    | 67   | G    | C4-C5-C6    | 7.03  | 123.02      | 118.80   |
| 35  | BB    | 1019 | U    | O4'-C1'-N1  | 7.03  | 113.82      | 108.20   |
| 35  | BB    | 1166 | G    | C4-C5-N7    | -7.03 | 107.99      | 110.80   |
| 1   | AA    | 609  | A    | C5-C6-N6    | -7.03 | 118.08      | 123.70   |
| 35  | BB    | 75   | G    | C6-N1-C2    | 7.03  | 129.32      | 125.10   |
| 35  | BB    | 729  | G    | C4-C5-C6    | 7.03  | 123.02      | 118.80   |
| 35  | BB    | 1227 | G    | O4'-C1'-N9  | 7.03  | 113.82      | 108.20   |
| 35  | BB    | 2833 | U    | C2-N1-C1'   | 7.03  | 126.13      | 117.70   |
| 1   | AA    | 68   | G    | C6-N1-C2    | -7.03 | 120.89      | 125.10   |
| 35  | BB    | 238  | C    | N3-C4-N4    | 7.03  | 122.92      | 118.00   |
| 35  | BB    | 822  | G    | O4'-C1'-N9  | 7.03  | 113.82      | 108.20   |
| 35  | BB    | 1055 | G    | N1-C2-N3    | -7.03 | 119.69      | 123.90   |
| 35  | BB    | 1233 | C    | N3-C2-O2    | 7.03  | 126.82      | 121.90   |
| 35  | BB    | 1397 | U    | O4'-C1'-N1  | 7.03  | 113.82      | 108.20   |
| 35  | BB    | 1856 | U    | C5-C6-N1    | 7.03  | 126.21      | 122.70   |
| 35  | BB    | 1910 | G    | N9-C4-C5    | -7.03 | 102.59      | 105.40   |
| 35  | BB    | 2052 | A    | C5-C6-N6    | -7.03 | 118.08      | 123.70   |
| 35  | BB    | 2512 | C    | O4'-C1'-N1  | 7.03  | 113.82      | 108.20   |
| 1   | AA    | 730  | G    | O4'-C1'-N9  | 7.02  | 113.82      | 108.20   |
| 22  | AV    | 1    | C    | N3-C4-N4    | 7.02  | 122.92      | 118.00   |
| 35  | BB    | 525  | U    | N3-C2-O2    | 7.02  | 127.12      | 122.20   |
| 1   | AA    | 225  | C    | O4'-C1'-N1  | 7.02  | 113.82      | 108.20   |
| 1   | AA    | 484  | G    | C6-N1-C2    | 7.02  | 129.31      | 125.10   |
| 1   | AA    | 826  | C    | C1'-O4'-C4' | 7.02  | 115.52      | 109.90   |
| 1   | AA    | 926  | G    | N3-C4-N9    | -7.02 | 121.79      | 126.00   |
| 1   | AA    | 977  | A    | N3-C4-C5    | -7.02 | 121.88      | 126.80   |
| 1   | AA    | 1306 | A    | N7-C8-N9    | -7.02 | 110.29      | 113.80   |
| 35  | BB    | 101  | A    | O4'-C1'-N9  | 7.02  | 113.82      | 108.20   |
| 35  | BB    | 781  | A    | O4'-C1'-N9  | 7.02  | 113.82      | 108.20   |
| 35  | BB    | 902  | C    | N3-C4-N4    | 7.02  | 122.92      | 118.00   |
| 35  | BB    | 1033 | U    | O4'-C1'-N1  | 7.02  | 113.82      | 108.20   |
| 35  | BB    | 1274 | A    | N7-C8-N9    | -7.02 | 110.29      | 113.80   |
| 1   | AA    | 149  | A    | N1-C6-N6    | 7.02  | 122.81      | 118.60   |
| 1   | AA    | 481  | G    | C2-N3-C4    | 7.02  | 115.41      | 111.90   |
| 35  | BB    | 401  | A    | N3-C4-C5    | -7.02 | 121.89      | 126.80   |
| 35  | BB    | 1152 | C    | N3-C4-N4    | 7.02  | 122.91      | 118.00   |
| 35  | BB    | 2764 | A    | N3-C4-N9    | 7.02  | 133.02      | 127.40   |
| 35  | BB    | 2814 | A    | C6-C5-N7    | -7.02 | 127.39      | 132.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2247 | A    | C5-N7-C8    | 7.02  | 107.41      | 103.90   |
| 35  | BB    | 2482 | A    | C4-C5-N7    | -7.02 | 107.19      | 110.70   |
| 1   | AA    | 1078 | U    | N1-C2-O2    | 7.02  | 127.71      | 122.80   |
| 1   | AA    | 1215 | G    | N7-C8-N9    | 7.02  | 116.61      | 113.10   |
| 35  | BB    | 386  | G    | N1-C6-O6    | 7.02  | 124.11      | 119.90   |
| 35  | BB    | 1888 | G    | C4-C5-N7    | -7.02 | 107.99      | 110.80   |
| 35  | BB    | 2545 | G    | N1-C6-O6    | 7.02  | 124.11      | 119.90   |
| 50  | BQ    | 91   | ARG  | NE-CZ-NH2   | -7.02 | 116.79      | 120.30   |
| 1   | AA    | 788  | U    | C5-C4-O4    | -7.02 | 121.69      | 125.90   |
| 1   | AA    | 842  | U    | C2-N3-C4    | 7.02  | 131.21      | 127.00   |
| 1   | AA    | 1129 | C    | C6-N1-C2    | -7.02 | 117.49      | 120.30   |
| 35  | BB    | 1072 | C    | O4'-C1'-N1  | 7.02  | 113.81      | 108.20   |
| 35  | BB    | 1970 | A    | N9-C4-C5    | 7.02  | 108.61      | 105.80   |
| 1   | AA    | 398  | U    | N3-C4-C5    | -7.01 | 110.39      | 114.60   |
| 1   | AA    | 983  | A    | C5-C6-N6    | -7.01 | 118.09      | 123.70   |
| 35  | BB    | 223  | A    | C5-C6-N1    | -7.01 | 114.19      | 117.70   |
| 35  | BB    | 425  | G    | C5-C6-O6    | -7.01 | 124.39      | 128.60   |
| 35  | BB    | 1553 | A    | C5-C6-N1    | -7.01 | 114.19      | 117.70   |
| 35  | BB    | 1933 | G    | O4'-C1'-N9  | 7.01  | 113.81      | 108.20   |
| 35  | BB    | 2558 | C    | O4'-C1'-N1  | 7.01  | 113.81      | 108.20   |
| 1   | AA    | 177  | G    | C5-C6-O6    | -7.01 | 124.39      | 128.60   |
| 1   | AA    | 513  | C    | C5-C4-N4    | -7.01 | 115.29      | 120.20   |
| 1   | AA    | 1217 | C    | C6-N1-C2    | 7.01  | 123.11      | 120.30   |
| 1   | AA    | 1473 | G    | C6-N1-C2    | -7.01 | 120.89      | 125.10   |
| 35  | BB    | 834  | G    | N1-C6-O6    | 7.01  | 124.11      | 119.90   |
| 35  | BB    | 1699 | G    | C5-C6-O6    | -7.01 | 124.39      | 128.60   |
| 1   | AA    | 1279 | G    | C4-C5-N7    | 7.01  | 113.60      | 110.80   |
| 1   | AA    | 1331 | G    | C6-C5-N7    | -7.01 | 126.19      | 130.40   |
| 29  | B4    | 5    | ARG  | NE-CZ-NH2   | -7.01 | 116.79      | 120.30   |
| 35  | BB    | 826  | U    | N3-C4-C5    | -7.01 | 110.39      | 114.60   |
| 35  | BB    | 1071 | G    | N1-C2-N3    | -7.01 | 119.69      | 123.90   |
| 35  | BB    | 1163 | G    | N1-C2-N3    | -7.01 | 119.69      | 123.90   |
| 35  | BB    | 1874 | C    | P-O5'-C5'   | 7.01  | 132.12      | 120.90   |
| 35  | BB    | 1955 | U    | O4'-C1'-N1  | 7.01  | 113.81      | 108.20   |
| 35  | BB    | 2132 | U    | C3'-C2'-C1' | -7.01 | 95.89       | 101.50   |
| 35  | BB    | 2157 | G    | N9-C4-C5    | -7.01 | 102.59      | 105.40   |
| 35  | BB    | 2270 | A    | C2-N3-C4    | -7.01 | 107.09      | 110.60   |
| 35  | BB    | 2642 | G    | C8-N9-C1'   | 7.01  | 136.11      | 127.00   |
| 54  | BU    | 72   | PHE  | CB-CG-CD2   | -7.01 | 115.89      | 120.80   |
| 1   | AA    | 562  | U    | C5'-C4'-C3' | 7.01  | 127.21      | 116.00   |
| 1   | AA    | 1047 | G    | N3-C2-N2    | 7.01  | 124.81      | 119.90   |
| 1   | AA    | 1206 | G    | N9-C4-C5    | -7.01 | 102.60      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 355  | U    | C5-C6-N1   | 7.01  | 126.20      | 122.70   |
| 35  | BB    | 1115 | G    | O4'-C1'-N9 | 7.01  | 113.81      | 108.20   |
| 35  | BB    | 2738 | A    | C6-C5-N7   | -7.01 | 127.39      | 132.30   |
| 43  | BJ    | 130  | HIS  | CA-CB-CG   | -7.01 | 101.68      | 113.60   |
| 1   | AA    | 507  | C    | O4'-C1'-N1 | 7.01  | 113.81      | 108.20   |
| 1   | AA    | 1143 | G    | N3-C2-N2   | 7.01  | 124.81      | 119.90   |
| 35  | BB    | 288  | U    | N3-C2-O2   | 7.01  | 127.11      | 122.20   |
| 35  | BB    | 379  | G    | C8-N9-C4   | -7.01 | 103.60      | 106.40   |
| 35  | BB    | 1248 | G    | C8-N9-C4   | 7.01  | 109.20      | 106.40   |
| 35  | BB    | 1913 | A    | N1-C2-N3   | 7.01  | 132.80      | 129.30   |
| 1   | AA    | 354  | G    | N1-C2-N3   | -7.01 | 119.70      | 123.90   |
| 35  | BB    | 364  | C    | N1-C2-O2   | 7.01  | 123.10      | 118.90   |
| 35  | BB    | 869  | G    | C5-C6-O6   | -7.01 | 124.40      | 128.60   |
| 35  | BB    | 1131 | G    | C4-C5-C6   | 7.01  | 123.00      | 118.80   |
| 35  | BB    | 1212 | G    | C5-C6-O6   | -7.01 | 124.40      | 128.60   |
| 1   | AA    | 1534 | A    | N1-C6-N6   | 7.00  | 122.80      | 118.60   |
| 1   | AA    | 235  | C    | C5-C6-N1   | 7.00  | 124.50      | 121.00   |
| 1   | AA    | 725  | G    | N1-C2-N3   | -7.00 | 119.70      | 123.90   |
| 1   | AA    | 962  | C    | O4'-C1'-N1 | 7.00  | 113.80      | 108.20   |
| 1   | AA    | 1070 | U    | N1-C2-O2   | -7.00 | 117.90      | 122.80   |
| 34  | BA    | 41   | G    | N9-C4-C5   | 7.00  | 108.20      | 105.40   |
| 35  | BB    | 125  | A    | C5-C6-N1   | -7.00 | 114.20      | 117.70   |
| 35  | BB    | 2792 | A    | C6-C5-N7   | -7.00 | 127.40      | 132.30   |
| 35  | BB    | 2797 | U    | C5-C6-N1   | 7.00  | 126.20      | 122.70   |
| 35  | BB    | 2810 | A    | N1-C6-N6   | 7.00  | 122.80      | 118.60   |
| 36  | BC    | 160  | TYR  | CB-CG-CD1  | -7.00 | 116.80      | 121.00   |
| 1   | AA    | 466  | A    | C5-N7-C8   | 7.00  | 107.40      | 103.90   |
| 35  | BB    | 240  | C    | N3-C4-N4   | 7.00  | 122.90      | 118.00   |
| 35  | BB    | 607  | U    | N1-C2-N3   | 7.00  | 119.10      | 114.90   |
| 35  | BB    | 729  | G    | O4'-C1'-N9 | 7.00  | 113.80      | 108.20   |
| 35  | BB    | 741  | U    | P-O3'-C3'  | -7.00 | 111.30      | 119.70   |
| 35  | BB    | 1846 | G    | N3-C2-N2   | 7.00  | 124.80      | 119.90   |
| 35  | BB    | 2643 | G    | C5-C6-N1   | 7.00  | 115.00      | 111.50   |
| 35  | BB    | 1077 | A    | C6-N1-C2   | 7.00  | 122.80      | 118.60   |
| 35  | BB    | 2541 | A    | N1-C6-N6   | 7.00  | 122.80      | 118.60   |
| 1   | AA    | 1112 | C    | N1-C2-O2   | -7.00 | 114.70      | 118.90   |
| 2   | AB    | 107  | ARG  | NE-CZ-NH2  | 7.00  | 123.80      | 120.30   |
| 35  | BB    | 638  | G    | N9-C4-C5   | 7.00  | 108.20      | 105.40   |
| 35  | BB    | 2312 | U    | N3-C4-C5   | -7.00 | 110.40      | 114.60   |
| 35  | BB    | 2369 | A    | C5-C6-N6   | -7.00 | 118.10      | 123.70   |
| 35  | BB    | 2628 | C    | C2-N3-C4   | 7.00  | 123.40      | 119.90   |
| 35  | BB    | 2756 | U    | C5-C4-O4   | -7.00 | 121.70      | 125.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 38  | BE    | 49   | ARG  | NE-CZ-NH2   | 7.00  | 123.80      | 120.30   |
| 38  | BE    | 69   | ARG  | NE-CZ-NH2   | -7.00 | 116.80      | 120.30   |
| 3   | AC    | 168  | ARG  | NE-CZ-NH1   | 7.00  | 123.80      | 120.30   |
| 23  | AX    | 16   | C    | C6-N1-C1'   | -7.00 | 112.41      | 120.80   |
| 35  | BB    | 88   | G    | C8-N9-C4    | -7.00 | 103.60      | 106.40   |
| 35  | BB    | 180  | G    | C4-C5-C6    | 7.00  | 123.00      | 118.80   |
| 35  | BB    | 194  | G    | N1-C2-N3    | -7.00 | 119.70      | 123.90   |
| 35  | BB    | 1830 | C    | N1-C2-N3    | -7.00 | 114.30      | 119.20   |
| 35  | BB    | 2050 | C    | C4-C5-C6    | 7.00  | 120.90      | 117.40   |
| 35  | BB    | 2247 | A    | C5-C6-N6    | -7.00 | 118.10      | 123.70   |
| 35  | BB    | 1112 | G    | O4'-C4'-C3' | -7.00 | 97.00       | 104.00   |
| 35  | BB    | 1348 | C    | N3-C4-C5    | -7.00 | 119.10      | 121.90   |
| 35  | BB    | 1471 | G    | N3-C4-C5    | -7.00 | 125.10      | 128.60   |
| 35  | BB    | 2539 | C    | C6-N1-C2    | 7.00  | 123.10      | 120.30   |
| 1   | AA    | 720  | C    | N1-C2-N3    | 6.99  | 124.09      | 119.20   |
| 1   | AA    | 1128 | C    | C2-N1-C1'   | 6.99  | 126.49      | 118.80   |
| 35  | BB    | 471  | A    | C2-N3-C4    | -6.99 | 107.10      | 110.60   |
| 35  | BB    | 1070 | A    | C6-C5-N7    | -6.99 | 127.40      | 132.30   |
| 35  | BB    | 1197 | G    | N3-C2-N2    | 6.99  | 124.80      | 119.90   |
| 35  | BB    | 1428 | C    | N1-C2-O2    | 6.99  | 123.10      | 118.90   |
| 1   | AA    | 1008 | U    | C4-C5-C6    | -6.99 | 115.50      | 119.70   |
| 35  | BB    | 447  | A    | N1-C2-N3    | 6.99  | 132.80      | 129.30   |
| 35  | BB    | 1239 | G    | N3-C4-C5    | -6.99 | 125.10      | 128.60   |
| 35  | BB    | 1499 | C    | O4'-C1'-N1  | 6.99  | 113.79      | 108.20   |
| 35  | BB    | 2754 | U    | C5-C4-O4    | -6.99 | 121.70      | 125.90   |
| 1   | AA    | 118  | U    | N3-C2-O2    | 6.99  | 127.09      | 122.20   |
| 1   | AA    | 550  | G    | N7-C8-N9    | 6.99  | 116.59      | 113.10   |
| 1   | AA    | 1002 | G    | C4-C5-C6    | 6.99  | 122.99      | 118.80   |
| 1   | AA    | 1210 | C    | C6-N1-C2    | -6.99 | 117.50      | 120.30   |
| 35  | BB    | 723  | C    | N3-C4-C5    | -6.99 | 119.10      | 121.90   |
| 35  | BB    | 1980 | G    | N3-C4-C5    | -6.99 | 125.11      | 128.60   |
| 35  | BB    | 2097 | A    | C5-C6-N6    | -6.99 | 118.11      | 123.70   |
| 35  | BB    | 2136 | G    | P-O5'-C5'   | 6.99  | 132.09      | 120.90   |
| 35  | BB    | 2345 | G    | C5-C6-O6    | -6.99 | 124.41      | 128.60   |
| 35  | BB    | 2482 | A    | C6-N1-C2    | -6.99 | 114.41      | 118.60   |
| 1   | AA    | 707  | U    | N3-C4-C5    | -6.99 | 110.41      | 114.60   |
| 35  | BB    | 156  | A    | O4'-C1'-N9  | 6.99  | 113.79      | 108.20   |
| 35  | BB    | 1771 | C    | O4'-C1'-C2' | 6.99  | 113.89      | 107.60   |
| 35  | BB    | 2895 | G    | C4-C5-C6    | 6.99  | 122.99      | 118.80   |
| 35  | BB    | 727  | A    | C4-C5-C6    | 6.99  | 120.49      | 117.00   |
| 35  | BB    | 2679 | A    | C4-C5-C6    | 6.99  | 120.49      | 117.00   |
| 1   | AA    | 76   | G    | N7-C8-N9    | -6.99 | 109.61      | 113.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 802  | A    | O4'-C1'-N9  | 6.99  | 113.79      | 108.20   |
| 1   | AA    | 912  | C    | N3-C4-C5    | -6.99 | 119.11      | 121.90   |
| 35  | BB    | 2053 | G    | N3-C4-C5    | 6.99  | 132.09      | 128.60   |
| 1   | AA    | 874  | G    | N9-C4-C5    | 6.98  | 108.19      | 105.40   |
| 1   | AA    | 109  | A    | C4-C5-N7    | 6.98  | 114.19      | 110.70   |
| 1   | AA    | 237  | G    | N3-C2-N2    | 6.98  | 124.79      | 119.90   |
| 1   | AA    | 1143 | G    | C6-C5-N7    | -6.98 | 126.21      | 130.40   |
| 28  | B3    | 43   | THR  | CA-CB-CG2   | -6.98 | 102.62      | 112.40   |
| 35  | BB    | 298  | G    | C8-N9-C4    | 6.98  | 109.19      | 106.40   |
| 35  | BB    | 442  | G    | C4-C5-N7    | -6.98 | 108.01      | 110.80   |
| 35  | BB    | 620  | G    | P-O5'-C5'   | -6.98 | 109.73      | 120.90   |
| 35  | BB    | 1767 | G    | O4'-C1'-N9  | 6.98  | 113.79      | 108.20   |
| 35  | BB    | 2175 | C    | C5'-C4'-O4' | 6.98  | 117.48      | 109.10   |
| 35  | BB    | 2490 | G    | OP2-P-O3'   | 6.98  | 120.56      | 105.20   |
| 35  | BB    | 2759 | G    | C5-C6-N1    | -6.98 | 108.01      | 111.50   |
| 1   | AA    | 703  | G    | C5-C6-O6    | -6.98 | 124.41      | 128.60   |
| 13  | AM    | 112  | ARG  | NE-CZ-NH2   | -6.98 | 116.81      | 120.30   |
| 35  | BB    | 166  | U    | C2-N3-C4    | 6.98  | 131.19      | 127.00   |
| 35  | BB    | 1215 | G    | N9-C4-C5    | 6.98  | 108.19      | 105.40   |
| 35  | BB    | 2477 | U    | C5-C6-N1    | -6.98 | 119.21      | 122.70   |
| 55  | BW    | 17   | SER  | N-CA-CB     | 6.98  | 120.97      | 110.50   |
| 1   | AA    | 450  | G    | N9-C4-C5    | 6.98  | 108.19      | 105.40   |
| 1   | AA    | 642  | A    | C5'-C4'-O4' | 6.98  | 117.47      | 109.10   |
| 1   | AA    | 956  | U    | P-O3'-C3'   | -6.98 | 111.33      | 119.70   |
| 1   | AA    | 1491 | G    | C6-N1-C2    | 6.98  | 129.29      | 125.10   |
| 4   | AD    | 28   | ASP  | CB-CG-OD2   | 6.98  | 124.58      | 118.30   |
| 35  | BB    | 555  | G    | N9-C4-C5    | -6.98 | 102.61      | 105.40   |
| 1   | AA    | 888  | G    | C6-C5-N7    | -6.98 | 126.21      | 130.40   |
| 34  | BA    | 23   | G    | N3-C2-N2    | 6.98  | 124.78      | 119.90   |
| 34  | BA    | 94   | A    | C1'-O4'-C4' | 6.98  | 115.48      | 109.90   |
| 35  | BB    | 329  | G    | C6-N1-C2    | 6.98  | 129.29      | 125.10   |
| 35  | BB    | 960  | A    | N7-C8-N9    | 6.98  | 117.29      | 113.80   |
| 35  | BB    | 1128 | G    | C4'-C3'-C2' | -6.98 | 95.62       | 102.60   |
| 35  | BB    | 1437 | C    | N3-C4-C5    | -6.98 | 119.11      | 121.90   |
| 35  | BB    | 1523 | U    | N3-C2-O2    | -6.98 | 117.31      | 122.20   |
| 35  | BB    | 1751 | U    | P-O3'-C3'   | -6.98 | 111.33      | 119.70   |
| 35  | BB    | 2027 | G    | C4-C5-N7    | 6.98  | 113.59      | 110.80   |
| 35  | BB    | 2077 | A    | C5-C6-N1    | -6.98 | 114.21      | 117.70   |
| 35  | BB    | 2154 | A    | C6-N1-C2    | -6.98 | 114.41      | 118.60   |
| 35  | BB    | 2342 | C    | C4'-C3'-C2' | -6.98 | 95.62       | 102.60   |
| 31  | B6    | 34   | ARG  | NE-CZ-NH1   | 6.98  | 123.79      | 120.30   |
| 35  | BB    | 727  | A    | C6-C5-N7    | -6.98 | 127.42      | 132.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1027 | A    | C6-C5-N7    | -6.98 | 127.42      | 132.30   |
| 35  | BB    | 1435 | G    | N3-C2-N2    | 6.98  | 124.78      | 119.90   |
| 35  | BB    | 2432 | A    | C4-C5-N7    | -6.98 | 107.21      | 110.70   |
| 33  | B8    | 20   | ASP  | CB-CG-OD1   | 6.97  | 124.58      | 118.30   |
| 35  | BB    | 335  | C    | N3-C4-N4    | 6.97  | 122.88      | 118.00   |
| 35  | BB    | 432  | A    | C2-N3-C4    | -6.97 | 107.11      | 110.60   |
| 35  | BB    | 523  | C    | N1-C2-N3    | -6.97 | 114.32      | 119.20   |
| 35  | BB    | 834  | G    | C4-C5-N7    | 6.97  | 113.59      | 110.80   |
| 35  | BB    | 1055 | G    | C5'-C4'-O4' | 6.97  | 117.47      | 109.10   |
| 35  | BB    | 1407 | G    | C8-N9-C4    | -6.97 | 103.61      | 106.40   |
| 35  | BB    | 2040 | G    | C4-C5-N7    | 6.97  | 113.59      | 110.80   |
| 35  | BB    | 2592 | G    | P-O5'-C5'   | 6.97  | 132.06      | 120.90   |
| 35  | BB    | 2701 | U    | N1-C2-N3    | 6.97  | 119.08      | 114.90   |
| 1   | AA    | 706  | A    | C4-C5-C6    | 6.97  | 120.49      | 117.00   |
| 1   | AA    | 1165 | U    | C5-C4-O4    | -6.97 | 121.72      | 125.90   |
| 1   | AA    | 1421 | G    | N1-C2-N3    | -6.97 | 119.72      | 123.90   |
| 3   | AC    | 202  | PHE  | CB-CG-CD1   | 6.97  | 125.68      | 120.80   |
| 35  | BB    | 490  | C    | N3-C4-C5    | -6.97 | 119.11      | 121.90   |
| 35  | BB    | 808  | G    | C8-N9-C4    | -6.97 | 103.61      | 106.40   |
| 35  | BB    | 2148 | G    | O4'-C1'-N9  | 6.97  | 113.78      | 108.20   |
| 35  | BB    | 2454 | G    | C5-C6-N1    | -6.97 | 108.01      | 111.50   |
| 35  | BB    | 2550 | G    | O4'-C1'-N9  | 6.97  | 113.78      | 108.20   |
| 35  | BB    | 2609 | U    | O4'-C1'-N1  | 6.97  | 113.78      | 108.20   |
| 35  | BB    | 2615 | U    | C5-C6-N1    | 6.97  | 126.19      | 122.70   |
| 1   | AA    | 240  | G    | C4'-C3'-C2' | -6.97 | 95.63       | 102.60   |
| 1   | AA    | 382  | A    | C4-C5-N7    | -6.97 | 107.22      | 110.70   |
| 1   | AA    | 864  | A    | C4-C5-N7    | -6.97 | 107.21      | 110.70   |
| 35  | BB    | 353  | C    | O4'-C1'-N1  | 6.97  | 113.78      | 108.20   |
| 35  | BB    | 2425 | A    | N9-C4-C5    | 6.97  | 108.59      | 105.80   |
| 1   | AA    | 675  | A    | O4'-C1'-N9  | 6.97  | 113.78      | 108.20   |
| 1   | AA    | 1411 | C    | O4'-C1'-N1  | 6.97  | 113.78      | 108.20   |
| 34  | BA    | 78   | A    | C4-C5-N7    | -6.97 | 107.22      | 110.70   |
| 35  | BB    | 823  | C    | C2-N3-C4    | -6.97 | 116.42      | 119.90   |
| 35  | BB    | 1556 | C    | C6-N1-C2    | -6.97 | 117.51      | 120.30   |
| 35  | BB    | 1753 | G    | N9-C4-C5    | 6.97  | 108.19      | 105.40   |
| 35  | BB    | 2269 | G    | C2-N3-C4    | -6.97 | 108.42      | 111.90   |
| 35  | BB    | 2767 | C    | C5-C4-N4    | -6.97 | 115.32      | 120.20   |
| 1   | AA    | 256  | U    | O4'-C1'-N1  | 6.97  | 113.78      | 108.20   |
| 22  | AV    | 67   | G    | C6-C5-N7    | -6.97 | 126.22      | 130.40   |
| 35  | BB    | 692  | C    | N3-C4-N4    | 6.97  | 122.88      | 118.00   |
| 35  | BB    | 761  | A    | N1-C6-N6    | 6.97  | 122.78      | 118.60   |
| 35  | BB    | 1964 | G    | P-O3'-C3'   | 6.97  | 128.06      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 515  | G    | C5-C6-O6    | -6.97 | 124.42      | 128.60   |
| 1   | AA    | 739  | C    | O4'-C1'-N1  | 6.97  | 113.77      | 108.20   |
| 1   | AA    | 947  | G    | C8-N9-C4    | -6.97 | 103.61      | 106.40   |
| 35  | BB    | 876  | C    | C5-C4-N4    | -6.97 | 115.32      | 120.20   |
| 35  | BB    | 1297 | C    | N1-C2-O2    | -6.97 | 114.72      | 118.90   |
| 35  | BB    | 1552 | A    | C8-N9-C4    | 6.97  | 108.59      | 105.80   |
| 35  | BB    | 1983 | G    | N1-C2-N3    | -6.97 | 119.72      | 123.90   |
| 35  | BB    | 2029 | G    | C5-C6-N1    | 6.97  | 114.98      | 111.50   |
| 35  | BB    | 2094 | A    | N3-C4-C5    | -6.97 | 121.92      | 126.80   |
| 35  | BB    | 2247 | A    | N1-C2-N3    | 6.97  | 132.78      | 129.30   |
| 35  | BB    | 2475 | C    | C2-N3-C4    | 6.97  | 123.38      | 119.90   |
| 35  | BB    | 2747 | G    | N1-C2-N3    | -6.97 | 119.72      | 123.90   |
| 35  | BB    | 2770 | G    | N1-C2-N2    | -6.97 | 109.93      | 116.20   |
| 1   | AA    | 1205 | U    | C5-C4-O4    | -6.96 | 121.72      | 125.90   |
| 1   | AA    | 1258 | G    | N3-C2-N2    | 6.96  | 124.78      | 119.90   |
| 35  | BB    | 39   | G    | C2-N3-C4    | 6.96  | 115.38      | 111.90   |
| 35  | BB    | 695  | G    | N9-C4-C5    | 6.96  | 108.19      | 105.40   |
| 35  | BB    | 1599 | U    | O4'-C1'-N1  | 6.96  | 113.77      | 108.20   |
| 35  | BB    | 2886 | A    | C5-C6-N6    | -6.96 | 118.13      | 123.70   |
| 1   | AA    | 510  | A    | C4-C5-C6    | 6.96  | 120.48      | 117.00   |
| 1   | AA    | 676  | A    | N3-C4-N9    | 6.96  | 132.97      | 127.40   |
| 1   | AA    | 779  | C    | C2-N1-C1'   | 6.96  | 126.46      | 118.80   |
| 35  | BB    | 2062 | A    | C3'-C2'-C1' | 6.96  | 107.07      | 101.50   |
| 35  | BB    | 2333 | A    | O4'-C1'-N9  | 6.96  | 113.77      | 108.20   |
| 1   | AA    | 627  | G    | C6-N1-C2    | 6.96  | 129.28      | 125.10   |
| 1   | AA    | 1332 | A    | C5-C6-N1    | -6.96 | 114.22      | 117.70   |
| 8   | AH    | 70   | VAL  | CA-CB-CG1   | -6.96 | 100.46      | 110.90   |
| 34  | BA    | 56   | G    | C6-N1-C2    | -6.96 | 120.92      | 125.10   |
| 35  | BB    | 16   | C    | C6-N1-C2    | 6.96  | 123.08      | 120.30   |
| 35  | BB    | 378  | C    | C5-C4-N4    | -6.96 | 115.33      | 120.20   |
| 35  | BB    | 654  | A    | C5-N7-C8    | 6.96  | 107.38      | 103.90   |
| 35  | BB    | 2594 | C    | P-O3'-C3'   | -6.96 | 111.35      | 119.70   |
| 35  | BB    | 2856 | A    | N7-C8-N9    | -6.96 | 110.32      | 113.80   |
| 1   | AA    | 805  | C    | C4-C5-C6    | -6.96 | 113.92      | 117.40   |
| 1   | AA    | 1259 | C    | C5-C4-N4    | -6.96 | 115.33      | 120.20   |
| 35  | BB    | 342  | A    | N1-C2-N3    | 6.96  | 132.78      | 129.30   |
| 1   | AA    | 331  | G    | C8-N9-C4    | -6.96 | 103.62      | 106.40   |
| 34  | BA    | 59   | A    | C5-C6-N1    | -6.96 | 114.22      | 117.70   |
| 35  | BB    | 333  | G    | C6-N1-C2    | 6.96  | 129.28      | 125.10   |
| 35  | BB    | 914  | G    | N7-C8-N9    | 6.96  | 116.58      | 113.10   |
| 35  | BB    | 1075 | C    | N3-C4-N4    | 6.96  | 122.87      | 118.00   |
| 35  | BB    | 1253 | A    | C2-N3-C4    | -6.96 | 107.12      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1642 | G    | C4-C5-C6    | 6.96  | 122.97      | 118.80   |
| 35  | BB    | 1790 | C    | C5-C6-N1    | 6.96  | 124.48      | 121.00   |
| 35  | BB    | 2238 | G    | O4'-C1'-N9  | 6.96  | 113.77      | 108.20   |
| 35  | BB    | 2798 | U    | N3-C4-O4    | 6.96  | 124.27      | 119.40   |
| 1   | AA    | 713  | G    | N3-C4-C5    | -6.96 | 125.12      | 128.60   |
| 34  | BA    | 51   | G    | C4-C5-N7    | 6.96  | 113.58      | 110.80   |
| 35  | BB    | 968  | C    | O4'-C1'-N1  | 6.96  | 113.77      | 108.20   |
| 35  | BB    | 1153 | C    | C2-N3-C4    | -6.96 | 116.42      | 119.90   |
| 35  | BB    | 1513 | U    | P-O3'-C3'   | -6.96 | 111.35      | 119.70   |
| 35  | BB    | 1797 | G    | C8-N9-C1'   | 6.96  | 136.04      | 127.00   |
| 35  | BB    | 2434 | A    | N9-C4-C5    | 6.96  | 108.58      | 105.80   |
| 35  | BB    | 1037 | G    | P-O3'-C3'   | -6.96 | 111.36      | 119.70   |
| 35  | BB    | 1063 | G    | O4'-C1'-N9  | 6.96  | 113.76      | 108.20   |
| 35  | BB    | 1854 | A    | N1-C2-N3    | -6.96 | 125.82      | 129.30   |
| 35  | BB    | 2114 | A    | O5'-P-OP1   | -6.96 | 99.44       | 105.70   |
| 1   | AA    | 34   | C    | N3-C2-O2    | 6.95  | 126.77      | 121.90   |
| 1   | AA    | 660  | C    | N1-C2-O2    | 6.95  | 123.07      | 118.90   |
| 1   | AA    | 1090 | U    | O4'-C1'-N1  | 6.95  | 113.76      | 108.20   |
| 1   | AA    | 1152 | A    | C5-C6-N1    | -6.95 | 114.22      | 117.70   |
| 22  | AV    | 7    | G    | OP1-P-O3'   | 6.95  | 120.50      | 105.20   |
| 35  | BB    | 170  | U    | N3-C2-O2    | 6.95  | 127.07      | 122.20   |
| 35  | BB    | 308  | G    | C3'-C2'-C1' | 6.95  | 107.06      | 101.50   |
| 35  | BB    | 648  | G    | N1-C2-N3    | -6.95 | 119.73      | 123.90   |
| 35  | BB    | 682  | G    | C4-C5-C6    | 6.95  | 122.97      | 118.80   |
| 35  | BB    | 962  | G    | N1-C6-O6    | 6.95  | 124.07      | 119.90   |
| 35  | BB    | 1074 | G    | C5-N7-C8    | 6.95  | 107.78      | 104.30   |
| 35  | BB    | 1479 | G    | P-O5'-C5'   | 6.95  | 132.03      | 120.90   |
| 35  | BB    | 1592 | C    | N3-C4-C5    | -6.95 | 119.12      | 121.90   |
| 35  | BB    | 1826 | G    | P-O3'-C3'   | -6.95 | 111.36      | 119.70   |
| 35  | BB    | 2252 | G    | C5-N7-C8    | 6.95  | 107.78      | 104.30   |
| 35  | BB    | 2658 | C    | C6-N1-C2    | 6.95  | 123.08      | 120.30   |
| 1   | AA    | 330  | C    | C6-N1-C2    | 6.95  | 123.08      | 120.30   |
| 1   | AA    | 666  | G    | C5-C6-O6    | -6.95 | 124.43      | 128.60   |
| 1   | AA    | 1148 | U    | N3-C2-O2    | 6.95  | 127.07      | 122.20   |
| 1   | AA    | 141  | G    | N9-C4-C5    | 6.95  | 108.18      | 105.40   |
| 1   | AA    | 303  | A    | N9-C4-C5    | -6.95 | 103.02      | 105.80   |
| 1   | AA    | 1170 | A    | C8-N9-C4    | -6.95 | 103.02      | 105.80   |
| 34  | BA    | 96   | G    | C8-N9-C4    | -6.95 | 103.62      | 106.40   |
| 43  | BJ    | 89   | PHE  | CB-CG-CD1   | -6.95 | 115.94      | 120.80   |
| 1   | AA    | 408  | A    | C5'-C4'-C3' | -6.95 | 104.88      | 116.00   |
| 1   | AA    | 548  | G    | O4'-C4'-C3' | -6.95 | 97.05       | 104.00   |
| 1   | AA    | 1405 | G    | N1-C2-N3    | -6.95 | 119.73      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1528 | U    | C4-C5-C6    | 6.95  | 123.87      | 119.70   |
| 5   | AE    | 67   | ARG  | NE-CZ-NH2   | -6.95 | 116.83      | 120.30   |
| 22  | AV    | 50   | G    | C5-C6-O6    | -6.95 | 124.43      | 128.60   |
| 34  | BA    | 28   | C    | C4'-C3'-C2' | -6.95 | 95.65       | 102.60   |
| 35  | BB    | 1036 | G    | C5-C6-O6    | -6.95 | 124.43      | 128.60   |
| 35  | BB    | 1181 | U    | P-O3'-C3'   | -6.95 | 111.36      | 119.70   |
| 35  | BB    | 2535 | G    | C5-N7-C8    | 6.95  | 107.78      | 104.30   |
| 35  | BB    | 2744 | G    | C4-C5-C6    | 6.95  | 122.97      | 118.80   |
| 35  | BB    | 2887 | A    | C6-N1-C2    | -6.95 | 114.43      | 118.60   |
| 1   | AA    | 721  | G    | O4'-C1'-N9  | 6.95  | 113.76      | 108.20   |
| 34  | BA    | 108  | A    | C5-C6-N1    | -6.95 | 114.23      | 117.70   |
| 35  | BB    | 862  | G    | N3-C4-C5    | 6.95  | 132.07      | 128.60   |
| 35  | BB    | 2241 | A    | C5-C6-N6    | -6.95 | 118.14      | 123.70   |
| 36  | BC    | 38   | LYS  | N-CA-CB     | 6.95  | 123.11      | 110.60   |
| 1   | AA    | 406  | G    | C8-N9-C4    | -6.95 | 103.62      | 106.40   |
| 1   | AA    | 731  | G    | C4-C5-C6    | 6.95  | 122.97      | 118.80   |
| 22  | AV    | 8    | U    | O4'-C1'-N1  | 6.95  | 113.76      | 108.20   |
| 35  | BB    | 380  | G    | C4-C5-C6    | 6.95  | 122.97      | 118.80   |
| 35  | BB    | 572  | A    | C1'-O4'-C4' | 6.95  | 115.46      | 109.90   |
| 35  | BB    | 1099 | G    | C5'-C4'-C3' | -6.95 | 104.89      | 116.00   |
| 35  | BB    | 2185 | U    | C3'-C2'-C1' | -6.95 | 95.94       | 101.50   |
| 1   | AA    | 940  | C    | C4-C5-C6    | 6.94  | 120.87      | 117.40   |
| 1   | AA    | 1297 | G    | N1-C6-O6    | 6.94  | 124.07      | 119.90   |
| 1   | AA    | 654  | G    | C6-C5-N7    | -6.94 | 126.23      | 130.40   |
| 22  | AV    | 42   | G    | C5-C6-O6    | -6.94 | 124.44      | 128.60   |
| 34  | BA    | 73   | A    | C8-N9-C4    | -6.94 | 103.02      | 105.80   |
| 35  | BB    | 313  | G    | N3-C4-C5    | -6.94 | 125.13      | 128.60   |
| 35  | BB    | 385  | C    | C5-C4-N4    | -6.94 | 115.34      | 120.20   |
| 35  | BB    | 1416 | G    | O4'-C1'-C2' | -6.94 | 98.86       | 105.80   |
| 35  | BB    | 1700 | A    | O4'-C1'-N9  | 6.94  | 113.75      | 108.20   |
| 35  | BB    | 2149 | U    | C2-N3-C4    | -6.94 | 122.83      | 127.00   |
| 35  | BB    | 2556 | C    | O5'-P-OP1   | 6.94  | 119.03      | 110.70   |
| 1   | AA    | 47   | C    | C4'-C3'-C2' | -6.94 | 95.66       | 102.60   |
| 35  | BB    | 2245 | U    | C4-C5-C6    | -6.94 | 115.54      | 119.70   |
| 35  | BB    | 2254 | C    | C6-N1-C2    | 6.94  | 123.08      | 120.30   |
| 35  | BB    | 2485 | G    | C5-C6-O6    | -6.94 | 124.44      | 128.60   |
| 35  | BB    | 2816 | G    | N1-C6-O6    | 6.94  | 124.06      | 119.90   |
| 17  | AQ    | 49   | ASN  | N-CA-CB     | 6.94  | 123.09      | 110.60   |
| 35  | BB    | 11   | C    | C5-C4-N4    | -6.94 | 115.34      | 120.20   |
| 35  | BB    | 352  | A    | O4'-C1'-N9  | 6.94  | 113.75      | 108.20   |
| 35  | BB    | 776  | G    | C6-C5-N7    | 6.94  | 134.56      | 130.40   |
| 35  | BB    | 1217 | U    | C6-N1-C2    | 6.94  | 125.16      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1023 | U    | O4'-C1'-N1  | 6.94  | 113.75      | 108.20   |
| 35  | BB    | 44   | A    | N9-C4-C5    | -6.94 | 103.03      | 105.80   |
| 35  | BB    | 532  | A    | C5-C6-N1    | -6.94 | 114.23      | 117.70   |
| 35  | BB    | 1127 | A    | C5-C6-N1    | -6.94 | 114.23      | 117.70   |
| 35  | BB    | 1204 | A    | O4'-C1'-N9  | 6.94  | 113.75      | 108.20   |
| 35  | BB    | 1324 | G    | C5-C6-O6    | -6.94 | 124.44      | 128.60   |
| 35  | BB    | 1439 | A    | C5-C6-N6    | 6.94  | 129.25      | 123.70   |
| 35  | BB    | 1520 | U    | C5-C6-N1    | 6.94  | 126.17      | 122.70   |
| 1   | AA    | 921  | U    | O4'-C1'-N1  | 6.94  | 113.75      | 108.20   |
| 1   | AA    | 1533 | C    | C6-N1-C1'   | -6.94 | 112.48      | 120.80   |
| 1   | AA    | 334  | C    | C6-N1-C2    | -6.93 | 117.53      | 120.30   |
| 34  | BA    | 75   | G    | N3-C2-N2    | 6.93  | 124.75      | 119.90   |
| 35  | BB    | 450  | G    | P-O3'-C3'   | -6.93 | 111.38      | 119.70   |
| 35  | BB    | 1156 | A    | N1-C6-N6    | 6.93  | 122.76      | 118.60   |
| 35  | BB    | 1420 | A    | P-O5'-C5'   | -6.93 | 109.81      | 120.90   |
| 35  | BB    | 1896 | G    | C2-N3-C4    | 6.93  | 115.37      | 111.90   |
| 35  | BB    | 2519 | U    | N3-C2-O2    | 6.93  | 127.05      | 122.20   |
| 35  | BB    | 2572 | A    | C4-C5-C6    | 6.93  | 120.47      | 117.00   |
| 47  | BN    | 103  | ARG  | NE-CZ-NH1   | 6.93  | 123.77      | 120.30   |
| 1   | AA    | 310  | G    | C4-C5-C6    | 6.93  | 122.96      | 118.80   |
| 1   | AA    | 511  | C    | O4'-C1'-N1  | 6.93  | 113.75      | 108.20   |
| 1   | AA    | 578  | C    | C6-N1-C2    | -6.93 | 117.53      | 120.30   |
| 1   | AA    | 639  | G    | P-O3'-C3'   | -6.93 | 111.38      | 119.70   |
| 34  | BA    | 104  | A    | C4'-C3'-C2' | -6.93 | 95.67       | 102.60   |
| 35  | BB    | 782  | A    | N1-C6-N6    | 6.93  | 122.76      | 118.60   |
| 35  | BB    | 1061 | U    | C6-N1-C2    | -6.93 | 116.84      | 121.00   |
| 35  | BB    | 2186 | G    | N3-C4-C5    | 6.93  | 132.07      | 128.60   |
| 35  | BB    | 2661 | G    | C5-C6-O6    | -6.93 | 124.44      | 128.60   |
| 35  | BB    | 2730 | C    | N3-C4-N4    | 6.93  | 122.85      | 118.00   |
| 48  | BO    | 72   | ALA  | N-CA-CB     | 6.93  | 119.81      | 110.10   |
| 1   | AA    | 887  | G    | C6-C5-N7    | -6.93 | 126.24      | 130.40   |
| 1   | AA    | 888  | G    | C2-N3-C4    | -6.93 | 108.44      | 111.90   |
| 1   | AA    | 1400 | C    | O4'-C1'-N1  | 6.93  | 113.75      | 108.20   |
| 1   | AA    | 1412 | C    | C5-C4-N4    | -6.93 | 115.35      | 120.20   |
| 35  | BB    | 542  | C    | O4'-C1'-N1  | 6.93  | 113.75      | 108.20   |
| 35  | BB    | 2130 | U    | N3-C4-O4    | 6.93  | 124.25      | 119.40   |
| 35  | BB    | 2229 | U    | C5-C4-O4    | -6.93 | 121.74      | 125.90   |
| 1   | AA    | 441  | A    | O4'-C1'-N9  | 6.93  | 113.74      | 108.20   |
| 35  | BB    | 636  | G    | N3-C2-N2    | 6.93  | 124.75      | 119.90   |
| 35  | BB    | 756  | A    | N1-C2-N3    | -6.93 | 125.83      | 129.30   |
| 35  | BB    | 1380 | G    | C5-N7-C8    | -6.93 | 100.84      | 104.30   |
| 35  | BB    | 2766 | A    | N3-C4-N9    | 6.93  | 132.94      | 127.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 232  | G    | N1-C2-N3   | -6.93 | 119.74      | 123.90   |
| 1   | AA    | 773  | G    | N1-C2-N3   | -6.93 | 119.74      | 123.90   |
| 1   | AA    | 788  | U    | N3-C4-O4   | 6.93  | 124.25      | 119.40   |
| 35  | BB    | 294  | A    | N9-C4-C5   | 6.93  | 108.57      | 105.80   |
| 35  | BB    | 339  | U    | C6-N1-C2   | -6.93 | 116.84      | 121.00   |
| 35  | BB    | 474  | G    | N1-C6-O6   | 6.93  | 124.06      | 119.90   |
| 35  | BB    | 1323 | C    | C2-N3-C4   | 6.93  | 123.36      | 119.90   |
| 35  | BB    | 1383 | A    | N1-C2-N3   | 6.93  | 132.76      | 129.30   |
| 35  | BB    | 1479 | G    | C5-N7-C8   | 6.93  | 107.76      | 104.30   |
| 35  | BB    | 2160 | C    | N3-C4-C5   | -6.93 | 119.13      | 121.90   |
| 35  | BB    | 2757 | A    | N1-C2-N3   | -6.93 | 125.84      | 129.30   |
| 1   | AA    | 408  | A    | C6-C5-N7   | -6.92 | 127.45      | 132.30   |
| 1   | AA    | 682  | G    | O4'-C1'-N9 | 6.92  | 113.74      | 108.20   |
| 35  | BB    | 561  | G    | N3-C4-N9   | -6.92 | 121.84      | 126.00   |
| 35  | BB    | 1093 | G    | N3-C4-C5   | -6.92 | 125.14      | 128.60   |
| 35  | BB    | 1129 | A    | C6-N1-C2   | 6.92  | 122.75      | 118.60   |
| 35  | BB    | 1997 | C    | C5-C4-N4   | -6.92 | 115.35      | 120.20   |
| 1   | AA    | 299  | G    | C4-C5-N7   | 6.92  | 113.57      | 110.80   |
| 1   | AA    | 310  | G    | C5-C6-N1   | -6.92 | 108.04      | 111.50   |
| 1   | AA    | 378  | G    | C2-N3-C4   | 6.92  | 115.36      | 111.90   |
| 35  | BB    | 2450 | A    | C8-N9-C4   | 6.92  | 108.57      | 105.80   |
| 35  | BB    | 2560 | A    | O4'-C1'-N9 | 6.92  | 113.74      | 108.20   |
| 1   | AA    | 502  | A    | N9-C1'-C2' | -6.92 | 104.39      | 112.00   |
| 1   | AA    | 505  | G    | N1-C2-N3   | -6.92 | 119.75      | 123.90   |
| 1   | AA    | 1369 | C    | C6-N1-C2   | 6.92  | 123.07      | 120.30   |
| 22  | AV    | 2    | G    | C6-C5-N7   | -6.92 | 126.25      | 130.40   |
| 35  | BB    | 294  | A    | N7-C8-N9   | -6.92 | 110.34      | 113.80   |
| 35  | BB    | 759  | G    | C2-N3-C4   | 6.92  | 115.36      | 111.90   |
| 35  | BB    | 1459 | G    | O4'-C1'-N9 | 6.92  | 113.74      | 108.20   |
| 35  | BB    | 1463 | C    | N3-C4-C5   | -6.92 | 119.13      | 121.90   |
| 35  | BB    | 2283 | C    | N3-C4-C5   | -6.92 | 119.13      | 121.90   |
| 35  | BB    | 2302 | U    | C5-C4-O4   | -6.92 | 121.75      | 125.90   |
| 35  | BB    | 2577 | A    | C6-C5-N7   | -6.92 | 127.45      | 132.30   |
| 35  | BB    | 2883 | A    | C5-N7-C8   | 6.92  | 107.36      | 103.90   |
| 1   | AA    | 316  | C    | O4'-C1'-N1 | 6.92  | 113.74      | 108.20   |
| 35  | BB    | 521  | U    | C6-N1-C2   | -6.92 | 116.85      | 121.00   |
| 35  | BB    | 1057 | A    | C4-C5-C6   | 6.92  | 120.46      | 117.00   |
| 35  | BB    | 1608 | A    | C8-N9-C4   | 6.92  | 108.57      | 105.80   |
| 35  | BB    | 1675 | C    | C5-C4-N4   | -6.92 | 115.36      | 120.20   |
| 1   | AA    | 97   | G    | C8-N9-C4   | -6.92 | 103.63      | 106.40   |
| 1   | AA    | 328  | C    | C5-C6-N1   | 6.92  | 124.46      | 121.00   |
| 1   | AA    | 447  | G    | N9-C4-C5   | 6.92  | 108.17      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 716  | A    | C8-N9-C4    | -6.92 | 103.03      | 105.80   |
| 1   | AA    | 1390 | U    | C5-C4-O4    | 6.92  | 130.05      | 125.90   |
| 7   | AG    | 97   | ALA  | N-CA-CB     | 6.92  | 119.78      | 110.10   |
| 35  | BB    | 276  | U    | N1-C2-O2    | -6.92 | 117.96      | 122.80   |
| 35  | BB    | 338  | G    | C3'-C2'-C1' | 6.92  | 107.03      | 101.50   |
| 35  | BB    | 428  | A    | C6-C5-N7    | -6.92 | 127.46      | 132.30   |
| 35  | BB    | 455  | C    | N3-C4-N4    | 6.92  | 122.84      | 118.00   |
| 35  | BB    | 1287 | A    | C5-N7-C8    | 6.92  | 107.36      | 103.90   |
| 35  | BB    | 1373 | A    | C6-N1-C2    | -6.92 | 114.45      | 118.60   |
| 35  | BB    | 2273 | A    | C5'-C4'-C3' | -6.92 | 104.93      | 116.00   |
| 35  | BB    | 2341 | G    | C6-C5-N7    | -6.92 | 126.25      | 130.40   |
| 35  | BB    | 2472 | G    | N7-C8-N9    | 6.92  | 116.56      | 113.10   |
| 35  | BB    | 2760 | C    | P-O3'-C3'   | -6.92 | 111.40      | 119.70   |
| 35  | BB    | 2886 | A    | C8-N9-C4    | -6.92 | 103.03      | 105.80   |
| 1   | AA    | 771  | G    | C8-N9-C4    | 6.92  | 109.17      | 106.40   |
| 1   | AA    | 1304 | G    | C4-C5-N7    | 6.92  | 113.57      | 110.80   |
| 1   | AA    | 1379 | G    | C8-N9-C4    | -6.92 | 103.63      | 106.40   |
| 35  | BB    | 709  | U    | P-O5'-C5'   | 6.92  | 131.97      | 120.90   |
| 35  | BB    | 789  | A    | OP1-P-OP2   | -6.92 | 109.22      | 119.60   |
| 35  | BB    | 1396 | U    | N1-C2-N3    | 6.92  | 119.05      | 114.90   |
| 35  | BB    | 1957 | C    | C6-N1-C2    | -6.92 | 117.53      | 120.30   |
| 35  | BB    | 2350 | C    | C2-N3-C4    | 6.92  | 123.36      | 119.90   |
| 35  | BB    | 2393 | U    | O4'-C4'-C3' | -6.92 | 97.08       | 104.00   |
| 35  | BB    | 2593 | U    | O4'-C1'-N1  | 6.92  | 113.73      | 108.20   |
| 1   | AA    | 1496 | C    | O4'-C1'-N1  | 6.92  | 113.73      | 108.20   |
| 35  | BB    | 1327 | A    | C5-C6-N1    | -6.92 | 114.24      | 117.70   |
| 1   | AA    | 46   | G    | C5-C6-O6    | -6.91 | 124.45      | 128.60   |
| 1   | AA    | 1436 | U    | C5-C6-N1    | 6.91  | 126.16      | 122.70   |
| 35  | BB    | 1317 | G    | C5-C6-O6    | -6.91 | 124.45      | 128.60   |
| 35  | BB    | 1415 | U    | N3-C4-O4    | 6.91  | 124.24      | 119.40   |
| 35  | BB    | 2557 | G    | C4-C5-N7    | -6.91 | 108.03      | 110.80   |
| 35  | BB    | 2644 | G    | N3-C4-N9    | 6.91  | 130.15      | 126.00   |
| 1   | AA    | 438  | U    | C2-N3-C4    | -6.91 | 122.85      | 127.00   |
| 1   | AA    | 1446 | A    | C5-C6-N6    | -6.91 | 118.17      | 123.70   |
| 35  | BB    | 759  | G    | N3-C4-N9    | 6.91  | 130.15      | 126.00   |
| 35  | BB    | 1092 | C    | N1-C2-O2    | 6.91  | 123.05      | 118.90   |
| 35  | BB    | 1346 | G    | C5-C6-O6    | -6.91 | 124.45      | 128.60   |
| 35  | BB    | 1795 | C    | C5-C6-N1    | 6.91  | 124.46      | 121.00   |
| 1   | AA    | 942  | G    | N9-C4-C5    | -6.91 | 102.64      | 105.40   |
| 1   | AA    | 1061 | G    | C6-C5-N7    | -6.91 | 126.25      | 130.40   |
| 1   | AA    | 1463 | U    | N3-C4-C5    | -6.91 | 110.45      | 114.60   |
| 35  | BB    | 451  | U    | N3-C2-O2    | -6.91 | 117.36      | 122.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1079 | C    | C5-C4-N4    | -6.91 | 115.36      | 120.20   |
| 35  | BB    | 1090 | A    | O4'-C1'-N9  | 6.91  | 113.73      | 108.20   |
| 35  | BB    | 1328 | A    | C2'-C3'-O3' | 6.91  | 124.76      | 113.70   |
| 35  | BB    | 1785 | A    | C5-C6-N6    | -6.91 | 118.17      | 123.70   |
| 35  | BB    | 2541 | A    | C8-N9-C4    | -6.91 | 103.03      | 105.80   |
| 1   | AA    | 255  | G    | N1-C2-N3    | -6.91 | 119.75      | 123.90   |
| 35  | BB    | 1025 | G    | N9-C4-C5    | -6.91 | 102.64      | 105.40   |
| 35  | BB    | 1368 | G    | C5-N7-C8    | 6.91  | 107.75      | 104.30   |
| 35  | BB    | 1482 | G    | C5-C6-O6    | -6.91 | 124.45      | 128.60   |
| 1   | AA    | 530  | G    | C5-C6-N1    | -6.91 | 108.05      | 111.50   |
| 1   | AA    | 888  | G    | C8-N9-C4    | -6.91 | 103.64      | 106.40   |
| 35  | BB    | 1086 | A    | N1-C6-N6    | 6.91  | 122.74      | 118.60   |
| 35  | BB    | 2883 | A    | C5-C6-N1    | -6.91 | 114.25      | 117.70   |
| 1   | AA    | 261  | U    | N3-C4-O4    | 6.91  | 124.23      | 119.40   |
| 1   | AA    | 907  | A    | O4'-C1'-N9  | 6.91  | 113.72      | 108.20   |
| 1   | AA    | 1528 | U    | O4'-C1'-N1  | 6.91  | 113.72      | 108.20   |
| 22  | AV    | 60   | U    | O4'-C1'-N1  | 6.91  | 113.72      | 108.20   |
| 35  | BB    | 370  | G    | N1-C6-O6    | 6.91  | 124.04      | 119.90   |
| 35  | BB    | 1047 | G    | C2-N3-C4    | 6.91  | 115.35      | 111.90   |
| 35  | BB    | 1131 | G    | C6-C5-N7    | -6.91 | 126.26      | 130.40   |
| 35  | BB    | 1287 | A    | N9-C4-C5    | 6.91  | 108.56      | 105.80   |
| 35  | BB    | 1594 | U    | N1-C2-N3    | 6.91  | 119.04      | 114.90   |
| 35  | BB    | 1830 | C    | N1-C2-O2    | 6.91  | 123.04      | 118.90   |
| 35  | BB    | 2666 | C    | O4'-C1'-N1  | 6.91  | 113.72      | 108.20   |
| 35  | BB    | 761  | A    | N7-C8-N9    | 6.90  | 117.25      | 113.80   |
| 35  | BB    | 2055 | C    | C2-N3-C4    | -6.90 | 116.45      | 119.90   |
| 35  | BB    | 2312 | U    | N3-C4-O4    | 6.90  | 124.23      | 119.40   |
| 1   | AA    | 167  | A    | O4'-C1'-N9  | 6.90  | 113.72      | 108.20   |
| 1   | AA    | 579  | A    | N1-C2-N3    | 6.90  | 132.75      | 129.30   |
| 35  | BB    | 1072 | C    | P-O3'-C3'   | -6.90 | 111.42      | 119.70   |
| 35  | BB    | 1305 | C    | C5-C4-N4    | -6.90 | 115.37      | 120.20   |
| 35  | BB    | 2359 | C    | C5-C4-N4    | -6.90 | 115.37      | 120.20   |
| 35  | BB    | 2370 | G    | C5-C6-O6    | -6.90 | 124.46      | 128.60   |
| 1   | AA    | 299  | G    | N1-C2-N2    | -6.90 | 109.99      | 116.20   |
| 8   | AH    | 101  | ALA  | N-CA-CB     | 6.90  | 119.76      | 110.10   |
| 35  | BB    | 65   | U    | N1-C2-O2    | -6.90 | 117.97      | 122.80   |
| 35  | BB    | 326  | G    | O4'-C1'-N9  | 6.90  | 113.72      | 108.20   |
| 35  | BB    | 353  | C    | N3-C4-N4    | 6.90  | 122.83      | 118.00   |
| 35  | BB    | 723  | C    | O4'-C1'-N1  | 6.90  | 113.72      | 108.20   |
| 35  | BB    | 970  | U    | O4'-C1'-N1  | 6.90  | 113.72      | 108.20   |
| 35  | BB    | 2495 | G    | N3-C2-N2    | 6.90  | 124.73      | 119.90   |
| 35  | BB    | 2841 | C    | C5-C4-N4    | -6.90 | 115.37      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 37  | BD    | 61   | THR  | CA-CB-CG2  | -6.90 | 102.74      | 112.40   |
| 1   | AA    | 9    | G    | P-O3'-C3'  | -6.90 | 111.42      | 119.70   |
| 1   | AA    | 705  | G    | C4-C5-N7   | 6.90  | 113.56      | 110.80   |
| 1   | AA    | 1170 | A    | C5-N7-C8   | 6.90  | 107.35      | 103.90   |
| 1   | AA    | 1329 | A    | C5-N7-C8   | 6.90  | 107.35      | 103.90   |
| 35  | BB    | 1697 | G    | C6-C5-N7   | -6.90 | 126.26      | 130.40   |
| 35  | BB    | 2419 | U    | N3-C4-C5   | -6.90 | 110.46      | 114.60   |
| 1   | AA    | 400  | C    | C5-C6-N1   | 6.90  | 124.45      | 121.00   |
| 1   | AA    | 826  | C    | N3-C4-N4   | 6.90  | 122.83      | 118.00   |
| 35  | BB    | 432  | A    | C8-N9-C4   | -6.90 | 103.04      | 105.80   |
| 35  | BB    | 690  | G    | O4'-C1'-N9 | 6.90  | 113.72      | 108.20   |
| 35  | BB    | 1009 | A    | N7-C8-N9   | -6.90 | 110.35      | 113.80   |
| 35  | BB    | 2508 | G    | C2-N3-C4   | 6.90  | 115.35      | 111.90   |
| 35  | BB    | 2877 | G    | O4'-C1'-N9 | 6.90  | 113.72      | 108.20   |
| 1   | AA    | 644  | U    | C6-N1-C2   | -6.90 | 116.86      | 121.00   |
| 1   | AA    | 878  | A    | N1-C2-N3   | 6.90  | 132.75      | 129.30   |
| 35  | BB    | 57   | C    | C5-C6-N1   | 6.90  | 124.45      | 121.00   |
| 35  | BB    | 1186 | G    | C5-N7-C8   | -6.90 | 100.85      | 104.30   |
| 35  | BB    | 2180 | U    | P-O5'-C5'  | 6.90  | 131.93      | 120.90   |
| 1   | AA    | 1068 | G    | N7-C8-N9   | -6.89 | 109.65      | 113.10   |
| 1   | AA    | 1179 | A    | N7-C8-N9   | -6.89 | 110.35      | 113.80   |
| 35  | BB    | 442  | G    | N1-C2-N3   | -6.89 | 119.76      | 123.90   |
| 1   | AA    | 112  | G    | N3-C2-N2   | 6.89  | 124.72      | 119.90   |
| 1   | AA    | 351  | G    | O4'-C1'-N9 | 6.89  | 113.71      | 108.20   |
| 1   | AA    | 537  | G    | N7-C8-N9   | 6.89  | 116.55      | 113.10   |
| 1   | AA    | 1149 | C    | C5-C4-N4   | -6.89 | 115.38      | 120.20   |
| 1   | AA    | 1309 | G    | C8-N9-C4   | -6.89 | 103.64      | 106.40   |
| 35  | BB    | 582  | A    | C6-N1-C2   | 6.89  | 122.74      | 118.60   |
| 35  | BB    | 1141 | U    | C2-N1-C1'  | -6.89 | 109.43      | 117.70   |
| 35  | BB    | 1516 | G    | N1-C2-N3   | -6.89 | 119.76      | 123.90   |
| 35  | BB    | 1601 | G    | C5-C6-O6   | -6.89 | 124.47      | 128.60   |
| 35  | BB    | 1990 | C    | N3-C4-N4   | 6.89  | 122.83      | 118.00   |
| 35  | BB    | 2386 | A    | N1-C6-N6   | 6.89  | 122.73      | 118.60   |
| 35  | BB    | 232  | G    | N1-C6-O6   | 6.89  | 124.03      | 119.90   |
| 35  | BB    | 245  | G    | O4'-C1'-N9 | 6.89  | 113.71      | 108.20   |
| 35  | BB    | 301  | G    | N9-C4-C5   | 6.89  | 108.16      | 105.40   |
| 35  | BB    | 500  | G    | C5-C6-N1   | -6.89 | 108.05      | 111.50   |
| 35  | BB    | 853  | C    | N1-C2-O2   | 6.89  | 123.03      | 118.90   |
| 35  | BB    | 1126 | A    | C5-C6-N6   | -6.89 | 118.19      | 123.70   |
| 1   | AA    | 776  | G    | C5-N7-C8   | -6.89 | 100.86      | 104.30   |
| 35  | BB    | 72   | U    | C4-C5-C6   | 6.89  | 123.83      | 119.70   |
| 35  | BB    | 548  | G    | N3-C2-N2   | 6.89  | 124.72      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 611  | C    | N3-C4-N4    | 6.89  | 122.82      | 118.00   |
| 35  | BB    | 905  | A    | C6-C5-N7    | -6.89 | 127.48      | 132.30   |
| 35  | BB    | 1385 | A    | C5-C6-N1    | -6.89 | 114.26      | 117.70   |
| 35  | BB    | 2411 | A    | N1-C6-N6    | 6.89  | 122.73      | 118.60   |
| 35  | BB    | 2472 | G    | N1-C6-O6    | 6.89  | 124.03      | 119.90   |
| 35  | BB    | 2492 | U    | O5'-P-OP2   | -6.89 | 99.50       | 105.70   |
| 1   | AA    | 433  | G    | N1-C2-N3    | -6.89 | 119.77      | 123.90   |
| 35  | BB    | 605  | G    | O4'-C1'-N9  | 6.89  | 113.71      | 108.20   |
| 1   | AA    | 949  | A    | C6-C5-N7    | -6.89 | 127.48      | 132.30   |
| 1   | AA    | 1500 | A    | N1-C2-N3    | 6.89  | 132.74      | 129.30   |
| 33  | B8    | 24   | ARG  | NE-CZ-NH2   | 6.89  | 123.74      | 120.30   |
| 35  | BB    | 25   | U    | C5-C6-N1    | 6.89  | 126.14      | 122.70   |
| 35  | BB    | 482  | A    | C8-N9-C4    | -6.89 | 103.05      | 105.80   |
| 35  | BB    | 1117 | C    | N1-C2-O2    | -6.89 | 114.77      | 118.90   |
| 35  | BB    | 1665 | A    | C6-C5-N7    | -6.89 | 127.48      | 132.30   |
| 35  | BB    | 1813 | G    | O4'-C1'-N9  | 6.89  | 113.71      | 108.20   |
| 35  | BB    | 2637 | U    | N3-C4-C5    | -6.89 | 110.47      | 114.60   |
| 35  | BB    | 2840 | C    | O4'-C1'-N1  | 6.89  | 113.71      | 108.20   |
| 1   | AA    | 8    | A    | C5-C6-N1    | 6.88  | 121.14      | 117.70   |
| 1   | AA    | 1000 | A    | O4'-C1'-N9  | 6.88  | 113.71      | 108.20   |
| 1   | AA    | 1060 | U    | C4-C5-C6    | -6.88 | 115.57      | 119.70   |
| 1   | AA    | 1105 | A    | O4'-C1'-N9  | 6.88  | 113.71      | 108.20   |
| 1   | AA    | 1208 | C    | C5-C4-N4    | -6.88 | 115.38      | 120.20   |
| 1   | AA    | 1215 | G    | N3-C4-C5    | -6.88 | 125.16      | 128.60   |
| 1   | AA    | 1439 | G    | O4'-C1'-N9  | 6.88  | 113.71      | 108.20   |
| 4   | AD    | 72   | ARG  | NE-CZ-NH2   | -6.88 | 116.86      | 120.30   |
| 34  | BA    | 53   | A    | C5'-C4'-C3' | 6.88  | 127.02      | 116.00   |
| 34  | BA    | 56   | G    | C4-C5-C6    | 6.88  | 122.93      | 118.80   |
| 35  | BB    | 88   | G    | C4-C5-C6    | 6.88  | 122.93      | 118.80   |
| 35  | BB    | 199  | A    | C4-C5-C6    | 6.88  | 120.44      | 117.00   |
| 35  | BB    | 218  | A    | N9-C4-C5    | 6.88  | 108.55      | 105.80   |
| 35  | BB    | 480  | A    | N9-C4-C5    | 6.88  | 108.55      | 105.80   |
| 35  | BB    | 713  | G    | C4-C5-N7    | 6.88  | 113.55      | 110.80   |
| 35  | BB    | 919  | U    | C5-C6-N1    | 6.88  | 126.14      | 122.70   |
| 35  | BB    | 1227 | G    | N3-C2-N2    | 6.88  | 124.72      | 119.90   |
| 35  | BB    | 1628 | G    | N9-C4-C5    | -6.88 | 102.65      | 105.40   |
| 35  | BB    | 1793 | C    | N3-C4-C5    | -6.88 | 119.15      | 121.90   |
| 35  | BB    | 1835 | G    | O4'-C1'-N9  | 6.88  | 113.71      | 108.20   |
| 35  | BB    | 2044 | C    | O4'-C1'-N1  | 6.88  | 113.71      | 108.20   |
| 35  | BB    | 2547 | A    | C2-N3-C4    | -6.88 | 107.16      | 110.60   |
| 1   | AA    | 973  | G    | N1-C6-O6    | 6.88  | 124.03      | 119.90   |
| 22  | AV    | 7    | G    | N1-C2-N3    | -6.88 | 119.77      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 287  | G    | N1-C6-O6    | 6.88  | 124.03      | 119.90   |
| 35  | BB    | 469  | G    | C5-C6-O6    | -6.88 | 124.47      | 128.60   |
| 35  | BB    | 728  | G    | N1-C2-N3    | -6.88 | 119.77      | 123.90   |
| 35  | BB    | 974  | G    | O4'-C1'-N9  | 6.88  | 113.71      | 108.20   |
| 35  | BB    | 1982 | U    | C2-N3-C4    | -6.88 | 122.87      | 127.00   |
| 35  | BB    | 1995 | U    | O4'-C1'-N1  | 6.88  | 113.71      | 108.20   |
| 1   | AA    | 39   | G    | C8-N9-C4    | 6.88  | 109.15      | 106.40   |
| 35  | BB    | 493  | G    | P-O3'-C3'   | -6.88 | 111.44      | 119.70   |
| 35  | BB    | 551  | G    | O4'-C1'-N9  | 6.88  | 113.70      | 108.20   |
| 35  | BB    | 719  | C    | N1-C2-O2    | -6.88 | 114.77      | 118.90   |
| 35  | BB    | 2196 | C    | N3-C4-C5    | -6.88 | 119.15      | 121.90   |
| 35  | BB    | 2404 | U    | O4'-C1'-N1  | 6.88  | 113.70      | 108.20   |
| 35  | BB    | 2886 | A    | N1-C2-N3    | 6.88  | 132.74      | 129.30   |
| 1   | AA    | 1003 | G    | C5-C6-N1    | -6.88 | 108.06      | 111.50   |
| 1   | AA    | 1147 | C    | C2-N3-C4    | 6.88  | 123.34      | 119.90   |
| 35  | BB    | 883  | G    | N3-C4-C5    | 6.88  | 132.04      | 128.60   |
| 35  | BB    | 1249 | U    | N3-C4-O4    | 6.88  | 124.22      | 119.40   |
| 35  | BB    | 1466 | U    | N1-C2-N3    | 6.88  | 119.03      | 114.90   |
| 35  | BB    | 2018 | G    | O4'-C1'-N9  | 6.88  | 113.70      | 108.20   |
| 1   | AA    | 873  | A    | C2-N3-C4    | 6.88  | 114.04      | 110.60   |
| 35  | BB    | 407  | G    | N7-C8-N9    | 6.88  | 116.54      | 113.10   |
| 35  | BB    | 999  | U    | C1'-O4'-C4' | 6.88  | 115.40      | 109.90   |
| 35  | BB    | 1156 | A    | C6-C5-N7    | -6.88 | 127.48      | 132.30   |
| 35  | BB    | 1288 | G    | O4'-C1'-N9  | 6.88  | 113.70      | 108.20   |
| 35  | BB    | 1620 | G    | N3-C2-N2    | 6.88  | 124.71      | 119.90   |
| 35  | BB    | 1695 | G    | C4-N9-C1'   | 6.88  | 135.44      | 126.50   |
| 35  | BB    | 1737 | G    | N9-C4-C5    | -6.88 | 102.65      | 105.40   |
| 35  | BB    | 2361 | G    | N9-C4-C5    | 6.88  | 108.15      | 105.40   |
| 35  | BB    | 2872 | A    | C5-C6-N1    | -6.88 | 114.26      | 117.70   |
| 1   | AA    | 232  | G    | N3-C2-N2    | 6.88  | 124.71      | 119.90   |
| 1   | AA    | 391  | G    | N1-C2-N3    | -6.88 | 119.78      | 123.90   |
| 1   | AA    | 405  | U    | C2-N3-C4    | -6.88 | 122.87      | 127.00   |
| 1   | AA    | 1029 | U    | C4-C5-C6    | -6.88 | 115.57      | 119.70   |
| 1   | AA    | 1040 | U    | C5-C4-O4    | -6.88 | 121.77      | 125.90   |
| 1   | AA    | 1511 | G    | C3'-C2'-C1' | -6.88 | 96.00       | 101.50   |
| 1   | AA    | 1512 | U    | C5-C4-O4    | -6.88 | 121.77      | 125.90   |
| 11  | AK    | 26   | PHE  | CB-CG-CD2   | -6.88 | 115.99      | 120.80   |
| 35  | BB    | 33   | C    | C5-C4-N4    | -6.88 | 115.39      | 120.20   |
| 35  | BB    | 415  | A    | C5-C6-N6    | -6.88 | 118.20      | 123.70   |
| 35  | BB    | 1153 | C    | N1-C2-N3    | 6.88  | 124.01      | 119.20   |
| 35  | BB    | 1699 | G    | C1'-O4'-C4' | -6.88 | 104.40      | 109.90   |
| 35  | BB    | 2210 | U    | N3-C2-O2    | 6.88  | 127.01      | 122.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2347 | C    | N3-C4-C5    | -6.88 | 119.15      | 121.90   |
| 38  | BE    | 78   | TRP  | CB-CG-CD2   | -6.88 | 117.66      | 126.60   |
| 1   | AA    | 1003 | G    | C6-C5-N7    | -6.88 | 126.28      | 130.40   |
| 1   | AA    | 54   | C    | C6-N1-C2    | -6.87 | 117.55      | 120.30   |
| 1   | AA    | 70   | U    | N3-C4-O4    | 6.87  | 124.21      | 119.40   |
| 1   | AA    | 199  | A    | C5-C6-N6    | -6.87 | 118.20      | 123.70   |
| 1   | AA    | 662  | U    | C3'-C2'-C1' | -6.87 | 96.00       | 101.50   |
| 1   | AA    | 788  | U    | O4'-C1'-N1  | 6.87  | 113.70      | 108.20   |
| 1   | AA    | 959  | A    | C5-C6-N6    | -6.87 | 118.20      | 123.70   |
| 12  | AL    | 3    | VAL  | CA-CB-CG2   | 6.87  | 121.21      | 110.90   |
| 14  | AN    | 19   | TYR  | CB-CG-CD1   | -6.87 | 116.88      | 121.00   |
| 35  | BB    | 812  | C    | O4'-C1'-N1  | 6.87  | 113.70      | 108.20   |
| 35  | BB    | 1007 | C    | N3-C4-C5    | -6.87 | 119.15      | 121.90   |
| 35  | BB    | 1211 | C    | C5-C4-N4    | -6.87 | 115.39      | 120.20   |
| 35  | BB    | 1710 | G    | N3-C2-N2    | 6.87  | 124.71      | 119.90   |
| 35  | BB    | 2117 | A    | N1-C2-N3    | 6.87  | 132.74      | 129.30   |
| 43  | BJ    | 34   | ARG  | NE-CZ-NH2   | 6.87  | 123.74      | 120.30   |
| 1   | AA    | 143  | A    | C5-N7-C8    | 6.87  | 107.34      | 103.90   |
| 1   | AA    | 1097 | C    | C5-C4-N4    | -6.87 | 115.39      | 120.20   |
| 22  | AV    | 37   | G    | C8-N9-C4    | -6.87 | 103.65      | 106.40   |
| 35  | BB    | 1014 | A    | C2-N3-C4    | 6.87  | 114.04      | 110.60   |
| 35  | BB    | 2433 | A    | N1-C2-N3    | 6.87  | 132.74      | 129.30   |
| 35  | BB    | 2744 | G    | C2-N3-C4    | 6.87  | 115.33      | 111.90   |
| 1   | AA    | 662  | U    | O4'-C1'-N1  | 6.87  | 113.70      | 108.20   |
| 35  | BB    | 404  | A    | C4-C5-C6    | 6.87  | 120.44      | 117.00   |
| 35  | BB    | 2114 | A    | N3-C4-C5    | -6.87 | 121.99      | 126.80   |
| 35  | BB    | 2319 | G    | P-O3'-C3'   | 6.87  | 127.94      | 119.70   |
| 1   | AA    | 138  | G    | N1-C6-O6    | 6.87  | 124.02      | 119.90   |
| 1   | AA    | 292  | G    | O4'-C1'-N9  | 6.87  | 113.69      | 108.20   |
| 22  | AV    | 3    | G    | O4'-C1'-N9  | 6.87  | 113.69      | 108.20   |
| 35  | BB    | 79   | C    | N3-C4-N4    | 6.87  | 122.81      | 118.00   |
| 35  | BB    | 187  | G    | C5-C6-N1    | 6.87  | 114.93      | 111.50   |
| 35  | BB    | 256  | A    | C2-N3-C4    | -6.87 | 107.17      | 110.60   |
| 35  | BB    | 1073 | A    | C5-N7-C8    | 6.87  | 107.33      | 103.90   |
| 35  | BB    | 1087 | G    | C8-N9-C4    | -6.87 | 103.65      | 106.40   |
| 35  | BB    | 1180 | U    | C3'-C2'-C1' | 6.87  | 107.00      | 101.50   |
| 35  | BB    | 1509 | A    | N7-C8-N9    | 6.87  | 117.23      | 113.80   |
| 35  | BB    | 1636 | U    | O4'-C1'-N1  | 6.87  | 113.69      | 108.20   |
| 35  | BB    | 1680 | U    | O4'-C1'-N1  | 6.87  | 113.69      | 108.20   |
| 35  | BB    | 1689 | A    | N3-C4-N9    | 6.87  | 132.90      | 127.40   |
| 35  | BB    | 1913 | A    | N1-C6-N6    | 6.87  | 122.72      | 118.60   |
| 35  | BB    | 2447 | G    | N3-C4-N9    | -6.87 | 121.88      | 126.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 196  | A    | N1-C2-N3    | 6.87  | 132.73      | 129.30   |
| 1   | AA    | 1423 | G    | P-O3'-C3'   | -6.87 | 111.46      | 119.70   |
| 35  | BB    | 184  | C    | C4-C5-C6    | -6.87 | 113.97      | 117.40   |
| 35  | BB    | 1236 | G    | N3-C2-N2    | 6.87  | 124.71      | 119.90   |
| 35  | BB    | 1511 | G    | N1-C6-O6    | 6.87  | 124.02      | 119.90   |
| 35  | BB    | 2450 | A    | C5-C6-N1    | -6.87 | 114.27      | 117.70   |
| 1   | AA    | 1474 | U    | O4'-C1'-N1  | 6.87  | 113.69      | 108.20   |
| 35  | BB    | 789  | A    | N1-C2-N3    | 6.87  | 132.73      | 129.30   |
| 35  | BB    | 1164 | C    | C6-N1-C2    | -6.87 | 117.55      | 120.30   |
| 35  | BB    | 1719 | G    | N3-C2-N2    | 6.87  | 124.71      | 119.90   |
| 35  | BB    | 2492 | U    | O4'-C1'-N1  | 6.87  | 113.69      | 108.20   |
| 36  | BC    | 261  | ARG  | NE-CZ-NH2   | 6.87  | 123.73      | 120.30   |
| 36  | BC    | 261  | ARG  | NH1-CZ-NH2  | -6.87 | 111.85      | 119.40   |
| 1   | AA    | 22   | G    | C4-C5-C6    | 6.86  | 122.92      | 118.80   |
| 1   | AA    | 525  | C    | N3-C4-C5    | -6.86 | 119.16      | 121.90   |
| 1   | AA    | 990  | C    | O4'-C1'-N1  | 6.86  | 113.69      | 108.20   |
| 35  | BB    | 2129 | C    | C6-N1-C1'   | -6.86 | 112.56      | 120.80   |
| 35  | BB    | 2324 | U    | C5-C4-O4    | -6.86 | 121.78      | 125.90   |
| 35  | BB    | 2428 | G    | P-O3'-C3'   | 6.86  | 127.94      | 119.70   |
| 1   | AA    | 443  | C    | O4'-C1'-N1  | 6.86  | 113.69      | 108.20   |
| 1   | AA    | 566  | G    | O4'-C1'-N9  | 6.86  | 113.69      | 108.20   |
| 35  | BB    | 764  | A    | O4'-C1'-N9  | 6.86  | 113.69      | 108.20   |
| 1   | AA    | 596  | A    | C6-C5-N7    | -6.86 | 127.50      | 132.30   |
| 35  | BB    | 324  | A    | C8-N9-C4    | -6.86 | 103.06      | 105.80   |
| 35  | BB    | 979  | A    | C4-C5-C6    | 6.86  | 120.43      | 117.00   |
| 35  | BB    | 1493 | C    | C2-N1-C1'   | 6.86  | 126.35      | 118.80   |
| 35  | BB    | 2016 | U    | C5-C6-N1    | 6.86  | 126.13      | 122.70   |
| 35  | BB    | 2763 | G    | O4'-C1'-N9  | 6.86  | 113.69      | 108.20   |
| 35  | BB    | 2809 | A    | C6-N1-C2    | 6.86  | 122.72      | 118.60   |
| 1   | AA    | 254  | G    | N9-C1'-C2'  | -6.86 | 104.46      | 112.00   |
| 1   | AA    | 430  | A    | C8-N9-C4    | -6.86 | 103.06      | 105.80   |
| 6   | AF    | 5    | GLU  | OE1-CD-OE2  | 6.86  | 131.53      | 123.30   |
| 35  | BB    | 90   | U    | O4'-C1'-N1  | 6.86  | 113.69      | 108.20   |
| 35  | BB    | 873  | C    | O4'-C1'-N1  | 6.86  | 113.69      | 108.20   |
| 35  | BB    | 1064 | C    | N3-C4-N4    | 6.86  | 122.80      | 118.00   |
| 35  | BB    | 1332 | G    | N9-C4-C5    | -6.86 | 102.66      | 105.40   |
| 35  | BB    | 1518 | C    | O4'-C1'-N1  | 6.86  | 113.69      | 108.20   |
| 35  | BB    | 1857 | G    | C4'-C3'-C2' | 6.86  | 109.46      | 102.60   |
| 35  | BB    | 2283 | C    | N3-C4-N4    | 6.86  | 122.80      | 118.00   |
| 46  | BM    | 66   | ARG  | NE-CZ-NH2   | -6.86 | 116.87      | 120.30   |
| 1   | AA    | 794  | A    | N7-C8-N9    | 6.86  | 117.23      | 113.80   |
| 1   | AA    | 903  | G    | C1'-O4'-C4' | -6.86 | 104.42      | 109.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1295 | U    | N3-C4-C5    | -6.86 | 110.49      | 114.60   |
| 1   | AA    | 1454 | G    | C8-N9-C1'   | 6.86  | 135.91      | 127.00   |
| 35  | BB    | 114  | U    | C5-C6-N1    | 6.86  | 126.13      | 122.70   |
| 35  | BB    | 1154 | G    | C8-N9-C4    | -6.86 | 103.66      | 106.40   |
| 35  | BB    | 1472 | C    | C5-C4-N4    | -6.86 | 115.40      | 120.20   |
| 35  | BB    | 2298 | A    | C4-C5-C6    | 6.86  | 120.43      | 117.00   |
| 35  | BB    | 2686 | G    | C5-N7-C8    | 6.86  | 107.73      | 104.30   |
| 1   | AA    | 272  | C    | N3-C4-N4    | 6.85  | 122.80      | 118.00   |
| 35  | BB    | 138  | U    | C4'-C3'-C2' | -6.85 | 95.75       | 102.60   |
| 35  | BB    | 605  | G    | N3-C2-N2    | 6.85  | 124.70      | 119.90   |
| 35  | BB    | 1524 | G    | C2-N3-C4    | 6.85  | 115.33      | 111.90   |
| 1   | AA    | 668  | G    | C5-N7-C8    | 6.85  | 107.73      | 104.30   |
| 1   | AA    | 958  | A    | C6-C5-N7    | -6.85 | 127.50      | 132.30   |
| 1   | AA    | 977  | A    | C4-C5-N7    | -6.85 | 107.27      | 110.70   |
| 7   | AG    | 142  | ARG  | NE-CZ-NH1   | 6.85  | 123.73      | 120.30   |
| 34  | BA    | 78   | A    | C5-C6-N6    | -6.85 | 118.22      | 123.70   |
| 35  | BB    | 331  | C    | C6-N1-C2    | -6.85 | 117.56      | 120.30   |
| 35  | BB    | 521  | U    | N3-C4-O4    | 6.85  | 124.20      | 119.40   |
| 35  | BB    | 721  | A    | C5-C6-N1    | -6.85 | 114.27      | 117.70   |
| 35  | BB    | 1432 | G    | N3-C4-C5    | 6.85  | 132.03      | 128.60   |
| 35  | BB    | 2024 | G    | O4'-C1'-N9  | 6.85  | 113.68      | 108.20   |
| 35  | BB    | 2171 | A    | C6-C5-N7    | -6.85 | 127.50      | 132.30   |
| 35  | BB    | 2212 | A    | C2-N3-C4    | 6.85  | 114.03      | 110.60   |
| 35  | BB    | 2514 | U    | O4'-C1'-N1  | 6.85  | 113.68      | 108.20   |
| 1   | AA    | 1491 | G    | N7-C8-N9    | 6.85  | 116.53      | 113.10   |
| 35  | BB    | 515  | A    | C5-C6-N1    | -6.85 | 114.27      | 117.70   |
| 1   | AA    | 1275 | A    | O4'-C1'-N9  | 6.85  | 113.68      | 108.20   |
| 35  | BB    | 341  | C    | C2-N3-C4    | -6.85 | 116.48      | 119.90   |
| 35  | BB    | 2040 | G    | C2-N3-C4    | -6.85 | 108.47      | 111.90   |
| 35  | BB    | 2558 | C    | N3-C4-N4    | 6.85  | 122.80      | 118.00   |
| 22  | AV    | 69   | G    | N3-C4-C5    | 6.85  | 132.02      | 128.60   |
| 30  | B5    | 168  | ASN  | CA-CB-CG    | -6.85 | 98.34       | 113.40   |
| 35  | BB    | 149  | A    | N1-C6-N6    | 6.85  | 122.71      | 118.60   |
| 35  | BB    | 1370 | C    | C5-C4-N4    | 6.85  | 124.99      | 120.20   |
| 35  | BB    | 2827 | C    | C5-C4-N4    | -6.85 | 115.41      | 120.20   |
| 35  | BB    | 242  | G    | P-O3'-C3'   | 6.85  | 127.92      | 119.70   |
| 35  | BB    | 435  | C    | C2-N3-C4    | 6.85  | 123.32      | 119.90   |
| 35  | BB    | 797  | G    | N1-C2-N3    | -6.85 | 119.79      | 123.90   |
| 1   | AA    | 474  | G    | C5-N7-C8    | 6.84  | 107.72      | 104.30   |
| 17  | AQ    | 36   | PHE  | CB-CG-CD2   | 6.84  | 125.59      | 120.80   |
| 35  | BB    | 386  | G    | C8-N9-C4    | -6.84 | 103.66      | 106.40   |
| 35  | BB    | 557  | C    | C2-N3-C4    | 6.84  | 123.32      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 1524 | G    | C6-N1-C2   | 6.84  | 129.21      | 125.10   |
| 35  | BB    | 1808 | A    | C5-C6-N6   | -6.84 | 118.22      | 123.70   |
| 35  | BB    | 1965 | C    | N3-C4-N4   | 6.84  | 122.79      | 118.00   |
| 35  | BB    | 2718 | G    | C8-N9-C4   | -6.84 | 103.66      | 106.40   |
| 44  | BK    | 33   | ALA  | N-CA-CB    | 6.84  | 119.68      | 110.10   |
| 1   | AA    | 723  | U    | C5-C6-N1   | 6.84  | 126.12      | 122.70   |
| 1   | AA    | 823  | C    | C6-N1-C2   | 6.84  | 123.04      | 120.30   |
| 1   | AA    | 1021 | A    | C5-N7-C8   | 6.84  | 107.32      | 103.90   |
| 1   | AA    | 1134 | G    | C6-C5-N7   | -6.84 | 126.29      | 130.40   |
| 35  | BB    | 423  | A    | N9-C4-C5   | 6.84  | 108.54      | 105.80   |
| 35  | BB    | 2789 | C    | N3-C4-C5   | -6.84 | 119.16      | 121.90   |
| 1   | AA    | 47   | C    | C6-N1-C1'  | -6.84 | 112.59      | 120.80   |
| 1   | AA    | 982  | U    | N3-C4-O4   | 6.84  | 124.19      | 119.40   |
| 2   | AB    | 186  | VAL  | N-CA-C     | -6.84 | 92.53       | 111.00   |
| 34  | BA    | 82   | U    | C4-C5-C6   | -6.84 | 115.59      | 119.70   |
| 35  | BB    | 799  | G    | O4'-C1'-N9 | 6.84  | 113.67      | 108.20   |
| 35  | BB    | 1344 | U    | N3-C4-O4   | 6.84  | 124.19      | 119.40   |
| 35  | BB    | 1926 | U    | P-O5'-C5'  | 6.84  | 131.85      | 120.90   |
| 35  | BB    | 2564 | A    | N3-C4-C5   | -6.84 | 122.01      | 126.80   |
| 35  | BB    | 2663 | G    | N7-C8-N9   | -6.84 | 109.68      | 113.10   |
| 35  | BB    | 2837 | A    | C6-N1-C2   | 6.84  | 122.70      | 118.60   |
| 1   | AA    | 320  | A    | C5-C6-N6   | -6.84 | 118.23      | 123.70   |
| 1   | AA    | 1039 | G    | C8-N9-C4   | -6.84 | 103.67      | 106.40   |
| 1   | AA    | 1341 | U    | O4'-C1'-N1 | 6.84  | 113.67      | 108.20   |
| 1   | AA    | 1404 | C    | C5-C4-N4   | -6.84 | 115.41      | 120.20   |
| 35  | BB    | 1262 | A    | C5-C6-N1   | -6.84 | 114.28      | 117.70   |
| 35  | BB    | 1287 | A    | C4-C5-C6   | 6.84  | 120.42      | 117.00   |
| 38  | BE    | 69   | ARG  | NE-CZ-NH1  | 6.84  | 123.72      | 120.30   |
| 35  | BB    | 371  | A    | C8-N9-C4   | -6.84 | 103.06      | 105.80   |
| 35  | BB    | 829  | A    | C2-N3-C4   | 6.84  | 114.02      | 110.60   |
| 35  | BB    | 1871 | A    | C8-N9-C4   | -6.84 | 103.06      | 105.80   |
| 35  | BB    | 2417 | C    | C2-N3-C4   | 6.84  | 123.32      | 119.90   |
| 35  | BB    | 2509 | G    | P-O3'-C3'  | -6.84 | 111.50      | 119.70   |
| 39  | BF    | 141  | ASP  | CB-CG-OD1  | -6.84 | 112.15      | 118.30   |
| 1   | AA    | 1018 | G    | C2-N3-C4   | 6.84  | 115.32      | 111.90   |
| 1   | AA    | 1071 | C    | P-O3'-C3'  | -6.84 | 111.50      | 119.70   |
| 1   | AA    | 1105 | A    | N7-C8-N9   | -6.84 | 110.38      | 113.80   |
| 1   | AA    | 1459 | G    | N1-C2-N3   | -6.84 | 119.80      | 123.90   |
| 7   | AG    | 84   | TYR  | CB-CG-CD1  | 6.84  | 125.10      | 121.00   |
| 35  | BB    | 781  | A    | N3-C4-C5   | -6.84 | 122.01      | 126.80   |
| 35  | BB    | 944  | C    | O4'-C1'-N1 | 6.84  | 113.67      | 108.20   |
| 35  | BB    | 1046 | A    | C5-C6-N1   | -6.84 | 114.28      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1285 | A    | N1-C6-N6    | 6.84  | 122.70      | 118.60   |
| 35  | BB    | 1983 | G    | C6-C5-N7    | -6.84 | 126.30      | 130.40   |
| 35  | BB    | 2335 | A    | N9-C4-C5    | 6.84  | 108.53      | 105.80   |
| 1   | AA    | 680  | C    | O4'-C1'-N1  | 6.83  | 113.67      | 108.20   |
| 35  | BB    | 15   | G    | N7-C8-N9    | 6.83  | 116.52      | 113.10   |
| 35  | BB    | 518  | G    | N3-C4-C5    | 6.83  | 132.02      | 128.60   |
| 35  | BB    | 731  | C    | P-O3'-C3'   | -6.83 | 111.50      | 119.70   |
| 35  | BB    | 980  | A    | P-O3'-C3'   | 6.83  | 127.90      | 119.70   |
| 35  | BB    | 1763 | G    | N1-C2-N3    | -6.83 | 119.80      | 123.90   |
| 35  | BB    | 1893 | C    | C6-N1-C2    | -6.83 | 117.57      | 120.30   |
| 1   | AA    | 270  | A    | O4'-C1'-N9  | 6.83  | 113.67      | 108.20   |
| 1   | AA    | 408  | A    | N1-C6-N6    | 6.83  | 122.70      | 118.60   |
| 1   | AA    | 710  | G    | P-O3'-C3'   | -6.83 | 111.50      | 119.70   |
| 1   | AA    | 826  | C    | N3-C2-O2    | -6.83 | 117.12      | 121.90   |
| 1   | AA    | 983  | A    | N1-C2-N3    | 6.83  | 132.72      | 129.30   |
| 35  | BB    | 607  | U    | O4'-C1'-N1  | 6.83  | 113.67      | 108.20   |
| 35  | BB    | 1144 | A    | C5-N7-C8    | 6.83  | 107.32      | 103.90   |
| 35  | BB    | 2533 | U    | O4'-C1'-N1  | 6.83  | 113.67      | 108.20   |
| 1   | AA    | 159  | G    | N1-C6-O6    | 6.83  | 124.00      | 119.90   |
| 1   | AA    | 622  | A    | C6-C5-N7    | -6.83 | 127.52      | 132.30   |
| 1   | AA    | 978  | A    | N3-C4-C5    | -6.83 | 122.02      | 126.80   |
| 1   | AA    | 1421 | G    | N1-C6-O6    | 6.83  | 124.00      | 119.90   |
| 1   | AA    | 1454 | G    | N1-C2-N3    | -6.83 | 119.80      | 123.90   |
| 35  | BB    | 464  | U    | C5-C6-N1    | 6.83  | 126.11      | 122.70   |
| 35  | BB    | 935  | C    | O4'-C1'-N1  | 6.83  | 113.67      | 108.20   |
| 35  | BB    | 1047 | G    | N3-C2-N2    | 6.83  | 124.68      | 119.90   |
| 35  | BB    | 1654 | A    | P-O3'-C3'   | -6.83 | 111.50      | 119.70   |
| 35  | BB    | 1906 | G    | N1-C6-O6    | 6.83  | 124.00      | 119.90   |
| 35  | BB    | 1970 | A    | N1-C6-N6    | 6.83  | 122.70      | 118.60   |
| 35  | BB    | 2070 | A    | N1-C6-N6    | 6.83  | 122.70      | 118.60   |
| 35  | BB    | 2444 | G    | C4-C5-N7    | -6.83 | 108.07      | 110.80   |
| 31  | B6    | 18   | PHE  | CB-CG-CD2   | -6.83 | 116.02      | 120.80   |
| 35  | BB    | 362  | A    | C1'-O4'-C4' | 6.83  | 115.36      | 109.90   |
| 35  | BB    | 816  | C    | C5-C4-N4    | -6.83 | 115.42      | 120.20   |
| 35  | BB    | 1631 | G    | N9-C4-C5    | -6.83 | 102.67      | 105.40   |
| 35  | BB    | 2443 | C    | C5-C4-N4    | -6.83 | 115.42      | 120.20   |
| 1   | AA    | 289  | G    | C2-N3-C4    | 6.83  | 115.31      | 111.90   |
| 1   | AA    | 890  | G    | N3-C4-C5    | -6.83 | 125.19      | 128.60   |
| 1   | AA    | 1442 | G    | C6-C5-N7    | -6.83 | 126.30      | 130.40   |
| 35  | BB    | 74   | A    | C8-N9-C4    | -6.83 | 103.07      | 105.80   |
| 35  | BB    | 123  | G    | N1-C2-N3    | -6.83 | 119.80      | 123.90   |
| 35  | BB    | 485  | C    | C1'-O4'-C4' | -6.83 | 104.44      | 109.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 519  | U    | C5-C6-N1    | 6.83  | 126.11      | 122.70   |
| 35  | BB    | 892  | A    | N3-C4-N9    | 6.83  | 132.86      | 127.40   |
| 35  | BB    | 1866 | A    | N9-C4-C5    | 6.83  | 108.53      | 105.80   |
| 35  | BB    | 2284 | A    | C5-C6-N6    | -6.83 | 118.24      | 123.70   |
| 35  | BB    | 2450 | A    | C4-C5-C6    | 6.83  | 120.41      | 117.00   |
| 1   | AA    | 846  | G    | N3-C4-N9    | 6.83  | 130.10      | 126.00   |
| 35  | BB    | 1541 | C    | N3-C4-N4    | 6.83  | 122.78      | 118.00   |
| 35  | BB    | 2448 | A    | C8-N9-C4    | -6.83 | 103.07      | 105.80   |
| 1   | AA    | 141  | G    | C4-C5-C6    | 6.83  | 122.89      | 118.80   |
| 1   | AA    | 147  | G    | C5-C6-O6    | -6.83 | 124.50      | 128.60   |
| 1   | AA    | 557  | G    | C4-C5-N7    | -6.83 | 108.07      | 110.80   |
| 1   | AA    | 559  | A    | O4'-C1'-N9  | 6.83  | 113.66      | 108.20   |
| 1   | AA    | 1046 | A    | N1-C2-N3    | 6.83  | 132.71      | 129.30   |
| 1   | AA    | 1066 | C    | O4'-C1'-N1  | 6.83  | 113.66      | 108.20   |
| 1   | AA    | 1452 | C    | C5-C6-N1    | 6.83  | 124.41      | 121.00   |
| 22  | AV    | 14   | A    | C4-C5-C6    | 6.83  | 120.41      | 117.00   |
| 35  | BB    | 310  | A    | C1'-O4'-C4' | -6.83 | 104.44      | 109.90   |
| 35  | BB    | 640  | C    | C3'-C2'-C1' | -6.83 | 96.04       | 101.50   |
| 35  | BB    | 743  | A    | C8-N9-C4    | 6.83  | 108.53      | 105.80   |
| 35  | BB    | 1410 | G    | C5-C6-O6    | -6.83 | 124.50      | 128.60   |
| 35  | BB    | 2102 | G    | C8-N9-C4    | 6.83  | 109.13      | 106.40   |
| 35  | BB    | 2775 | G    | N1-C6-O6    | 6.83  | 124.00      | 119.90   |
| 1   | AA    | 44   | A    | C6-N1-C2    | -6.82 | 114.51      | 118.60   |
| 1   | AA    | 630  | A    | N1-C6-N6    | 6.82  | 122.69      | 118.60   |
| 1   | AA    | 869  | G    | C6-C5-N7    | -6.82 | 126.31      | 130.40   |
| 1   | AA    | 1099 | G    | C5-C6-O6    | -6.82 | 124.51      | 128.60   |
| 22  | AV    | 76   | A    | N1-C6-N6    | 6.82  | 122.69      | 118.60   |
| 35  | BB    | 80   | G    | O4'-C1'-N9  | 6.82  | 113.66      | 108.20   |
| 35  | BB    | 1312 | U    | C5-C6-N1    | -6.82 | 119.29      | 122.70   |
| 35  | BB    | 2239 | G    | C6-C5-N7    | -6.82 | 126.31      | 130.40   |
| 35  | BB    | 2440 | C    | C5-C4-N4    | -6.82 | 115.42      | 120.20   |
| 35  | BB    | 2784 | U    | N1-C2-O2    | 6.82  | 127.58      | 122.80   |
| 1   | AA    | 234  | C    | O4'-C1'-N1  | 6.82  | 113.66      | 108.20   |
| 35  | BB    | 874  | G    | C4-N9-C1'   | 6.82  | 135.37      | 126.50   |
| 35  | BB    | 1793 | C    | O4'-C1'-N1  | 6.82  | 113.66      | 108.20   |
| 35  | BB    | 1928 | A    | N1-C2-N3    | 6.82  | 132.71      | 129.30   |
| 35  | BB    | 2004 | G    | C5-C6-N1    | -6.82 | 108.09      | 111.50   |
| 1   | AA    | 1218 | C    | C5-C6-N1    | 6.82  | 124.41      | 121.00   |
| 1   | AA    | 1230 | C    | N3-C4-C5    | -6.82 | 119.17      | 121.90   |
| 1   | AA    | 1275 | A    | C5-C6-N1    | -6.82 | 114.29      | 117.70   |
| 35  | BB    | 339  | U    | C1'-O4'-C4' | -6.82 | 104.44      | 109.90   |
| 35  | BB    | 1287 | A    | C5-C6-N1    | -6.82 | 114.29      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1434 | A    | C5-N7-C8    | 6.82  | 107.31      | 103.90   |
| 35  | BB    | 1694 | C    | C6-N1-C1'   | -6.82 | 112.62      | 120.80   |
| 35  | BB    | 1845 | G    | N3-C2-N2    | 6.82  | 124.67      | 119.90   |
| 35  | BB    | 1978 | A    | N9-C4-C5    | -6.82 | 103.07      | 105.80   |
| 35  | BB    | 2565 | A    | C6-N1-C2    | 6.82  | 122.69      | 118.60   |
| 35  | BB    | 2617 | U    | N3-C2-O2    | 6.82  | 126.97      | 122.20   |
| 1   | AA    | 1226 | C    | C5-C6-N1    | 6.82  | 124.41      | 121.00   |
| 35  | BB    | 1699 | G    | O4'-C1'-C2' | -6.82 | 98.98       | 105.80   |
| 35  | BB    | 1851 | U    | C5'-C4'-O4' | 6.82  | 117.28      | 109.10   |
| 1   | AA    | 138  | G    | N3-C4-C5    | 6.82  | 132.01      | 128.60   |
| 1   | AA    | 408  | A    | C4'-C3'-C2' | -6.82 | 95.78       | 102.60   |
| 1   | AA    | 497  | G    | N1-C2-N3    | -6.82 | 119.81      | 123.90   |
| 1   | AA    | 639  | G    | N1-C2-N3    | -6.82 | 119.81      | 123.90   |
| 2   | AB    | 166  | ASP  | CB-CG-OD1   | -6.82 | 112.17      | 118.30   |
| 22  | AV    | 29   | G    | C5-C6-O6    | -6.82 | 124.51      | 128.60   |
| 35  | BB    | 888  | C    | N3-C4-C5    | -6.82 | 119.17      | 121.90   |
| 35  | BB    | 1015 | U    | N3-C4-O4    | 6.82  | 124.17      | 119.40   |
| 35  | BB    | 1034 | G    | C4-C5-N7    | 6.82  | 113.53      | 110.80   |
| 35  | BB    | 1899 | A    | C8-N9-C4    | -6.82 | 103.07      | 105.80   |
| 1   | AA    | 94   | G    | C5-C6-O6    | -6.82 | 124.51      | 128.60   |
| 1   | AA    | 161  | A    | C8-N9-C4    | -6.82 | 103.07      | 105.80   |
| 1   | AA    | 199  | A    | C5-C6-N1    | -6.82 | 114.29      | 117.70   |
| 1   | AA    | 445  | G    | O4'-C1'-N9  | 6.82  | 113.65      | 108.20   |
| 1   | AA    | 685  | G    | N1-C6-O6    | 6.82  | 123.99      | 119.90   |
| 1   | AA    | 755  | G    | P-O5'-C5'   | -6.82 | 110.00      | 120.90   |
| 1   | AA    | 1431 | A    | C5-C6-N1    | -6.82 | 114.29      | 117.70   |
| 1   | AA    | 1491 | G    | N1-C2-N3    | -6.82 | 119.81      | 123.90   |
| 35  | BB    | 98   | G    | C4-C5-N7    | -6.82 | 108.07      | 110.80   |
| 35  | BB    | 997  | G    | N3-C2-N2    | 6.82  | 124.67      | 119.90   |
| 35  | BB    | 2017 | U    | C1'-O4'-C4' | -6.82 | 104.45      | 109.90   |
| 1   | AA    | 974  | A    | C5'-C4'-C3' | -6.81 | 105.10      | 116.00   |
| 35  | BB    | 765  | C    | O4'-C1'-N1  | 6.81  | 113.65      | 108.20   |
| 35  | BB    | 1878 | G    | O4'-C1'-N9  | 6.81  | 113.65      | 108.20   |
| 35  | BB    | 2153 | C    | O4'-C1'-N1  | 6.81  | 113.65      | 108.20   |
| 35  | BB    | 2738 | A    | N3-C4-N9    | 6.81  | 132.85      | 127.40   |
| 1   | AA    | 49   | U    | N3-C4-C5    | -6.81 | 110.51      | 114.60   |
| 1   | AA    | 144  | G    | C5-C6-O6    | -6.81 | 124.51      | 128.60   |
| 1   | AA    | 592  | G    | C6-N1-C2    | 6.81  | 129.19      | 125.10   |
| 1   | AA    | 616  | G    | C6-C5-N7    | -6.81 | 126.31      | 130.40   |
| 1   | AA    | 806  | C    | C5-C4-N4    | -6.81 | 115.43      | 120.20   |
| 1   | AA    | 971  | G    | C5-C6-O6    | -6.81 | 124.51      | 128.60   |
| 1   | AA    | 975  | A    | N9-C4-C5    | 6.81  | 108.53      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1442 | G    | C4-C5-C6    | 6.81  | 122.89      | 118.80   |
| 35  | BB    | 560  | C    | O4'-C1'-N1  | 6.81  | 113.65      | 108.20   |
| 35  | BB    | 2292 | U    | N3-C4-C5    | -6.81 | 110.51      | 114.60   |
| 1   | AA    | 171  | A    | N7-C8-N9    | -6.81 | 110.39      | 113.80   |
| 35  | BB    | 2699 | C    | N3-C4-C5    | -6.81 | 119.18      | 121.90   |
| 35  | BB    | 2754 | U    | N3-C4-C5    | 6.81  | 118.69      | 114.60   |
| 1   | AA    | 511  | C    | C6-N1-C2    | 6.81  | 123.02      | 120.30   |
| 1   | AA    | 743  | A    | C4-C5-C6    | 6.81  | 120.41      | 117.00   |
| 1   | AA    | 823  | C    | N3-C4-C5    | -6.81 | 119.18      | 121.90   |
| 1   | AA    | 833  | G    | N7-C8-N9    | -6.81 | 109.69      | 113.10   |
| 35  | BB    | 1836 | C    | O4'-C1'-N1  | 6.81  | 113.65      | 108.20   |
| 35  | BB    | 2821 | A    | C2-N3-C4    | 6.81  | 114.00      | 110.60   |
| 35  | BB    | 2888 | C    | N3-C4-C5    | -6.81 | 119.18      | 121.90   |
| 1   | AA    | 834  | U    | N3-C2-O2    | 6.81  | 126.97      | 122.20   |
| 35  | BB    | 246  | C    | C6-N1-C2    | 6.81  | 123.02      | 120.30   |
| 35  | BB    | 445  | C    | C6-N1-C2    | -6.81 | 117.58      | 120.30   |
| 35  | BB    | 894  | U    | C5-C4-O4    | 6.81  | 129.98      | 125.90   |
| 35  | BB    | 1202 | G    | N9-C4-C5    | 6.81  | 108.12      | 105.40   |
| 35  | BB    | 1371 | G    | C5-N7-C8    | -6.81 | 100.90      | 104.30   |
| 35  | BB    | 1581 | G    | O4'-C1'-N9  | 6.81  | 113.65      | 108.20   |
| 35  | BB    | 1891 | G    | N1-C2-N2    | -6.81 | 110.07      | 116.20   |
| 35  | BB    | 2017 | U    | O4'-C1'-N1  | 6.81  | 113.64      | 108.20   |
| 35  | BB    | 2345 | G    | C8-N9-C4    | 6.81  | 109.12      | 106.40   |
| 35  | BB    | 2413 | G    | C6-C5-N7    | -6.81 | 126.32      | 130.40   |
| 35  | BB    | 2675 | A    | C5-C6-N6    | -6.81 | 118.25      | 123.70   |
| 35  | BB    | 2693 | G    | C5-C6-O6    | -6.81 | 124.52      | 128.60   |
| 1   | AA    | 931  | C    | P-O3'-C3'   | -6.81 | 111.53      | 119.70   |
| 1   | AA    | 1332 | A    | N1-C6-N6    | 6.81  | 122.68      | 118.60   |
| 35  | BB    | 282  | A    | C5-C6-N1    | -6.81 | 114.30      | 117.70   |
| 35  | BB    | 2645 | G    | N9-C4-C5    | -6.81 | 102.68      | 105.40   |
| 1   | AA    | 73   | C    | C5-C4-N4    | -6.80 | 115.44      | 120.20   |
| 1   | AA    | 121  | U    | C4'-C3'-C2' | -6.80 | 95.80       | 102.60   |
| 1   | AA    | 1290 | G    | N1-C2-N3    | -6.80 | 119.82      | 123.90   |
| 1   | AA    | 1352 | C    | P-O3'-C3'   | 6.80  | 127.87      | 119.70   |
| 30  | B5    | 122  | ARG  | NE-CZ-NH1   | 6.80  | 123.70      | 120.30   |
| 35  | BB    | 265  | A    | N7-C8-N9    | -6.80 | 110.40      | 113.80   |
| 35  | BB    | 292  | U    | N3-C4-O4    | 6.80  | 124.16      | 119.40   |
| 35  | BB    | 777  | G    | N7-C8-N9    | -6.80 | 109.70      | 113.10   |
| 35  | BB    | 857  | G    | C2-N3-C4    | 6.80  | 115.30      | 111.90   |
| 35  | BB    | 1354 | A    | C5-C6-N1    | -6.80 | 114.30      | 117.70   |
| 35  | BB    | 1447 | C    | P-O3'-C3'   | -6.80 | 111.54      | 119.70   |
| 35  | BB    | 1602 | U    | C5'-C4'-O4' | 6.80  | 117.27      | 109.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1645 | G    | C6-C5-N7    | -6.80 | 126.32      | 130.40   |
| 35  | BB    | 2067 | G    | N1-C6-O6    | 6.80  | 123.98      | 119.90   |
| 34  | BA    | 10   | G    | O4'-C1'-N9  | 6.80  | 113.64      | 108.20   |
| 35  | BB    | 973  | A    | C8-N9-C4    | -6.80 | 103.08      | 105.80   |
| 35  | BB    | 1095 | A    | C4-C5-C6    | 6.80  | 120.40      | 117.00   |
| 35  | BB    | 1287 | A    | P-O5'-C5'   | 6.80  | 131.78      | 120.90   |
| 36  | BC    | 42   | ARG  | NE-CZ-NH2   | -6.80 | 116.90      | 120.30   |
| 1   | AA    | 334  | C    | C2-N3-C4    | -6.80 | 116.50      | 119.90   |
| 1   | AA    | 616  | G    | C4-N9-C1'   | 6.80  | 135.34      | 126.50   |
| 1   | AA    | 690  | G    | C5-C6-O6    | -6.80 | 124.52      | 128.60   |
| 1   | AA    | 1212 | U    | C4-C5-C6    | 6.80  | 123.78      | 119.70   |
| 35  | BB    | 88   | G    | C6-C5-N7    | -6.80 | 126.32      | 130.40   |
| 35  | BB    | 120  | U    | N3-C4-C5    | -6.80 | 110.52      | 114.60   |
| 35  | BB    | 523  | C    | N3-C4-N4    | 6.80  | 122.76      | 118.00   |
| 35  | BB    | 633  | A    | C4-C5-C6    | 6.80  | 120.40      | 117.00   |
| 35  | BB    | 654  | A    | C8-N9-C4    | -6.80 | 103.08      | 105.80   |
| 35  | BB    | 1168 | G    | N1-C2-N2    | -6.80 | 110.08      | 116.20   |
| 35  | BB    | 1920 | C    | P-O5'-C5'   | 6.80  | 131.78      | 120.90   |
| 35  | BB    | 2205 | A    | C5-C6-N1    | -6.80 | 114.30      | 117.70   |
| 47  | BN    | 87   | PHE  | CB-CG-CD2   | 6.80  | 125.56      | 120.80   |
| 51  | BR    | 13   | ARG  | NE-CZ-NH1   | -6.80 | 116.90      | 120.30   |
| 35  | BB    | 91   | A    | C8-N9-C4    | 6.80  | 108.52      | 105.80   |
| 35  | BB    | 266  | G    | C4-C5-C6    | 6.80  | 122.88      | 118.80   |
| 35  | BB    | 365  | U    | N3-C4-O4    | 6.80  | 124.16      | 119.40   |
| 35  | BB    | 1852 | U    | C5-C4-O4    | -6.80 | 121.82      | 125.90   |
| 35  | BB    | 2145 | C    | C4'-C3'-C2' | 6.80  | 109.40      | 102.60   |
| 1   | AA    | 705  | G    | C4'-C3'-C2' | -6.80 | 95.80       | 102.60   |
| 1   | AA    | 1111 | A    | C5-C6-N1    | -6.80 | 114.30      | 117.70   |
| 4   | AD    | 163  | GLN  | N-CA-CB     | 6.80  | 122.84      | 110.60   |
| 35  | BB    | 322  | A    | C5-C6-N6    | -6.80 | 118.26      | 123.70   |
| 35  | BB    | 1074 | G    | N1-C2-N3    | -6.80 | 119.82      | 123.90   |
| 35  | BB    | 2399 | G    | C6-N1-C2    | 6.80  | 129.18      | 125.10   |
| 1   | AA    | 210  | C    | C3'-C2'-C1' | -6.80 | 96.06       | 101.50   |
| 1   | AA    | 364  | A    | O4'-C4'-C3' | -6.80 | 97.20       | 104.00   |
| 1   | AA    | 769  | G    | C8-N9-C4    | 6.80  | 109.12      | 106.40   |
| 1   | AA    | 1345 | U    | N1-C2-N3    | 6.80  | 118.98      | 114.90   |
| 17  | AQ    | 10   | ARG  | NE-CZ-NH2   | -6.80 | 116.90      | 120.30   |
| 35  | BB    | 333  | G    | C6-C5-N7    | -6.80 | 126.32      | 130.40   |
| 35  | BB    | 348  | A    | C2-N3-C4    | 6.80  | 114.00      | 110.60   |
| 35  | BB    | 644  | A    | C5-N7-C8    | 6.80  | 107.30      | 103.90   |
| 35  | BB    | 1639 | C    | O4'-C1'-N1  | 6.80  | 113.64      | 108.20   |
| 35  | BB    | 1643 | G    | O4'-C1'-N9  | 6.80  | 113.64      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1728 | C    | O4'-C1'-N1  | 6.80  | 113.64      | 108.20   |
| 35  | BB    | 1825 | U    | OP1-P-OP2   | -6.80 | 109.41      | 119.60   |
| 35  | BB    | 2482 | A    | C5-N7-C8    | 6.80  | 107.30      | 103.90   |
| 35  | BB    | 2556 | C    | N3-C2-O2    | 6.80  | 126.66      | 121.90   |
| 1   | AA    | 720  | C    | O4'-C1'-N1  | 6.79  | 113.64      | 108.20   |
| 1   | AA    | 1010 | U    | C3'-C2'-C1' | -6.79 | 96.06       | 101.50   |
| 1   | AA    | 1285 | A    | C4-C5-C6    | 6.79  | 120.40      | 117.00   |
| 35  | BB    | 291  | G    | C4-C5-N7    | 6.79  | 113.52      | 110.80   |
| 35  | BB    | 414  | C    | N3-C4-N4    | 6.79  | 122.76      | 118.00   |
| 35  | BB    | 632  | A    | N1-C2-N3    | 6.79  | 132.70      | 129.30   |
| 35  | BB    | 1001 | A    | C8-N9-C4    | -6.79 | 103.08      | 105.80   |
| 35  | BB    | 1038 | G    | N3-C4-N9    | 6.79  | 130.08      | 126.00   |
| 35  | BB    | 1080 | A    | O4'-C1'-N9  | 6.79  | 113.64      | 108.20   |
| 1   | AA    | 275  | G    | C8-N9-C4    | 6.79  | 109.12      | 106.40   |
| 1   | AA    | 583  | A    | C5-C6-N1    | -6.79 | 114.30      | 117.70   |
| 1   | AA    | 1461 | G    | O4'-C1'-N9  | 6.79  | 113.64      | 108.20   |
| 35  | BB    | 232  | G    | N3-C2-N2    | 6.79  | 124.66      | 119.90   |
| 35  | BB    | 289  | G    | O4'-C1'-N9  | 6.79  | 113.64      | 108.20   |
| 35  | BB    | 689  | A    | C8-N9-C4    | 6.79  | 108.52      | 105.80   |
| 35  | BB    | 967  | U    | N3-C4-O4    | 6.79  | 124.16      | 119.40   |
| 35  | BB    | 1246 | A    | N1-C2-N3    | 6.79  | 132.70      | 129.30   |
| 35  | BB    | 1966 | A    | C6-C5-N7    | -6.79 | 127.54      | 132.30   |
| 1   | AA    | 156  | C    | C1'-O4'-C4' | 6.79  | 115.33      | 109.90   |
| 1   | AA    | 171  | A    | C5-N7-C8    | 6.79  | 107.30      | 103.90   |
| 1   | AA    | 342  | C    | O4'-C1'-N1  | 6.79  | 113.63      | 108.20   |
| 1   | AA    | 466  | A    | C5'-C4'-O4' | 6.79  | 117.25      | 109.10   |
| 1   | AA    | 1385 | G    | N3-C2-N2    | -6.79 | 115.14      | 119.90   |
| 3   | AC    | 22   | PHE  | CB-CG-CD1   | -6.79 | 116.05      | 120.80   |
| 16  | AP    | 25   | ARG  | NE-CZ-NH2   | -6.79 | 116.90      | 120.30   |
| 35  | BB    | 215  | G    | N1-C2-N3    | -6.79 | 119.83      | 123.90   |
| 35  | BB    | 216  | A    | N3-C4-N9    | 6.79  | 132.83      | 127.40   |
| 35  | BB    | 329  | G    | C5-N7-C8    | -6.79 | 100.91      | 104.30   |
| 35  | BB    | 1112 | G    | C4-C5-C6    | 6.79  | 122.88      | 118.80   |
| 35  | BB    | 1394 | U    | C3'-C2'-C1' | 6.79  | 106.93      | 101.50   |
| 35  | BB    | 1785 | A    | O4'-C1'-N9  | 6.79  | 113.63      | 108.20   |
| 35  | BB    | 1913 | A    | N3-C4-N9    | 6.79  | 132.83      | 127.40   |
| 35  | BB    | 2636 | C    | N3-C2-O2    | 6.79  | 126.65      | 121.90   |
| 1   | AA    | 66   | A    | C4-C5-C6    | 6.79  | 120.39      | 117.00   |
| 1   | AA    | 655  | A    | C6-C5-N7    | -6.79 | 127.55      | 132.30   |
| 1   | AA    | 816  | A    | N9-C4-C5    | 6.79  | 108.52      | 105.80   |
| 1   | AA    | 352  | C    | C5-C6-N1    | 6.79  | 124.39      | 121.00   |
| 1   | AA    | 944  | G    | N1-C6-O6    | 6.79  | 123.97      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 983  | A    | C4-C5-C6    | 6.79  | 120.39      | 117.00   |
| 1   | AA    | 1025 | U    | C5-C6-N1    | -6.79 | 119.31      | 122.70   |
| 1   | AA    | 1316 | G    | C5-C6-N1    | -6.79 | 108.11      | 111.50   |
| 35  | BB    | 518  | G    | C6-N1-C2    | -6.79 | 121.03      | 125.10   |
| 35  | BB    | 1212 | G    | C3'-C2'-C1' | 6.79  | 106.93      | 101.50   |
| 35  | BB    | 1361 | G    | C5-C6-O6    | -6.79 | 124.53      | 128.60   |
| 35  | BB    | 2276 | G    | N9-C4-C5    | -6.79 | 102.69      | 105.40   |
| 1   | AA    | 736  | C    | C3'-C2'-C1' | -6.79 | 96.07       | 101.50   |
| 1   | AA    | 1468 | A    | C8-N9-C4    | -6.79 | 103.08      | 105.80   |
| 1   | AA    | 1494 | G    | C4'-C3'-C2' | -6.79 | 95.81       | 102.60   |
| 35  | BB    | 267  | C    | C2-N3-C4    | 6.79  | 123.29      | 119.90   |
| 35  | BB    | 992  | C    | N3-C4-C5    | -6.79 | 119.19      | 121.90   |
| 35  | BB    | 1196 | C    | C4-C5-C6    | 6.79  | 120.79      | 117.40   |
| 1   | AA    | 40   | C    | C6-N1-C2    | -6.79 | 117.59      | 120.30   |
| 1   | AA    | 286  | C    | C2-N1-C1'   | 6.79  | 126.26      | 118.80   |
| 1   | AA    | 517  | G    | N1-C2-N3    | -6.79 | 119.83      | 123.90   |
| 4   | AD    | 28   | ASP  | CB-CG-OD1   | -6.79 | 112.19      | 118.30   |
| 35  | BB    | 64   | A    | O4'-C4'-C3' | -6.79 | 97.21       | 104.00   |
| 35  | BB    | 886  | A    | N7-C8-N9    | -6.79 | 110.41      | 113.80   |
| 35  | BB    | 975  | A    | C4-C5-C6    | 6.79  | 120.39      | 117.00   |
| 35  | BB    | 1030 | C    | N3-C2-O2    | -6.79 | 117.15      | 121.90   |
| 35  | BB    | 1129 | A    | C5-N7-C8    | 6.79  | 107.29      | 103.90   |
| 35  | BB    | 2193 | G    | N3-C4-C5    | -6.79 | 125.21      | 128.60   |
| 35  | BB    | 2197 | U    | O4'-C1'-N1  | 6.79  | 113.63      | 108.20   |
| 35  | BB    | 2766 | A    | C6-C5-N7    | -6.79 | 127.55      | 132.30   |
| 35  | BB    | 2816 | G    | C4-C5-N7    | -6.79 | 108.09      | 110.80   |
| 1   | AA    | 727  | G    | C8-N9-C4    | -6.78 | 103.69      | 106.40   |
| 35  | BB    | 864  | G    | N1-C2-N3    | -6.78 | 119.83      | 123.90   |
| 35  | BB    | 1471 | G    | C6-C5-N7    | -6.78 | 126.33      | 130.40   |
| 35  | BB    | 1577 | C    | C6-N1-C2    | -6.78 | 117.59      | 120.30   |
| 35  | BB    | 1731 | G    | C5-N7-C8    | 6.78  | 107.69      | 104.30   |
| 35  | BB    | 2151 | U    | O4'-C1'-N1  | 6.78  | 113.63      | 108.20   |
| 35  | BB    | 2370 | G    | N9-C4-C5    | -6.78 | 102.69      | 105.40   |
| 1   | AA    | 21   | G    | C4'-C3'-C2' | -6.78 | 95.82       | 102.60   |
| 1   | AA    | 196  | A    | C5-C6-N1    | -6.78 | 114.31      | 117.70   |
| 1   | AA    | 229  | U    | C5-C4-O4    | -6.78 | 121.83      | 125.90   |
| 1   | AA    | 636  | U    | O4'-C1'-N1  | 6.78  | 113.62      | 108.20   |
| 1   | AA    | 742  | G    | C4'-C3'-C2' | -6.78 | 95.82       | 102.60   |
| 1   | AA    | 929  | G    | C5-N7-C8    | 6.78  | 107.69      | 104.30   |
| 1   | AA    | 1214 | C    | P-O3'-C3'   | 6.78  | 127.84      | 119.70   |
| 1   | AA    | 1255 | G    | N3-C2-N2    | 6.78  | 124.65      | 119.90   |
| 35  | BB    | 1574 | C    | N1-C2-O2    | -6.78 | 114.83      | 118.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2479 | U    | C2-N3-C4    | -6.78 | 122.93      | 127.00   |
| 35  | BB    | 2894 | G    | C6-C5-N7    | -6.78 | 126.33      | 130.40   |
| 35  | BB    | 2758 | A    | C5-N7-C8    | 6.78  | 107.29      | 103.90   |
| 1   | AA    | 40   | C    | OP2-P-O3'   | 6.78  | 120.11      | 105.20   |
| 1   | AA    | 353  | A    | O4'-C1'-N9  | 6.78  | 113.62      | 108.20   |
| 1   | AA    | 1146 | A    | P-O3'-C3'   | -6.78 | 111.57      | 119.70   |
| 9   | AI    | 17   | ARG  | NE-CZ-NH1   | 6.78  | 123.69      | 120.30   |
| 35  | BB    | 1136 | G    | C4-C5-N7    | -6.78 | 108.09      | 110.80   |
| 35  | BB    | 1168 | G    | C5-C6-O6    | -6.78 | 124.53      | 128.60   |
| 35  | BB    | 2619 | C    | N3-C4-N4    | 6.78  | 122.75      | 118.00   |
| 35  | BB    | 2709 | G    | O4'-C4'-C3' | -6.78 | 97.22       | 104.00   |
| 1   | AA    | 101  | A    | N7-C8-N9    | 6.78  | 117.19      | 113.80   |
| 1   | AA    | 966  | G    | N7-C8-N9    | -6.78 | 109.71      | 113.10   |
| 1   | AA    | 1038 | C    | C5-C4-N4    | -6.78 | 115.46      | 120.20   |
| 1   | AA    | 1074 | G    | C5-N7-C8    | -6.78 | 100.91      | 104.30   |
| 1   | AA    | 1170 | A    | O4'-C1'-N9  | 6.78  | 113.62      | 108.20   |
| 1   | AA    | 1397 | C    | O4'-C1'-N1  | 6.78  | 113.62      | 108.20   |
| 1   | AA    | 1437 | A    | C5-C6-N6    | -6.78 | 118.28      | 123.70   |
| 1   | AA    | 1523 | G    | C2-N3-C4    | -6.78 | 108.51      | 111.90   |
| 35  | BB    | 103  | A    | C2-N3-C4    | 6.78  | 113.99      | 110.60   |
| 35  | BB    | 1416 | G    | P-O3'-C3'   | 6.78  | 127.83      | 119.70   |
| 35  | BB    | 2596 | U    | N3-C4-O4    | 6.78  | 124.14      | 119.40   |
| 35  | BB    | 2822 | G    | C4-C5-N7    | -6.78 | 108.09      | 110.80   |
| 1   | AA    | 631  | C    | N3-C4-N4    | 6.77  | 122.74      | 118.00   |
| 1   | AA    | 1284 | C    | N3-C4-N4    | 6.77  | 122.74      | 118.00   |
| 35  | BB    | 35   | G    | N1-C6-O6    | 6.77  | 123.96      | 119.90   |
| 35  | BB    | 1294 | U    | O4'-C1'-N1  | 6.77  | 113.62      | 108.20   |
| 35  | BB    | 1448 | G    | N1-C2-N2    | -6.77 | 110.10      | 116.20   |
| 35  | BB    | 1840 | G    | N9-C4-C5    | -6.77 | 102.69      | 105.40   |
| 36  | BC    | 269  | ARG  | NE-CZ-NH2   | -6.77 | 116.91      | 120.30   |
| 1   | AA    | 878  | A    | C2-N3-C4    | -6.77 | 107.21      | 110.60   |
| 1   | AA    | 1198 | G    | C5-N7-C8    | 6.77  | 107.69      | 104.30   |
| 22  | AV    | 66   | C    | N3-C4-C5    | -6.77 | 119.19      | 121.90   |
| 35  | BB    | 205  | G    | C6-N1-C2    | -6.77 | 121.04      | 125.10   |
| 35  | BB    | 491  | G    | O4'-C1'-N9  | 6.77  | 113.62      | 108.20   |
| 35  | BB    | 791  | C    | C4'-C3'-C2' | -6.77 | 95.83       | 102.60   |
| 35  | BB    | 1630 | A    | P-O3'-C3'   | -6.77 | 111.57      | 119.70   |
| 35  | BB    | 2176 | A    | C8-N9-C4    | -6.77 | 103.09      | 105.80   |
| 35  | BB    | 2247 | A    | C2-N3-C4    | -6.77 | 107.21      | 110.60   |
| 1   | AA    | 389  | A    | N1-C6-N6    | 6.77  | 122.66      | 118.60   |
| 1   | AA    | 529  | G    | C6-N1-C2    | 6.77  | 129.16      | 125.10   |
| 1   | AA    | 625  | U    | P-O3'-C3'   | 6.77  | 127.83      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1193 | G    | C6-N1-C2    | -6.77 | 121.04      | 125.10   |
| 35  | BB    | 221  | A    | C5-C6-N1    | -6.77 | 114.31      | 117.70   |
| 35  | BB    | 979  | A    | O4'-C1'-N9  | 6.77  | 113.62      | 108.20   |
| 35  | BB    | 1376 | C    | N3-C4-N4    | 6.77  | 122.74      | 118.00   |
| 35  | BB    | 1848 | A    | N3-C4-N9    | 6.77  | 132.82      | 127.40   |
| 35  | BB    | 2755 | C    | C5-C6-N1    | 6.77  | 124.39      | 121.00   |
| 1   | AA    | 720  | C    | C2-N3-C4    | -6.77 | 116.52      | 119.90   |
| 1   | AA    | 925  | G    | N3-C4-N9    | 6.77  | 130.06      | 126.00   |
| 4   | AD    | 127  | ARG  | NE-CZ-NH1   | 6.77  | 123.69      | 120.30   |
| 22  | AV    | 69   | G    | N9-C4-C5    | -6.77 | 102.69      | 105.40   |
| 35  | BB    | 278  | A    | C5-N7-C8    | 6.77  | 107.28      | 103.90   |
| 35  | BB    | 416  | U    | N3-C2-O2    | -6.77 | 117.46      | 122.20   |
| 35  | BB    | 592  | A    | N1-C6-N6    | 6.77  | 122.66      | 118.60   |
| 35  | BB    | 922  | C    | C5-C4-N4    | -6.77 | 115.46      | 120.20   |
| 35  | BB    | 924  | G    | C5-C6-O6    | -6.77 | 124.54      | 128.60   |
| 35  | BB    | 1337 | G    | C1'-O4'-C4' | 6.77  | 115.32      | 109.90   |
| 35  | BB    | 2289 | G    | O4'-C1'-N9  | 6.77  | 113.62      | 108.20   |
| 35  | BB    | 2804 | U    | O4'-C1'-N1  | 6.77  | 113.61      | 108.20   |
| 50  | BQ    | 112  | ALA  | N-CA-CB     | 6.77  | 119.58      | 110.10   |
| 1   | AA    | 267  | C    | N3-C4-C5    | -6.77 | 119.19      | 121.90   |
| 35  | BB    | 491  | G    | C2-N3-C4    | 6.77  | 115.28      | 111.90   |
| 35  | BB    | 520  | G    | C8-N9-C4    | -6.77 | 103.69      | 106.40   |
| 35  | BB    | 1396 | U    | C6-N1-C2    | -6.77 | 116.94      | 121.00   |
| 35  | BB    | 1664 | A    | C1'-O4'-C4' | -6.77 | 104.49      | 109.90   |
| 35  | BB    | 1928 | A    | N3-C4-C5    | -6.77 | 122.06      | 126.80   |
| 35  | BB    | 2799 | A    | C4-C5-N7    | -6.77 | 107.32      | 110.70   |
| 1   | AA    | 1308 | U    | C4-C5-C6    | 6.77  | 123.76      | 119.70   |
| 7   | AG    | 2    | ARG  | NE-CZ-NH1   | 6.77  | 123.68      | 120.30   |
| 35  | BB    | 6    | A    | C8-N9-C4    | -6.77 | 103.09      | 105.80   |
| 35  | BB    | 1580 | A    | C4'-C3'-C2' | -6.77 | 95.83       | 102.60   |
| 35  | BB    | 2826 | A    | C6-N1-C2    | -6.77 | 114.54      | 118.60   |
| 1   | AA    | 334  | C    | C5-C6-N1    | 6.76  | 124.38      | 121.00   |
| 1   | AA    | 1022 | A    | C5-C6-N1    | -6.76 | 114.32      | 117.70   |
| 35  | BB    | 545  | U    | C5-C6-N1    | -6.76 | 119.32      | 122.70   |
| 35  | BB    | 645  | C    | C2'-C3'-O3' | 6.76  | 124.52      | 113.70   |
| 35  | BB    | 1018 | U    | N3-C4-C5    | 6.76  | 118.66      | 114.60   |
| 35  | BB    | 1051 | G    | C5-C6-N1    | -6.76 | 108.12      | 111.50   |
| 35  | BB    | 1360 | G    | N3-C4-C5    | 6.76  | 131.98      | 128.60   |
| 35  | BB    | 1427 | A    | C8-N9-C4    | -6.76 | 103.09      | 105.80   |
| 35  | BB    | 1500 | G    | P-O3'-C3'   | -6.76 | 111.58      | 119.70   |
| 35  | BB    | 1527 | G    | C1'-O4'-C4' | 6.76  | 115.31      | 109.90   |
| 35  | BB    | 1897 | G    | N3-C2-N2    | 6.76  | 124.64      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1956 | U    | C4'-C3'-C2' | -6.76 | 95.83       | 102.60   |
| 35  | BB    | 2201 | G    | C8-N9-C4    | 6.76  | 109.11      | 106.40   |
| 35  | BB    | 2225 | A    | C6-C5-N7    | -6.76 | 127.56      | 132.30   |
| 1   | AA    | 359  | G    | N3-C4-C5    | 6.76  | 131.98      | 128.60   |
| 1   | AA    | 1108 | G    | C4-C5-N7    | -6.76 | 108.09      | 110.80   |
| 35  | BB    | 381  | G    | O4'-C1'-N9  | 6.76  | 113.61      | 108.20   |
| 35  | BB    | 1425 | G    | N1-C6-O6    | 6.76  | 123.96      | 119.90   |
| 1   | AA    | 614  | C    | C2-N1-C1'   | 6.76  | 126.24      | 118.80   |
| 1   | AA    | 834  | U    | C6-N1-C2    | -6.76 | 116.94      | 121.00   |
| 35  | BB    | 845  | A    | C5-C6-N1    | -6.76 | 114.32      | 117.70   |
| 35  | BB    | 2095 | A    | C4-C5-N7    | 6.76  | 114.08      | 110.70   |
| 35  | BB    | 2536 | G    | N7-C8-N9    | 6.76  | 116.48      | 113.10   |
| 35  | BB    | 2753 | A    | O4'-C1'-N9  | 6.76  | 113.61      | 108.20   |
| 35  | BB    | 540  | C    | N3-C4-C5    | -6.76 | 119.20      | 121.90   |
| 35  | BB    | 596  | U    | O4'-C1'-N1  | 6.76  | 113.61      | 108.20   |
| 35  | BB    | 2509 | G    | C4-C5-C6    | 6.76  | 122.86      | 118.80   |
| 35  | BB    | 2725 | A    | C5-N7-C8    | 6.76  | 107.28      | 103.90   |
| 35  | BB    | 2831 | G    | N1-C6-O6    | 6.76  | 123.96      | 119.90   |
| 35  | BB    | 2885 | G    | O4'-C1'-N9  | 6.76  | 113.61      | 108.20   |
| 35  | BB    | 2891 | U    | C4-C5-C6    | -6.76 | 115.64      | 119.70   |
| 1   | AA    | 526  | C    | O4'-C1'-N1  | 6.76  | 113.61      | 108.20   |
| 1   | AA    | 619  | U    | C3'-C2'-C1' | 6.76  | 106.91      | 101.50   |
| 1   | AA    | 1172 | C    | N1-C2-O2    | -6.76 | 114.84      | 118.90   |
| 35  | BB    | 71   | A    | C3'-C2'-C1' | -6.76 | 96.09       | 101.50   |
| 35  | BB    | 114  | U    | C4-C5-C6    | -6.76 | 115.64      | 119.70   |
| 55  | BW    | 57   | TYR  | CG-CD1-CE1  | -6.76 | 115.89      | 121.30   |
| 1   | AA    | 765  | G    | C5'-C4'-O4' | 6.76  | 117.21      | 109.10   |
| 1   | AA    | 829  | G    | N3-C2-N2    | 6.76  | 124.63      | 119.90   |
| 1   | AA    | 984  | C    | O4'-C1'-N1  | 6.76  | 113.61      | 108.20   |
| 1   | AA    | 1097 | C    | N3-C4-C5    | -6.76 | 119.20      | 121.90   |
| 1   | AA    | 1480 | A    | C4-C5-C6    | 6.76  | 120.38      | 117.00   |
| 35  | BB    | 31   | C    | P-O3'-C3'   | -6.76 | 111.59      | 119.70   |
| 35  | BB    | 320  | A    | C5-C6-N1    | -6.76 | 114.32      | 117.70   |
| 35  | BB    | 826  | U    | O4'-C1'-N1  | 6.76  | 113.61      | 108.20   |
| 35  | BB    | 2340 | A    | O4'-C4'-C3' | -6.76 | 97.24       | 104.00   |
| 35  | BB    | 2542 | A    | C4-C5-C6    | 6.76  | 120.38      | 117.00   |
| 48  | BO    | 16   | ARG  | NE-CZ-NH1   | 6.76  | 123.68      | 120.30   |
| 1   | AA    | 12   | U    | C5-C4-O4    | -6.75 | 121.85      | 125.90   |
| 1   | AA    | 205  | A    | C4-C5-N7    | -6.75 | 107.32      | 110.70   |
| 1   | AA    | 574  | A    | C4-C5-C6    | 6.75  | 120.38      | 117.00   |
| 13  | AM    | 105  | ALA  | N-CA-CB     | 6.75  | 119.56      | 110.10   |
| 35  | BB    | 1131 | G    | N3-C4-C5    | -6.75 | 125.22      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1603 | A    | N7-C8-N9    | -6.75 | 110.42      | 113.80   |
| 35  | BB    | 2753 | A    | N3-C4-C5    | -6.75 | 122.07      | 126.80   |
| 1   | AA    | 1402 | C    | O4'-C1'-N1  | 6.75  | 113.60      | 108.20   |
| 1   | AA    | 1492 | A    | C8-N9-C4    | -6.75 | 103.10      | 105.80   |
| 34  | BA    | 99   | A    | N1-C6-N6    | 6.75  | 122.65      | 118.60   |
| 35  | BB    | 51   | G    | N1-C6-O6    | 6.75  | 123.95      | 119.90   |
| 35  | BB    | 821  | A    | O4'-C1'-N9  | 6.75  | 113.60      | 108.20   |
| 35  | BB    | 1663 | G    | N3-C2-N2    | 6.75  | 124.63      | 119.90   |
| 35  | BB    | 2152 | G    | O4'-C1'-N9  | 6.75  | 113.60      | 108.20   |
| 35  | BB    | 2177 | C    | N3-C4-C5    | -6.75 | 119.20      | 121.90   |
| 1   | AA    | 103  | U    | N3-C4-O4    | 6.75  | 124.13      | 119.40   |
| 1   | AA    | 158  | G    | C4-C5-N7    | -6.75 | 108.10      | 110.80   |
| 35  | BB    | 308  | G    | N1-C6-O6    | 6.75  | 123.95      | 119.90   |
| 35  | BB    | 464  | U    | C5-C4-O4    | -6.75 | 121.85      | 125.90   |
| 35  | BB    | 1115 | G    | O5'-C5'-C4' | -6.75 | 98.87       | 111.70   |
| 35  | BB    | 1237 | A    | C6-N1-C2    | 6.75  | 122.65      | 118.60   |
| 35  | BB    | 1240 | U    | C2-N3-C4    | 6.75  | 131.05      | 127.00   |
| 35  | BB    | 1645 | G    | N1-C2-N3    | -6.75 | 119.85      | 123.90   |
| 35  | BB    | 2297 | A    | C8-N9-C4    | -6.75 | 103.10      | 105.80   |
| 35  | BB    | 2569 | G    | C5-C6-O6    | -6.75 | 124.55      | 128.60   |
| 35  | BB    | 2726 | A    | N7-C8-N9    | -6.75 | 110.42      | 113.80   |
| 37  | BD    | 161  | MET  | N-CA-CB     | 6.75  | 122.75      | 110.60   |
| 1   | AA    | 1139 | G    | O4'-C1'-N9  | -6.75 | 102.80      | 108.20   |
| 1   | AA    | 1231 | G    | C6-N1-C2    | -6.75 | 121.05      | 125.10   |
| 35  | BB    | 2023 | C    | N1-C2-N3    | 6.75  | 123.92      | 119.20   |
| 35  | BB    | 2679 | A    | P-O5'-C5'   | -6.75 | 110.10      | 120.90   |
| 1   | AA    | 457  | G    | C5-N7-C8    | 6.75  | 107.67      | 104.30   |
| 1   | AA    | 478  | A    | N1-C6-N6    | 6.75  | 122.65      | 118.60   |
| 1   | AA    | 664  | G    | C8-N9-C4    | -6.75 | 103.70      | 106.40   |
| 1   | AA    | 665  | A    | C8-N9-C4    | 6.75  | 108.50      | 105.80   |
| 1   | AA    | 1300 | G    | C8-N9-C4    | 6.75  | 109.10      | 106.40   |
| 34  | BA    | 104  | A    | C6-C5-N7    | -6.75 | 127.58      | 132.30   |
| 35  | BB    | 31   | C    | N3-C4-N4    | 6.75  | 122.72      | 118.00   |
| 35  | BB    | 247  | G    | C4-C5-C6    | 6.75  | 122.85      | 118.80   |
| 35  | BB    | 844  | A    | C1'-O4'-C4' | -6.75 | 104.50      | 109.90   |
| 35  | BB    | 1143 | A    | C2-N3-C4    | 6.75  | 113.97      | 110.60   |
| 35  | BB    | 2037 | A    | C2-N3-C4    | -6.75 | 107.23      | 110.60   |
| 1   | AA    | 495  | A    | N3-C4-C5    | -6.75 | 122.08      | 126.80   |
| 1   | AA    | 1025 | U    | C4'-C3'-C2' | -6.75 | 95.85       | 102.60   |
| 1   | AA    | 1369 | C    | N3-C4-N4    | 6.75  | 122.72      | 118.00   |
| 35  | BB    | 1076 | C    | N3-C2-O2    | 6.75  | 126.62      | 121.90   |
| 35  | BB    | 1146 | C    | C2-N3-C4    | 6.75  | 123.27      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1260 | A    | C8-N9-C4    | -6.75 | 103.10      | 105.80   |
| 35  | BB    | 2162 | G    | N1-C2-N3    | -6.75 | 119.85      | 123.90   |
| 35  | BB    | 2709 | G    | N7-C8-N9    | -6.75 | 109.73      | 113.10   |
| 1   | AA    | 110  | C    | C5-C4-N4    | -6.75 | 115.48      | 120.20   |
| 15  | AO    | 68   | TYR  | CB-CG-CD1   | -6.75 | 116.95      | 121.00   |
| 35  | BB    | 517  | C    | P-O5'-C5'   | 6.75  | 131.69      | 120.90   |
| 35  | BB    | 839  | U    | C3'-C2'-C1' | -6.75 | 96.10       | 101.50   |
| 35  | BB    | 1109 | C    | C2-N1-C1'   | 6.75  | 126.22      | 118.80   |
| 35  | BB    | 1771 | C    | O4'-C1'-N1  | 6.75  | 113.60      | 108.20   |
| 35  | BB    | 2094 | A    | C5-C6-N1    | -6.75 | 114.33      | 117.70   |
| 35  | BB    | 2461 | A    | O4'-C1'-N9  | 6.75  | 113.60      | 108.20   |
| 1   | AA    | 82   | G    | O4'-C1'-N9  | 6.74  | 113.59      | 108.20   |
| 1   | AA    | 640  | A    | C5-C6-N1    | -6.74 | 114.33      | 117.70   |
| 1   | AA    | 993  | G    | N3-C2-N2    | 6.74  | 124.62      | 119.90   |
| 1   | AA    | 1157 | A    | O4'-C1'-N9  | 6.74  | 113.59      | 108.20   |
| 22  | AV    | 52   | G    | C5-C6-O6    | -6.74 | 124.55      | 128.60   |
| 35  | BB    | 686  | U    | O5'-P-OP1   | 6.74  | 118.79      | 110.70   |
| 35  | BB    | 922  | C    | C6-N1-C2    | 6.74  | 123.00      | 120.30   |
| 35  | BB    | 1275 | A    | C8-N9-C1'   | -6.74 | 115.56      | 127.70   |
| 35  | BB    | 1279 | G    | C4-C5-N7    | -6.74 | 108.10      | 110.80   |
| 35  | BB    | 1598 | A    | N1-C2-N3    | 6.74  | 132.67      | 129.30   |
| 35  | BB    | 2282 | G    | C2'-C3'-O3' | 6.74  | 124.49      | 113.70   |
| 35  | BB    | 2293 | G    | C8-N9-C4    | 6.74  | 109.10      | 106.40   |
| 1   | AA    | 1515 | G    | C4-C5-C6    | 6.74  | 122.84      | 118.80   |
| 35  | BB    | 1017 | G    | C4-C5-N7    | 6.74  | 113.50      | 110.80   |
| 35  | BB    | 1338 | G    | C4-C5-C6    | 6.74  | 122.84      | 118.80   |
| 35  | BB    | 2267 | A    | N9-C4-C5    | 6.74  | 108.50      | 105.80   |
| 35  | BB    | 2333 | A    | C4-C5-N7    | -6.74 | 107.33      | 110.70   |
| 1   | AA    | 435  | A    | N3-C4-C5    | -6.74 | 122.08      | 126.80   |
| 1   | AA    | 758  | C    | C5-C6-N1    | 6.74  | 124.37      | 121.00   |
| 1   | AA    | 1067 | A    | C5'-C4'-O4' | 6.74  | 117.19      | 109.10   |
| 35  | BB    | 1471 | G    | C4-N9-C1'   | -6.74 | 117.74      | 126.50   |
| 35  | BB    | 1553 | A    | P-O5'-C5'   | -6.74 | 110.11      | 120.90   |
| 35  | BB    | 1568 | G    | P-O5'-C5'   | 6.74  | 131.68      | 120.90   |
| 35  | BB    | 2253 | G    | C5-C6-N1    | 6.74  | 114.87      | 111.50   |
| 35  | BB    | 2368 | C    | O4'-C1'-N1  | 6.74  | 113.59      | 108.20   |
| 1   | AA    | 257  | G    | O4'-C1'-N9  | 6.74  | 113.59      | 108.20   |
| 1   | AA    | 1358 | U    | N1-C2-N3    | 6.74  | 118.94      | 114.90   |
| 34  | BA    | 63   | C    | C5-C4-N4    | -6.74 | 115.48      | 120.20   |
| 35  | BB    | 307  | G    | O4'-C1'-N9  | 6.74  | 113.59      | 108.20   |
| 35  | BB    | 440  | C    | N1-C2-O2    | 6.74  | 122.94      | 118.90   |
| 35  | BB    | 1107 | G    | C8-N9-C4    | -6.74 | 103.70      | 106.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1304 | A    | C1'-O4'-C4' | 6.74  | 115.29      | 109.90   |
| 35  | BB    | 1379 | U    | N3-C4-C5    | -6.74 | 110.56      | 114.60   |
| 35  | BB    | 1614 | A    | C5-C6-N6    | -6.74 | 118.31      | 123.70   |
| 35  | BB    | 2193 | G    | N9-C4-C5    | 6.74  | 108.09      | 105.40   |
| 48  | BO    | 10   | ARG  | NE-CZ-NH2   | -6.74 | 116.93      | 120.30   |
| 54  | BU    | 86   | PHE  | CB-CG-CD2   | 6.74  | 125.52      | 120.80   |
| 1   | AA    | 1018 | G    | O4'-C1'-N9  | 6.74  | 113.59      | 108.20   |
| 1   | AA    | 1024 | G    | C6-C5-N7    | -6.74 | 126.36      | 130.40   |
| 1   | AA    | 1141 | C    | C5-C6-N1    | 6.74  | 124.37      | 121.00   |
| 35  | BB    | 452  | G    | N1-C2-N2    | -6.74 | 110.14      | 116.20   |
| 35  | BB    | 800  | A    | N1-C2-N3    | 6.74  | 132.67      | 129.30   |
| 35  | BB    | 954  | G    | C4-C5-N7    | -6.74 | 108.11      | 110.80   |
| 35  | BB    | 1942 | C    | C5-C6-N1    | 6.74  | 124.37      | 121.00   |
| 1   | AA    | 544  | G    | C4-C5-C6    | 6.74  | 122.84      | 118.80   |
| 1   | AA    | 782  | A    | O4'-C4'-C3' | -6.74 | 97.27       | 104.00   |
| 1   | AA    | 895  | G    | C4'-C3'-C2' | -6.74 | 95.86       | 102.60   |
| 1   | AA    | 954  | G    | C5-N7-C8    | 6.74  | 107.67      | 104.30   |
| 1   | AA    | 1477 | U    | N3-C2-O2    | 6.74  | 126.92      | 122.20   |
| 35  | BB    | 30   | G    | N1-C2-N3    | -6.74 | 119.86      | 123.90   |
| 35  | BB    | 522  | A    | C4-C5-C6    | 6.74  | 120.37      | 117.00   |
| 35  | BB    | 588  | U    | C5-C6-N1    | 6.74  | 126.07      | 122.70   |
| 35  | BB    | 834  | G    | C5-C6-O6    | -6.74 | 124.56      | 128.60   |
| 35  | BB    | 1588 | G    | C5-C6-N1    | -6.74 | 108.13      | 111.50   |
| 35  | BB    | 1641 | A    | O4'-C1'-N9  | 6.74  | 113.59      | 108.20   |
| 35  | BB    | 2641 | G    | O4'-C1'-N9  | 6.74  | 113.59      | 108.20   |
| 1   | AA    | 1175 | G    | N9-C4-C5    | -6.73 | 102.71      | 105.40   |
| 1   | AA    | 1355 | G    | C4-C5-N7    | 6.73  | 113.49      | 110.80   |
| 35  | BB    | 1755 | A    | O4'-C1'-N9  | 6.73  | 113.59      | 108.20   |
| 35  | BB    | 2406 | A    | C5-C6-N1    | -6.73 | 114.33      | 117.70   |
| 1   | AA    | 14   | U    | C5-C4-O4    | -6.73 | 121.86      | 125.90   |
| 1   | AA    | 15   | G    | N7-C8-N9    | 6.73  | 116.47      | 113.10   |
| 35  | BB    | 385  | C    | C2-N3-C4    | 6.73  | 123.27      | 119.90   |
| 35  | BB    | 1672 | A    | C6-C5-N7    | -6.73 | 127.59      | 132.30   |
| 35  | BB    | 2050 | C    | C5-C4-N4    | -6.73 | 115.49      | 120.20   |
| 35  | BB    | 2158 | A    | O4'-C1'-N9  | 6.73  | 113.59      | 108.20   |
| 35  | BB    | 2159 | G    | N1-C2-N3    | -6.73 | 119.86      | 123.90   |
| 35  | BB    | 2235 | G    | N3-C4-C5    | -6.73 | 125.23      | 128.60   |
| 35  | BB    | 2293 | G    | O4'-C1'-N9  | 6.73  | 113.59      | 108.20   |
| 35  | BB    | 2319 | G    | N1-C6-O6    | 6.73  | 123.94      | 119.90   |
| 1   | AA    | 1488 | G    | N1-C2-N3    | -6.73 | 119.86      | 123.90   |
| 2   | AB    | 26   | MET  | CG-SD-CE    | 6.73  | 110.97      | 100.20   |
| 35  | BB    | 567  | U    | O4'-C1'-N1  | 6.73  | 113.58      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1783 | A    | N3-C4-N9    | 6.73  | 132.78      | 127.40   |
| 35  | BB    | 2357 | G    | N9-C4-C5    | 6.73  | 108.09      | 105.40   |
| 35  | BB    | 2595 | G    | C4-C5-N7    | -6.73 | 108.11      | 110.80   |
| 1   | AA    | 238  | A    | C8-N9-C4    | -6.73 | 103.11      | 105.80   |
| 1   | AA    | 875  | U    | N1-C2-O2    | -6.73 | 118.09      | 122.80   |
| 35  | BB    | 1493 | C    | C6-N1-C1'   | -6.73 | 112.72      | 120.80   |
| 1   | AA    | 808  | C    | N3-C2-O2    | 6.73  | 126.61      | 121.90   |
| 1   | AA    | 860  | A    | C5-N7-C8    | 6.73  | 107.26      | 103.90   |
| 1   | AA    | 1088 | G    | O4'-C1'-N9  | 6.73  | 113.58      | 108.20   |
| 17  | AQ    | 64   | ARG  | NE-CZ-NH2   | -6.73 | 116.94      | 120.30   |
| 34  | BA    | 25   | U    | N1-C2-O2    | -6.73 | 118.09      | 122.80   |
| 35  | BB    | 549  | G    | N3-C2-N2    | 6.73  | 124.61      | 119.90   |
| 35  | BB    | 943  | A    | O4'-C1'-N9  | 6.73  | 113.58      | 108.20   |
| 35  | BB    | 1542 | U    | C2-N3-C4    | -6.73 | 122.96      | 127.00   |
| 35  | BB    | 1636 | U    | C5-C6-N1    | 6.73  | 126.06      | 122.70   |
| 35  | BB    | 2830 | C    | N3-C4-N4    | 6.73  | 122.71      | 118.00   |
| 1   | AA    | 928  | G    | C5-C6-O6    | -6.73 | 124.56      | 128.60   |
| 1   | AA    | 1306 | A    | C8-N9-C4    | 6.73  | 108.49      | 105.80   |
| 35  | BB    | 34   | U    | N3-C4-O4    | 6.73  | 124.11      | 119.40   |
| 35  | BB    | 1291 | C    | N3-C4-C5    | -6.73 | 119.21      | 121.90   |
| 35  | BB    | 2030 | A    | N1-C2-N3    | 6.73  | 132.66      | 129.30   |
| 35  | BB    | 2066 | C    | C4-C5-C6    | 6.73  | 120.76      | 117.40   |
| 35  | BB    | 2870 | C    | C4-C5-C6    | 6.73  | 120.76      | 117.40   |
| 35  | BB    | 2893 | A    | O4'-C1'-N9  | 6.73  | 113.58      | 108.20   |
| 1   | AA    | 75   | G    | C5'-C4'-C3' | -6.72 | 105.24      | 116.00   |
| 1   | AA    | 372  | C    | C5-C6-N1    | 6.72  | 124.36      | 121.00   |
| 1   | AA    | 583  | A    | N7-C8-N9    | -6.72 | 110.44      | 113.80   |
| 1   | AA    | 649  | A    | C3'-C2'-C1' | -6.72 | 96.12       | 101.50   |
| 1   | AA    | 741  | G    | C6-N1-C2    | 6.72  | 129.13      | 125.10   |
| 35  | BB    | 810  | U    | N1-C2-O2    | 6.72  | 127.51      | 122.80   |
| 35  | BB    | 1361 | G    | C2-N3-C4    | 6.72  | 115.26      | 111.90   |
| 35  | BB    | 1581 | G    | N1-C2-N3    | -6.72 | 119.87      | 123.90   |
| 35  | BB    | 2276 | G    | C4'-C3'-C2' | -6.72 | 95.88       | 102.60   |
| 35  | BB    | 2563 | U    | N3-C4-C5    | -6.72 | 110.57      | 114.60   |
| 35  | BB    | 2747 | G    | P-O5'-C5'   | 6.72  | 131.66      | 120.90   |
| 35  | BB    | 2783 | U    | O4'-C1'-N1  | 6.72  | 113.58      | 108.20   |
| 1   | AA    | 223  | A    | C4-C5-N7    | -6.72 | 107.34      | 110.70   |
| 1   | AA    | 1002 | G    | C4'-C3'-C2' | -6.72 | 95.88       | 102.60   |
| 1   | AA    | 1022 | A    | C4-C5-N7    | -6.72 | 107.34      | 110.70   |
| 1   | AA    | 1201 | A    | C8-N9-C4    | -6.72 | 103.11      | 105.80   |
| 1   | AA    | 1450 | U    | N1-C2-N3    | 6.72  | 118.93      | 114.90   |
| 35  | BB    | 763  | G    | N3-C2-N2    | 6.72  | 124.61      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 831  | G    | C5-C6-O6    | -6.72 | 124.57      | 128.60   |
| 35  | BB    | 1489 | C    | C6-N1-C1'   | -6.72 | 112.73      | 120.80   |
| 35  | BB    | 1552 | A    | N9-C4-C5    | -6.72 | 103.11      | 105.80   |
| 35  | BB    | 1658 | C    | N3-C4-N4    | 6.72  | 122.70      | 118.00   |
| 35  | BB    | 2115 | G    | C6-C5-N7    | -6.72 | 126.37      | 130.40   |
| 35  | BB    | 2273 | A    | N3-C4-C5    | -6.72 | 122.09      | 126.80   |
| 35  | BB    | 2476 | A    | N3-C4-C5    | -6.72 | 122.09      | 126.80   |
| 35  | BB    | 2661 | G    | C8-N9-C4    | 6.72  | 109.09      | 106.40   |
| 35  | BB    | 2692 | G    | C6-C5-N7    | -6.72 | 126.37      | 130.40   |
| 56  | BY    | 59   | PHE  | CB-CG-CD1   | 6.72  | 125.51      | 120.80   |
| 35  | BB    | 13   | A    | N9-C4-C5    | 6.72  | 108.49      | 105.80   |
| 35  | BB    | 2325 | G    | C5-C6-N1    | -6.72 | 108.14      | 111.50   |
| 35  | BB    | 2353 | G    | O4'-C1'-N9  | 6.72  | 113.58      | 108.20   |
| 35  | BB    | 2403 | C    | P-O5'-C5'   | -6.72 | 110.15      | 120.90   |
| 35  | BB    | 2605 | U    | C4'-C3'-C2' | -6.72 | 95.88       | 102.60   |
| 35  | BB    | 2846 | G    | N9-C4-C5    | -6.72 | 102.71      | 105.40   |
| 1   | AA    | 589  | U    | N1-C2-O2    | -6.72 | 118.10      | 122.80   |
| 1   | AA    | 700  | G    | N1-C2-N3    | -6.72 | 119.87      | 123.90   |
| 1   | AA    | 1246 | A    | C4'-C3'-C2' | -6.72 | 95.88       | 102.60   |
| 13  | AM    | 69   | ARG  | NE-CZ-NH2   | -6.72 | 116.94      | 120.30   |
| 35  | BB    | 42   | A    | N7-C8-N9    | 6.72  | 117.16      | 113.80   |
| 35  | BB    | 897  | C    | C4'-C3'-C2' | -6.72 | 95.88       | 102.60   |
| 35  | BB    | 1410 | G    | N3-C4-N9    | -6.72 | 121.97      | 126.00   |
| 35  | BB    | 1538 | G    | C5-N7-C8    | -6.72 | 100.94      | 104.30   |
| 1   | AA    | 1104 | G    | C6-C5-N7    | -6.72 | 126.37      | 130.40   |
| 1   | AA    | 1360 | A    | C6-C5-N7    | -6.72 | 127.60      | 132.30   |
| 22  | AV    | 24   | G    | C5-C6-O6    | -6.72 | 124.57      | 128.60   |
| 34  | BA    | 26   | C    | N3-C4-C5    | -6.72 | 119.21      | 121.90   |
| 35  | BB    | 195  | A    | C5-C6-N1    | -6.72 | 114.34      | 117.70   |
| 35  | BB    | 1302 | A    | N1-C6-N6    | 6.72  | 122.63      | 118.60   |
| 35  | BB    | 1309 | G    | C8-N9-C4    | -6.72 | 103.71      | 106.40   |
| 35  | BB    | 1715 | G    | C6-C5-N7    | -6.72 | 126.37      | 130.40   |
| 35  | BB    | 2432 | A    | C5-C6-N6    | -6.72 | 118.33      | 123.70   |
| 35  | BB    | 2466 | C    | N3-C2-O2    | 6.72  | 126.60      | 121.90   |
| 44  | BK    | 70   | ARG  | NE-CZ-NH2   | -6.72 | 116.94      | 120.30   |
| 1   | AA    | 590  | U    | C5-C4-O4    | -6.72 | 121.87      | 125.90   |
| 1   | AA    | 849  | G    | C6-C5-N7    | -6.72 | 126.37      | 130.40   |
| 1   | AA    | 1055 | A    | C5-C6-N6    | -6.72 | 118.33      | 123.70   |
| 35  | BB    | 1199 | U    | C6-N1-C2    | 6.72  | 125.03      | 121.00   |
| 35  | BB    | 1389 | G    | C5-C6-N1    | -6.72 | 108.14      | 111.50   |
| 35  | BB    | 1505 | A    | C5-C6-N6    | -6.72 | 118.33      | 123.70   |
| 35  | BB    | 1510 | G    | O4'-C1'-N9  | 6.72  | 113.57      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 229  | U    | N3-C4-O4    | 6.71  | 124.10      | 119.40   |
| 1   | AA    | 979  | C    | C6-N1-C2    | -6.71 | 117.61      | 120.30   |
| 1   | AA    | 1182 | G    | N3-C4-C5    | -6.71 | 125.24      | 128.60   |
| 1   | AA    | 1261 | A    | N1-C2-N3    | -6.71 | 125.94      | 129.30   |
| 4   | AD    | 192  | ALA  | N-CA-CB     | 6.71  | 119.50      | 110.10   |
| 35  | BB    | 10   | A    | C4-C5-N7    | -6.71 | 107.34      | 110.70   |
| 35  | BB    | 524  | G    | C4-C5-C6    | 6.71  | 122.83      | 118.80   |
| 35  | BB    | 589  | U    | C5-C4-O4    | -6.71 | 121.87      | 125.90   |
| 35  | BB    | 840  | C    | O4'-C1'-N1  | 6.71  | 113.57      | 108.20   |
| 35  | BB    | 1274 | A    | N9-C4-C5    | -6.71 | 103.11      | 105.80   |
| 35  | BB    | 1297 | C    | N3-C4-C5    | -6.71 | 119.21      | 121.90   |
| 35  | BB    | 1407 | G    | C4'-C3'-C2' | -6.71 | 95.89       | 102.60   |
| 35  | BB    | 2142 | A    | C5-C6-N6    | -6.71 | 118.33      | 123.70   |
| 1   | AA    | 1430 | A    | C5-C6-N6    | -6.71 | 118.33      | 123.70   |
| 35  | BB    | 55   | G    | N1-C6-O6    | 6.71  | 123.93      | 119.90   |
| 35  | BB    | 196  | A    | C5-C6-N1    | -6.71 | 114.34      | 117.70   |
| 35  | BB    | 1935 | G    | N7-C8-N9    | 6.71  | 116.46      | 113.10   |
| 35  | BB    | 2433 | A    | N7-C8-N9    | -6.71 | 110.44      | 113.80   |
| 1   | AA    | 171  | A    | O4'-C1'-N9  | 6.71  | 113.57      | 108.20   |
| 1   | AA    | 232  | G    | C4-C5-N7    | 6.71  | 113.48      | 110.80   |
| 30  | B5    | 21   | TYR  | CB-CG-CD1   | -6.71 | 116.97      | 121.00   |
| 35  | BB    | 1589 | U    | C4-C5-C6    | -6.71 | 115.67      | 119.70   |
| 35  | BB    | 654  | A    | C2-N3-C4    | 6.71  | 113.95      | 110.60   |
| 35  | BB    | 1032 | A    | C6-N1-C2    | 6.71  | 122.63      | 118.60   |
| 35  | BB    | 2423 | U    | C4-C5-C6    | 6.71  | 123.73      | 119.70   |
| 1   | AA    | 81   | A    | C6-C5-N7    | -6.71 | 127.60      | 132.30   |
| 12  | AL    | 40   | THR  | CA-CB-CG2   | -6.71 | 103.01      | 112.40   |
| 35  | BB    | 1406 | U    | C6-N1-C2    | -6.71 | 116.97      | 121.00   |
| 35  | BB    | 2086 | U    | O4'-C1'-N1  | 6.71  | 113.57      | 108.20   |
| 35  | BB    | 2392 | A    | O4'-C1'-N9  | 6.71  | 113.57      | 108.20   |
| 35  | BB    | 2862 | G    | C6-N1-C2    | 6.71  | 129.12      | 125.10   |
| 1   | AA    | 246  | A    | C2-N3-C4    | -6.71 | 107.25      | 110.60   |
| 1   | AA    | 794  | A    | C5-C6-N1    | -6.71 | 114.35      | 117.70   |
| 1   | AA    | 841  | C    | C5-C4-N4    | -6.71 | 115.51      | 120.20   |
| 1   | AA    | 1518 | A    | O4'-C1'-N9  | 6.71  | 113.57      | 108.20   |
| 35  | BB    | 90   | U    | N3-C4-O4    | 6.71  | 124.09      | 119.40   |
| 35  | BB    | 1756 | G    | C4-C5-N7    | 6.71  | 113.48      | 110.80   |
| 35  | BB    | 1793 | C    | N3-C4-N4    | 6.71  | 122.69      | 118.00   |
| 35  | BB    | 1989 | G    | C4-C5-C6    | 6.71  | 122.82      | 118.80   |
| 35  | BB    | 2280 | G    | N9-C4-C5    | -6.71 | 102.72      | 105.40   |
| 35  | BB    | 2362 | C    | C5-C4-N4    | -6.71 | 115.50      | 120.20   |
| 1   | AA    | 331  | G    | C4-C5-N7    | -6.71 | 108.12      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 753  | A    | N7-C8-N9    | 6.71  | 117.15      | 113.80   |
| 35  | BB    | 1510 | G    | C8-N9-C4    | 6.71  | 109.08      | 106.40   |
| 35  | BB    | 2708 | G    | N1-C2-N3    | -6.71 | 119.88      | 123.90   |
| 35  | BB    | 2767 | C    | O4'-C1'-N1  | 6.71  | 113.56      | 108.20   |
| 35  | BB    | 2860 | A    | N9-C4-C5    | -6.71 | 103.12      | 105.80   |
| 56  | BY    | 44   | PHE  | CB-CG-CD1   | 6.71  | 125.49      | 120.80   |
| 1   | AA    | 561  | U    | O4'-C1'-N1  | 6.70  | 113.56      | 108.20   |
| 1   | AA    | 792  | A    | C3'-C2'-C1' | -6.70 | 96.14       | 101.50   |
| 1   | AA    | 1020 | G    | C4-C5-N7    | -6.70 | 108.12      | 110.80   |
| 35  | BB    | 42   | A    | C8-N9-C4    | -6.70 | 103.12      | 105.80   |
| 35  | BB    | 249  | C    | O4'-C1'-N1  | 6.70  | 113.56      | 108.20   |
| 35  | BB    | 356  | G    | C4-C5-N7    | 6.70  | 113.48      | 110.80   |
| 35  | BB    | 450  | G    | N1-C6-O6    | 6.70  | 123.92      | 119.90   |
| 35  | BB    | 546  | U    | O4'-C1'-N1  | 6.70  | 113.56      | 108.20   |
| 35  | BB    | 1622 | G    | O4'-C1'-N9  | 6.70  | 113.56      | 108.20   |
| 1   | AA    | 482  | A    | N3-C4-N9    | 6.70  | 132.76      | 127.40   |
| 35  | BB    | 718  | A    | C5'-C4'-C3' | 6.70  | 126.72      | 116.00   |
| 35  | BB    | 1220 | G    | N1-C6-O6    | 6.70  | 123.92      | 119.90   |
| 35  | BB    | 1395 | A    | C6-C5-N7    | -6.70 | 127.61      | 132.30   |
| 35  | BB    | 2332 | C    | N3-C4-N4    | 6.70  | 122.69      | 118.00   |
| 35  | BB    | 2654 | A    | C4-C5-N7    | -6.70 | 107.35      | 110.70   |
| 1   | AA    | 404  | G    | C8-N9-C4    | -6.70 | 103.72      | 106.40   |
| 1   | AA    | 465  | A    | C5-C6-N6    | -6.70 | 118.34      | 123.70   |
| 1   | AA    | 727  | G    | O4'-C1'-N9  | 6.70  | 113.56      | 108.20   |
| 1   | AA    | 782  | A    | N7-C8-N9    | -6.70 | 110.45      | 113.80   |
| 1   | AA    | 1479 | C    | C2-N1-C1'   | 6.70  | 126.17      | 118.80   |
| 35  | BB    | 675  | A    | N1-C6-N6    | 6.70  | 122.62      | 118.60   |
| 35  | BB    | 899  | A    | C5-C6-N6    | -6.70 | 118.34      | 123.70   |
| 35  | BB    | 943  | A    | N3-C4-C5    | -6.70 | 122.11      | 126.80   |
| 35  | BB    | 2119 | A    | C6-C5-N7    | -6.70 | 127.61      | 132.30   |
| 35  | BB    | 2225 | A    | C5-C6-N1    | -6.70 | 114.35      | 117.70   |
| 35  | BB    | 2235 | G    | C2-N3-C4    | 6.70  | 115.25      | 111.90   |
| 1   | AA    | 158  | G    | N1-C2-N3    | -6.70 | 119.88      | 123.90   |
| 1   | AA    | 177  | G    | N3-C4-N9    | 6.70  | 130.02      | 126.00   |
| 1   | AA    | 904  | U    | C3'-C2'-C1' | -6.70 | 96.14       | 101.50   |
| 34  | BA    | 14   | U    | C5-C4-O4    | 6.70  | 129.92      | 125.90   |
| 35  | BB    | 347  | A    | O4'-C1'-N9  | 6.70  | 113.56      | 108.20   |
| 35  | BB    | 887  | U    | N3-C4-O4    | 6.70  | 124.09      | 119.40   |
| 35  | BB    | 974  | G    | N3-C2-N2    | 6.70  | 124.59      | 119.90   |
| 35  | BB    | 1615 | C    | N3-C4-C5    | 6.70  | 124.58      | 121.90   |
| 35  | BB    | 1757 | A    | N1-C2-N3    | 6.70  | 132.65      | 129.30   |
| 35  | BB    | 2188 | U    | C4-C5-C6    | 6.70  | 123.72      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BU    | 39   | ASN  | CB-CA-C     | -6.70 | 97.00       | 110.40   |
| 1   | AA    | 27   | G    | P-O3'-C3'   | -6.70 | 111.66      | 119.70   |
| 1   | AA    | 505  | G    | C4-C5-N7    | 6.70  | 113.48      | 110.80   |
| 1   | AA    | 1068 | G    | C5-N7-C8    | 6.70  | 107.65      | 104.30   |
| 35  | BB    | 1077 | A    | N3-C4-N9    | 6.70  | 132.76      | 127.40   |
| 35  | BB    | 1268 | A    | O4'-C1'-N9  | 6.70  | 113.56      | 108.20   |
| 35  | BB    | 1951 | U    | N3-C4-O4    | 6.70  | 124.09      | 119.40   |
| 35  | BB    | 2009 | A    | C8-N9-C4    | 6.70  | 108.48      | 105.80   |
| 35  | BB    | 2427 | C    | P-O3'-C3'   | 6.70  | 127.74      | 119.70   |
| 35  | BB    | 2745 | C    | C5-C4-N4    | -6.70 | 115.51      | 120.20   |
| 1   | AA    | 15   | G    | C1'-O4'-C4' | 6.70  | 115.26      | 109.90   |
| 1   | AA    | 817  | C    | C2-N1-C1'   | 6.70  | 126.17      | 118.80   |
| 35  | BB    | 83   | A    | C4-C5-N7    | -6.70 | 107.35      | 110.70   |
| 35  | BB    | 564  | C    | C4'-C3'-C2' | -6.70 | 95.91       | 102.60   |
| 35  | BB    | 978  | G    | P-O3'-C3'   | -6.70 | 111.66      | 119.70   |
| 35  | BB    | 1104 | C    | P-O3'-C3'   | 6.70  | 127.73      | 119.70   |
| 35  | BB    | 1115 | G    | P-O3'-C3'   | 6.70  | 127.73      | 119.70   |
| 35  | BB    | 1396 | U    | C2-N3-C4    | -6.70 | 122.98      | 127.00   |
| 35  | BB    | 1570 | A    | N7-C8-N9    | -6.70 | 110.45      | 113.80   |
| 34  | BA    | 22   | U    | O4'-C1'-N1  | 6.69  | 113.56      | 108.20   |
| 35  | BB    | 2552 | U    | C5-C6-N1    | -6.69 | 119.35      | 122.70   |
| 35  | BB    | 2736 | A    | C8-N9-C4    | -6.69 | 103.12      | 105.80   |
| 35  | BB    | 2838 | G    | N1-C2-N3    | -6.69 | 119.88      | 123.90   |
| 1   | AA    | 1288 | A    | N9-C4-C5    | 6.69  | 108.48      | 105.80   |
| 1   | AA    | 1492 | A    | C5-N7-C8    | 6.69  | 107.25      | 103.90   |
| 35  | BB    | 405  | U    | N1-C2-O2    | 6.69  | 127.48      | 122.80   |
| 35  | BB    | 746  | U    | C2-N3-C4    | -6.69 | 122.98      | 127.00   |
| 35  | BB    | 749  | A    | N1-C6-N6    | 6.69  | 122.61      | 118.60   |
| 35  | BB    | 1169 | A    | C5-C6-N1    | -6.69 | 114.35      | 117.70   |
| 35  | BB    | 1338 | G    | C5-C6-N1    | -6.69 | 108.15      | 111.50   |
| 35  | BB    | 2121 | G    | N1-C6-O6    | 6.69  | 123.92      | 119.90   |
| 1   | AA    | 228  | A    | C2-N3-C4    | 6.69  | 113.94      | 110.60   |
| 1   | AA    | 300  | A    | C5-N7-C8    | 6.69  | 107.25      | 103.90   |
| 35  | BB    | 5    | A    | C5'-C4'-C3' | -6.69 | 105.29      | 116.00   |
| 35  | BB    | 686  | U    | O5'-C5'-C4' | -6.69 | 98.99       | 111.70   |
| 35  | BB    | 924  | G    | C4-C5-C6    | 6.69  | 122.81      | 118.80   |
| 35  | BB    | 1283 | G    | N1-C6-O6    | 6.69  | 123.91      | 119.90   |
| 35  | BB    | 1352 | U    | C5-C4-O4    | -6.69 | 121.89      | 125.90   |
| 35  | BB    | 1461 | C    | N3-C4-C5    | -6.69 | 119.22      | 121.90   |
| 35  | BB    | 1532 | A    | C5-C6-N1    | -6.69 | 114.36      | 117.70   |
| 35  | BB    | 1746 | A    | N3-C4-C5    | -6.69 | 122.12      | 126.80   |
| 35  | BB    | 2149 | U    | O4'-C1'-N1  | 6.69  | 113.55      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2212 | A    | N1-C2-N3    | -6.69 | 125.95      | 129.30   |
| 3   | AC    | 125  | ARG  | NE-CZ-NH2   | -6.69 | 116.95      | 120.30   |
| 35  | BB    | 558  | U    | P-O3'-C3'   | -6.69 | 111.67      | 119.70   |
| 1   | AA    | 285  | C    | C6-N1-C2    | -6.69 | 117.62      | 120.30   |
| 1   | AA    | 785  | G    | O5'-C5'-C4' | -6.69 | 98.99       | 111.70   |
| 1   | AA    | 960  | U    | N3-C2-O2    | 6.69  | 126.88      | 122.20   |
| 1   | AA    | 989  | U    | C5-C4-O4    | -6.69 | 121.89      | 125.90   |
| 1   | AA    | 1036 | A    | C2-N3-C4    | -6.69 | 107.26      | 110.60   |
| 12  | AL    | 6    | LEU  | CB-CG-CD2   | 6.69  | 122.37      | 111.00   |
| 35  | BB    | 1530 | G    | C5-N7-C8    | 6.69  | 107.64      | 104.30   |
| 12  | AL    | 37   | TYR  | CB-CG-CD2   | -6.69 | 116.99      | 121.00   |
| 34  | BA    | 41   | G    | C4-C5-C6    | 6.69  | 122.81      | 118.80   |
| 34  | BA    | 65   | U    | N3-C2-O2    | 6.69  | 126.88      | 122.20   |
| 35  | BB    | 705  | A    | O4'-C1'-N9  | 6.69  | 113.55      | 108.20   |
| 35  | BB    | 1679 | A    | N3-C4-N9    | -6.69 | 122.05      | 127.40   |
| 35  | BB    | 1749 | A    | P-O3'-C3'   | -6.69 | 111.68      | 119.70   |
| 25  | B0    | 17   | ARG  | NE-CZ-NH2   | 6.68  | 123.64      | 120.30   |
| 34  | BA    | 67   | G    | O4'-C1'-N9  | 6.68  | 113.55      | 108.20   |
| 35  | BB    | 74   | A    | C5-C6-N1    | -6.68 | 114.36      | 117.70   |
| 35  | BB    | 911  | A    | C5-N7-C8    | 6.68  | 107.24      | 103.90   |
| 35  | BB    | 1186 | G    | C4-C5-N7    | 6.68  | 113.47      | 110.80   |
| 35  | BB    | 1631 | G    | C6-N1-C2    | 6.68  | 129.11      | 125.10   |
| 35  | BB    | 1645 | G    | C4-C5-N7    | 6.68  | 113.47      | 110.80   |
| 35  | BB    | 2343 | U    | C5-C4-O4    | -6.68 | 121.89      | 125.90   |
| 35  | BB    | 2598 | A    | O4'-C1'-N9  | 6.68  | 113.55      | 108.20   |
| 35  | BB    | 2819 | G    | C4-C5-C6    | 6.68  | 122.81      | 118.80   |
| 1   | AA    | 292  | G    | N3-C2-N2    | 6.68  | 124.58      | 119.90   |
| 1   | AA    | 559  | A    | C2-N3-C4    | 6.68  | 113.94      | 110.60   |
| 1   | AA    | 1319 | A    | N1-C2-N3    | 6.68  | 132.64      | 129.30   |
| 1   | AA    | 1397 | C    | C6-N1-C1'   | -6.68 | 112.78      | 120.80   |
| 22  | AV    | 6    | C    | C4'-C3'-C2' | -6.68 | 95.92       | 102.60   |
| 30  | B5    | 8    | MET  | CG-SD-CE    | -6.68 | 89.51       | 100.20   |
| 35  | BB    | 509  | C    | O4'-C1'-N1  | 6.68  | 113.55      | 108.20   |
| 35  | BB    | 673  | C    | C2-N1-C1'   | 6.68  | 126.15      | 118.80   |
| 35  | BB    | 2414 | G    | N3-C4-N9    | -6.68 | 121.99      | 126.00   |
| 35  | BB    | 2710 | C    | N3-C4-N4    | 6.68  | 122.68      | 118.00   |
| 29  | B4    | 43   | ARG  | NE-CZ-NH2   | -6.68 | 116.96      | 120.30   |
| 35  | BB    | 1944 | U    | N3-C4-C5    | -6.68 | 110.59      | 114.60   |
| 1   | AA    | 957  | U    | O4'-C1'-N1  | 6.68  | 113.54      | 108.20   |
| 1   | AA    | 1111 | A    | C5-N7-C8    | 6.68  | 107.24      | 103.90   |
| 12  | AL    | 108  | ASP  | CB-CG-OD1   | -6.68 | 112.29      | 118.30   |
| 35  | BB    | 2132 | U    | C4'-C3'-O3' | 6.68  | 126.36      | 113.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 230  | G    | N3-C2-N2    | 6.68  | 124.58      | 119.90   |
| 1   | AA    | 1284 | C    | C5-C6-N1    | -6.68 | 117.66      | 121.00   |
| 30  | B5    | 7    | ARG  | NE-CZ-NH2   | -6.68 | 116.96      | 120.30   |
| 35  | BB    | 588  | U    | C3'-C2'-C1' | 6.68  | 106.84      | 101.50   |
| 35  | BB    | 1840 | G    | N9-C1'-C2'  | -6.68 | 104.65      | 112.00   |
| 35  | BB    | 2152 | G    | N1-C2-N3    | -6.68 | 119.89      | 123.90   |
| 52  | BS    | 82   | MET  | CA-CB-CG    | 6.68  | 124.65      | 113.30   |
| 1   | AA    | 57   | G    | O4'-C1'-N9  | 6.68  | 113.54      | 108.20   |
| 1   | AA    | 1502 | A    | N9-C4-C5    | 6.68  | 108.47      | 105.80   |
| 1   | AA    | 1523 | G    | C4-C5-C6    | 6.68  | 122.81      | 118.80   |
| 26  | B1    | 49   | ASP  | CB-CG-OD1   | -6.68 | 112.29      | 118.30   |
| 32  | B7    | 48   | MET  | CA-CB-CG    | 6.68  | 124.65      | 113.30   |
| 35  | BB    | 366  | C    | N3-C4-N4    | 6.68  | 122.67      | 118.00   |
| 35  | BB    | 422  | A    | C4-C5-C6    | 6.68  | 120.34      | 117.00   |
| 35  | BB    | 779  | U    | C4-C5-C6    | -6.68 | 115.69      | 119.70   |
| 35  | BB    | 935  | C    | C5-C6-N1    | 6.68  | 124.34      | 121.00   |
| 35  | BB    | 1267 | U    | C5-C6-N1    | 6.68  | 126.04      | 122.70   |
| 35  | BB    | 1535 | A    | C5-N7-C8    | -6.68 | 100.56      | 103.90   |
| 35  | BB    | 1739 | A    | C8-N9-C4    | -6.68 | 103.13      | 105.80   |
| 35  | BB    | 1857 | G    | N7-C8-N9    | 6.68  | 116.44      | 113.10   |
| 35  | BB    | 2577 | A    | C4-C5-C6    | 6.68  | 120.34      | 117.00   |
| 47  | BN    | 72   | ASP  | CB-CG-OD1   | -6.68 | 112.29      | 118.30   |
| 35  | BB    | 1148 | U    | O4'-C1'-N1  | 6.67  | 113.54      | 108.20   |
| 35  | BB    | 2124 | G    | N1-C2-N3    | -6.67 | 119.89      | 123.90   |
| 1   | AA    | 109  | A    | C6-N1-C2    | 6.67  | 122.60      | 118.60   |
| 35  | BB    | 1039 | A    | N3-C4-C5    | -6.67 | 122.13      | 126.80   |
| 35  | BB    | 1139 | G    | C2-N3-C4    | 6.67  | 115.24      | 111.90   |
| 35  | BB    | 1278 | C    | C4-C5-C6    | 6.67  | 120.74      | 117.40   |
| 35  | BB    | 1412 | U    | O4'-C4'-C3' | -6.67 | 97.33       | 104.00   |
| 1   | AA    | 222  | C    | P-O3'-C3'   | -6.67 | 111.69      | 119.70   |
| 1   | AA    | 408  | A    | C5-C6-N1    | -6.67 | 114.36      | 117.70   |
| 1   | AA    | 1246 | A    | C4-C5-C6    | 6.67  | 120.34      | 117.00   |
| 1   | AA    | 1483 | A    | C6-C5-N7    | -6.67 | 127.63      | 132.30   |
| 35  | BB    | 400  | G    | N1-C2-N2    | -6.67 | 110.20      | 116.20   |
| 35  | BB    | 1416 | G    | C6-N1-C2    | 6.67  | 129.10      | 125.10   |
| 35  | BB    | 1652 | A    | O4'-C1'-N9  | 6.67  | 113.54      | 108.20   |
| 35  | BB    | 1696 | G    | N1-C2-N3    | -6.67 | 119.90      | 123.90   |
| 35  | BB    | 1819 | A    | O4'-C1'-N9  | 6.67  | 113.54      | 108.20   |
| 35  | BB    | 2815 | C    | C5-C4-N4    | -6.67 | 115.53      | 120.20   |
| 1   | AA    | 417  | G    | C6-C5-N7    | -6.67 | 126.40      | 130.40   |
| 1   | AA    | 832  | G    | P-O3'-C3'   | -6.67 | 111.70      | 119.70   |
| 1   | AA    | 1197 | A    | C5-C6-N6    | -6.67 | 118.36      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BB    | 2729 | G    | N3-C2-N2   | 6.67  | 124.57      | 119.90   |
| 1   | AA    | 379  | C    | P-O3'-C3'  | -6.67 | 111.70      | 119.70   |
| 1   | AA    | 707  | U    | N3-C4-O4   | 6.67  | 124.07      | 119.40   |
| 1   | AA    | 923  | A    | C6-N1-C2   | -6.67 | 114.60      | 118.60   |
| 1   | AA    | 937  | A    | C5-C6-N1   | -6.67 | 114.37      | 117.70   |
| 1   | AA    | 1326 | U    | P-O3'-C3'  | -6.67 | 111.70      | 119.70   |
| 35  | BB    | 1115 | G    | P-O5'-C5'  | -6.67 | 110.23      | 120.90   |
| 35  | BB    | 1631 | G    | N1-C2-N3   | -6.67 | 119.90      | 123.90   |
| 35  | BB    | 2281 | A    | N7-C8-N9   | 6.67  | 117.14      | 113.80   |
| 35  | BB    | 2497 | A    | C5-N7-C8   | 6.67  | 107.23      | 103.90   |
| 35  | BB    | 2623 | G    | O4'-C1'-N9 | 6.67  | 113.53      | 108.20   |
| 35  | BB    | 2798 | U    | P-O5'-C5'  | 6.67  | 131.57      | 120.90   |
| 22  | AV    | 36   | G    | P-O5'-C5'  | -6.67 | 110.23      | 120.90   |
| 35  | BB    | 698  | C    | N3-C2-O2   | -6.67 | 117.23      | 121.90   |
| 35  | BB    | 1412 | U    | N3-C4-C5   | 6.67  | 118.60      | 114.60   |
| 35  | BB    | 1594 | U    | C5-C4-O4   | -6.67 | 121.90      | 125.90   |
| 35  | BB    | 2327 | A    | C4-C5-C6   | 6.67  | 120.33      | 117.00   |
| 1   | AA    | 1270 | G    | C8-N9-C4   | -6.67 | 103.73      | 106.40   |
| 35  | BB    | 39   | G    | N1-C2-N3   | -6.67 | 119.90      | 123.90   |
| 35  | BB    | 1349 | C    | N3-C4-C5   | -6.67 | 119.23      | 121.90   |
| 35  | BB    | 1964 | G    | C5-N7-C8   | 6.67  | 107.63      | 104.30   |
| 35  | BB    | 2195 | U    | N1-C2-O2   | -6.67 | 118.14      | 122.80   |
| 46  | BM    | 31   | PHE  | CB-CG-CD2  | -6.67 | 116.14      | 120.80   |
| 1   | AA    | 100  | G    | O4'-C1'-N9 | 6.66  | 113.53      | 108.20   |
| 1   | AA    | 324  | G    | N3-C2-N2   | 6.66  | 124.56      | 119.90   |
| 1   | AA    | 452  | A    | N1-C6-N6   | 6.66  | 122.60      | 118.60   |
| 1   | AA    | 1167 | A    | N1-C2-N3   | 6.66  | 132.63      | 129.30   |
| 16  | AP    | 32   | PHE  | CB-CA-C    | -6.66 | 97.07       | 110.40   |
| 35  | BB    | 815  | C    | C6-N1-C2   | -6.66 | 117.64      | 120.30   |
| 35  | BB    | 1869 | G    | O4'-C1'-N9 | 6.66  | 113.53      | 108.20   |
| 35  | BB    | 2094 | A    | O4'-C1'-N9 | 6.66  | 113.53      | 108.20   |
| 35  | BB    | 2121 | G    | C6-N1-C2   | 6.66  | 129.10      | 125.10   |
| 35  | BB    | 2277 | G    | N9-C4-C5   | -6.66 | 102.73      | 105.40   |
| 35  | BB    | 2903 | U    | N3-C2-O2   | -6.66 | 117.53      | 122.20   |
| 1   | AA    | 1152 | A    | N9-C4-C5   | 6.66  | 108.47      | 105.80   |
| 7   | AG    | 17   | PHE  | CB-CG-CD2  | -6.66 | 116.14      | 120.80   |
| 22  | AV    | 1    | C    | O4'-C1'-N1 | 6.66  | 113.53      | 108.20   |
| 49  | BP    | 98   | TYR  | CB-CG-CD1  | -6.66 | 117.00      | 121.00   |
| 13  | AM    | 10   | ASP  | CB-CG-OD2  | -6.66 | 112.31      | 118.30   |
| 35  | BB    | 164  | C    | N1-C1'-C2' | -6.66 | 104.67      | 112.00   |
| 35  | BB    | 576  | U    | C5-C6-N1   | 6.66  | 126.03      | 122.70   |
| 35  | BB    | 784  | G    | C2-N3-C4   | 6.66  | 115.23      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1071 | G    | O4'-C1'-N9  | 6.66  | 113.53      | 108.20   |
| 35  | BB    | 1091 | G    | N3-C2-N2    | 6.66  | 124.56      | 119.90   |
| 35  | BB    | 1187 | G    | C1'-O4'-C4' | 6.66  | 115.23      | 109.90   |
| 1   | AA    | 48   | C    | N3-C4-N4    | 6.66  | 122.66      | 118.00   |
| 1   | AA    | 160  | A    | C4-C5-C6    | 6.66  | 120.33      | 117.00   |
| 1   | AA    | 518  | C    | N1-C2-O2    | 6.66  | 122.89      | 118.90   |
| 1   | AA    | 720  | C    | C5-C6-N1    | 6.66  | 124.33      | 121.00   |
| 1   | AA    | 763  | G    | C5-C6-N1    | 6.66  | 114.83      | 111.50   |
| 1   | AA    | 852  | G    | C5-N7-C8    | 6.66  | 107.63      | 104.30   |
| 1   | AA    | 1032 | G    | O4'-C1'-N9  | 6.66  | 113.53      | 108.20   |
| 1   | AA    | 1428 | A    | N1-C6-N6    | 6.66  | 122.59      | 118.60   |
| 1   | AA    | 1472 | U    | C4'-C3'-C2' | -6.66 | 95.94       | 102.60   |
| 34  | BA    | 22   | U    | P-O3'-C3'   | -6.66 | 111.71      | 119.70   |
| 35  | BB    | 141  | G    | C8-N9-C4    | 6.66  | 109.06      | 106.40   |
| 35  | BB    | 333  | G    | N1-C2-N3    | -6.66 | 119.91      | 123.90   |
| 35  | BB    | 433  | C    | N3-C4-N4    | 6.66  | 122.66      | 118.00   |
| 35  | BB    | 1014 | A    | P-O3'-C3'   | -6.66 | 111.71      | 119.70   |
| 35  | BB    | 1030 | C    | C6-N1-C2    | -6.66 | 117.64      | 120.30   |
| 35  | BB    | 1388 | G    | O4'-C1'-N9  | 6.66  | 113.53      | 108.20   |
| 35  | BB    | 1395 | A    | C4-C5-C6    | 6.66  | 120.33      | 117.00   |
| 35  | BB    | 1557 | C    | C6-N1-C2    | 6.66  | 122.96      | 120.30   |
| 35  | BB    | 1773 | A    | O4'-C1'-N9  | 6.66  | 113.53      | 108.20   |
| 35  | BB    | 1813 | G    | C4'-C3'-C2' | -6.66 | 95.94       | 102.60   |
| 35  | BB    | 1902 | C    | N3-C4-N4    | 6.66  | 122.66      | 118.00   |
| 35  | BB    | 2242 | G    | C3'-C2'-C1' | 6.66  | 106.83      | 101.50   |
| 35  | BB    | 2773 | C    | O4'-C1'-N1  | 6.66  | 113.53      | 108.20   |
| 35  | BB    | 2801 | G    | N1-C2-N3    | -6.66 | 119.91      | 123.90   |
| 1   | AA    | 502  | A    | C1'-O4'-C4' | 6.66  | 115.23      | 109.90   |
| 1   | AA    | 1000 | A    | C5-C6-N6    | -6.66 | 118.37      | 123.70   |
| 35  | BB    | 570  | G    | C1'-O4'-C4' | -6.66 | 104.58      | 109.90   |
| 1   | AA    | 231  | U    | N1-C2-O2    | 6.66  | 127.46      | 122.80   |
| 1   | AA    | 255  | G    | O4'-C1'-N9  | 6.66  | 113.52      | 108.20   |
| 34  | BA    | 46   | A    | C2-N3-C4    | -6.66 | 107.27      | 110.60   |
| 35  | BB    | 1994 | C    | C5-C4-N4    | -6.66 | 115.54      | 120.20   |
| 35  | BB    | 2342 | C    | C6-N1-C2    | 6.66  | 122.96      | 120.30   |
| 35  | BB    | 2414 | G    | N3-C4-C5    | 6.66  | 131.93      | 128.60   |
| 1   | AA    | 559  | A    | N1-C6-N6    | 6.65  | 122.59      | 118.60   |
| 22  | AV    | 3    | G    | N9-C4-C5    | -6.65 | 102.74      | 105.40   |
| 1   | AA    | 321  | A    | C5-C6-N6    | -6.65 | 118.38      | 123.70   |
| 1   | AA    | 358  | U    | O4'-C1'-N1  | 6.65  | 113.52      | 108.20   |
| 1   | AA    | 396  | C    | N3-C2-O2    | 6.65  | 126.56      | 121.90   |
| 1   | AA    | 517  | G    | C2-N3-C4    | 6.65  | 115.23      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 597  | G    | C8-N9-C4    | 6.65  | 109.06      | 106.40   |
| 35  | BB    | 370  | G    | N1-C2-N3    | -6.65 | 119.91      | 123.90   |
| 35  | BB    | 741  | U    | C6-N1-C2    | -6.65 | 117.01      | 121.00   |
| 35  | BB    | 2092 | U    | C2-N1-C1'   | 6.65  | 125.68      | 117.70   |
| 35  | BB    | 2265 | U    | C4-C5-C6    | -6.65 | 115.71      | 119.70   |
| 35  | BB    | 2502 | G    | C5-C6-O6    | -6.65 | 124.61      | 128.60   |
| 1   | AA    | 65   | A    | C4-C5-C6    | 6.65  | 120.33      | 117.00   |
| 1   | AA    | 134  | G    | C5-N7-C8    | -6.65 | 100.97      | 104.30   |
| 1   | AA    | 494  | G    | C5-C6-O6    | -6.65 | 124.61      | 128.60   |
| 1   | AA    | 1089 | G    | C4-C5-N7    | -6.65 | 108.14      | 110.80   |
| 35  | BB    | 26   | G    | N3-C4-N9    | 6.65  | 129.99      | 126.00   |
| 35  | BB    | 385  | C    | N3-C4-N4    | 6.65  | 122.66      | 118.00   |
| 35  | BB    | 547  | A    | C5-N7-C8    | 6.65  | 107.22      | 103.90   |
| 35  | BB    | 617  | G    | N1-C6-O6    | 6.65  | 123.89      | 119.90   |
| 35  | BB    | 807  | U    | C5-C4-O4    | 6.65  | 129.89      | 125.90   |
| 35  | BB    | 1054 | A    | C5-N7-C8    | 6.65  | 107.22      | 103.90   |
| 35  | BB    | 1478 | G    | C5-C6-O6    | -6.65 | 124.61      | 128.60   |
| 35  | BB    | 2297 | A    | P-O3'-C3'   | -6.65 | 111.72      | 119.70   |
| 35  | BB    | 2302 | U    | N1-C2-N3    | -6.65 | 110.91      | 114.90   |
| 35  | BB    | 2438 | U    | C5-C4-O4    | -6.65 | 121.91      | 125.90   |
| 35  | BB    | 2530 | A    | C5'-C4'-O4' | 6.65  | 117.08      | 109.10   |
| 35  | BB    | 2778 | A    | N9-C4-C5    | -6.65 | 103.14      | 105.80   |
| 1   | AA    | 441  | A    | N9-C4-C5    | 6.65  | 108.46      | 105.80   |
| 1   | AA    | 996  | A    | C5-C6-N6    | -6.65 | 118.38      | 123.70   |
| 35  | BB    | 919  | U    | N1-C2-O2    | -6.65 | 118.14      | 122.80   |
| 35  | BB    | 2189 | U    | C2-N3-C4    | -6.65 | 123.01      | 127.00   |
| 35  | BB    | 2246 | G    | N3-C2-N2    | 6.65  | 124.55      | 119.90   |
| 1   | AA    | 208  | U    | C5'-C4'-C3' | 6.65  | 126.64      | 116.00   |
| 1   | AA    | 276  | G    | C4-C5-N7    | 6.65  | 113.46      | 110.80   |
| 1   | AA    | 350  | G    | N1-C6-O6    | 6.65  | 123.89      | 119.90   |
| 1   | AA    | 631  | C    | N1-C2-N3    | -6.65 | 114.55      | 119.20   |
| 1   | AA    | 790  | A    | C5-C6-N1    | -6.65 | 114.38      | 117.70   |
| 1   | AA    | 1081 | A    | C6-C5-N7    | -6.65 | 127.65      | 132.30   |
| 1   | AA    | 1232 | U    | C5-C4-O4    | -6.65 | 121.91      | 125.90   |
| 1   | AA    | 1347 | G    | C4-N9-C1'   | -6.65 | 117.86      | 126.50   |
| 35  | BB    | 354  | A    | C8-N9-C4    | -6.65 | 103.14      | 105.80   |
| 35  | BB    | 535  | G    | C4-C5-N7    | -6.65 | 108.14      | 110.80   |
| 35  | BB    | 790  | U    | C5'-C4'-O4' | 6.65  | 117.08      | 109.10   |
| 35  | BB    | 904  | G    | N1-C2-N3    | -6.65 | 119.91      | 123.90   |
| 35  | BB    | 1042 | G    | N9-C4-C5    | 6.65  | 108.06      | 105.40   |
| 35  | BB    | 1854 | A    | O4'-C1'-N9  | 6.65  | 113.52      | 108.20   |
| 35  | BB    | 2019 | A    | O4'-C1'-N9  | 6.65  | 113.52      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2450 | A    | C5-N7-C8    | 6.65  | 107.22      | 103.90   |
| 35  | BB    | 2739 | U    | C2-N3-C4    | -6.65 | 123.01      | 127.00   |
| 1   | AA    | 720  | C    | N1-C2-O2    | -6.65 | 114.91      | 118.90   |
| 1   | AA    | 1367 | C    | N3-C4-N4    | 6.65  | 122.65      | 118.00   |
| 35  | BB    | 346  | A    | O4'-C1'-N9  | 6.65  | 113.52      | 108.20   |
| 35  | BB    | 2156 | G    | N3-C4-N9    | -6.65 | 122.01      | 126.00   |
| 1   | AA    | 123  | U    | P-O5'-C5'   | -6.64 | 110.27      | 120.90   |
| 1   | AA    | 409  | U    | N1-C2-O2    | -6.64 | 118.15      | 122.80   |
| 1   | AA    | 572  | A    | C5-C6-N6    | -6.64 | 118.39      | 123.70   |
| 1   | AA    | 839  | C    | C4-C5-C6    | 6.64  | 120.72      | 117.40   |
| 1   | AA    | 861  | G    | N3-C4-C5    | -6.64 | 125.28      | 128.60   |
| 35  | BB    | 320  | A    | N7-C8-N9    | 6.64  | 117.12      | 113.80   |
| 35  | BB    | 1111 | A    | C6-C5-N7    | -6.64 | 127.65      | 132.30   |
| 35  | BB    | 1441 | G    | C6-C5-N7    | -6.64 | 126.41      | 130.40   |
| 35  | BB    | 2313 | C    | C6-N1-C2    | -6.64 | 117.64      | 120.30   |
| 35  | BB    | 2864 | G    | C6-C5-N7    | -6.64 | 126.41      | 130.40   |
| 35  | BB    | 1300 | G    | N1-C6-O6    | 6.64  | 123.89      | 119.90   |
| 35  | BB    | 1382 | G    | O4'-C1'-N9  | 6.64  | 113.51      | 108.20   |
| 35  | BB    | 1559 | U    | O4'-C1'-N1  | 6.64  | 113.51      | 108.20   |
| 35  | BB    | 2162 | G    | O4'-C4'-C3' | -6.64 | 97.36       | 104.00   |
| 35  | BB    | 2466 | C    | C6-N1-C2    | -6.64 | 117.64      | 120.30   |
| 35  | BB    | 2667 | C    | C4-C5-C6    | 6.64  | 120.72      | 117.40   |
| 35  | BB    | 2725 | A    | O4'-C1'-N9  | 6.64  | 113.52      | 108.20   |
| 38  | BE    | 106  | LYS  | CB-CA-C     | -6.64 | 97.11       | 110.40   |
| 1   | AA    | 816  | A    | C4-C5-C6    | 6.64  | 120.32      | 117.00   |
| 35  | BB    | 170  | U    | O4'-C1'-N1  | 6.64  | 113.51      | 108.20   |
| 35  | BB    | 1189 | A    | O4'-C1'-N9  | 6.64  | 113.51      | 108.20   |
| 50  | BQ    | 46   | TYR  | CB-CG-CD2   | -6.64 | 117.02      | 121.00   |
| 1   | AA    | 752  | G    | C5-C6-O6    | -6.64 | 124.62      | 128.60   |
| 1   | AA    | 875  | U    | N1-C2-N3    | 6.64  | 118.88      | 114.90   |
| 1   | AA    | 889  | A    | C2-N3-C4    | 6.64  | 113.92      | 110.60   |
| 1   | AA    | 1189 | U    | O4'-C1'-N1  | 6.64  | 113.51      | 108.20   |
| 26  | B1    | 26   | PHE  | CB-CG-CD1   | -6.64 | 116.15      | 120.80   |
| 35  | BB    | 218  | A    | C8-N9-C4    | -6.64 | 103.14      | 105.80   |
| 35  | BB    | 436  | C    | O4'-C1'-N1  | 6.64  | 113.51      | 108.20   |
| 35  | BB    | 1508 | A    | C5-C6-N1    | 6.64  | 121.02      | 117.70   |
| 35  | BB    | 2429 | G    | N7-C8-N9    | -6.64 | 109.78      | 113.10   |
| 47  | BN    | 118  | ARG  | NE-CZ-NH2   | -6.64 | 116.98      | 120.30   |
| 1   | AA    | 128  | G    | C4'-C3'-C2' | -6.64 | 95.96       | 102.60   |
| 35  | BB    | 172  | A    | C4-C5-C6    | 6.64  | 120.32      | 117.00   |
| 35  | BB    | 276  | U    | C1'-O4'-C4' | 6.64  | 115.21      | 109.90   |
| 35  | BB    | 1097 | U    | C4-C5-C6    | 6.64  | 123.68      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1527 | G    | C6-N1-C2    | 6.64  | 129.08      | 125.10   |
| 35  | BB    | 2077 | A    | C6-C5-N7    | -6.64 | 127.65      | 132.30   |
| 1   | AA    | 315  | A    | C5-C6-N6    | -6.64 | 118.39      | 123.70   |
| 1   | AA    | 529  | G    | C2-N3-C4    | 6.64  | 115.22      | 111.90   |
| 1   | AA    | 1406 | U    | C4-C5-C6    | 6.64  | 123.68      | 119.70   |
| 35  | BB    | 35   | G    | O4'-C1'-N9  | 6.64  | 113.51      | 108.20   |
| 35  | BB    | 355  | U    | O4'-C1'-N1  | 6.64  | 113.51      | 108.20   |
| 35  | BB    | 991  | C    | P-O3'-C3'   | 6.64  | 127.66      | 119.70   |
| 35  | BB    | 2560 | A    | N3-C4-N9    | -6.64 | 122.09      | 127.40   |
| 46  | BM    | 6    | ARG  | NE-CZ-NH2   | -6.64 | 116.98      | 120.30   |
| 1   | AA    | 354  | G    | N3-C4-C5    | -6.63 | 125.28      | 128.60   |
| 1   | AA    | 437  | U    | P-O3'-C3'   | 6.63  | 127.66      | 119.70   |
| 1   | AA    | 927  | G    | C6-C5-N7    | -6.63 | 126.42      | 130.40   |
| 22  | AV    | 48   | C    | O4'-C1'-N1  | 6.63  | 113.51      | 108.20   |
| 35  | BB    | 466  | A    | C4'-C3'-C2' | -6.63 | 95.97       | 102.60   |
| 35  | BB    | 473  | G    | N1-C2-N2    | -6.63 | 110.23      | 116.20   |
| 35  | BB    | 1434 | A    | C5-C6-N1    | -6.63 | 114.38      | 117.70   |
| 35  | BB    | 1903 | G    | N3-C4-C5    | 6.63  | 131.92      | 128.60   |
| 35  | BB    | 2198 | A    | C5-C6-N1    | -6.63 | 114.38      | 117.70   |
| 1   | AA    | 916  | U    | O4'-C4'-C3' | -6.63 | 97.37       | 104.00   |
| 1   | AA    | 1363 | A    | P-O3'-C3'   | 6.63  | 127.66      | 119.70   |
| 1   | AA    | 1408 | A    | N7-C8-N9    | -6.63 | 110.48      | 113.80   |
| 35  | BB    | 160  | A    | C5-C6-N1    | -6.63 | 114.38      | 117.70   |
| 35  | BB    | 1907 | G    | C6-C5-N7    | -6.63 | 126.42      | 130.40   |
| 35  | BB    | 2233 | U    | N3-C4-O4    | 6.63  | 124.04      | 119.40   |
| 35  | BB    | 2670 | A    | N9-C4-C5    | -6.63 | 103.15      | 105.80   |
| 1   | AA    | 537  | G    | C4-C5-C6    | 6.63  | 122.78      | 118.80   |
| 1   | AA    | 1273 | C    | OP1-P-OP2   | -6.63 | 109.65      | 119.60   |
| 22  | AV    | 47   | U    | O4'-C1'-N1  | 6.63  | 113.50      | 108.20   |
| 35  | BB    | 124  | G    | C4-C5-C6    | 6.63  | 122.78      | 118.80   |
| 35  | BB    | 923  | G    | N1-C6-O6    | 6.63  | 123.88      | 119.90   |
| 35  | BB    | 1861 | G    | C2-N3-C4    | 6.63  | 115.22      | 111.90   |
| 35  | BB    | 1878 | G    | C6-C5-N7    | -6.63 | 126.42      | 130.40   |
| 1   | AA    | 601  | G    | O4'-C1'-N9  | 6.63  | 113.50      | 108.20   |
| 1   | AA    | 1034 | G    | C8-N9-C4    | -6.63 | 103.75      | 106.40   |
| 1   | AA    | 1127 | G    | C5-C6-N1    | -6.63 | 108.19      | 111.50   |
| 35  | BB    | 20   | C    | N3-C4-N4    | 6.63  | 122.64      | 118.00   |
| 35  | BB    | 169  | G    | C5-C6-N1    | -6.63 | 108.19      | 111.50   |
| 35  | BB    | 1203 | U    | OP1-P-OP2   | -6.63 | 109.66      | 119.60   |
| 35  | BB    | 2249 | U    | C5'-C4'-O4' | 6.63  | 117.05      | 109.10   |
| 1   | AA    | 504  | C    | P-O3'-C3'   | -6.63 | 111.75      | 119.70   |
| 1   | AA    | 904  | U    | N3-C2-O2    | 6.63  | 126.84      | 122.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 922  | G    | N9-C4-C5    | -6.63 | 102.75      | 105.40   |
| 1   | AA    | 1077 | G    | N1-C2-N3    | -6.63 | 119.92      | 123.90   |
| 1   | AA    | 1209 | C    | N1-C2-O2    | 6.63  | 122.88      | 118.90   |
| 1   | AA    | 1489 | G    | N7-C8-N9    | -6.63 | 109.79      | 113.10   |
| 35  | BB    | 248  | G    | C2-N3-C4    | 6.63  | 115.21      | 111.90   |
| 35  | BB    | 856  | G    | O4'-C1'-N9  | 6.63  | 113.50      | 108.20   |
| 35  | BB    | 1112 | G    | N7-C8-N9    | -6.63 | 109.79      | 113.10   |
| 35  | BB    | 1259 | G    | C5-C6-N1    | -6.63 | 108.19      | 111.50   |
| 35  | BB    | 2239 | G    | N1-C6-O6    | 6.63  | 123.88      | 119.90   |
| 35  | BB    | 2488 | G    | C6-C5-N7    | -6.63 | 126.42      | 130.40   |
| 36  | BC    | 263  | ASP  | CB-CG-OD1   | -6.63 | 112.34      | 118.30   |
| 1   | AA    | 1280 | A    | C4-C5-N7    | -6.62 | 107.39      | 110.70   |
| 1   | AA    | 1457 | G    | C5-C6-O6    | -6.62 | 124.62      | 128.60   |
| 1   | AA    | 1465 | A    | N1-C2-N3    | 6.62  | 132.61      | 129.30   |
| 35  | BB    | 1644 | C    | C5-C4-N4    | -6.62 | 115.56      | 120.20   |
| 35  | BB    | 2170 | A    | C6-N1-C2    | 6.62  | 122.58      | 118.60   |
| 35  | BB    | 2830 | C    | C2-N1-C1'   | 6.62  | 126.09      | 118.80   |
| 1   | AA    | 437  | U    | O4'-C1'-N1  | 6.62  | 113.50      | 108.20   |
| 1   | AA    | 558  | G    | C5-C6-N1    | -6.62 | 108.19      | 111.50   |
| 1   | AA    | 911  | U    | C5-C6-N1    | -6.62 | 119.39      | 122.70   |
| 1   | AA    | 1164 | G    | O4'-C1'-N9  | 6.62  | 113.50      | 108.20   |
| 1   | AA    | 1232 | U    | O4'-C1'-N1  | 6.62  | 113.50      | 108.20   |
| 1   | AA    | 1360 | A    | N1-C2-N3    | 6.62  | 132.61      | 129.30   |
| 1   | AA    | 1443 | C    | C6-N1-C1'   | -6.62 | 112.85      | 120.80   |
| 35  | BB    | 195  | A    | O4'-C1'-N9  | 6.62  | 113.50      | 108.20   |
| 35  | BB    | 598  | U    | N1-C2-O2    | -6.62 | 118.16      | 122.80   |
| 35  | BB    | 1046 | A    | C5'-C4'-C3' | -6.62 | 105.40      | 116.00   |
| 35  | BB    | 1071 | G    | C2-N3-C4    | 6.62  | 115.21      | 111.90   |
| 35  | BB    | 1143 | A    | C4-C5-N7    | -6.62 | 107.39      | 110.70   |
| 35  | BB    | 1272 | A    | O4'-C1'-N9  | 6.62  | 113.50      | 108.20   |
| 35  | BB    | 2559 | C    | C5-C6-N1    | 6.62  | 124.31      | 121.00   |
| 35  | BB    | 2641 | G    | C3'-C2'-C1' | -6.62 | 96.20       | 101.50   |
| 1   | AA    | 349  | A    | C8-N9-C4    | -6.62 | 103.15      | 105.80   |
| 1   | AA    | 735  | C    | N3-C2-O2    | 6.62  | 126.53      | 121.90   |
| 1   | AA    | 909  | A    | N3-C4-C5    | -6.62 | 122.17      | 126.80   |
| 1   | AA    | 1363 | A    | N9-C4-C5    | -6.62 | 103.15      | 105.80   |
| 35  | BB    | 175  | G    | C2-N3-C4    | -6.62 | 108.59      | 111.90   |
| 35  | BB    | 2326 | C    | C6-N1-C2    | 6.62  | 122.95      | 120.30   |
| 35  | BB    | 2357 | G    | C8-N9-C4    | -6.62 | 103.75      | 106.40   |
| 48  | BO    | 9    | ARG  | NE-CZ-NH2   | -6.62 | 116.99      | 120.30   |
| 1   | AA    | 374  | A    | O4'-C1'-N9  | 6.62  | 113.50      | 108.20   |
| 1   | AA    | 1083 | U    | O4'-C4'-C3' | -6.62 | 97.38       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26  | B1    | 47   | ARG  | NE-CZ-NH2   | 6.62  | 123.61      | 120.30   |
| 35  | BB    | 384  | A    | C5-N7-C8    | 6.62  | 107.21      | 103.90   |
| 35  | BB    | 1563 | U    | C5-C4-O4    | -6.62 | 121.93      | 125.90   |
| 35  | BB    | 2039 | U    | C5-C6-N1    | 6.62  | 126.01      | 122.70   |
| 1   | AA    | 485  | U    | C5-C6-N1    | -6.62 | 119.39      | 122.70   |
| 1   | AA    | 566  | G    | N9-C4-C5    | 6.62  | 108.05      | 105.40   |
| 1   | AA    | 1383 | C    | O4'-C1'-N1  | 6.62  | 113.50      | 108.20   |
| 35  | BB    | 56   | A    | C4'-C3'-C2' | -6.62 | 95.98       | 102.60   |
| 35  | BB    | 136  | G    | C4-C5-C6    | 6.62  | 122.77      | 118.80   |
| 35  | BB    | 1434 | A    | N7-C8-N9    | -6.62 | 110.49      | 113.80   |
| 35  | BB    | 1684 | G    | N3-C2-N2    | 6.62  | 124.53      | 119.90   |
| 35  | BB    | 1711 | A    | C2-N3-C4    | -6.62 | 107.29      | 110.60   |
| 35  | BB    | 1845 | G    | P-O5'-C5'   | 6.62  | 131.49      | 120.90   |
| 35  | BB    | 2205 | A    | P-O5'-C5'   | -6.62 | 110.31      | 120.90   |
| 1   | AA    | 1067 | A    | P-O5'-C5'   | 6.62  | 131.49      | 120.90   |
| 34  | BA    | 81   | G    | O4'-C1'-N9  | 6.62  | 113.49      | 108.20   |
| 35  | BB    | 1884 | G    | N3-C2-N2    | 6.62  | 124.53      | 119.90   |
| 35  | BB    | 2259 | U    | N1-C2-N3    | 6.62  | 118.87      | 114.90   |
| 35  | BB    | 2352 | A    | C4-C5-N7    | 6.62  | 114.01      | 110.70   |
| 46  | BM    | 1    | MET  | CG-SD-CE    | -6.62 | 89.61       | 100.20   |
| 1   | AA    | 253  | A    | C4-C5-C6    | 6.62  | 120.31      | 117.00   |
| 1   | AA    | 380  | G    | N9-C4-C5    | -6.62 | 102.75      | 105.40   |
| 1   | AA    | 558  | G    | C1'-O4'-C4' | 6.62  | 115.19      | 109.90   |
| 1   | AA    | 855  | U    | N3-C4-O4    | 6.62  | 124.03      | 119.40   |
| 35  | BB    | 749  | A    | C4-C5-C6    | 6.62  | 120.31      | 117.00   |
| 35  | BB    | 1022 | G    | C3'-C2'-C1' | -6.62 | 96.21       | 101.50   |
| 35  | BB    | 1271 | G    | P-O3'-C3'   | -6.62 | 111.76      | 119.70   |
| 35  | BB    | 1361 | G    | N7-C8-N9    | 6.62  | 116.41      | 113.10   |
| 35  | BB    | 1700 | A    | N1-C6-N6    | 6.62  | 122.57      | 118.60   |
| 35  | BB    | 1852 | U    | C2-N1-C1'   | 6.62  | 125.64      | 117.70   |
| 35  | BB    | 2544 | G    | O4'-C1'-N9  | 6.62  | 113.49      | 108.20   |
| 1   | AA    | 472  | U    | C5'-C4'-O4' | 6.61  | 117.04      | 109.10   |
| 1   | AA    | 1476 | A    | C4-C5-C6    | 6.61  | 120.31      | 117.00   |
| 1   | AA    | 1502 | A    | C4-C5-N7    | -6.61 | 107.39      | 110.70   |
| 22  | AV    | 12   | G    | C5-C6-O6    | -6.61 | 124.63      | 128.60   |
| 35  | BB    | 2150 | C    | N3-C4-N4    | 6.61  | 122.63      | 118.00   |
| 38  | BE    | 183  | PHE  | N-CA-CB     | 6.61  | 122.50      | 110.60   |
| 1   | AA    | 446  | G    | C5-C6-N1    | -6.61 | 108.19      | 111.50   |
| 1   | AA    | 681  | A    | C4-C5-C6    | 6.61  | 120.31      | 117.00   |
| 1   | AA    | 840  | C    | O4'-C1'-N1  | 6.61  | 113.49      | 108.20   |
| 1   | AA    | 1454 | G    | P-O5'-C5'   | 6.61  | 131.48      | 120.90   |
| 35  | BB    | 409  | G    | N3-C4-C5    | -6.61 | 125.29      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 802  | A    | N1-C6-N6    | 6.61  | 122.57      | 118.60   |
| 35  | BB    | 845  | A    | C6-C5-N7    | -6.61 | 127.67      | 132.30   |
| 35  | BB    | 1533 | C    | N3-C4-N4    | 6.61  | 122.63      | 118.00   |
| 35  | BB    | 2748 | A    | C3'-C2'-C1' | -6.61 | 96.21       | 101.50   |
| 53  | BT    | 92   | ASN  | N-CA-CB     | 6.61  | 122.50      | 110.60   |
| 1   | AA    | 197  | A    | C5-C6-N1    | -6.61 | 114.39      | 117.70   |
| 1   | AA    | 564  | C    | N3-C4-N4    | 6.61  | 122.63      | 118.00   |
| 1   | AA    | 592  | G    | O4'-C1'-N9  | 6.61  | 113.49      | 108.20   |
| 1   | AA    | 654  | G    | C5-C6-O6    | -6.61 | 124.63      | 128.60   |
| 1   | AA    | 747  | A    | C3'-C2'-C1' | -6.61 | 96.21       | 101.50   |
| 1   | AA    | 834  | U    | O4'-C1'-N1  | 6.61  | 113.49      | 108.20   |
| 1   | AA    | 1144 | G    | N1-C2-N3    | -6.61 | 119.93      | 123.90   |
| 1   | AA    | 1269 | A    | O4'-C1'-N9  | 6.61  | 113.49      | 108.20   |
| 35  | BB    | 164  | C    | C6-N1-C2    | -6.61 | 117.66      | 120.30   |
| 35  | BB    | 265  | A    | N1-C2-N3    | -6.61 | 125.99      | 129.30   |
| 35  | BB    | 825  | A    | O4'-C1'-N9  | 6.61  | 113.49      | 108.20   |
| 35  | BB    | 1561 | C    | C4-C5-C6    | 6.61  | 120.70      | 117.40   |
| 35  | BB    | 1744 | A    | C4-C5-C6    | 6.61  | 120.31      | 117.00   |
| 35  | BB    | 1757 | A    | N9-C4-C5    | -6.61 | 103.16      | 105.80   |
| 35  | BB    | 1776 | G    | C4-C5-C6    | 6.61  | 122.77      | 118.80   |
| 35  | BB    | 2286 | G    | C5-C6-O6    | -6.61 | 124.63      | 128.60   |
| 35  | BB    | 2865 | U    | C4'-C3'-C2' | -6.61 | 95.99       | 102.60   |
| 1   | AA    | 447  | G    | C5-C6-N1    | -6.61 | 108.20      | 111.50   |
| 1   | AA    | 621  | A    | C5'-C4'-O4' | -6.61 | 101.17      | 109.10   |
| 1   | AA    | 1234 | C    | N3-C4-N4    | 6.61  | 122.63      | 118.00   |
| 35  | BB    | 518  | G    | C5-C6-N1    | 6.61  | 114.81      | 111.50   |
| 35  | BB    | 981  | A    | C8-N9-C4    | 6.61  | 108.44      | 105.80   |
| 1   | AA    | 644  | U    | N1-C2-N3    | 6.61  | 118.86      | 114.90   |
| 1   | AA    | 820  | U    | C2-N3-C4    | 6.61  | 130.97      | 127.00   |
| 1   | AA    | 821  | G    | C5-N7-C8    | 6.61  | 107.60      | 104.30   |
| 1   | AA    | 840  | C    | C5-C6-N1    | 6.61  | 124.30      | 121.00   |
| 1   | AA    | 843  | U    | C1'-O4'-C4' | -6.61 | 104.61      | 109.90   |
| 1   | AA    | 1334 | G    | C4-C5-C6    | 6.61  | 122.76      | 118.80   |
| 1   | AA    | 1523 | G    | C5-N7-C8    | 6.61  | 107.60      | 104.30   |
| 34  | BA    | 81   | G    | N1-C6-O6    | 6.61  | 123.86      | 119.90   |
| 35  | BB    | 279  | A    | C5-N7-C8    | -6.61 | 100.60      | 103.90   |
| 35  | BB    | 680  | C    | C4-C5-C6    | -6.61 | 114.10      | 117.40   |
| 35  | BB    | 810  | U    | N3-C2-O2    | -6.61 | 117.58      | 122.20   |
| 35  | BB    | 1168 | G    | P-O3'-C3'   | -6.61 | 111.77      | 119.70   |
| 35  | BB    | 1268 | A    | N7-C8-N9    | -6.61 | 110.50      | 113.80   |
| 35  | BB    | 1479 | G    | N1-C2-N3    | -6.61 | 119.94      | 123.90   |
| 35  | BB    | 1679 | A    | O4'-C1'-N9  | 6.61  | 113.49      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2621 | G    | N1-C6-O6    | 6.61  | 123.86      | 119.90   |
| 35  | BB    | 2803 | G    | C8-N9-C1'   | 6.61  | 135.59      | 127.00   |
| 1   | AA    | 81   | A    | C4-C5-C6    | 6.61  | 120.30      | 117.00   |
| 1   | AA    | 262  | A    | C1'-O4'-C4' | -6.61 | 104.61      | 109.90   |
| 1   | AA    | 318  | G    | N9-C4-C5    | -6.61 | 102.76      | 105.40   |
| 1   | AA    | 348  | G    | O4'-C1'-N9  | 6.61  | 113.48      | 108.20   |
| 1   | AA    | 665  | A    | N7-C8-N9    | -6.61 | 110.50      | 113.80   |
| 1   | AA    | 829  | G    | C1'-O4'-C4' | -6.61 | 104.62      | 109.90   |
| 1   | AA    | 1004 | A    | N1-C2-N3    | 6.61  | 132.60      | 129.30   |
| 1   | AA    | 1008 | U    | C5-C4-O4    | -6.61 | 121.94      | 125.90   |
| 1   | AA    | 1143 | G    | C4-C5-C6    | 6.61  | 122.76      | 118.80   |
| 1   | AA    | 1346 | A    | C1'-O4'-C4' | 6.61  | 115.18      | 109.90   |
| 35  | BB    | 473  | G    | C4-C5-C6    | 6.61  | 122.76      | 118.80   |
| 35  | BB    | 706  | A    | C4-C5-N7    | 6.61  | 114.00      | 110.70   |
| 35  | BB    | 1649 | G    | N3-C4-C5    | -6.61 | 125.30      | 128.60   |
| 35  | BB    | 2035 | G    | C6-C5-N7    | -6.61 | 126.44      | 130.40   |
| 35  | BB    | 2288 | A    | C5-N7-C8    | 6.61  | 107.20      | 103.90   |
| 50  | BQ    | 63   | ARG  | NE-CZ-NH1   | 6.61  | 123.60      | 120.30   |
| 1   | AA    | 452  | A    | C8-N9-C4    | -6.60 | 103.16      | 105.80   |
| 1   | AA    | 1069 | C    | N3-C4-C5    | -6.60 | 119.26      | 121.90   |
| 35  | BB    | 62   | U    | C4'-C3'-C2' | -6.60 | 96.00       | 102.60   |
| 35  | BB    | 429  | A    | O4'-C1'-N9  | 6.60  | 113.48      | 108.20   |
| 35  | BB    | 1778 | U    | C2-N3-C4    | -6.60 | 123.04      | 127.00   |
| 1   | AA    | 730  | G    | N3-C4-C5    | -6.60 | 125.30      | 128.60   |
| 1   | AA    | 973  | G    | N3-C4-C5    | -6.60 | 125.30      | 128.60   |
| 35  | BB    | 172  | A    | C5-C6-N1    | -6.60 | 114.40      | 117.70   |
| 35  | BB    | 496  | G    | C5-C6-O6    | -6.60 | 124.64      | 128.60   |
| 35  | BB    | 1250 | G    | N9-C4-C5    | 6.60  | 108.04      | 105.40   |
| 35  | BB    | 2455 | G    | C4-C5-N7    | -6.60 | 108.16      | 110.80   |
| 1   | AA    | 68   | G    | C5-C6-N1    | 6.60  | 114.80      | 111.50   |
| 1   | AA    | 476  | U    | O4'-C1'-N1  | 6.60  | 113.48      | 108.20   |
| 35  | BB    | 37   | C    | N3-C4-C5    | -6.60 | 119.26      | 121.90   |
| 35  | BB    | 1842 | G    | C6-N1-C2    | 6.60  | 129.06      | 125.10   |
| 35  | BB    | 2183 | A    | C5-C6-N6    | -6.60 | 118.42      | 123.70   |
| 35  | BB    | 2302 | U    | C2-N3-C4    | 6.60  | 130.96      | 127.00   |
| 35  | BB    | 2336 | A    | N1-C6-N6    | 6.60  | 122.56      | 118.60   |
| 35  | BB    | 2694 | G    | O4'-C1'-N9  | 6.60  | 113.48      | 108.20   |
| 1   | AA    | 65   | A    | O4'-C1'-N9  | 6.60  | 113.48      | 108.20   |
| 1   | AA    | 132  | C    | N3-C4-N4    | 6.60  | 122.62      | 118.00   |
| 1   | AA    | 202  | G    | N1-C2-N3    | -6.60 | 119.94      | 123.90   |
| 1   | AA    | 1054 | C    | C2-N1-C1'   | 6.60  | 126.06      | 118.80   |
| 35  | BB    | 43   | G    | C4-C5-C6    | 6.60  | 122.76      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 788  | A    | C4-C5-N7    | -6.60 | 107.40      | 110.70   |
| 35  | BB    | 2770 | G    | C5-N7-C8    | -6.60 | 101.00      | 104.30   |
| 1   | AA    | 105  | G    | O4'-C1'-N9  | 6.60  | 113.48      | 108.20   |
| 1   | AA    | 220  | G    | O4'-C4'-C3' | -6.60 | 97.40       | 104.00   |
| 1   | AA    | 411  | A    | C5-N7-C8    | 6.60  | 107.20      | 103.90   |
| 1   | AA    | 646  | G    | C1'-O4'-C4' | -6.60 | 104.62      | 109.90   |
| 1   | AA    | 904  | U    | P-O5'-C5'   | 6.60  | 131.46      | 120.90   |
| 1   | AA    | 947  | G    | N1-C2-N2    | -6.60 | 110.26      | 116.20   |
| 1   | AA    | 1275 | A    | C4-C5-C6    | 6.60  | 120.30      | 117.00   |
| 2   | AB    | 49   | PHE  | CB-CG-CD2   | 6.60  | 125.42      | 120.80   |
| 19  | AS    | 79   | TYR  | CG-CD2-CE2  | -6.60 | 116.02      | 121.30   |
| 35  | BB    | 526  | A    | C5-C6-N6    | -6.60 | 118.42      | 123.70   |
| 35  | BB    | 2293 | G    | C4-C5-N7    | 6.60  | 113.44      | 110.80   |
| 1   | AA    | 134  | G    | C8-N9-C4    | 6.60  | 109.04      | 106.40   |
| 1   | AA    | 710  | G    | N9-C4-C5    | 6.60  | 108.04      | 105.40   |
| 1   | AA    | 910  | C    | O4'-C1'-N1  | 6.60  | 113.48      | 108.20   |
| 1   | AA    | 1082 | A    | C5-C6-N1    | -6.60 | 114.40      | 117.70   |
| 1   | AA    | 1096 | C    | N3-C4-C5    | 6.60  | 124.54      | 121.90   |
| 1   | AA    | 1455 | G    | C4-C5-C6    | 6.60  | 122.76      | 118.80   |
| 35  | BB    | 317  | G    | N9-C4-C5    | -6.60 | 102.76      | 105.40   |
| 1   | AA    | 202  | G    | C2-N3-C4    | 6.59  | 115.20      | 111.90   |
| 1   | AA    | 1016 | A    | C6-C5-N7    | -6.59 | 127.68      | 132.30   |
| 1   | AA    | 1213 | A    | C5-N7-C8    | 6.59  | 107.20      | 103.90   |
| 34  | BA    | 61   | G    | N3-C2-N2    | 6.59  | 124.52      | 119.90   |
| 35  | BB    | 72   | U    | N3-C4-C5    | -6.59 | 110.64      | 114.60   |
| 35  | BB    | 291  | G    | N3-C2-N2    | 6.59  | 124.52      | 119.90   |
| 35  | BB    | 416  | U    | N1-C2-O2    | 6.59  | 127.42      | 122.80   |
| 35  | BB    | 843  | G    | C5'-C4'-O4' | 6.59  | 117.01      | 109.10   |
| 35  | BB    | 1156 | A    | C4-C5-N7    | 6.59  | 114.00      | 110.70   |
| 35  | BB    | 1710 | G    | C5-C6-N1    | -6.59 | 108.20      | 111.50   |
| 35  | BB    | 1810 | A    | C5-C6-N1    | -6.59 | 114.40      | 117.70   |
| 35  | BB    | 1865 | U    | N1-C2-O2    | -6.59 | 118.18      | 122.80   |
| 35  | BB    | 2299 | U    | O4'-C1'-N1  | 6.59  | 113.47      | 108.20   |
| 35  | BB    | 2553 | G    | N3-C2-N2    | 6.59  | 124.52      | 119.90   |
| 35  | BB    | 2772 | C    | N3-C4-C5    | -6.59 | 119.26      | 121.90   |
| 52  | BS    | 53   | SER  | N-CA-C      | -6.59 | 93.19       | 111.00   |
| 1   | AA    | 359  | G    | C5-C6-O6    | -6.59 | 124.64      | 128.60   |
| 1   | AA    | 411  | A    | C6-N1-C2    | 6.59  | 122.56      | 118.60   |
| 34  | BA    | 49   | C    | O4'-C1'-N1  | 6.59  | 113.47      | 108.20   |
| 1   | AA    | 319  | G    | C4-C5-C6    | 6.59  | 122.75      | 118.80   |
| 1   | AA    | 735  | C    | N3-C4-C5    | 6.59  | 124.54      | 121.90   |
| 1   | AA    | 1356 | G    | C6-C5-N7    | -6.59 | 126.45      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | AV    | 40   | U    | O4'-C1'-N1  | 6.59  | 113.47      | 108.20   |
| 34  | BA    | 5    | U    | N3-C4-O4    | 6.59  | 124.01      | 119.40   |
| 35  | BB    | 810  | U    | C5-C6-N1    | -6.59 | 119.41      | 122.70   |
| 1   | AA    | 205  | A    | N9-C4-C5    | 6.59  | 108.44      | 105.80   |
| 1   | AA    | 592  | G    | C6-C5-N7    | -6.59 | 126.45      | 130.40   |
| 1   | AA    | 848  | C    | C2-N1-C1'   | 6.59  | 126.05      | 118.80   |
| 14  | AN    | 64   | ARG  | NE-CZ-NH1   | -6.59 | 117.00      | 120.30   |
| 30  | B5    | 53   | ARG  | NE-CZ-NH1   | 6.59  | 123.59      | 120.30   |
| 35  | BB    | 287  | G    | C5-N7-C8    | -6.59 | 101.00      | 104.30   |
| 35  | BB    | 544  | C    | N3-C4-C5    | -6.59 | 119.26      | 121.90   |
| 35  | BB    | 1126 | A    | N7-C8-N9    | -6.59 | 110.51      | 113.80   |
| 35  | BB    | 1229 | C    | C5-C4-N4    | -6.59 | 115.59      | 120.20   |
| 35  | BB    | 1364 | G    | P-O5'-C5'   | 6.59  | 131.44      | 120.90   |
| 35  | BB    | 1529 | G    | N1-C6-O6    | 6.59  | 123.85      | 119.90   |
| 35  | BB    | 1769 | U    | N3-C2-O2    | 6.59  | 126.81      | 122.20   |
| 35  | BB    | 2033 | A    | N1-C6-N6    | 6.59  | 122.55      | 118.60   |
| 35  | BB    | 2459 | A    | C5-C6-N1    | -6.59 | 114.41      | 117.70   |
| 1   | AA    | 1407 | C    | O4'-C1'-N1  | 6.59  | 113.47      | 108.20   |
| 35  | BB    | 273  | G    | C4-C5-N7    | -6.59 | 108.17      | 110.80   |
| 35  | BB    | 2460 | U    | P-O3'-C3'   | -6.59 | 111.79      | 119.70   |
| 1   | AA    | 41   | G    | C6-N1-C2    | 6.59  | 129.05      | 125.10   |
| 1   | AA    | 278  | G    | N3-C4-C5    | -6.59 | 125.31      | 128.60   |
| 1   | AA    | 297  | G    | N1-C2-N2    | -6.59 | 110.27      | 116.20   |
| 1   | AA    | 517  | G    | O4'-C1'-N9  | 6.59  | 113.47      | 108.20   |
| 1   | AA    | 682  | G    | C4-C5-C6    | 6.59  | 122.75      | 118.80   |
| 1   | AA    | 1169 | A    | C6-N1-C2    | 6.59  | 122.55      | 118.60   |
| 1   | AA    | 1336 | C    | C4-C5-C6    | 6.59  | 120.69      | 117.40   |
| 34  | BA    | 52   | A    | C6-C5-N7    | -6.59 | 127.69      | 132.30   |
| 34  | BA    | 70   | C    | N3-C4-N4    | 6.59  | 122.61      | 118.00   |
| 35  | BB    | 30   | G    | N3-C2-N2    | 6.59  | 124.51      | 119.90   |
| 35  | BB    | 168  | G    | C4-C5-C6    | 6.59  | 122.75      | 118.80   |
| 35  | BB    | 938  | G    | C1'-O4'-C4' | 6.59  | 115.17      | 109.90   |
| 35  | BB    | 2602 | A    | C5-C6-N6    | -6.59 | 118.43      | 123.70   |
| 54  | BU    | 80   | ASP  | CB-CG-OD1   | 6.59  | 124.23      | 118.30   |
| 1   | AA    | 282  | A    | N1-C6-N6    | 6.58  | 122.55      | 118.60   |
| 1   | AA    | 288  | A    | C5-C6-N1    | -6.58 | 114.41      | 117.70   |
| 1   | AA    | 1491 | G    | C5-C6-N1    | -6.58 | 108.21      | 111.50   |
| 1   | AA    | 1519 | A    | C2-N3-C4    | 6.58  | 113.89      | 110.60   |
| 35  | BB    | 176  | A    | C5-C6-N1    | -6.58 | 114.41      | 117.70   |
| 35  | BB    | 1412 | U    | N1-C2-N3    | 6.58  | 118.85      | 114.90   |
| 35  | BB    | 1452 | G    | O4'-C1'-N9  | 6.58  | 113.47      | 108.20   |
| 35  | BB    | 1844 | C    | C4-C5-C6    | -6.58 | 114.11      | 117.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2682 | A    | P-O3'-C3'   | -6.58 | 111.80      | 119.70   |
| 1   | AA    | 563  | A    | N3-C4-C5    | -6.58 | 122.19      | 126.80   |
| 1   | AA    | 1095 | U    | P-O5'-C5'   | -6.58 | 110.37      | 120.90   |
| 22  | AV    | 45   | G    | C5-C6-O6    | -6.58 | 124.65      | 128.60   |
| 34  | BA    | 12   | C    | P-O3'-C3'   | 6.58  | 127.60      | 119.70   |
| 35  | BB    | 201  | C    | C1'-O4'-C4' | 6.58  | 115.17      | 109.90   |
| 35  | BB    | 635  | C    | C6-N1-C2    | -6.58 | 117.67      | 120.30   |
| 35  | BB    | 1531 | C    | P-O3'-C3'   | 6.58  | 127.60      | 119.70   |
| 35  | BB    | 1605 | C    | C6-N1-C2    | -6.58 | 117.67      | 120.30   |
| 35  | BB    | 2741 | A    | C2-N3-C4    | -6.58 | 107.31      | 110.60   |
| 35  | BB    | 2746 | U    | C6-N1-C2    | -6.58 | 117.05      | 121.00   |
| 1   | AA    | 377  | G    | N3-C4-C5    | 6.58  | 131.89      | 128.60   |
| 1   | AA    | 837  | U    | C1'-O4'-C4' | 6.58  | 115.17      | 109.90   |
| 1   | AA    | 1179 | A    | C5-C6-N6    | -6.58 | 118.44      | 123.70   |
| 1   | AA    | 1307 | U    | O4'-C1'-N1  | 6.58  | 113.47      | 108.20   |
| 34  | BA    | 12   | C    | C5-C4-N4    | -6.58 | 115.59      | 120.20   |
| 34  | BA    | 75   | G    | C8-N9-C4    | 6.58  | 109.03      | 106.40   |
| 35  | BB    | 524  | G    | O4'-C1'-N9  | 6.58  | 113.47      | 108.20   |
| 35  | BB    | 631  | A    | C5-N7-C8    | 6.58  | 107.19      | 103.90   |
| 35  | BB    | 1134 | A    | C4-C5-N7    | -6.58 | 107.41      | 110.70   |
| 35  | BB    | 1138 | G    | C5-N7-C8    | 6.58  | 107.59      | 104.30   |
| 35  | BB    | 1636 | U    | C6-N1-C2    | -6.58 | 117.05      | 121.00   |
| 35  | BB    | 2193 | G    | P-O3'-C3'   | -6.58 | 111.80      | 119.70   |
| 35  | BB    | 2216 | G    | O4'-C1'-N9  | 6.58  | 113.47      | 108.20   |
| 35  | BB    | 2768 | U    | C4'-C3'-C2' | -6.58 | 96.02       | 102.60   |
| 1   | AA    | 858  | G    | C6-C5-N7    | -6.58 | 126.45      | 130.40   |
| 1   | AA    | 1318 | A    | C2-N3-C4    | 6.58  | 113.89      | 110.60   |
| 35  | BB    | 804  | A    | O4'-C1'-N9  | 6.58  | 113.46      | 108.20   |
| 35  | BB    | 1038 | G    | O4'-C1'-N9  | 6.58  | 113.46      | 108.20   |
| 35  | BB    | 1984 | G    | C6-C5-N7    | -6.58 | 126.45      | 130.40   |
| 1   | AA    | 41   | G    | C4'-C3'-C2' | -6.58 | 96.02       | 102.60   |
| 1   | AA    | 120  | A    | N1-C2-N3    | 6.58  | 132.59      | 129.30   |
| 1   | AA    | 337  | G    | N3-C2-N2    | 6.58  | 124.50      | 119.90   |
| 1   | AA    | 1094 | G    | N3-C2-N2    | 6.58  | 124.50      | 119.90   |
| 1   | AA    | 1145 | A    | O4'-C1'-N9  | 6.58  | 113.46      | 108.20   |
| 1   | AA    | 1274 | A    | C6-N1-C2    | 6.58  | 122.55      | 118.60   |
| 35  | BB    | 8    | C    | N1-C2-O2    | -6.58 | 114.95      | 118.90   |
| 35  | BB    | 1019 | U    | N3-C4-C5    | -6.58 | 110.65      | 114.60   |
| 35  | BB    | 1264 | A    | N1-C2-N3    | -6.58 | 126.01      | 129.30   |
| 35  | BB    | 1949 | G    | C6-C5-N7    | -6.58 | 126.45      | 130.40   |
| 35  | BB    | 1998 | A    | C4-C5-N7    | -6.58 | 107.41      | 110.70   |
| 35  | BB    | 2234 | G    | N3-C2-N2    | 6.58  | 124.50      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2305 | U    | C6-N1-C2    | -6.58 | 117.05      | 121.00   |
| 45  | BL    | 126  | ARG  | NH1-CZ-NH2  | -6.58 | 112.16      | 119.40   |
| 1   | AA    | 285  | C    | P-O3'-C3'   | -6.58 | 111.81      | 119.70   |
| 1   | AA    | 572  | A    | N7-C8-N9    | -6.58 | 110.51      | 113.80   |
| 34  | BA    | 54   | G    | O4'-C1'-N9  | 6.58  | 113.46      | 108.20   |
| 35  | BB    | 11   | C    | C5'-C4'-C3' | 6.58  | 126.52      | 116.00   |
| 35  | BB    | 364  | C    | C5-C6-N1    | 6.58  | 124.29      | 121.00   |
| 35  | BB    | 1649 | G    | N1-C2-N3    | -6.58 | 119.95      | 123.90   |
| 35  | BB    | 1855 | U    | O4'-C1'-N1  | 6.58  | 113.46      | 108.20   |
| 1   | AA    | 153  | C    | C1'-O4'-C4' | 6.58  | 115.16      | 109.90   |
| 1   | AA    | 377  | G    | N3-C4-N9    | -6.58 | 122.06      | 126.00   |
| 1   | AA    | 377  | G    | O4'-C1'-N9  | 6.58  | 113.46      | 108.20   |
| 1   | AA    | 963  | G    | C5-C6-O6    | -6.58 | 124.65      | 128.60   |
| 35  | BB    | 347  | A    | C8-N9-C4    | -6.58 | 103.17      | 105.80   |
| 35  | BB    | 467  | G    | C5-C6-O6    | -6.58 | 124.66      | 128.60   |
| 35  | BB    | 573  | U    | C6-N1-C2    | -6.58 | 117.05      | 121.00   |
| 35  | BB    | 1190 | G    | O4'-C1'-N9  | 6.58  | 113.46      | 108.20   |
| 35  | BB    | 1254 | A    | C5-N7-C8    | 6.58  | 107.19      | 103.90   |
| 35  | BB    | 1320 | C    | C5-C6-N1    | 6.58  | 124.29      | 121.00   |
| 35  | BB    | 1369 | G    | C6-C5-N7    | -6.58 | 126.45      | 130.40   |
| 35  | BB    | 1371 | G    | C8-N9-C1'   | 6.58  | 135.55      | 127.00   |
| 35  | BB    | 2072 | C    | O4'-C1'-N1  | 6.58  | 113.46      | 108.20   |
| 35  | BB    | 2902 | C    | OP2-P-O3'   | 6.58  | 119.67      | 105.20   |
| 1   | AA    | 587  | G    | O4'-C1'-N9  | 6.57  | 113.46      | 108.20   |
| 1   | AA    | 936  | C    | C5-C4-N4    | -6.57 | 115.60      | 120.20   |
| 35  | BB    | 386  | G    | C4-C5-N7    | 6.57  | 113.43      | 110.80   |
| 35  | BB    | 858  | G    | C6-N1-C2    | 6.57  | 129.04      | 125.10   |
| 35  | BB    | 991  | C    | C6-N1-C2    | 6.57  | 122.93      | 120.30   |
| 35  | BB    | 1065 | U    | C5-C6-N1    | -6.57 | 119.41      | 122.70   |
| 35  | BB    | 1143 | A    | C5'-C4'-O4' | 6.57  | 116.99      | 109.10   |
| 35  | BB    | 1734 | G    | N7-C8-N9    | -6.57 | 109.81      | 113.10   |
| 35  | BB    | 1752 | C    | N3-C4-N4    | 6.57  | 122.60      | 118.00   |
| 35  | BB    | 2047 | C    | C5-C4-N4    | -6.57 | 115.60      | 120.20   |
| 54  | BU    | 41   | VAL  | N-CA-CB     | 6.57  | 125.96      | 111.50   |
| 1   | AA    | 50   | A    | C6-N1-C2    | 6.57  | 122.54      | 118.60   |
| 1   | AA    | 243  | A    | C5-C6-N1    | -6.57 | 114.41      | 117.70   |
| 1   | AA    | 366  | A    | P-O3'-C3'   | 6.57  | 127.59      | 119.70   |
| 1   | AA    | 601  | G    | C5-C6-N1    | 6.57  | 114.79      | 111.50   |
| 1   | AA    | 1219 | A    | C2-N3-C4    | 6.57  | 113.89      | 110.60   |
| 35  | BB    | 2674 | G    | C2-N3-C4    | 6.57  | 115.19      | 111.90   |
| 1   | AA    | 745  | G    | C4-N9-C1'   | -6.57 | 117.96      | 126.50   |
| 34  | BA    | 69   | G    | C5-C6-O6    | -6.57 | 124.66      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 89   | A    | O4'-C1'-N9  | 6.57  | 113.46      | 108.20   |
| 35  | BB    | 668  | A    | N3-C4-C5    | -6.57 | 122.20      | 126.80   |
| 35  | BB    | 2168 | G    | C4-C5-N7    | 6.57  | 113.43      | 110.80   |
| 36  | BC    | 215  | VAL  | CG1-CB-CG2  | -6.57 | 100.39      | 110.90   |
| 39  | BF    | 9    | ASP  | N-CA-CB     | 6.57  | 122.42      | 110.60   |
| 49  | BP    | 97   | TYR  | CG-CD1-CE1  | -6.57 | 116.04      | 121.30   |
| 50  | BQ    | 87   | VAL  | CA-CB-CG1   | -6.57 | 101.05      | 110.90   |
| 1   | AA    | 556  | C    | N3-C4-N4    | 6.57  | 122.60      | 118.00   |
| 35  | BB    | 149  | A    | C1'-O4'-C4' | 6.57  | 115.16      | 109.90   |
| 35  | BB    | 742  | A    | C4-C5-N7    | -6.57 | 107.42      | 110.70   |
| 35  | BB    | 1651 | G    | C2-N3-C4    | 6.57  | 115.18      | 111.90   |
| 35  | BB    | 1769 | U    | N1-C2-O2    | -6.57 | 118.20      | 122.80   |
| 35  | BB    | 2269 | G    | P-O5'-C5'   | -6.57 | 110.39      | 120.90   |
| 35  | BB    | 2721 | A    | C5-C6-N1    | -6.57 | 114.42      | 117.70   |
| 1   | AA    | 136  | C    | C1'-O4'-C4' | -6.57 | 104.65      | 109.90   |
| 1   | AA    | 408  | A    | N1-C2-N3    | 6.57  | 132.58      | 129.30   |
| 1   | AA    | 444  | G    | N1-C6-O6    | 6.57  | 123.84      | 119.90   |
| 1   | AA    | 1080 | A    | O4'-C1'-N9  | 6.57  | 113.45      | 108.20   |
| 17  | AQ    | 33   | TYR  | N-CA-CB     | 6.57  | 122.42      | 110.60   |
| 23  | AX    | 19   | A    | O4'-C1'-N9  | 6.57  | 113.45      | 108.20   |
| 35  | BB    | 75   | G    | N3-C2-N2    | 6.57  | 124.50      | 119.90   |
| 35  | BB    | 1297 | C    | C6-N1-C2    | -6.57 | 117.67      | 120.30   |
| 1   | AA    | 966  | G    | N3-C2-N2    | 6.57  | 124.50      | 119.90   |
| 35  | BB    | 107  | G    | C2-N3-C4    | 6.57  | 115.18      | 111.90   |
| 35  | BB    | 620  | G    | C5-C6-O6    | -6.57 | 124.66      | 128.60   |
| 35  | BB    | 800  | A    | N9-C4-C5    | -6.57 | 103.17      | 105.80   |
| 35  | BB    | 1127 | A    | N9-C4-C5    | -6.57 | 103.17      | 105.80   |
| 35  | BB    | 1545 | A    | N3-C4-C5    | -6.57 | 122.20      | 126.80   |
| 35  | BB    | 1595 | C    | O4'-C4'-C3' | -6.57 | 97.44       | 104.00   |
| 35  | BB    | 1681 | G    | C4-C5-C6    | 6.57  | 122.74      | 118.80   |
| 35  | BB    | 1860 | G    | N1-C6-O6    | 6.57  | 123.84      | 119.90   |
| 35  | BB    | 2076 | U    | C3'-C2'-C1' | -6.57 | 96.25       | 101.50   |
| 35  | BB    | 2218 | G    | N7-C8-N9    | -6.57 | 109.82      | 113.10   |
| 35  | BB    | 2627 | G    | C4-C5-C6    | 6.57  | 122.74      | 118.80   |
| 38  | BE    | 91   | ASP  | CB-CG-OD2   | -6.57 | 112.39      | 118.30   |
| 1   | AA    | 1267 | C    | C4-C5-C6    | 6.56  | 120.68      | 117.40   |
| 35  | BB    | 949  | G    | C6-C5-N7    | -6.56 | 126.46      | 130.40   |
| 1   | AA    | 118  | U    | C6-N1-C2    | -6.56 | 117.06      | 121.00   |
| 1   | AA    | 1012 | A    | C6-N1-C2    | -6.56 | 114.66      | 118.60   |
| 35  | BB    | 98   | G    | O4'-C1'-N9  | 6.56  | 113.45      | 108.20   |
| 35  | BB    | 191  | A    | N9-C4-C5    | 6.56  | 108.42      | 105.80   |
| 35  | BB    | 535  | G    | N3-C4-C5    | -6.56 | 125.32      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 874  | G    | N7-C8-N9    | 6.56  | 116.38      | 113.10   |
| 35  | BB    | 1224 | U    | C5-C4-O4    | -6.56 | 121.96      | 125.90   |
| 35  | BB    | 1559 | U    | N3-C4-O4    | 6.56  | 123.99      | 119.40   |
| 35  | BB    | 1608 | A    | N1-C6-N6    | 6.56  | 122.54      | 118.60   |
| 40  | BG    | 93   | TYR  | CB-CG-CD2   | 6.56  | 124.94      | 121.00   |
| 1   | AA    | 955  | U    | O4'-C1'-N1  | 6.56  | 113.45      | 108.20   |
| 35  | BB    | 106  | C    | O4'-C4'-C3' | -6.56 | 97.44       | 104.00   |
| 35  | BB    | 1507 | C    | O4'-C1'-N1  | 6.56  | 113.45      | 108.20   |
| 35  | BB    | 1696 | G    | C5-C6-N1    | 6.56  | 114.78      | 111.50   |
| 35  | BB    | 2448 | A    | C5-C6-N6    | -6.56 | 118.45      | 123.70   |
| 1   | AA    | 908  | A    | C4'-C3'-C2' | -6.56 | 96.04       | 102.60   |
| 1   | AA    | 1154 | G    | C5-C6-N1    | -6.56 | 108.22      | 111.50   |
| 1   | AA    | 1167 | A    | C5-C6-N1    | -6.56 | 114.42      | 117.70   |
| 35  | BB    | 298  | G    | N1-C2-N3    | -6.56 | 119.96      | 123.90   |
| 35  | BB    | 311  | A    | N9-C4-C5    | 6.56  | 108.42      | 105.80   |
| 35  | BB    | 366  | C    | C4'-C3'-C2' | -6.56 | 96.04       | 102.60   |
| 35  | BB    | 422  | A    | C6-C5-N7    | -6.56 | 127.71      | 132.30   |
| 35  | BB    | 763  | G    | C8-N9-C1'   | 6.56  | 135.53      | 127.00   |
| 35  | BB    | 1215 | G    | N7-C8-N9    | -6.56 | 109.82      | 113.10   |
| 35  | BB    | 1406 | U    | N3-C4-O4    | 6.56  | 123.99      | 119.40   |
| 1   | AA    | 385  | C    | N1-C2-O2    | -6.56 | 114.97      | 118.90   |
| 1   | AA    | 733  | G    | C4'-C3'-C2' | -6.56 | 96.04       | 102.60   |
| 1   | AA    | 1009 | U    | N3-C2-O2    | -6.56 | 117.61      | 122.20   |
| 3   | AC    | 71   | ARG  | NE-CZ-NH2   | -6.56 | 117.02      | 120.30   |
| 5   | AE    | 44   | ARG  | N-CA-CB     | 6.56  | 122.41      | 110.60   |
| 35  | BB    | 950  | G    | O4'-C4'-C3' | -6.56 | 97.44       | 104.00   |
| 35  | BB    | 983  | A    | C3'-C2'-C1' | 6.56  | 106.75      | 101.50   |
| 35  | BB    | 1449 | G    | C4'-C3'-C2' | -6.56 | 96.04       | 102.60   |
| 35  | BB    | 1864 | U    | P-O3'-C3'   | 6.56  | 127.57      | 119.70   |
| 35  | BB    | 1930 | G    | N3-C4-C5    | 6.56  | 131.88      | 128.60   |
| 35  | BB    | 2108 | A    | O4'-C1'-N9  | 6.56  | 113.45      | 108.20   |
| 35  | BB    | 2225 | A    | C8-N9-C4    | -6.56 | 103.18      | 105.80   |
| 35  | BB    | 2658 | C    | O4'-C1'-N1  | 6.56  | 113.45      | 108.20   |
| 35  | BB    | 2765 | A    | C5-C6-N1    | -6.56 | 114.42      | 117.70   |
| 1   | AA    | 951  | G    | P-O5'-C5'   | -6.56 | 110.41      | 120.90   |
| 35  | BB    | 1902 | C    | O4'-C1'-N1  | 6.56  | 113.44      | 108.20   |
| 35  | BB    | 2108 | A    | N1-C2-N3    | 6.56  | 132.58      | 129.30   |
| 1   | AA    | 542  | G    | C5-C6-N1    | -6.55 | 108.22      | 111.50   |
| 1   | AA    | 992  | U    | C5-C4-O4    | -6.55 | 121.97      | 125.90   |
| 23  | AX    | 16   | C    | O4'-C1'-N1  | 6.55  | 113.44      | 108.20   |
| 35  | BB    | 320  | A    | N1-C6-N6    | 6.55  | 122.53      | 118.60   |
| 35  | BB    | 1960 | A    | C1'-O4'-C4' | 6.55  | 115.14      | 109.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2137 | U    | N3-C2-O2    | 6.55  | 126.79      | 122.20   |
| 35  | BB    | 180  | G    | C2-N3-C4    | 6.55  | 115.18      | 111.90   |
| 35  | BB    | 2891 | U    | O4'-C1'-N1  | 6.55  | 113.44      | 108.20   |
| 20  | AT    | 24   | ARG  | NE-CZ-NH1   | -6.55 | 117.02      | 120.30   |
| 35  | BB    | 1632 | A    | O4'-C1'-N9  | 6.55  | 113.44      | 108.20   |
| 35  | BB    | 2131 | U    | C6-N1-C2    | -6.55 | 117.07      | 121.00   |
| 35  | BB    | 2286 | G    | N3-C4-C5    | -6.55 | 125.33      | 128.60   |
| 35  | BB    | 2385 | C    | O4'-C1'-N1  | 6.55  | 113.44      | 108.20   |
| 35  | BB    | 27   | G    | C4-C5-C6    | 6.55  | 122.73      | 118.80   |
| 35  | BB    | 123  | G    | N7-C8-N9    | -6.55 | 109.83      | 113.10   |
| 35  | BB    | 414  | C    | N3-C4-C5    | -6.55 | 119.28      | 121.90   |
| 35  | BB    | 445  | C    | C2-N3-C4    | 6.55  | 123.17      | 119.90   |
| 35  | BB    | 888  | C    | C2-N3-C4    | 6.55  | 123.17      | 119.90   |
| 35  | BB    | 1032 | A    | C5-C6-N1    | -6.55 | 114.42      | 117.70   |
| 35  | BB    | 1210 | G    | N9-C4-C5    | 6.55  | 108.02      | 105.40   |
| 35  | BB    | 1294 | U    | N1-C2-O2    | -6.55 | 118.22      | 122.80   |
| 35  | BB    | 1608 | A    | C5-N7-C8    | -6.55 | 100.62      | 103.90   |
| 1   | AA    | 382  | A    | C5-C6-N6    | -6.55 | 118.46      | 123.70   |
| 35  | BB    | 493  | G    | C5-C6-O6    | -6.55 | 124.67      | 128.60   |
| 35  | BB    | 1011 | G    | N1-C6-O6    | 6.55  | 123.83      | 119.90   |
| 35  | BB    | 2176 | A    | C4-C5-N7    | -6.55 | 107.43      | 110.70   |
| 1   | AA    | 863  | U    | O3'-P-O5'   | -6.55 | 91.56       | 104.00   |
| 1   | AA    | 1401 | G    | O4'-C1'-N9  | 6.55  | 113.44      | 108.20   |
| 1   | AA    | 1459 | G    | N3-C2-N2    | 6.55  | 124.48      | 119.90   |
| 34  | BA    | 105  | G    | N1-C2-N3    | -6.55 | 119.97      | 123.90   |
| 35  | BB    | 237  | C    | N3-C4-C5    | -6.55 | 119.28      | 121.90   |
| 35  | BB    | 1413 | A    | C4-C5-N7    | -6.55 | 107.43      | 110.70   |
| 35  | BB    | 1576 | U    | C4'-C3'-C2' | -6.55 | 96.05       | 102.60   |
| 35  | BB    | 1807 | G    | C2-N3-C4    | -6.55 | 108.63      | 111.90   |
| 35  | BB    | 2146 | C    | C6-N1-C2    | -6.55 | 117.68      | 120.30   |
| 35  | BB    | 2275 | C    | N1-C2-N3    | -6.55 | 114.62      | 119.20   |
| 35  | BB    | 2846 | G    | C5-C6-N1    | -6.55 | 108.23      | 111.50   |
| 35  | BB    | 801  | G    | C2-N3-C4    | -6.54 | 108.63      | 111.90   |
| 35  | BB    | 937  | C    | P-O5'-C5'   | 6.54  | 131.37      | 120.90   |
| 35  | BB    | 1389 | G    | C4-C5-C6    | 6.54  | 122.73      | 118.80   |
| 35  | BB    | 2174 | C    | N3-C4-C5    | -6.54 | 119.28      | 121.90   |
| 35  | BB    | 2250 | G    | O4'-C1'-N9  | 6.54  | 113.44      | 108.20   |
| 1   | AA    | 183  | C    | C2-N3-C4    | 6.54  | 123.17      | 119.90   |
| 1   | AA    | 289  | G    | N3-C4-C5    | -6.54 | 125.33      | 128.60   |
| 1   | AA    | 576  | C    | C6-N1-C2    | -6.54 | 117.68      | 120.30   |
| 1   | AA    | 907  | A    | C4-C5-C6    | 6.54  | 120.27      | 117.00   |
| 1   | AA    | 1167 | A    | C2-N3-C4    | -6.54 | 107.33      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1202 | U    | C6-N1-C2    | -6.54 | 117.07      | 121.00   |
| 1   | AA    | 1466 | C    | N3-C4-N4    | 6.54  | 122.58      | 118.00   |
| 35  | BB    | 891  | G    | N1-C2-N3    | -6.54 | 119.97      | 123.90   |
| 35  | BB    | 1773 | A    | C4-C5-N7    | -6.54 | 107.43      | 110.70   |
| 35  | BB    | 1867 | G    | O4'-C1'-N9  | 6.54  | 113.43      | 108.20   |
| 35  | BB    | 2209 | G    | C6-C5-N7    | -6.54 | 126.47      | 130.40   |
| 35  | BB    | 2801 | G    | N3-C4-C5    | -6.54 | 125.33      | 128.60   |
| 35  | BB    | 2848 | G    | C6-N1-C2    | 6.54  | 129.03      | 125.10   |
| 1   | AA    | 72   | A    | C1'-O4'-C4' | -6.54 | 104.67      | 109.90   |
| 1   | AA    | 1266 | G    | N7-C8-N9    | 6.54  | 116.37      | 113.10   |
| 1   | AA    | 1270 | G    | N3-C4-C5    | -6.54 | 125.33      | 128.60   |
| 1   | AA    | 1493 | A    | C5-N7-C8    | 6.54  | 107.17      | 103.90   |
| 35  | BB    | 155  | A    | C4-C5-C6    | 6.54  | 120.27      | 117.00   |
| 35  | BB    | 261  | G    | N7-C8-N9    | 6.54  | 116.37      | 113.10   |
| 35  | BB    | 968  | C    | C5-C4-N4    | -6.54 | 115.62      | 120.20   |
| 35  | BB    | 1622 | G    | C4-C5-C6    | 6.54  | 122.72      | 118.80   |
| 35  | BB    | 2033 | A    | C4-C5-C6    | 6.54  | 120.27      | 117.00   |
| 35  | BB    | 2360 | G    | N1-C2-N3    | -6.54 | 119.97      | 123.90   |
| 1   | AA    | 656  | G    | N1-C2-N3    | -6.54 | 119.98      | 123.90   |
| 1   | AA    | 1068 | G    | N3-C4-N9    | 6.54  | 129.92      | 126.00   |
| 35  | BB    | 1051 | G    | O4'-C1'-N9  | 6.54  | 113.43      | 108.20   |
| 35  | BB    | 1595 | C    | O4'-C1'-N1  | 6.54  | 113.43      | 108.20   |
| 1   | AA    | 326  | G    | O4'-C1'-N9  | 6.54  | 113.43      | 108.20   |
| 35  | BB    | 41   | C    | C4-C5-C6    | 6.54  | 120.67      | 117.40   |
| 35  | BB    | 186  | G    | O4'-C1'-N9  | 6.54  | 113.43      | 108.20   |
| 35  | BB    | 619  | G    | N3-C2-N2    | 6.54  | 124.48      | 119.90   |
| 35  | BB    | 751  | A    | C4-C5-C6    | 6.54  | 120.27      | 117.00   |
| 35  | BB    | 1055 | G    | N1-C6-O6    | 6.54  | 123.82      | 119.90   |
| 35  | BB    | 1804 | C    | C5-C4-N4    | -6.54 | 115.62      | 120.20   |
| 35  | BB    | 1999 | C    | C2-N3-C4    | 6.54  | 123.17      | 119.90   |
| 35  | BB    | 2664 | G    | C6-C5-N7    | -6.54 | 126.48      | 130.40   |
| 1   | AA    | 429  | U    | C5-C4-O4    | -6.54 | 121.98      | 125.90   |
| 11  | AK    | 110  | THR  | N-CA-CB     | 6.54  | 122.72      | 110.30   |
| 35  | BB    | 597  | G    | N3-C4-C5    | -6.54 | 125.33      | 128.60   |
| 35  | BB    | 785  | G    | C6-N1-C2    | 6.54  | 129.02      | 125.10   |
| 35  | BB    | 807  | U    | C4-C5-C6    | 6.54  | 123.62      | 119.70   |
| 35  | BB    | 2018 | G    | N9-C4-C5    | 6.54  | 108.02      | 105.40   |
| 35  | BB    | 2235 | G    | C6-C5-N7    | -6.54 | 126.48      | 130.40   |
| 35  | BB    | 2882 | A    | C4-C5-C6    | 6.54  | 120.27      | 117.00   |
| 1   | AA    | 669  | G    | N3-C4-C5    | -6.54 | 125.33      | 128.60   |
| 1   | AA    | 1476 | A    | N7-C8-N9    | -6.54 | 110.53      | 113.80   |
| 35  | BB    | 116  | C    | C4-C5-C6    | 6.54  | 120.67      | 117.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 189  | G    | N1-C6-O6    | 6.54  | 123.82      | 119.90   |
| 35  | BB    | 212  | G    | C5-N7-C8    | 6.54  | 107.57      | 104.30   |
| 35  | BB    | 572  | A    | C5-C6-N1    | -6.54 | 114.43      | 117.70   |
| 35  | BB    | 893  | C    | P-O3'-C3'   | -6.54 | 111.86      | 119.70   |
| 35  | BB    | 1393 | A    | C4-C5-C6    | 6.54  | 120.27      | 117.00   |
| 35  | BB    | 1424 | G    | C6-N1-C2    | 6.54  | 129.02      | 125.10   |
| 35  | BB    | 1993 | U    | C2-N3-C4    | -6.54 | 123.08      | 127.00   |
| 35  | BB    | 2342 | C    | N1-C2-N3    | -6.54 | 114.62      | 119.20   |
| 35  | BB    | 2408 | U    | N1-C2-N3    | 6.54  | 118.82      | 114.90   |
| 35  | BB    | 2692 | G    | O4'-C1'-N9  | 6.54  | 113.43      | 108.20   |
| 1   | AA    | 195  | A    | O4'-C1'-N9  | 6.53  | 113.43      | 108.20   |
| 1   | AA    | 899  | C    | C2-N3-C4    | 6.53  | 123.17      | 119.90   |
| 34  | BA    | 15   | A    | C2-N3-C4    | -6.53 | 107.33      | 110.60   |
| 35  | BB    | 1039 | A    | O4'-C1'-N9  | 6.53  | 113.43      | 108.20   |
| 35  | BB    | 1096 | A    | N1-C2-N3    | -6.53 | 126.03      | 129.30   |
| 35  | BB    | 1223 | G    | N7-C8-N9    | -6.53 | 109.83      | 113.10   |
| 35  | BB    | 1330 | C    | C6-N1-C2    | -6.53 | 117.69      | 120.30   |
| 35  | BB    | 1611 | C    | P-O5'-C5'   | -6.53 | 110.45      | 120.90   |
| 35  | BB    | 2441 | U    | O4'-C1'-N1  | 6.53  | 113.43      | 108.20   |
| 35  | BB    | 2714 | G    | C5-N7-C8    | 6.53  | 107.57      | 104.30   |
| 1   | AA    | 35   | G    | C2-N3-C4    | 6.53  | 115.17      | 111.90   |
| 1   | AA    | 833  | G    | C5-C6-N1    | -6.53 | 108.23      | 111.50   |
| 22  | AV    | 39   | G    | N3-C4-N9    | 6.53  | 129.92      | 126.00   |
| 34  | BA    | 44   | G    | O4'-C1'-N9  | 6.53  | 113.42      | 108.20   |
| 35  | BB    | 329  | G    | C6-C5-N7    | -6.53 | 126.48      | 130.40   |
| 35  | BB    | 818  | G    | C4-N9-C1'   | 6.53  | 134.99      | 126.50   |
| 35  | BB    | 1026 | G    | N1-C2-N3    | -6.53 | 119.98      | 123.90   |
| 35  | BB    | 2204 | G    | N9-C4-C5    | -6.53 | 102.79      | 105.40   |
| 35  | BB    | 2351 | G    | N7-C8-N9    | -6.53 | 109.83      | 113.10   |
| 34  | BA    | 99   | A    | C5-N7-C8    | 6.53  | 107.17      | 103.90   |
| 35  | BB    | 319  | G    | P-O3'-C3'   | -6.53 | 111.87      | 119.70   |
| 35  | BB    | 952  | G    | C4-N9-C1'   | -6.53 | 118.01      | 126.50   |
| 35  | BB    | 1116 | G    | C5'-C4'-O4' | 6.53  | 116.93      | 109.10   |
| 35  | BB    | 1419 | A    | C5-C6-N1    | -6.53 | 114.44      | 117.70   |
| 35  | BB    | 1455 | G    | C2-N3-C4    | -6.53 | 108.64      | 111.90   |
| 35  | BB    | 1489 | C    | C5-C6-N1    | 6.53  | 124.26      | 121.00   |
| 35  | BB    | 1715 | G    | C4-C5-C6    | 6.53  | 122.72      | 118.80   |
| 1   | AA    | 384  | G    | C6-C5-N7    | -6.53 | 126.48      | 130.40   |
| 1   | AA    | 885  | G    | C4-C5-C6    | 6.53  | 122.72      | 118.80   |
| 1   | AA    | 1128 | C    | C4'-C3'-C2' | -6.53 | 96.07       | 102.60   |
| 35  | BB    | 124  | G    | N3-C4-C5    | -6.53 | 125.34      | 128.60   |
| 35  | BB    | 156  | A    | C6-C5-N7    | -6.53 | 127.73      | 132.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1390 | U    | C5-C4-O4    | 6.53  | 129.82      | 125.90   |
| 35  | BB    | 1467 | U    | P-O3'-C3'   | -6.53 | 111.87      | 119.70   |
| 35  | BB    | 1593 | A    | O4'-C1'-N9  | 6.53  | 113.42      | 108.20   |
| 35  | BB    | 1651 | G    | N1-C2-N3    | -6.53 | 119.98      | 123.90   |
| 35  | BB    | 1746 | A    | C5-C6-N1    | -6.53 | 114.44      | 117.70   |
| 35  | BB    | 1930 | G    | N1-C6-O6    | 6.53  | 123.82      | 119.90   |
| 35  | BB    | 2451 | A    | C4-C5-C6    | 6.53  | 120.26      | 117.00   |
| 35  | BB    | 2856 | A    | C1'-O4'-C4' | -6.53 | 104.68      | 109.90   |
| 51  | BR    | 83   | TYR  | N-CA-CB     | 6.53  | 122.35      | 110.60   |
| 1   | AA    | 523  | A    | C4-C5-N7    | -6.53 | 107.44      | 110.70   |
| 1   | AA    | 868  | C    | C2-N3-C4    | -6.53 | 116.64      | 119.90   |
| 1   | AA    | 1023 | U    | C1'-O4'-C4' | 6.53  | 115.12      | 109.90   |
| 35  | BB    | 2479 | U    | C5-C4-O4    | -6.53 | 121.98      | 125.90   |
| 35  | BB    | 2623 | G    | C2-N3-C4    | 6.53  | 115.16      | 111.90   |
| 35  | BB    | 2639 | A    | O4'-C1'-N9  | 6.53  | 113.42      | 108.20   |
| 35  | BB    | 2818 | U    | O4'-C1'-N1  | 6.53  | 113.42      | 108.20   |
| 3   | AC    | 178  | ARG  | N-CA-C      | -6.52 | 93.38       | 111.00   |
| 9   | AI    | 118  | ARG  | NE-CZ-NH2   | -6.52 | 117.04      | 120.30   |
| 35  | BB    | 131  | A    | C4-C5-C6    | 6.52  | 120.26      | 117.00   |
| 35  | BB    | 217  | A    | C6-C5-N7    | -6.52 | 127.73      | 132.30   |
| 35  | BB    | 836  | G    | O4'-C1'-N9  | 6.52  | 113.42      | 108.20   |
| 35  | BB    | 1732 | C    | C6-N1-C2    | -6.52 | 117.69      | 120.30   |
| 35  | BB    | 2110 | G    | N1-C6-O6    | 6.52  | 123.81      | 119.90   |
| 35  | BB    | 2872 | A    | O4'-C1'-N9  | 6.52  | 113.42      | 108.20   |
| 1   | AA    | 321  | A    | C6-C5-N7    | -6.52 | 127.73      | 132.30   |
| 1   | AA    | 532  | A    | C5-N7-C8    | 6.52  | 107.16      | 103.90   |
| 1   | AA    | 743  | A    | N1-C2-N3    | 6.52  | 132.56      | 129.30   |
| 1   | AA    | 746  | A    | P-O3'-C3'   | -6.52 | 111.87      | 119.70   |
| 1   | AA    | 1191 | A    | N1-C6-N6    | 6.52  | 122.51      | 118.60   |
| 35  | BB    | 154  | U    | C5-C4-O4    | -6.52 | 121.99      | 125.90   |
| 35  | BB    | 352  | A    | C4-C5-C6    | 6.52  | 120.26      | 117.00   |
| 35  | BB    | 389  | G    | C6-C5-N7    | -6.52 | 126.49      | 130.40   |
| 35  | BB    | 1348 | C    | C5-C6-N1    | 6.52  | 124.26      | 121.00   |
| 35  | BB    | 1863 | G    | N1-C6-O6    | 6.52  | 123.81      | 119.90   |
| 35  | BB    | 2543 | G    | N1-C2-N2    | -6.52 | 110.33      | 116.20   |
| 35  | BB    | 2594 | C    | C5-C4-N4    | -6.52 | 115.63      | 120.20   |
| 35  | BB    | 2741 | A    | C6-N1-C2    | -6.52 | 114.69      | 118.60   |
| 1   | AA    | 799  | G    | N3-C4-C5    | -6.52 | 125.34      | 128.60   |
| 35  | BB    | 345  | A    | C5-C6-N1    | -6.52 | 114.44      | 117.70   |
| 35  | BB    | 524  | G    | C5-C6-O6    | -6.52 | 124.69      | 128.60   |
| 35  | BB    | 1857 | G    | C5'-C4'-O4' | 6.52  | 116.92      | 109.10   |
| 35  | BB    | 2347 | C    | N3-C4-N4    | 6.52  | 122.56      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 578  | C    | C4-C5-C6    | -6.52 | 114.14      | 117.40   |
| 1   | AA    | 951  | G    | N1-C6-O6    | 6.52  | 123.81      | 119.90   |
| 25  | B0    | 64   | ASP  | O-C-N       | 6.52  | 133.13      | 122.70   |
| 35  | BB    | 119  | A    | N7-C8-N9    | -6.52 | 110.54      | 113.80   |
| 35  | BB    | 1342 | A    | C6-C5-N7    | -6.52 | 127.74      | 132.30   |
| 35  | BB    | 2174 | C    | C2-N3-C4    | 6.52  | 123.16      | 119.90   |
| 35  | BB    | 2268 | A    | N1-C2-N3    | -6.52 | 126.04      | 129.30   |
| 1   | AA    | 595  | A    | C8-N9-C4    | 6.52  | 108.41      | 105.80   |
| 1   | AA    | 1228 | C    | C6-N1-C2    | 6.52  | 122.91      | 120.30   |
| 35  | BB    | 68   | G    | N1-C6-O6    | 6.52  | 123.81      | 119.90   |
| 35  | BB    | 159  | G    | P-O3'-C3'   | 6.52  | 127.52      | 119.70   |
| 35  | BB    | 393  | C    | N3-C4-C5    | -6.52 | 119.29      | 121.90   |
| 35  | BB    | 429  | A    | C5-C6-N6    | -6.52 | 118.48      | 123.70   |
| 35  | BB    | 2098 | U    | N1-C2-N3    | -6.52 | 110.99      | 114.90   |
| 1   | AA    | 1253 | G    | P-O3'-C3'   | -6.52 | 111.88      | 119.70   |
| 35  | BB    | 17   | G    | N1-C2-N3    | -6.52 | 119.99      | 123.90   |
| 35  | BB    | 51   | G    | N3-C2-N2    | 6.52  | 124.46      | 119.90   |
| 35  | BB    | 438  | G    | N1-C6-O6    | 6.52  | 123.81      | 119.90   |
| 35  | BB    | 2054 | A    | C5-C6-N1    | -6.52 | 114.44      | 117.70   |
| 34  | BA    | 11   | C    | N3-C2-O2    | 6.51  | 126.46      | 121.90   |
| 35  | BB    | 786  | C    | N3-C2-O2    | -6.51 | 117.34      | 121.90   |
| 35  | BB    | 969  | G    | N1-C2-N3    | -6.51 | 119.99      | 123.90   |
| 35  | BB    | 2857 | G    | C6-C5-N7    | -6.51 | 126.49      | 130.40   |
| 1   | AA    | 637  | C    | N3-C4-N4    | 6.51  | 122.56      | 118.00   |
| 1   | AA    | 1326 | U    | C5-C4-O4    | 6.51  | 129.81      | 125.90   |
| 1   | AA    | 1432 | G    | C4'-C3'-C2' | 6.51  | 109.11      | 102.60   |
| 35  | BB    | 570  | G    | N1-C6-O6    | -6.51 | 115.99      | 119.90   |
| 1   | AA    | 25   | C    | N3-C2-O2    | 6.51  | 126.46      | 121.90   |
| 1   | AA    | 811  | C    | N3-C4-C5    | -6.51 | 119.30      | 121.90   |
| 35  | BB    | 122  | G    | O4'-C1'-N9  | 6.51  | 113.41      | 108.20   |
| 35  | BB    | 234  | U    | O4'-C1'-N1  | 6.51  | 113.41      | 108.20   |
| 35  | BB    | 2744 | G    | N3-C4-C5    | -6.51 | 125.34      | 128.60   |
| 1   | AA    | 255  | G    | C6-N1-C2    | 6.51  | 129.00      | 125.10   |
| 1   | AA    | 396  | C    | C5-C6-N1    | 6.51  | 124.25      | 121.00   |
| 1   | AA    | 628  | G    | N3-C2-N2    | 6.51  | 124.46      | 119.90   |
| 1   | AA    | 726  | C    | N3-C4-N4    | 6.51  | 122.56      | 118.00   |
| 1   | AA    | 814  | A    | C5-N7-C8    | -6.51 | 100.64      | 103.90   |
| 1   | AA    | 1022 | A    | C5-C6-N6    | -6.51 | 118.49      | 123.70   |
| 1   | AA    | 1066 | C    | N3-C4-N4    | 6.51  | 122.56      | 118.00   |
| 1   | AA    | 1088 | G    | C5-C6-O6    | -6.51 | 124.69      | 128.60   |
| 35  | BB    | 627  | A    | C4'-C3'-C2' | -6.51 | 96.09       | 102.60   |
| 35  | BB    | 641  | U    | O4'-C1'-N1  | 6.51  | 113.41      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 859  | G    | C8-N9-C4    | 6.51  | 109.00      | 106.40   |
| 35  | BB    | 1391 | U    | N3-C2-O2    | -6.51 | 117.64      | 122.20   |
| 35  | BB    | 2299 | U    | N3-C4-O4    | 6.51  | 123.96      | 119.40   |
| 35  | BB    | 2324 | U    | N3-C4-O4    | 6.51  | 123.96      | 119.40   |
| 35  | BB    | 2817 | U    | O4'-C1'-N1  | 6.51  | 113.41      | 108.20   |
| 43  | BJ    | 35   | ARG  | NE-CZ-NH2   | -6.51 | 117.05      | 120.30   |
| 1   | AA    | 428  | G    | N3-C2-N2    | 6.51  | 124.45      | 119.90   |
| 35  | BB    | 220  | G    | N7-C8-N9    | -6.51 | 109.85      | 113.10   |
| 35  | BB    | 574  | A    | C2-N3-C4    | -6.51 | 107.35      | 110.60   |
| 35  | BB    | 1415 | U    | N1-C2-N3    | -6.51 | 111.00      | 114.90   |
| 1   | AA    | 298  | A    | N3-C4-C5    | -6.51 | 122.25      | 126.80   |
| 1   | AA    | 868  | C    | O4'-C1'-N1  | 6.51  | 113.40      | 108.20   |
| 1   | AA    | 1094 | G    | O4'-C1'-N9  | 6.51  | 113.41      | 108.20   |
| 35  | BB    | 30   | G    | N7-C8-N9    | -6.51 | 109.85      | 113.10   |
| 35  | BB    | 323  | C    | C5-C6-N1    | 6.51  | 124.25      | 121.00   |
| 35  | BB    | 412  | A    | C4-C5-C6    | 6.51  | 120.25      | 117.00   |
| 35  | BB    | 468  | G    | N1-C6-O6    | 6.51  | 123.80      | 119.90   |
| 35  | BB    | 882  | G    | P-O5'-C5'   | -6.51 | 110.49      | 120.90   |
| 35  | BB    | 911  | A    | C6-C5-N7    | -6.51 | 127.75      | 132.30   |
| 35  | BB    | 1213 | A    | C4-C5-C6    | 6.51  | 120.25      | 117.00   |
| 35  | BB    | 1327 | A    | C5-C6-N6    | -6.51 | 118.50      | 123.70   |
| 35  | BB    | 1739 | A    | N9-C4-C5    | 6.51  | 108.40      | 105.80   |
| 35  | BB    | 1842 | G    | C4-C5-N7    | -6.51 | 108.20      | 110.80   |
| 1   | AA    | 1433 | A    | C8-N9-C4    | 6.50  | 108.40      | 105.80   |
| 35  | BB    | 1221 | C    | C5-C4-N4    | -6.50 | 115.65      | 120.20   |
| 35  | BB    | 1708 | C    | N1-C2-O2    | -6.50 | 115.00      | 118.90   |
| 35  | BB    | 1920 | C    | P-O3'-C3'   | -6.50 | 111.89      | 119.70   |
| 35  | BB    | 2787 | C    | N3-C4-C5    | -6.50 | 119.30      | 121.90   |
| 35  | BB    | 2859 | G    | C4'-C3'-C2' | 6.50  | 109.11      | 102.60   |
| 1   | AA    | 773  | G    | N1-C6-O6    | 6.50  | 123.80      | 119.90   |
| 1   | AA    | 1192 | C    | C6-N1-C2    | 6.50  | 122.90      | 120.30   |
| 4   | AD    | 12   | ARG  | NE-CZ-NH2   | -6.50 | 117.05      | 120.30   |
| 22  | AV    | 44   | G    | C5-C6-O6    | -6.50 | 124.70      | 128.60   |
| 35  | BB    | 561  | G    | N1-C2-N3    | -6.50 | 120.00      | 123.90   |
| 35  | BB    | 934  | U    | C5-C6-N1    | 6.50  | 125.95      | 122.70   |
| 1   | AA    | 204  | G    | C5-N7-C8    | 6.50  | 107.55      | 104.30   |
| 1   | AA    | 369  | G    | C4'-C3'-C2' | -6.50 | 96.10       | 102.60   |
| 1   | AA    | 392  | C    | N3-C4-N4    | 6.50  | 122.55      | 118.00   |
| 1   | AA    | 424  | G    | C5-C6-O6    | -6.50 | 124.70      | 128.60   |
| 1   | AA    | 439  | U    | N1-C2-O2    | 6.50  | 127.35      | 122.80   |
| 35  | BB    | 31   | C    | C5-C4-N4    | -6.50 | 115.65      | 120.20   |
| 35  | BB    | 299  | A    | C5-N7-C8    | 6.50  | 107.15      | 103.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 655  | A    | C5-C6-N1    | -6.50 | 114.45      | 117.70   |
| 35  | BB    | 896  | A    | C5'-C4'-O4' | 6.50  | 116.90      | 109.10   |
| 35  | BB    | 983  | A    | N1-C6-N6    | 6.50  | 122.50      | 118.60   |
| 35  | BB    | 2400 | G    | C2-N3-C4    | 6.50  | 115.15      | 111.90   |
| 35  | BB    | 2828 | G    | C8-N9-C4    | 6.50  | 109.00      | 106.40   |
| 34  | BA    | 32   | U    | N3-C2-O2    | 6.50  | 126.75      | 122.20   |
| 35  | BB    | 2423 | U    | N3-C4-O4    | 6.50  | 123.95      | 119.40   |
| 35  | BB    | 2524 | G    | C4-C5-C6    | 6.50  | 122.70      | 118.80   |
| 35  | BB    | 2627 | G    | N3-C2-N2    | 6.50  | 124.45      | 119.90   |
| 1   | AA    | 558  | G    | N3-C4-C5    | -6.50 | 125.35      | 128.60   |
| 1   | AA    | 1265 | C    | O4'-C1'-N1  | 6.50  | 113.40      | 108.20   |
| 8   | AH    | 8    | ASP  | CB-CG-OD2   | -6.50 | 112.45      | 118.30   |
| 34  | BA    | 112  | G    | C6-N1-C2    | -6.50 | 121.20      | 125.10   |
| 35  | BB    | 247  | G    | C6-N1-C2    | 6.50  | 129.00      | 125.10   |
| 35  | BB    | 1510 | G    | N1-C2-N3    | -6.50 | 120.00      | 123.90   |
| 35  | BB    | 2054 | A    | C5-N7-C8    | 6.50  | 107.15      | 103.90   |
| 1   | AA    | 19   | A    | N9-C4-C5    | -6.50 | 103.20      | 105.80   |
| 1   | AA    | 87   | C    | C4-C5-C6    | 6.50  | 120.65      | 117.40   |
| 1   | AA    | 932  | C    | O4'-C1'-N1  | 6.50  | 113.40      | 108.20   |
| 1   | AA    | 948  | C    | N3-C4-N4    | 6.50  | 122.55      | 118.00   |
| 1   | AA    | 1258 | G    | N7-C8-N9    | -6.50 | 109.85      | 113.10   |
| 12  | AL    | 11   | ARG  | CB-CA-C     | -6.50 | 97.41       | 110.40   |
| 35  | BB    | 814  | C    | C5-C6-N1    | 6.50  | 124.25      | 121.00   |
| 35  | BB    | 1630 | A    | C2-N3-C4    | 6.50  | 113.85      | 110.60   |
| 35  | BB    | 1949 | G    | C4-C5-N7    | -6.50 | 108.20      | 110.80   |
| 35  | BB    | 2348 | U    | N3-C4-O4    | 6.50  | 123.95      | 119.40   |
| 35  | BB    | 2488 | G    | C3'-C2'-C1' | -6.50 | 96.30       | 101.50   |
| 35  | BB    | 2567 | G    | C5-C6-O6    | -6.50 | 124.70      | 128.60   |
| 1   | AA    | 927  | G    | C4-C5-C6    | 6.50  | 122.70      | 118.80   |
| 1   | AA    | 1470 | U    | C2-N3-C4    | 6.50  | 130.90      | 127.00   |
| 35  | BB    | 271  | G    | N3-C2-N2    | 6.50  | 124.45      | 119.90   |
| 35  | BB    | 294  | A    | N3-C4-C5    | -6.50 | 122.25      | 126.80   |
| 35  | BB    | 236  | C    | C6-N1-C1'   | -6.49 | 113.01      | 120.80   |
| 35  | BB    | 938  | G    | C4-C5-C6    | -6.49 | 114.90      | 118.80   |
| 35  | BB    | 1034 | G    | C6-C5-N7    | -6.49 | 126.50      | 130.40   |
| 35  | BB    | 1238 | G    | C6-C5-N7    | -6.49 | 126.50      | 130.40   |
| 35  | BB    | 1532 | A    | C2-N3-C4    | 6.49  | 113.85      | 110.60   |
| 35  | BB    | 1552 | A    | O4'-C1'-N9  | 6.49  | 113.39      | 108.20   |
| 35  | BB    | 2544 | G    | C6-C5-N7    | -6.49 | 126.50      | 130.40   |
| 1   | AA    | 239  | U    | N1-C1'-C2'  | -6.49 | 104.86      | 112.00   |
| 1   | AA    | 437  | U    | P-O5'-C5'   | -6.49 | 110.51      | 120.90   |
| 1   | AA    | 1363 | A    | C5-C6-N6    | -6.49 | 118.51      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | AD    | 76   | LYS  | CA-CB-CG    | 6.49  | 127.68      | 113.40   |
| 35  | BB    | 51   | G    | C4-C5-C6    | 6.49  | 122.69      | 118.80   |
| 35  | BB    | 309  | A    | C4-C5-C6    | 6.49  | 120.25      | 117.00   |
| 35  | BB    | 327  | G    | C6-N1-C2    | 6.49  | 129.00      | 125.10   |
| 35  | BB    | 504  | A    | C1'-O4'-C4' | 6.49  | 115.09      | 109.90   |
| 35  | BB    | 2467 | C    | C4'-C3'-C2' | -6.49 | 96.11       | 102.60   |
| 35  | BB    | 2673 | G    | N1-C2-N3    | -6.49 | 120.00      | 123.90   |
| 43  | BJ    | 53   | TYR  | CG-CD2-CE2  | -6.49 | 116.11      | 121.30   |
| 1   | AA    | 83   | C    | C5'-C4'-C3' | 6.49  | 126.39      | 116.00   |
| 1   | AA    | 276  | G    | P-O3'-C3'   | -6.49 | 111.91      | 119.70   |
| 1   | AA    | 449  | G    | C8-N9-C4    | -6.49 | 103.80      | 106.40   |
| 1   | AA    | 781  | A    | C8-N9-C4    | -6.49 | 103.20      | 105.80   |
| 1   | AA    | 1236 | A    | C4-C5-C6    | 6.49  | 120.25      | 117.00   |
| 35  | BB    | 471  | A    | C5-C6-N6    | -6.49 | 118.51      | 123.70   |
| 35  | BB    | 680  | C    | O5'-C5'-C4' | -6.49 | 99.37       | 111.70   |
| 35  | BB    | 1881 | C    | N1-C2-N3    | -6.49 | 114.66      | 119.20   |
| 35  | BB    | 2168 | G    | N1-C2-N3    | -6.49 | 120.01      | 123.90   |
| 35  | BB    | 2758 | A    | N1-C6-N6    | 6.49  | 122.49      | 118.60   |
| 1   | AA    | 286  | C    | OP1-P-OP2   | -6.49 | 109.87      | 119.60   |
| 1   | AA    | 1358 | U    | C4'-C3'-C2' | -6.49 | 96.11       | 102.60   |
| 1   | AA    | 1513 | A    | O4'-C1'-N9  | 6.49  | 113.39      | 108.20   |
| 35  | BB    | 273  | G    | N1-C6-O6    | 6.49  | 123.79      | 119.90   |
| 35  | BB    | 368  | A    | C8-N9-C4    | -6.49 | 103.20      | 105.80   |
| 35  | BB    | 743  | A    | C5-N7-C8    | 6.49  | 107.14      | 103.90   |
| 35  | BB    | 1624 | U    | N3-C4-O4    | 6.49  | 123.94      | 119.40   |
| 35  | BB    | 1844 | C    | C6-N1-C2    | 6.49  | 122.89      | 120.30   |
| 35  | BB    | 2110 | G    | C4-C5-N7    | 6.49  | 113.40      | 110.80   |
| 35  | BB    | 2471 | A    | O4'-C1'-N9  | 6.49  | 113.39      | 108.20   |
| 35  | BB    | 2645 | G    | N1-C2-N2    | -6.49 | 110.36      | 116.20   |
| 35  | BB    | 2816 | G    | N3-C2-N2    | 6.49  | 124.44      | 119.90   |
| 1   | AA    | 469  | C    | N3-C4-C5    | 6.49  | 124.50      | 121.90   |
| 1   | AA    | 837  | U    | C6-N1-C2    | -6.49 | 117.11      | 121.00   |
| 1   | AA    | 1382 | C    | C2-N3-C4    | 6.49  | 123.14      | 119.90   |
| 35  | BB    | 602  | A    | C6-C5-N7    | -6.49 | 127.76      | 132.30   |
| 35  | BB    | 1255 | U    | C1'-O4'-C4' | 6.49  | 115.09      | 109.90   |
| 1   | AA    | 971  | G    | C4-C5-N7    | 6.49  | 113.39      | 110.80   |
| 34  | BA    | 13   | G    | C2-N3-C4    | 6.49  | 115.14      | 111.90   |
| 35  | BB    | 1208 | C    | C5-C6-N1    | 6.49  | 124.24      | 121.00   |
| 35  | BB    | 1608 | A    | N9-C4-C5    | -6.49 | 103.21      | 105.80   |
| 35  | BB    | 1809 | A    | C5-N7-C8    | 6.49  | 107.14      | 103.90   |
| 35  | BB    | 1840 | G    | C6-N1-C2    | 6.49  | 128.99      | 125.10   |
| 35  | BB    | 2334 | U    | O4'-C1'-N1  | 6.49  | 113.39      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2549 | G    | C5-C6-O6    | -6.49 | 124.71      | 128.60   |
| 35  | BB    | 2897 | U    | N1-C2-O2    | 6.49  | 127.34      | 122.80   |
| 1   | AA    | 349  | A    | N1-C6-N6    | 6.48  | 122.49      | 118.60   |
| 35  | BB    | 532  | A    | N1-C2-N3    | -6.48 | 126.06      | 129.30   |
| 35  | BB    | 776  | G    | C3'-C2'-C1' | -6.48 | 96.31       | 101.50   |
| 35  | BB    | 2120 | G    | C5-C6-O6    | -6.48 | 124.71      | 128.60   |
| 35  | BB    | 2120 | G    | N1-C2-N3    | -6.48 | 120.01      | 123.90   |
| 35  | BB    | 2318 | G    | C5-N7-C8    | 6.48  | 107.54      | 104.30   |
| 1   | AA    | 73   | C    | C6-N1-C2    | -6.48 | 117.71      | 120.30   |
| 1   | AA    | 119  | A    | C5-C6-N6    | -6.48 | 118.52      | 123.70   |
| 1   | AA    | 239  | U    | C2-N3-C4    | 6.48  | 130.89      | 127.00   |
| 1   | AA    | 437  | U    | N3-C4-O4    | 6.48  | 123.94      | 119.40   |
| 1   | AA    | 734  | G    | C8-N9-C4    | -6.48 | 103.81      | 106.40   |
| 8   | AH    | 127  | TYR  | CB-CG-CD1   | -6.48 | 117.11      | 121.00   |
| 35  | BB    | 379  | G    | C5-C6-N1    | -6.48 | 108.26      | 111.50   |
| 35  | BB    | 441  | U    | C2-N3-C4    | 6.48  | 130.89      | 127.00   |
| 35  | BB    | 514  | A    | C3'-C2'-C1' | 6.48  | 106.69      | 101.50   |
| 35  | BB    | 825  | A    | C6-C5-N7    | -6.48 | 127.76      | 132.30   |
| 35  | BB    | 1281 | G    | O4'-C1'-N9  | 6.48  | 113.39      | 108.20   |
| 35  | BB    | 1341 | G    | N1-C6-O6    | 6.48  | 123.79      | 119.90   |
| 35  | BB    | 2595 | G    | N9-C4-C5    | 6.48  | 107.99      | 105.40   |
| 1   | AA    | 143  | A    | C4-C5-N7    | -6.48 | 107.46      | 110.70   |
| 1   | AA    | 594  | U    | N1-C2-O2    | -6.48 | 118.26      | 122.80   |
| 1   | AA    | 1186 | G    | C8-N9-C4    | -6.48 | 103.81      | 106.40   |
| 1   | AA    | 1238 | A    | N3-C4-C5    | -6.48 | 122.26      | 126.80   |
| 34  | BA    | 103  | U    | P-O5'-C5'   | 6.48  | 131.27      | 120.90   |
| 35  | BB    | 17   | G    | O4'-C1'-N9  | 6.48  | 113.39      | 108.20   |
| 35  | BB    | 492  | A    | O4'-C1'-N9  | 6.48  | 113.38      | 108.20   |
| 35  | BB    | 699  | A    | O4'-C4'-C3' | -6.48 | 97.52       | 104.00   |
| 35  | BB    | 1433 | A    | C5-C6-N6    | -6.48 | 118.52      | 123.70   |
| 35  | BB    | 1802 | A    | C6-C5-N7    | -6.48 | 127.76      | 132.30   |
| 35  | BB    | 1952 | A    | C2-N3-C4    | -6.48 | 107.36      | 110.60   |
| 35  | BB    | 2767 | C    | C6-N1-C2    | -6.48 | 117.71      | 120.30   |
| 35  | BB    | 2770 | G    | N9-C4-C5    | -6.48 | 102.81      | 105.40   |
| 35  | BB    | 2843 | G    | C8-N9-C4    | -6.48 | 103.81      | 106.40   |
| 35  | BB    | 62   | U    | O4'-C1'-N1  | 6.48  | 113.38      | 108.20   |
| 35  | BB    | 454  | A    | N3-C4-C5    | -6.48 | 122.27      | 126.80   |
| 35  | BB    | 1727 | C    | N3-C4-C5    | -6.48 | 119.31      | 121.90   |
| 35  | BB    | 2636 | C    | C4-C5-C6    | 6.48  | 120.64      | 117.40   |
| 1   | AA    | 553  | A    | C8-N9-C4    | -6.48 | 103.21      | 105.80   |
| 1   | AA    | 1039 | G    | N3-C4-N9    | 6.48  | 129.89      | 126.00   |
| 1   | AA    | 1386 | G    | C4'-C3'-C2' | -6.48 | 96.12       | 102.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 29   | U    | C5-C4-O4    | -6.48 | 122.01      | 125.90   |
| 35  | BB    | 1010 | A    | C4-C5-C6    | 6.48  | 120.24      | 117.00   |
| 35  | BB    | 1076 | C    | N3-C4-C5    | -6.48 | 119.31      | 121.90   |
| 35  | BB    | 1483 | G    | C5-N7-C8    | 6.48  | 107.54      | 104.30   |
| 35  | BB    | 1593 | A    | C2-N3-C4    | -6.48 | 107.36      | 110.60   |
| 35  | BB    | 1687 | G    | C6-C5-N7    | -6.48 | 126.51      | 130.40   |
| 35  | BB    | 879  | G    | N7-C8-N9    | 6.48  | 116.34      | 113.10   |
| 35  | BB    | 2110 | G    | C5-C6-O6    | -6.48 | 124.72      | 128.60   |
| 1   | AA    | 161  | A    | N1-C6-N6    | 6.47  | 122.48      | 118.60   |
| 1   | AA    | 449  | G    | C5-C6-O6    | -6.47 | 124.72      | 128.60   |
| 1   | AA    | 685  | G    | C2-N3-C4    | -6.47 | 108.66      | 111.90   |
| 1   | AA    | 942  | G    | N7-C8-N9    | -6.47 | 109.86      | 113.10   |
| 1   | AA    | 1080 | A    | C4-C5-C6    | 6.47  | 120.24      | 117.00   |
| 9   | AI    | 84   | ARG  | NE-CZ-NH2   | -6.47 | 117.06      | 120.30   |
| 22  | AV    | 72   | G    | N3-C2-N2    | 6.47  | 124.43      | 119.90   |
| 35  | BB    | 377  | G    | N1-C6-O6    | 6.47  | 123.78      | 119.90   |
| 35  | BB    | 465  | G    | N3-C4-N9    | -6.47 | 122.11      | 126.00   |
| 35  | BB    | 650  | C    | O4'-C1'-N1  | 6.47  | 113.38      | 108.20   |
| 35  | BB    | 704  | G    | N1-C6-O6    | 6.47  | 123.78      | 119.90   |
| 35  | BB    | 962  | G    | N1-C2-N3    | -6.47 | 120.02      | 123.90   |
| 35  | BB    | 1058 | U    | N3-C2-O2    | 6.47  | 126.73      | 122.20   |
| 35  | BB    | 1144 | A    | O4'-C1'-N9  | 6.47  | 113.38      | 108.20   |
| 35  | BB    | 1733 | G    | N9-C1'-C2'  | -6.47 | 104.88      | 112.00   |
| 35  | BB    | 1862 | G    | C8-N9-C1'   | 6.47  | 135.42      | 127.00   |
| 1   | AA    | 175  | C    | C5-C4-N4    | -6.47 | 115.67      | 120.20   |
| 1   | AA    | 220  | G    | C1'-O4'-C4' | 6.47  | 115.08      | 109.90   |
| 1   | AA    | 550  | G    | C6-N1-C2    | 6.47  | 128.98      | 125.10   |
| 1   | AA    | 793  | U    | C6-N1-C2    | -6.47 | 117.12      | 121.00   |
| 1   | AA    | 801  | U    | N1-C1'-C2'  | -6.47 | 104.88      | 112.00   |
| 3   | AC    | 20   | THR  | CA-CB-CG2   | -6.47 | 103.34      | 112.40   |
| 16  | AP    | 70   | ARG  | NE-CZ-NH2   | -6.47 | 117.06      | 120.30   |
| 35  | BB    | 1440 | U    | C4-C5-C6    | 6.47  | 123.58      | 119.70   |
| 35  | BB    | 1546 | G    | N1-C2-N3    | -6.47 | 120.02      | 123.90   |
| 35  | BB    | 1933 | G    | C6-N1-C2    | -6.47 | 121.22      | 125.10   |
| 35  | BB    | 2106 | U    | N1-C2-O2    | -6.47 | 118.27      | 122.80   |
| 1   | AA    | 828  | U    | C4-C5-C6    | -6.47 | 115.82      | 119.70   |
| 35  | BB    | 2010 | G    | N7-C8-N9    | -6.47 | 109.86      | 113.10   |
| 35  | BB    | 2506 | U    | C6-N1-C2    | -6.47 | 117.12      | 121.00   |
| 1   | AA    | 6    | G    | O4'-C1'-N9  | 6.47  | 113.38      | 108.20   |
| 1   | AA    | 165  | G    | N1-C2-N3    | -6.47 | 120.02      | 123.90   |
| 1   | AA    | 267  | C    | C5-C6-N1    | 6.47  | 124.23      | 121.00   |
| 1   | AA    | 298  | A    | C4-C5-N7    | -6.47 | 107.47      | 110.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 512  | U    | C6-N1-C2    | -6.47 | 117.12      | 121.00   |
| 1   | AA    | 807  | A    | C5-C6-N1    | -6.47 | 114.47      | 117.70   |
| 1   | AA    | 812  | G    | C6-C5-N7    | -6.47 | 126.52      | 130.40   |
| 1   | AA    | 1358 | U    | N3-C2-O2    | -6.47 | 117.67      | 122.20   |
| 35  | BB    | 83   | A    | O4'-C1'-N9  | 6.47  | 113.38      | 108.20   |
| 35  | BB    | 401  | A    | C5-N7-C8    | 6.47  | 107.14      | 103.90   |
| 35  | BB    | 714  | U    | O4'-C1'-N1  | 6.47  | 113.38      | 108.20   |
| 35  | BB    | 1420 | A    | N1-C6-N6    | 6.47  | 122.48      | 118.60   |
| 35  | BB    | 1424 | G    | C3'-C2'-C1' | 6.47  | 106.67      | 101.50   |
| 35  | BB    | 1500 | G    | O4'-C1'-N9  | 6.47  | 113.38      | 108.20   |
| 35  | BB    | 1619 | G    | C4-C5-N7    | 6.47  | 113.39      | 110.80   |
| 35  | BB    | 2099 | U    | N3-C2-O2    | 6.47  | 126.73      | 122.20   |
| 35  | BB    | 2258 | C    | N3-C4-C5    | -6.47 | 119.31      | 121.90   |
| 35  | BB    | 2364 | C    | C4'-C3'-C2' | -6.47 | 96.13       | 102.60   |
| 35  | BB    | 2451 | A    | O4'-C1'-N9  | 6.47  | 113.38      | 108.20   |
| 35  | BB    | 2686 | G    | N3-C4-C5    | 6.47  | 131.83      | 128.60   |
| 35  | BB    | 1507 | C    | C4-C5-C6    | -6.47 | 114.17      | 117.40   |
| 35  | BB    | 1749 | A    | C2-N3-C4    | -6.47 | 107.37      | 110.60   |
| 35  | BB    | 1983 | G    | C5-C6-O6    | -6.47 | 124.72      | 128.60   |
| 35  | BB    | 2421 | G    | C6-C5-N7    | -6.47 | 126.52      | 130.40   |
| 1   | AA    | 488  | C    | O4'-C4'-C3' | -6.47 | 97.53       | 104.00   |
| 1   | AA    | 582  | C    | C6-N1-C2    | -6.47 | 117.71      | 120.30   |
| 1   | AA    | 855  | U    | C5-C4-O4    | -6.47 | 122.02      | 125.90   |
| 1   | AA    | 1200 | C    | C4-C5-C6    | 6.47  | 120.63      | 117.40   |
| 35  | BB    | 541  | A    | N1-C2-N3    | 6.47  | 132.53      | 129.30   |
| 35  | BB    | 1393 | A    | O4'-C1'-N9  | 6.47  | 113.37      | 108.20   |
| 35  | BB    | 1519 | G    | N1-C2-N2    | -6.47 | 110.38      | 116.20   |
| 35  | BB    | 1639 | C    | C6-N1-C2    | -6.47 | 117.71      | 120.30   |
| 35  | BB    | 1841 | U    | C5-C6-N1    | 6.47  | 125.93      | 122.70   |
| 35  | BB    | 2519 | U    | O5'-P-OP1   | -6.47 | 99.88       | 105.70   |
| 35  | BB    | 2546 | U    | N3-C4-O4    | 6.47  | 123.93      | 119.40   |
| 35  | BB    | 2657 | A    | C5-C6-N1    | -6.47 | 114.47      | 117.70   |
| 40  | BG    | 96   | ALA  | N-CA-CB     | 6.47  | 119.15      | 110.10   |
| 1   | AA    | 17   | U    | N3-C4-O4    | 6.46  | 123.92      | 119.40   |
| 1   | AA    | 928  | G    | C6-C5-N7    | -6.46 | 126.52      | 130.40   |
| 1   | AA    | 1364 | U    | N1-C2-O2    | -6.46 | 118.28      | 122.80   |
| 8   | AH    | 85   | TYR  | N-CA-CB     | 6.46  | 122.24      | 110.60   |
| 35  | BB    | 881  | G    | C5-C6-N1    | -6.46 | 108.27      | 111.50   |
| 35  | BB    | 894  | U    | O4'-C1'-N1  | 6.46  | 113.37      | 108.20   |
| 35  | BB    | 1011 | G    | C5-C6-O6    | -6.46 | 124.72      | 128.60   |
| 35  | BB    | 1157 | G    | N3-C4-N9    | 6.46  | 129.88      | 126.00   |
| 35  | BB    | 2248 | C    | O4'-C1'-N1  | 6.46  | 113.37      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36  | BC    | 132  | ARG  | NE-CZ-NH1   | 6.46  | 123.53      | 120.30   |
| 1   | AA    | 406  | G    | C4-C5-N7    | -6.46 | 108.22      | 110.80   |
| 1   | AA    | 465  | A    | C5-N7-C8    | 6.46  | 107.13      | 103.90   |
| 1   | AA    | 812  | G    | O4'-C1'-N9  | 6.46  | 113.37      | 108.20   |
| 1   | AA    | 1058 | G    | N3-C2-N2    | 6.46  | 124.42      | 119.90   |
| 1   | AA    | 1079 | G    | C5-C6-O6    | -6.46 | 124.72      | 128.60   |
| 35  | BB    | 193  | U    | N3-C4-O4    | 6.46  | 123.92      | 119.40   |
| 35  | BB    | 740  | C    | O4'-C1'-N1  | 6.46  | 113.37      | 108.20   |
| 35  | BB    | 2553 | G    | C3'-C2'-C1' | -6.46 | 96.33       | 101.50   |
| 49  | BP    | 52   | ARG  | N-CA-CB     | 6.46  | 122.23      | 110.60   |
| 1   | AA    | 743  | A    | C5-C6-N6    | -6.46 | 118.53      | 123.70   |
| 1   | AA    | 976  | G    | C5'-C4'-O4' | 6.46  | 116.86      | 109.10   |
| 1   | AA    | 1044 | A    | C4-C5-C6    | 6.46  | 120.23      | 117.00   |
| 1   | AA    | 1441 | A    | C5-C6-N6    | -6.46 | 118.53      | 123.70   |
| 1   | AA    | 1446 | A    | P-O3'-C3'   | 6.46  | 127.45      | 119.70   |
| 35  | BB    | 384  | A    | C2-N3-C4    | 6.46  | 113.83      | 110.60   |
| 35  | BB    | 1100 | C    | O4'-C1'-N1  | 6.46  | 113.37      | 108.20   |
| 35  | BB    | 1195 | G    | O4'-C1'-N9  | 6.46  | 113.37      | 108.20   |
| 35  | BB    | 1381 | G    | P-O3'-C3'   | -6.46 | 111.95      | 119.70   |
| 35  | BB    | 1435 | G    | C1'-O4'-C4' | 6.46  | 115.07      | 109.90   |
| 35  | BB    | 1612 | C    | C6-N1-C2    | 6.46  | 122.89      | 120.30   |
| 35  | BB    | 1712 | U    | O4'-C1'-N1  | 6.46  | 113.37      | 108.20   |
| 35  | BB    | 2255 | G    | O4'-C1'-N9  | 6.46  | 113.37      | 108.20   |
| 53  | BT    | 50   | LEU  | CB-CG-CD1   | -6.46 | 100.02      | 111.00   |
| 1   | AA    | 222  | C    | C1'-O4'-C4' | -6.46 | 104.73      | 109.90   |
| 1   | AA    | 561  | U    | C6-N1-C1'   | -6.46 | 112.16      | 121.20   |
| 1   | AA    | 722  | G    | C5-C6-O6    | -6.46 | 124.72      | 128.60   |
| 1   | AA    | 1187 | G    | C5-C6-O6    | -6.46 | 124.72      | 128.60   |
| 35  | BB    | 81   | G    | N3-C2-N2    | -6.46 | 115.38      | 119.90   |
| 35  | BB    | 131  | A    | C5-C6-N1    | -6.46 | 114.47      | 117.70   |
| 35  | BB    | 216  | A    | O4'-C1'-N9  | 6.46  | 113.37      | 108.20   |
| 35  | BB    | 1633 | G    | C5-C6-N1    | -6.46 | 108.27      | 111.50   |
| 35  | BB    | 1803 | A    | N1-C6-N6    | 6.46  | 122.48      | 118.60   |
| 1   | AA    | 51   | A    | N1-C2-N3    | -6.46 | 126.07      | 129.30   |
| 1   | AA    | 127  | G    | C4-C5-C6    | 6.46  | 122.67      | 118.80   |
| 1   | AA    | 596  | A    | C5-C6-N6    | -6.46 | 118.53      | 123.70   |
| 34  | BA    | 107  | G    | C5-C6-O6    | -6.46 | 124.72      | 128.60   |
| 35  | BB    | 319  | G    | O4'-C1'-N9  | 6.46  | 113.37      | 108.20   |
| 35  | BB    | 363  | G    | C2-N3-C4    | -6.46 | 108.67      | 111.90   |
| 35  | BB    | 694  | U    | O4'-C1'-N1  | 6.46  | 113.37      | 108.20   |
| 35  | BB    | 1097 | U    | C4'-C3'-C2' | -6.46 | 96.14       | 102.60   |
| 35  | BB    | 1261 | C    | C5-C4-N4    | -6.46 | 115.68      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2789 | C    | C6-N1-C2    | 6.46  | 122.88      | 120.30   |
| 1   | AA    | 159  | G    | N1-C2-N3    | -6.46 | 120.03      | 123.90   |
| 1   | AA    | 1067 | A    | C8-N9-C4    | -6.46 | 103.22      | 105.80   |
| 35  | BB    | 148  | U    | N3-C4-O4    | 6.46  | 123.92      | 119.40   |
| 35  | BB    | 712  | G    | N3-C4-N9    | -6.46 | 122.13      | 126.00   |
| 35  | BB    | 912  | C    | O4'-C1'-N1  | 6.46  | 113.36      | 108.20   |
| 35  | BB    | 943  | A    | C5-C6-N1    | -6.46 | 114.47      | 117.70   |
| 35  | BB    | 1275 | A    | C4-N9-C1'   | 6.46  | 137.92      | 126.30   |
| 35  | BB    | 1391 | U    | C5'-C4'-O4' | 6.46  | 116.85      | 109.10   |
| 35  | BB    | 1703 | G    | N3-C4-N9    | -6.46 | 122.13      | 126.00   |
| 54  | BU    | 97   | SER  | N-CA-CB     | 6.46  | 120.19      | 110.50   |
| 1   | AA    | 1153 | G    | C4-C5-N7    | 6.46  | 113.38      | 110.80   |
| 35  | BB    | 265  | A    | C5-C6-N6    | -6.46 | 118.54      | 123.70   |
| 35  | BB    | 897  | C    | N3-C4-N4    | 6.46  | 122.52      | 118.00   |
| 35  | BB    | 1665 | A    | N7-C8-N9    | -6.46 | 110.57      | 113.80   |
| 35  | BB    | 2173 | A    | C5-N7-C8    | 6.46  | 107.13      | 103.90   |
| 1   | AA    | 46   | G    | C6-C5-N7    | -6.45 | 126.53      | 130.40   |
| 1   | AA    | 68   | G    | C6-C5-N7    | -6.45 | 126.53      | 130.40   |
| 1   | AA    | 400  | C    | C4'-C3'-C2' | -6.45 | 96.15       | 102.60   |
| 1   | AA    | 646  | G    | N1-C6-O6    | 6.45  | 123.77      | 119.90   |
| 1   | AA    | 1256 | A    | O4'-C1'-N9  | 6.45  | 113.36      | 108.20   |
| 8   | AH    | 53   | ASP  | CB-CG-OD1   | -6.45 | 112.49      | 118.30   |
| 22  | AV    | 21   | A    | C4-C5-C6    | 6.45  | 120.23      | 117.00   |
| 35  | BB    | 693  | A    | O4'-C1'-N9  | 6.45  | 113.36      | 108.20   |
| 35  | BB    | 1511 | G    | C5-C6-O6    | -6.45 | 124.73      | 128.60   |
| 1   | AA    | 540  | G    | C8-N9-C4    | -6.45 | 103.82      | 106.40   |
| 35  | BB    | 452  | G    | C5'-C4'-C3' | -6.45 | 105.68      | 116.00   |
| 35  | BB    | 698  | C    | C5-C4-N4    | -6.45 | 115.68      | 120.20   |
| 35  | BB    | 855  | G    | C5-C6-N1    | -6.45 | 108.27      | 111.50   |
| 1   | AA    | 148  | G    | N3-C2-N2    | 6.45  | 124.42      | 119.90   |
| 1   | AA    | 731  | G    | C4-C5-N7    | -6.45 | 108.22      | 110.80   |
| 1   | AA    | 814  | A    | C4-C5-N7    | 6.45  | 113.92      | 110.70   |
| 1   | AA    | 1337 | G    | P-O3'-C3'   | 6.45  | 127.44      | 119.70   |
| 35  | BB    | 89   | A    | C5-C6-N6    | -6.45 | 118.54      | 123.70   |
| 35  | BB    | 625  | G    | C5-C6-O6    | -6.45 | 124.73      | 128.60   |
| 35  | BB    | 952  | G    | C4'-C3'-C2' | -6.45 | 96.15       | 102.60   |
| 35  | BB    | 1842 | G    | N1-C6-O6    | 6.45  | 123.77      | 119.90   |
| 35  | BB    | 1900 | A    | C6-C5-N7    | -6.45 | 127.78      | 132.30   |
| 35  | BB    | 2494 | G    | N3-C2-N2    | 6.45  | 124.42      | 119.90   |
| 35  | BB    | 2606 | C    | C5-C4-N4    | -6.45 | 115.68      | 120.20   |
| 1   | AA    | 412  | A    | C8-N9-C4    | -6.45 | 103.22      | 105.80   |
| 1   | AA    | 471  | U    | P-O5'-C5'   | 6.45  | 131.22      | 120.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 624  | C    | N3-C4-N4    | 6.45  | 122.51      | 118.00   |
| 35  | BB    | 119  | A    | C5-C6-N1    | -6.45 | 114.48      | 117.70   |
| 35  | BB    | 1075 | C    | N3-C2-O2    | 6.45  | 126.41      | 121.90   |
| 35  | BB    | 1810 | A    | C5-N7-C8    | 6.45  | 107.12      | 103.90   |
| 35  | BB    | 2788 | C    | C4-C5-C6    | -6.45 | 114.18      | 117.40   |
| 35  | BB    | 2835 | A    | C4-C5-C6    | 6.45  | 120.22      | 117.00   |
| 1   | AA    | 1153 | G    | O4'-C1'-C2' | 6.45  | 113.40      | 107.60   |
| 35  | BB    | 1291 | C    | O4'-C4'-C3' | -6.45 | 97.55       | 104.00   |
| 35  | BB    | 1903 | G    | C1'-O4'-C4' | -6.45 | 104.74      | 109.90   |
| 35  | BB    | 2339 | C    | N3-C4-C5    | -6.45 | 119.32      | 121.90   |
| 51  | BR    | 58   | VAL  | CA-CB-CG1   | -6.45 | 101.23      | 110.90   |
| 1   | AA    | 874  | G    | N1-C2-N3    | -6.45 | 120.03      | 123.90   |
| 1   | AA    | 1270 | G    | N9-C4-C5    | 6.45  | 107.98      | 105.40   |
| 35  | BB    | 288  | U    | N3-C4-C5    | -6.45 | 110.73      | 114.60   |
| 35  | BB    | 313  | G    | N3-C2-N2    | 6.45  | 124.41      | 119.90   |
| 35  | BB    | 759  | G    | C5-C6-O6    | -6.45 | 124.73      | 128.60   |
| 35  | BB    | 1315 | C    | N3-C4-N4    | 6.45  | 122.51      | 118.00   |
| 35  | BB    | 1448 | G    | N9-C4-C5    | 6.45  | 107.98      | 105.40   |
| 35  | BB    | 1550 | C    | N1-C2-N3    | 6.45  | 123.71      | 119.20   |
| 35  | BB    | 1966 | A    | C5-N7-C8    | 6.45  | 107.12      | 103.90   |
| 35  | BB    | 2221 | G    | N3-C4-N9    | 6.45  | 129.87      | 126.00   |
| 1   | AA    | 85   | U    | N3-C4-C5    | -6.44 | 110.73      | 114.60   |
| 1   | AA    | 664  | G    | C6-N1-C2    | 6.44  | 128.97      | 125.10   |
| 35  | BB    | 2074 | U    | O4'-C1'-N1  | 6.44  | 113.36      | 108.20   |
| 1   | AA    | 445  | G    | C5-C6-O6    | -6.44 | 124.73      | 128.60   |
| 1   | AA    | 865  | A    | O4'-C1'-N9  | 6.44  | 113.36      | 108.20   |
| 1   | AA    | 1104 | G    | N1-C6-O6    | 6.44  | 123.77      | 119.90   |
| 35  | BB    | 701  | G    | N3-C4-N9    | -6.44 | 122.13      | 126.00   |
| 35  | BB    | 1027 | A    | C6-N1-C2    | -6.44 | 114.73      | 118.60   |
| 35  | BB    | 1237 | A    | C2-N3-C4    | 6.44  | 113.82      | 110.60   |
| 35  | BB    | 1358 | G    | N3-C4-C5    | 6.44  | 131.82      | 128.60   |
| 35  | BB    | 2782 | G    | C5-C6-N1    | 6.44  | 114.72      | 111.50   |
| 35  | BB    | 2843 | G    | O4'-C1'-N9  | 6.44  | 113.35      | 108.20   |
| 52  | BS    | 64   | ALA  | N-CA-CB     | 6.44  | 119.12      | 110.10   |
| 1   | AA    | 79   | G    | C2-N3-C4    | 6.44  | 115.12      | 111.90   |
| 1   | AA    | 1003 | G    | P-O3'-C3'   | 6.44  | 127.43      | 119.70   |
| 11  | AK    | 71   | ASP  | CB-CG-OD2   | -6.44 | 112.50      | 118.30   |
| 34  | BA    | 83   | G    | N1-C2-N3    | -6.44 | 120.04      | 123.90   |
| 35  | BB    | 409  | G    | P-O3'-C3'   | -6.44 | 111.97      | 119.70   |
| 35  | BB    | 649  | G    | N9-C4-C5    | 6.44  | 107.98      | 105.40   |
| 35  | BB    | 684  | G    | C2-N3-C4    | 6.44  | 115.12      | 111.90   |
| 35  | BB    | 827  | U    | P-O3'-C3'   | 6.44  | 127.43      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1976 | U    | N3-C4-O4    | 6.44  | 123.91      | 119.40   |
| 35  | BB    | 2425 | A    | C4-C5-C6    | 6.44  | 120.22      | 117.00   |
| 35  | BB    | 2523 | G    | P-O5'-C5'   | 6.44  | 131.21      | 120.90   |
| 1   | AA    | 1269 | A    | C5-C6-N1    | -6.44 | 114.48      | 117.70   |
| 1   | AA    | 1305 | G    | C8-N9-C4    | -6.44 | 103.82      | 106.40   |
| 35  | BB    | 411  | G    | C4-C5-N7    | -6.44 | 108.22      | 110.80   |
| 35  | BB    | 956  | G    | C4'-C3'-C2' | -6.44 | 96.16       | 102.60   |
| 35  | BB    | 1155 | A    | C5-C6-N1    | -6.44 | 114.48      | 117.70   |
| 35  | BB    | 1224 | U    | N1-C2-N3    | 6.44  | 118.76      | 114.90   |
| 35  | BB    | 1280 | G    | P-O3'-C3'   | -6.44 | 111.97      | 119.70   |
| 1   | AA    | 862  | C    | N3-C4-C5    | -6.44 | 119.33      | 121.90   |
| 1   | AA    | 962  | C    | C6-N1-C2    | 6.44  | 122.88      | 120.30   |
| 1   | AA    | 1138 | G    | N1-C6-O6    | 6.44  | 123.76      | 119.90   |
| 20  | AT    | 17   | ARG  | NE-CZ-NH1   | -6.44 | 117.08      | 120.30   |
| 35  | BB    | 52   | A    | C4-C5-N7    | -6.44 | 107.48      | 110.70   |
| 35  | BB    | 168  | G    | C6-N1-C2    | 6.44  | 128.96      | 125.10   |
| 35  | BB    | 178  | G    | C5-C6-O6    | -6.44 | 124.74      | 128.60   |
| 35  | BB    | 437  | U    | C2-N3-C4    | -6.44 | 123.14      | 127.00   |
| 35  | BB    | 831  | G    | N7-C8-N9    | -6.44 | 109.88      | 113.10   |
| 35  | BB    | 861  | A    | C5-C6-N6    | -6.44 | 118.55      | 123.70   |
| 35  | BB    | 1106 | G    | N1-C2-N3    | -6.44 | 120.04      | 123.90   |
| 22  | AV    | 3    | G    | P-O5'-C5'   | -6.44 | 110.60      | 120.90   |
| 35  | BB    | 710  | U    | O4'-C1'-N1  | 6.44  | 113.35      | 108.20   |
| 35  | BB    | 1711 | A    | N7-C8-N9    | -6.44 | 110.58      | 113.80   |
| 35  | BB    | 2331 | G    | O4'-C1'-N9  | 6.44  | 113.35      | 108.20   |
| 35  | BB    | 2698 | U    | C2-N3-C4    | 6.44  | 130.86      | 127.00   |
| 1   | AA    | 203  | G    | C2-N3-C4    | -6.43 | 108.68      | 111.90   |
| 1   | AA    | 468  | A    | C5-C6-N1    | 6.43  | 120.92      | 117.70   |
| 1   | AA    | 612  | C    | C5'-C4'-O4' | 6.43  | 116.82      | 109.10   |
| 1   | AA    | 846  | G    | O4'-C4'-C3' | -6.43 | 97.56       | 104.00   |
| 1   | AA    | 923  | A    | C2-N3-C4    | -6.43 | 107.38      | 110.60   |
| 1   | AA    | 1283 | U    | N3-C4-O4    | 6.43  | 123.91      | 119.40   |
| 1   | AA    | 1386 | G    | N1-C2-N3    | -6.43 | 120.04      | 123.90   |
| 1   | AA    | 1438 | G    | C5-C6-O6    | -6.43 | 124.74      | 128.60   |
| 34  | BA    | 71   | C    | C5-C6-N1    | 6.43  | 124.22      | 121.00   |
| 35  | BB    | 633  | A    | C4'-C3'-C2' | -6.43 | 96.17       | 102.60   |
| 35  | BB    | 2123 | G    | C5-C6-N1    | 6.43  | 114.72      | 111.50   |
| 35  | BB    | 2529 | G    | C5-C6-N1    | 6.43  | 114.72      | 111.50   |
| 35  | BB    | 2612 | C    | N3-C4-C5    | -6.43 | 119.33      | 121.90   |
| 35  | BB    | 2723 | C    | C1'-O4'-C4' | 6.43  | 115.05      | 109.90   |
| 1   | AA    | 16   | A    | C4-C5-N7    | -6.43 | 107.48      | 110.70   |
| 1   | AA    | 205  | A    | N1-C2-N3    | 6.43  | 132.52      | 129.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 563  | A    | P-O3'-C3'   | 6.43  | 127.42      | 119.70   |
| 1   | AA    | 1374 | A    | C2-N3-C4    | -6.43 | 107.38      | 110.60   |
| 3   | AC    | 62   | SER  | N-CA-CB     | 6.43  | 120.15      | 110.50   |
| 34  | BA    | 7    | G    | O5'-P-OP1   | -6.43 | 99.91       | 105.70   |
| 35  | BB    | 617  | G    | C5-N7-C8    | 6.43  | 107.52      | 104.30   |
| 35  | BB    | 913  | U    | N3-C2-O2    | 6.43  | 126.70      | 122.20   |
| 35  | BB    | 1254 | A    | C3'-C2'-C1' | 6.43  | 106.65      | 101.50   |
| 35  | BB    | 1542 | U    | C4-C5-C6    | -6.43 | 115.84      | 119.70   |
| 35  | BB    | 1617 | C    | N3-C4-N4    | 6.43  | 122.50      | 118.00   |
| 35  | BB    | 2199 | A    | C5-N7-C8    | 6.43  | 107.12      | 103.90   |
| 35  | BB    | 2328 | A    | C5-N7-C8    | 6.43  | 107.12      | 103.90   |
| 35  | BB    | 2766 | A    | C2-N3-C4    | 6.43  | 113.82      | 110.60   |
| 35  | BB    | 2894 | G    | C4-C5-C6    | 6.43  | 122.66      | 118.80   |
| 35  | BB    | 2897 | U    | N1-C2-N3    | -6.43 | 111.04      | 114.90   |
| 1   | AA    | 71   | A    | P-O3'-C3'   | -6.43 | 111.98      | 119.70   |
| 35  | BB    | 400  | G    | C4-C5-C6    | 6.43  | 122.66      | 118.80   |
| 35  | BB    | 1049 | C    | C5-C4-N4    | -6.43 | 115.70      | 120.20   |
| 35  | BB    | 2648 | G    | C5-C6-O6    | -6.43 | 124.74      | 128.60   |
| 1   | AA    | 677  | U    | C5-C4-O4    | -6.43 | 122.04      | 125.90   |
| 1   | AA    | 729  | A    | O4'-C1'-N9  | 6.43  | 113.34      | 108.20   |
| 1   | AA    | 769  | G    | N1-C2-N3    | -6.43 | 120.04      | 123.90   |
| 1   | AA    | 814  | A    | C6-N1-C2    | -6.43 | 114.74      | 118.60   |
| 1   | AA    | 1138 | G    | C6-N1-C2    | 6.43  | 128.96      | 125.10   |
| 1   | AA    | 1508 | A    | N7-C8-N9    | 6.43  | 117.02      | 113.80   |
| 35  | BB    | 443  | A    | C5-C6-N6    | -6.43 | 118.56      | 123.70   |
| 35  | BB    | 693  | A    | C6-N1-C2    | -6.43 | 114.74      | 118.60   |
| 35  | BB    | 788  | A    | C5-N7-C8    | 6.43  | 107.11      | 103.90   |
| 35  | BB    | 1895 | C    | O4'-C1'-N1  | 6.43  | 113.34      | 108.20   |
| 35  | BB    | 2554 | U    | O4'-C1'-N1  | 6.43  | 113.34      | 108.20   |
| 35  | BB    | 2635 | A    | C5-N7-C8    | -6.43 | 100.69      | 103.90   |
| 35  | BB    | 2721 | A    | C4-C5-C6    | 6.43  | 120.21      | 117.00   |
| 40  | BG    | 68   | ARG  | NE-CZ-NH1   | 6.43  | 123.52      | 120.30   |
| 1   | AA    | 150  | U    | N3-C4-O4    | 6.43  | 123.90      | 119.40   |
| 1   | AA    | 1072 | G    | C1'-O4'-C4' | 6.43  | 115.04      | 109.90   |
| 35  | BB    | 785  | G    | N3-C2-N2    | 6.43  | 124.40      | 119.90   |
| 48  | BO    | 41   | ALA  | CB-CA-C     | -6.43 | 100.46      | 110.10   |
| 1   | AA    | 1340 | A    | N7-C8-N9    | -6.43 | 110.59      | 113.80   |
| 1   | AA    | 1359 | C    | C6-N1-C1'   | -6.43 | 113.09      | 120.80   |
| 35  | BB    | 215  | G    | C6-C5-N7    | -6.43 | 126.54      | 130.40   |
| 35  | BB    | 984  | A    | C4-C5-C6    | 6.43  | 120.21      | 117.00   |
| 35  | BB    | 1065 | U    | O4'-C1'-N1  | 6.43  | 113.34      | 108.20   |
| 35  | BB    | 1387 | A    | C5-C6-N1    | -6.43 | 114.49      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1587 | G    | P-O3'-C3'   | -6.43 | 111.99      | 119.70   |
| 35  | BB    | 1703 | G    | C5-C6-O6    | -6.43 | 124.74      | 128.60   |
| 35  | BB    | 1834 | U    | P-O3'-C3'   | 6.43  | 127.41      | 119.70   |
| 38  | BE    | 130  | LYS  | N-CA-C      | -6.43 | 93.65       | 111.00   |
| 52  | BS    | 62   | ASP  | CB-CG-OD2   | -6.43 | 112.52      | 118.30   |
| 1   | AA    | 693  | G    | C5-N7-C8    | 6.42  | 107.51      | 104.30   |
| 1   | AA    | 1382 | C    | N3-C4-C5    | -6.42 | 119.33      | 121.90   |
| 35  | BB    | 205  | G    | N3-C2-N2    | -6.42 | 115.40      | 119.90   |
| 35  | BB    | 406  | G    | C5-C6-N1    | -6.42 | 108.29      | 111.50   |
| 35  | BB    | 455  | C    | C6-N1-C2    | 6.42  | 122.87      | 120.30   |
| 35  | BB    | 2036 | C    | C5'-C4'-C3' | -6.42 | 105.72      | 116.00   |
| 35  | BB    | 2166 | U    | O4'-C1'-N1  | 6.42  | 113.34      | 108.20   |
| 35  | BB    | 2189 | U    | OP1-P-OP2   | -6.42 | 109.96      | 119.60   |
| 35  | BB    | 2189 | U    | C5-C4-O4    | -6.42 | 122.05      | 125.90   |
| 35  | BB    | 2688 | G    | N1-C6-O6    | 6.42  | 123.75      | 119.90   |
| 35  | BB    | 2726 | A    | O4'-C1'-N9  | 6.42  | 113.34      | 108.20   |
| 1   | AA    | 335  | C    | N3-C4-C5    | -6.42 | 119.33      | 121.90   |
| 1   | AA    | 1255 | G    | C8-N9-C4    | -6.42 | 103.83      | 106.40   |
| 35  | BB    | 406  | G    | C4-C5-C6    | 6.42  | 122.65      | 118.80   |
| 35  | BB    | 1840 | G    | N3-C4-N9    | 6.42  | 129.85      | 126.00   |
| 35  | BB    | 2381 | A    | C4-C5-C6    | 6.42  | 120.21      | 117.00   |
| 35  | BB    | 2826 | A    | C5'-C4'-O4' | 6.42  | 116.81      | 109.10   |
| 39  | BF    | 142  | TYR  | CB-CG-CD1   | 6.42  | 124.85      | 121.00   |
| 1   | AA    | 161  | A    | C6-C5-N7    | -6.42 | 127.81      | 132.30   |
| 1   | AA    | 200  | G    | C5'-C4'-C3' | -6.42 | 105.72      | 116.00   |
| 1   | AA    | 209  | U    | P-O3'-C3'   | 6.42  | 127.41      | 119.70   |
| 1   | AA    | 239  | U    | N1-C2-N3    | -6.42 | 111.05      | 114.90   |
| 1   | AA    | 1528 | U    | N3-C4-O4    | 6.42  | 123.89      | 119.40   |
| 22  | AV    | 55   | U    | O4'-C1'-N1  | 6.42  | 113.34      | 108.20   |
| 35  | BB    | 12   | U    | N1-C2-N3    | 6.42  | 118.75      | 114.90   |
| 35  | BB    | 89   | A    | C2-N3-C4    | -6.42 | 107.39      | 110.60   |
| 35  | BB    | 338  | G    | N1-C6-O6    | 6.42  | 123.75      | 119.90   |
| 35  | BB    | 1376 | C    | C6-N1-C2    | -6.42 | 117.73      | 120.30   |
| 35  | BB    | 2476 | A    | N3-C4-N9    | 6.42  | 132.54      | 127.40   |
| 35  | BB    | 2484 | G    | N7-C8-N9    | -6.42 | 109.89      | 113.10   |
| 1   | AA    | 1202 | U    | P-O3'-C3'   | -6.42 | 112.00      | 119.70   |
| 35  | BB    | 2229 | U    | P-O3'-C3'   | -6.42 | 112.00      | 119.70   |
| 35  | BB    | 2592 | G    | C6-C5-N7    | -6.42 | 126.55      | 130.40   |
| 35  | BB    | 2744 | G    | N1-C2-N2    | 6.42  | 121.98      | 116.20   |
| 1   | AA    | 373  | A    | C5'-C4'-C3' | 6.42  | 126.27      | 116.00   |
| 1   | AA    | 427  | U    | C2-N3-C4    | 6.42  | 130.85      | 127.00   |
| 1   | AA    | 592  | G    | N3-C4-C5    | -6.42 | 125.39      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1206 | G    | N3-C2-N2    | 6.42  | 124.39      | 119.90   |
| 1   | AA    | 1223 | C    | O4'-C1'-N1  | 6.42  | 113.33      | 108.20   |
| 1   | AA    | 1322 | C    | O4'-C1'-N1  | 6.42  | 113.33      | 108.20   |
| 14  | AN    | 8    | ARG  | NE-CZ-NH1   | -6.42 | 117.09      | 120.30   |
| 15  | AO    | 76   | ARG  | NE-CZ-NH2   | -6.42 | 117.09      | 120.30   |
| 35  | BB    | 483  | A    | C8-N9-C4    | -6.42 | 103.23      | 105.80   |
| 35  | BB    | 591  | U    | N3-C4-C5    | 6.42  | 118.45      | 114.60   |
| 35  | BB    | 974  | G    | P-O3'-C3'   | 6.42  | 127.40      | 119.70   |
| 35  | BB    | 993  | G    | O5'-P-OP2   | -6.42 | 99.92       | 105.70   |
| 35  | BB    | 1307 | A    | C5-N7-C8    | 6.42  | 107.11      | 103.90   |
| 35  | BB    | 2134 | A    | C4'-C3'-C2' | -6.42 | 96.18       | 102.60   |
| 35  | BB    | 2699 | C    | P-O3'-C3'   | -6.42 | 112.00      | 119.70   |
| 35  | BB    | 2751 | G    | N3-C2-N2    | 6.42  | 124.39      | 119.90   |
| 1   | AA    | 29   | U    | N3-C4-C5    | 6.42  | 118.45      | 114.60   |
| 1   | AA    | 41   | G    | C5-C6-N1    | -6.42 | 108.29      | 111.50   |
| 1   | AA    | 194  | C    | C5-C4-N4    | -6.42 | 115.71      | 120.20   |
| 1   | AA    | 944  | G    | C2-N3-C4    | 6.42  | 115.11      | 111.90   |
| 1   | AA    | 1157 | A    | C6-C5-N7    | -6.42 | 127.81      | 132.30   |
| 22  | AV    | 6    | C    | C2-N3-C4    | 6.42  | 123.11      | 119.90   |
| 35  | BB    | 200  | U    | N3-C4-O4    | 6.42  | 123.89      | 119.40   |
| 35  | BB    | 788  | A    | N3-C4-C5    | -6.42 | 122.31      | 126.80   |
| 35  | BB    | 1059 | G    | C4'-C3'-C2' | -6.42 | 96.18       | 102.60   |
| 35  | BB    | 1274 | A    | C4'-C3'-C2' | -6.42 | 96.18       | 102.60   |
| 35  | BB    | 1975 | G    | C6-N1-C2    | 6.42  | 128.95      | 125.10   |
| 1   | AA    | 1066 | C    | C5-C4-N4    | -6.42 | 115.71      | 120.20   |
| 34  | BA    | 21   | G    | N3-C4-C5    | 6.42  | 131.81      | 128.60   |
| 1   | AA    | 130  | A    | N1-C6-N6    | 6.41  | 122.45      | 118.60   |
| 1   | AA    | 1307 | U    | N3-C4-O4    | 6.41  | 123.89      | 119.40   |
| 22  | AV    | 58   | A    | C4-C5-C6    | 6.41  | 120.21      | 117.00   |
| 35  | BB    | 308  | G    | C5-C6-O6    | -6.41 | 124.75      | 128.60   |
| 35  | BB    | 1149 | G    | C3'-C2'-C1' | 6.41  | 106.63      | 101.50   |
| 35  | BB    | 1972 | G    | O5'-C5'-C4' | -6.41 | 99.51       | 111.70   |
| 35  | BB    | 2610 | C    | N3-C4-C5    | -6.41 | 119.33      | 121.90   |
| 35  | BB    | 2664 | G    | C4'-C3'-C2' | -6.41 | 96.19       | 102.60   |
| 35  | BB    | 2761 | A    | C5-C6-N6    | -6.41 | 118.57      | 123.70   |
| 1   | AA    | 1037 | C    | C4'-C3'-C2' | -6.41 | 96.19       | 102.60   |
| 34  | BA    | 63   | C    | C4'-C3'-C2' | -6.41 | 96.19       | 102.60   |
| 35  | BB    | 144  | A    | C5-C6-N6    | -6.41 | 118.57      | 123.70   |
| 35  | BB    | 1083 | U    | C5'-C4'-C3' | -6.41 | 105.74      | 116.00   |
| 35  | BB    | 1886 | U    | O4'-C1'-N1  | 6.41  | 113.33      | 108.20   |
| 35  | BB    | 2576 | G    | C4-N9-C1'   | 6.41  | 134.83      | 126.50   |
| 1   | AA    | 13   | U    | N1-C2-N3    | -6.41 | 111.05      | 114.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 278  | G    | C6-N1-C2    | 6.41  | 128.94      | 125.10   |
| 1   | AA    | 1002 | G    | C4-C5-N7    | -6.41 | 108.24      | 110.80   |
| 1   | AA    | 1337 | G    | C8-N9-C4    | 6.41  | 108.96      | 106.40   |
| 35  | BB    | 143  | C    | O4'-C4'-C3' | -6.41 | 97.59       | 104.00   |
| 35  | BB    | 610  | C    | N3-C4-N4    | 6.41  | 122.49      | 118.00   |
| 35  | BB    | 681  | G    | C5-N7-C8    | 6.41  | 107.50      | 104.30   |
| 35  | BB    | 938  | G    | C5-C6-N1    | 6.41  | 114.70      | 111.50   |
| 35  | BB    | 960  | A    | N3-C4-C5    | -6.41 | 122.31      | 126.80   |
| 35  | BB    | 994  | C    | O4'-C1'-N1  | 6.41  | 113.33      | 108.20   |
| 35  | BB    | 1510 | G    | N3-C2-N2    | 6.41  | 124.39      | 119.90   |
| 35  | BB    | 1881 | C    | C6-N1-C2    | 6.41  | 122.86      | 120.30   |
| 35  | BB    | 2388 | A    | P-O5'-C5'   | 6.41  | 131.15      | 120.90   |
| 20  | AT    | 67   | HIS  | C-N-CA      | 6.41  | 137.72      | 121.70   |
| 35  | BB    | 1545 | A    | C2-N3-C4    | 6.41  | 113.80      | 110.60   |
| 1   | AA    | 583  | A    | C8-N9-C4    | 6.41  | 108.36      | 105.80   |
| 1   | AA    | 707  | U    | C2-N3-C4    | 6.41  | 130.84      | 127.00   |
| 1   | AA    | 1340 | A    | O4'-C1'-N9  | 6.41  | 113.33      | 108.20   |
| 35  | BB    | 1425 | G    | C1'-O4'-C4' | 6.41  | 115.02      | 109.90   |
| 35  | BB    | 1932 | A    | C5-N7-C8    | 6.41  | 107.10      | 103.90   |
| 35  | BB    | 2405 | G    | C2-N3-C4    | 6.41  | 115.10      | 111.90   |
| 44  | BK    | 37   | ASP  | CB-CG-OD2   | -6.41 | 112.53      | 118.30   |
| 1   | AA    | 642  | A    | C8-N9-C4    | -6.40 | 103.24      | 105.80   |
| 35  | BB    | 178  | G    | C2-N3-C4    | 6.40  | 115.10      | 111.90   |
| 35  | BB    | 546  | U    | C5'-C4'-O4' | 6.40  | 116.78      | 109.10   |
| 35  | BB    | 713  | G    | N7-C8-N9    | -6.40 | 109.90      | 113.10   |
| 35  | BB    | 757  | G    | P-O5'-C5'   | 6.40  | 131.15      | 120.90   |
| 35  | BB    | 1026 | G    | C2-N3-C4    | 6.40  | 115.10      | 111.90   |
| 35  | BB    | 2196 | C    | C1'-O4'-C4' | -6.40 | 104.78      | 109.90   |
| 1   | AA    | 206  | C    | C6-N1-C2    | 6.40  | 122.86      | 120.30   |
| 1   | AA    | 1201 | A    | C5-C6-N1    | -6.40 | 114.50      | 117.70   |
| 3   | AC    | 142  | ARG  | NE-CZ-NH2   | -6.40 | 117.10      | 120.30   |
| 35  | BB    | 86   | G    | C5-C6-O6    | -6.40 | 124.76      | 128.60   |
| 35  | BB    | 771  | G    | C8-N9-C4    | -6.40 | 103.84      | 106.40   |
| 35  | BB    | 1013 | C    | N3-C4-N4    | 6.40  | 122.48      | 118.00   |
| 35  | BB    | 1229 | C    | O4'-C1'-N1  | 6.40  | 113.32      | 108.20   |
| 35  | BB    | 1685 | C    | O4'-C4'-C3' | -6.40 | 97.60       | 104.00   |
| 35  | BB    | 2080 | A    | C6-C5-N7    | -6.40 | 127.82      | 132.30   |
| 35  | BB    | 2635 | A    | N1-C2-N3    | 6.40  | 132.50      | 129.30   |
| 35  | BB    | 2714 | G    | N3-C4-N9    | 6.40  | 129.84      | 126.00   |
| 35  | BB    | 2834 | G    | P-O5'-C5'   | -6.40 | 110.66      | 120.90   |
| 35  | BB    | 332  | A    | N7-C8-N9    | 6.40  | 117.00      | 113.80   |
| 35  | BB    | 544  | C    | O4'-C1'-N1  | 6.40  | 113.32      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 608  | A    | C8-N9-C4    | -6.40 | 103.24      | 105.80   |
| 35  | BB    | 629  | G    | N1-C2-N3    | -6.40 | 120.06      | 123.90   |
| 35  | BB    | 1898 | U    | O4'-C1'-N1  | 6.40  | 113.32      | 108.20   |
| 1   | AA    | 235  | C    | C2-N1-C1'   | 6.40  | 125.84      | 118.80   |
| 7   | AG    | 120  | ALA  | N-CA-CB     | 6.40  | 119.06      | 110.10   |
| 35  | BB    | 102  | U    | N3-C4-O4    | 6.40  | 123.88      | 119.40   |
| 35  | BB    | 291  | G    | C4'-C3'-C2' | -6.40 | 96.20       | 102.60   |
| 35  | BB    | 2581 | G    | N1-C6-O6    | 6.40  | 123.74      | 119.90   |
| 35  | BB    | 2674 | G    | C4-C5-C6    | 6.40  | 122.64      | 118.80   |
| 35  | BB    | 2746 | U    | N1-C1'-C2'  | -6.40 | 104.96      | 112.00   |
| 1   | AA    | 474  | G    | OP1-P-OP2   | -6.40 | 110.00      | 119.60   |
| 1   | AA    | 1057 | G    | N1-C2-N3    | -6.40 | 120.06      | 123.90   |
| 1   | AA    | 1346 | A    | N9-C4-C5    | 6.40  | 108.36      | 105.80   |
| 35  | BB    | 192  | C    | N1-C2-O2    | 6.40  | 122.74      | 118.90   |
| 35  | BB    | 686  | U    | C2-N3-C4    | 6.40  | 130.84      | 127.00   |
| 35  | BB    | 1445 | G    | O4'-C1'-N9  | 6.40  | 113.32      | 108.20   |
| 35  | BB    | 1799 | G    | N7-C8-N9    | 6.40  | 116.30      | 113.10   |
| 35  | BB    | 2027 | G    | C2-N3-C4    | 6.40  | 115.10      | 111.90   |
| 1   | AA    | 336  | A    | C5'-C4'-O4' | -6.40 | 101.42      | 109.10   |
| 1   | AA    | 532  | A    | C6-C5-N7    | -6.40 | 127.82      | 132.30   |
| 1   | AA    | 912  | C    | C5-C6-N1    | 6.40  | 124.20      | 121.00   |
| 35  | BB    | 1053 | C    | O4'-C1'-N1  | 6.40  | 113.32      | 108.20   |
| 1   | AA    | 1139 | G    | C4'-C3'-C2' | -6.39 | 96.21       | 102.60   |
| 34  | BA    | 114  | C    | N3-C4-C5    | 6.39  | 124.46      | 121.90   |
| 35  | BB    | 81   | G    | N9-C4-C5    | -6.39 | 102.84      | 105.40   |
| 35  | BB    | 372  | G    | C8-N9-C4    | -6.39 | 103.84      | 106.40   |
| 35  | BB    | 487  | C    | C1'-O4'-C4' | 6.39  | 115.02      | 109.90   |
| 35  | BB    | 523  | C    | C5-C4-N4    | -6.39 | 115.72      | 120.20   |
| 35  | BB    | 1182 | G    | O4'-C1'-N9  | 6.39  | 113.32      | 108.20   |
| 35  | BB    | 1857 | G    | C4-C5-N7    | 6.39  | 113.36      | 110.80   |
| 35  | BB    | 2273 | A    | N3-C4-N9    | 6.39  | 132.52      | 127.40   |
| 35  | BB    | 2557 | G    | C5-C6-N1    | -6.39 | 108.30      | 111.50   |
| 35  | BB    | 2776 | A    | C5-N7-C8    | 6.39  | 107.10      | 103.90   |
| 1   | AA    | 160  | A    | N1-C6-N6    | 6.39  | 122.44      | 118.60   |
| 1   | AA    | 285  | C    | N3-C4-C5    | -6.39 | 119.34      | 121.90   |
| 1   | AA    | 305  | G    | C5-C6-N1    | -6.39 | 108.30      | 111.50   |
| 1   | AA    | 706  | A    | P-O5'-C5'   | 6.39  | 131.13      | 120.90   |
| 1   | AA    | 962  | C    | N3-C4-C5    | -6.39 | 119.34      | 121.90   |
| 1   | AA    | 1087 | G    | N1-C2-N3    | -6.39 | 120.06      | 123.90   |
| 1   | AA    | 1093 | A    | N7-C8-N9    | -6.39 | 110.60      | 113.80   |
| 1   | AA    | 1234 | C    | N3-C4-C5    | -6.39 | 119.34      | 121.90   |
| 1   | AA    | 1292 | G    | C5-N7-C8    | 6.39  | 107.50      | 104.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 327  | G    | P-O3'-C3'   | -6.39 | 112.03      | 119.70   |
| 35  | BB    | 1109 | C    | N3-C4-C5    | -6.39 | 119.34      | 121.90   |
| 35  | BB    | 1185 | G    | C4-C5-N7    | -6.39 | 108.24      | 110.80   |
| 35  | BB    | 1709 | U    | C5-C4-O4    | -6.39 | 122.06      | 125.90   |
| 35  | BB    | 1889 | A    | C5-C6-N6    | -6.39 | 118.59      | 123.70   |
| 35  | BB    | 2324 | U    | C2-N3-C4    | -6.39 | 123.17      | 127.00   |
| 35  | BB    | 2355 | G    | C6-N1-C2    | -6.39 | 121.27      | 125.10   |
| 35  | BB    | 2392 | A    | N7-C8-N9    | 6.39  | 117.00      | 113.80   |
| 35  | BB    | 2421 | G    | C8-N9-C4    | 6.39  | 108.96      | 106.40   |
| 35  | BB    | 2536 | G    | C6-C5-N7    | -6.39 | 126.56      | 130.40   |
| 35  | BB    | 2697 | G    | N9-C1'-C2'  | -6.39 | 104.97      | 112.00   |
| 35  | BB    | 2892 | G    | C8-N9-C4    | 6.39  | 108.96      | 106.40   |
| 1   | AA    | 117  | G    | O4'-C4'-C3' | -6.39 | 97.61       | 104.00   |
| 1   | AA    | 236  | A    | O4'-C1'-N9  | 6.39  | 113.31      | 108.20   |
| 1   | AA    | 609  | A    | O4'-C1'-N9  | 6.39  | 113.31      | 108.20   |
| 1   | AA    | 1010 | U    | O4'-C1'-N1  | 6.39  | 113.31      | 108.20   |
| 1   | AA    | 1021 | A    | C5-C6-N6    | -6.39 | 118.59      | 123.70   |
| 1   | AA    | 1146 | A    | C5-C6-N1    | -6.39 | 114.50      | 117.70   |
| 1   | AA    | 1182 | G    | C2-N3-C4    | 6.39  | 115.10      | 111.90   |
| 1   | AA    | 1346 | A    | O4'-C1'-N9  | 6.39  | 113.31      | 108.20   |
| 35  | BB    | 102  | U    | C2-N3-C4    | 6.39  | 130.83      | 127.00   |
| 35  | BB    | 533  | G    | C8-N9-C4    | -6.39 | 103.84      | 106.40   |
| 35  | BB    | 853  | C    | C4'-C3'-C2' | -6.39 | 96.21       | 102.60   |
| 35  | BB    | 1003 | G    | C4-C5-C6    | 6.39  | 122.64      | 118.80   |
| 35  | BB    | 1688 | U    | O3'-P-O5'   | -6.39 | 91.86       | 104.00   |
| 35  | BB    | 1740 | G    | C2-N3-C4    | -6.39 | 108.70      | 111.90   |
| 35  | BB    | 1978 | A    | C8-N9-C4    | 6.39  | 108.36      | 105.80   |
| 35  | BB    | 2662 | A    | C4-C5-C6    | 6.39  | 120.19      | 117.00   |
| 1   | AA    | 759  | A    | O3'-P-O5'   | 6.39  | 116.14      | 104.00   |
| 1   | AA    | 797  | C    | C6-N1-C1'   | -6.39 | 113.13      | 120.80   |
| 1   | AA    | 902  | G    | O4'-C1'-N9  | 6.39  | 113.31      | 108.20   |
| 3   | AC    | 81   | GLU  | OE1-CD-OE2  | -6.39 | 115.63      | 123.30   |
| 12  | AL    | 118  | VAL  | CG1-CB-CG2  | 6.39  | 121.12      | 110.90   |
| 35  | BB    | 493  | G    | C8-N9-C1'   | 6.39  | 135.31      | 127.00   |
| 35  | BB    | 772  | C    | C6-N1-C2    | 6.39  | 122.86      | 120.30   |
| 35  | BB    | 1138 | G    | O4'-C1'-N9  | 6.39  | 113.31      | 108.20   |
| 35  | BB    | 1252 | G    | N7-C8-N9    | 6.39  | 116.30      | 113.10   |
| 35  | BB    | 1547 | C    | C5'-C4'-C3' | -6.39 | 105.78      | 116.00   |
| 35  | BB    | 1701 | A    | C6-C5-N7    | -6.39 | 127.83      | 132.30   |
| 35  | BB    | 2143 | C    | N3-C4-C5    | -6.39 | 119.34      | 121.90   |
| 35  | BB    | 2205 | A    | C4-C5-C6    | 6.39  | 120.19      | 117.00   |
| 35  | BB    | 2279 | G    | N3-C4-N9    | -6.39 | 122.17      | 126.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2352 | A    | C8-N9-C4    | -6.39 | 103.24      | 105.80   |
| 35  | BB    | 2518 | A    | N3-C4-C5    | -6.39 | 122.33      | 126.80   |
| 34  | BA    | 91   | C    | C1'-O4'-C4' | 6.39  | 115.01      | 109.90   |
| 35  | BB    | 1978 | A    | N1-C2-N3    | 6.39  | 132.49      | 129.30   |
| 35  | BB    | 2174 | C    | O5'-C5'-C4' | -6.39 | 99.56       | 111.70   |
| 44  | BK    | 29   | HIS  | N-CA-CB     | 6.39  | 122.10      | 110.60   |
| 1   | AA    | 630  | A    | O4'-C1'-N9  | 6.39  | 113.31      | 108.20   |
| 1   | AA    | 1311 | A    | P-O3'-C3'   | -6.39 | 112.04      | 119.70   |
| 35  | BB    | 825  | A    | C5-N7-C8    | 6.39  | 107.09      | 103.90   |
| 35  | BB    | 1910 | G    | C5-C6-O6    | -6.39 | 124.77      | 128.60   |
| 35  | BB    | 2583 | G    | C5-C6-N1    | -6.39 | 108.31      | 111.50   |
| 35  | BB    | 2777 | G    | O4'-C1'-N9  | 6.39  | 113.31      | 108.20   |
| 35  | BB    | 2893 | A    | N3-C4-N9    | -6.39 | 122.29      | 127.40   |
| 1   | AA    | 120  | A    | C5-C6-N6    | -6.38 | 118.59      | 123.70   |
| 1   | AA    | 444  | G    | C8-N9-C4    | -6.38 | 103.85      | 106.40   |
| 1   | AA    | 637  | C    | C4-C5-C6    | 6.38  | 120.59      | 117.40   |
| 1   | AA    | 777  | A    | P-O5'-C5'   | -6.38 | 110.69      | 120.90   |
| 1   | AA    | 1207 | G    | C5-N7-C8    | 6.38  | 107.49      | 104.30   |
| 1   | AA    | 1253 | G    | N7-C8-N9    | -6.38 | 109.91      | 113.10   |
| 1   | AA    | 1325 | C    | O4'-C1'-N1  | 6.38  | 113.31      | 108.20   |
| 34  | BA    | 87   | U    | N1-C2-O2    | 6.38  | 127.27      | 122.80   |
| 35  | BB    | 90   | U    | C5-C4-O4    | -6.38 | 122.07      | 125.90   |
| 35  | BB    | 103  | A    | C6-N1-C2    | 6.38  | 122.43      | 118.60   |
| 35  | BB    | 1027 | A    | O4'-C1'-N9  | 6.38  | 113.31      | 108.20   |
| 35  | BB    | 1189 | A    | N9-C4-C5    | 6.38  | 108.35      | 105.80   |
| 35  | BB    | 1426 | G    | N1-C2-N3    | -6.38 | 120.07      | 123.90   |
| 35  | BB    | 2021 | C    | O4'-C1'-N1  | 6.38  | 113.31      | 108.20   |
| 35  | BB    | 2410 | G    | C5-C6-O6    | -6.38 | 124.77      | 128.60   |
| 35  | BB    | 2490 | G    | C4-C5-C6    | 6.38  | 122.63      | 118.80   |
| 35  | BB    | 2674 | G    | P-O3'-C3'   | -6.38 | 112.04      | 119.70   |
| 1   | AA    | 595  | A    | OP1-P-OP2   | -6.38 | 110.03      | 119.60   |
| 35  | BB    | 425  | G    | N1-C2-N3    | -6.38 | 120.07      | 123.90   |
| 35  | BB    | 1115 | G    | C8-N9-C4    | -6.38 | 103.85      | 106.40   |
| 1   | AA    | 29   | U    | C2-N1-C1'   | -6.38 | 110.04      | 117.70   |
| 1   | AA    | 303  | A    | C5-C6-N1    | -6.38 | 114.51      | 117.70   |
| 1   | AA    | 504  | C    | C5-C4-N4    | -6.38 | 115.73      | 120.20   |
| 35  | BB    | 44   | A    | N9-C1'-C2'  | -6.38 | 104.98      | 112.00   |
| 35  | BB    | 532  | A    | O4'-C1'-N9  | 6.38  | 113.31      | 108.20   |
| 35  | BB    | 845  | A    | C6-N1-C2    | -6.38 | 114.77      | 118.60   |
| 35  | BB    | 1021 | A    | N9-C4-C5    | -6.38 | 103.25      | 105.80   |
| 35  | BB    | 1109 | C    | C5-C4-N4    | -6.38 | 115.73      | 120.20   |
| 35  | BB    | 1170 | C    | C5-C6-N1    | 6.38  | 124.19      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1447 | C    | O4'-C1'-N1  | 6.38  | 113.31      | 108.20   |
| 35  | BB    | 2578 | G    | N3-C4-C5    | -6.38 | 125.41      | 128.60   |
| 35  | BB    | 1013 | C    | N1-C2-N3    | -6.38 | 114.73      | 119.20   |
| 35  | BB    | 1396 | U    | C4'-C3'-C2' | 6.38  | 108.98      | 102.60   |
| 35  | BB    | 1989 | G    | C3'-C2'-C1' | -6.38 | 96.40       | 101.50   |
| 35  | BB    | 2900 | A    | C4-C5-C6    | 6.38  | 120.19      | 117.00   |
| 39  | BF    | 127  | TYR  | CB-CG-CD1   | 6.38  | 124.83      | 121.00   |
| 1   | AA    | 430  | A    | C5-C6-N1    | -6.38 | 114.51      | 117.70   |
| 1   | AA    | 1369 | C    | C5-C4-N4    | -6.38 | 115.73      | 120.20   |
| 35  | BB    | 389  | G    | C5'-C4'-O4' | 6.38  | 116.75      | 109.10   |
| 35  | BB    | 552  | U    | O4'-C1'-N1  | 6.38  | 113.30      | 108.20   |
| 35  | BB    | 789  | A    | C8-N9-C4    | -6.38 | 103.25      | 105.80   |
| 35  | BB    | 1230 | A    | C6-C5-N7    | -6.38 | 127.83      | 132.30   |
| 35  | BB    | 1655 | A    | C4-C5-C6    | 6.38  | 120.19      | 117.00   |
| 35  | BB    | 2083 | G    | C4-C5-C6    | 6.38  | 122.63      | 118.80   |
| 35  | BB    | 2450 | A    | N7-C8-N9    | -6.38 | 110.61      | 113.80   |
| 1   | AA    | 210  | C    | C5-C4-N4    | -6.38 | 115.74      | 120.20   |
| 1   | AA    | 952  | U    | N1-C2-N3    | 6.38  | 118.73      | 114.90   |
| 1   | AA    | 1074 | G    | C8-N9-C4    | -6.38 | 103.85      | 106.40   |
| 35  | BB    | 159  | G    | C8-N9-C4    | -6.38 | 103.85      | 106.40   |
| 35  | BB    | 477  | A    | N1-C2-N3    | -6.38 | 126.11      | 129.30   |
| 35  | BB    | 546  | U    | C6-N1-C2    | -6.38 | 117.17      | 121.00   |
| 35  | BB    | 559  | G    | N1-C2-N3    | -6.38 | 120.07      | 123.90   |
| 35  | BB    | 797  | G    | C8-N9-C4    | -6.38 | 103.85      | 106.40   |
| 35  | BB    | 1057 | A    | C3'-C2'-C1' | 6.38  | 106.60      | 101.50   |
| 35  | BB    | 1096 | A    | C6-C5-N7    | -6.38 | 127.84      | 132.30   |
| 35  | BB    | 1431 | A    | C8-N9-C4    | 6.38  | 108.35      | 105.80   |
| 35  | BB    | 1751 | U    | C2-N1-C1'   | 6.38  | 125.35      | 117.70   |
| 35  | BB    | 2168 | G    | C5'-C4'-C3' | 6.38  | 126.20      | 116.00   |
| 35  | BB    | 2286 | G    | C4-C5-N7    | -6.38 | 108.25      | 110.80   |
| 35  | BB    | 2469 | A    | N7-C8-N9    | -6.38 | 110.61      | 113.80   |
| 35  | BB    | 2535 | G    | N7-C8-N9    | -6.38 | 109.91      | 113.10   |
| 35  | BB    | 76   | C    | C5-C4-N4    | -6.38 | 115.74      | 120.20   |
| 35  | BB    | 1606 | C    | C2-N3-C4    | 6.38  | 123.09      | 119.90   |
| 35  | BB    | 2061 | G    | C4-C5-C6    | 6.38  | 122.62      | 118.80   |
| 35  | BB    | 2825 | G    | N3-C2-N2    | 6.38  | 124.36      | 119.90   |
| 1   | AA    | 297  | G    | N3-C2-N2    | 6.37  | 124.36      | 119.90   |
| 1   | AA    | 456  | A    | N1-C2-N3    | 6.37  | 132.49      | 129.30   |
| 22  | AV    | 19   | G    | C5-C6-O6    | -6.37 | 124.78      | 128.60   |
| 35  | BB    | 27   | G    | O4'-C4'-C3' | 6.37  | 111.20      | 106.10   |
| 35  | BB    | 446  | G    | N9-C4-C5    | -6.37 | 102.85      | 105.40   |
| 35  | BB    | 1124 | G    | O4'-C1'-N9  | 6.37  | 113.30      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 31   | G    | C8-N9-C4    | -6.37 | 103.85      | 106.40   |
| 1   | AA    | 497  | G    | C5-C6-O6    | -6.37 | 124.78      | 128.60   |
| 1   | AA    | 947  | G    | C5-C6-N1    | -6.37 | 108.31      | 111.50   |
| 1   | AA    | 1499 | A    | P-O5'-C5'   | 6.37  | 131.09      | 120.90   |
| 35  | BB    | 204  | A    | N1-C2-N3    | -6.37 | 126.11      | 129.30   |
| 35  | BB    | 507  | A    | C6-N1-C2    | -6.37 | 114.78      | 118.60   |
| 35  | BB    | 1079 | C    | P-O5'-C5'   | -6.37 | 110.71      | 120.90   |
| 35  | BB    | 1532 | A    | C8-N9-C4    | -6.37 | 103.25      | 105.80   |
| 35  | BB    | 1872 | A    | C5-C6-N6    | -6.37 | 118.60      | 123.70   |
| 35  | BB    | 1882 | U    | N3-C2-O2    | -6.37 | 117.74      | 122.20   |
| 35  | BB    | 2216 | G    | N1-C2-N2    | 6.37  | 121.94      | 116.20   |
| 35  | BB    | 2534 | A    | C3'-C2'-C1' | -6.37 | 96.40       | 101.50   |
| 35  | BB    | 2542 | A    | C4-C5-N7    | -6.37 | 107.51      | 110.70   |
| 1   | AA    | 1479 | C    | C2-N3-C4    | 6.37  | 123.08      | 119.90   |
| 35  | BB    | 1065 | U    | C6-N1-C2    | 6.37  | 124.82      | 121.00   |
| 35  | BB    | 2375 | G    | C6-N1-C2    | -6.37 | 121.28      | 125.10   |
| 1   | AA    | 104  | G    | C5-C6-O6    | -6.37 | 124.78      | 128.60   |
| 1   | AA    | 310  | G    | C2-N3-C4    | -6.37 | 108.72      | 111.90   |
| 1   | AA    | 739  | C    | C5-C6-N1    | 6.37  | 124.18      | 121.00   |
| 35  | BB    | 281  | C    | C4-C5-C6    | 6.37  | 120.58      | 117.40   |
| 35  | BB    | 480  | A    | C4-C5-N7    | -6.37 | 107.52      | 110.70   |
| 35  | BB    | 782  | A    | O4'-C1'-N9  | 6.37  | 113.30      | 108.20   |
| 35  | BB    | 893  | C    | N3-C4-C5    | -6.37 | 119.35      | 121.90   |
| 35  | BB    | 1780 | A    | C5-C6-N1    | -6.37 | 114.52      | 117.70   |
| 37  | BD    | 46   | ARG  | NE-CZ-NH2   | -6.37 | 117.12      | 120.30   |
| 1   | AA    | 328  | C    | C1'-O4'-C4' | -6.37 | 104.81      | 109.90   |
| 1   | AA    | 626  | G    | N1-C6-O6    | 6.37  | 123.72      | 119.90   |
| 1   | AA    | 795  | C    | C6-N1-C2    | -6.37 | 117.75      | 120.30   |
| 4   | AD    | 64   | TYR  | CB-CG-CD2   | -6.37 | 117.18      | 121.00   |
| 35  | BB    | 885  | C    | C5'-C4'-O4' | 6.37  | 116.74      | 109.10   |
| 35  | BB    | 1344 | U    | P-O3'-C3'   | -6.37 | 112.06      | 119.70   |
| 35  | BB    | 1820 | U    | C5-C6-N1    | -6.37 | 119.52      | 122.70   |
| 35  | BB    | 2050 | C    | C2-N3-C4    | 6.37  | 123.08      | 119.90   |
| 35  | BB    | 2156 | G    | C3'-C2'-C1' | -6.37 | 96.41       | 101.50   |
| 35  | BB    | 2335 | A    | C4-C5-N7    | -6.37 | 107.52      | 110.70   |
| 1   | AA    | 889  | A    | N3-C4-C5    | -6.37 | 122.34      | 126.80   |
| 34  | BA    | 7    | G    | N7-C8-N9    | -6.37 | 109.92      | 113.10   |
| 35  | BB    | 1459 | G    | N1-C2-N3    | -6.37 | 120.08      | 123.90   |
| 35  | BB    | 1889 | A    | C4-C5-C6    | 6.37  | 120.18      | 117.00   |
| 35  | BB    | 2494 | G    | C5-C6-O6    | -6.37 | 124.78      | 128.60   |
| 35  | BB    | 2533 | U    | N3-C4-C5    | 6.37  | 118.42      | 114.60   |
| 35  | BB    | 2772 | C    | C6-N1-C2    | -6.37 | 117.75      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2841 | C    | C6-N1-C2    | -6.37 | 117.75      | 120.30   |
| 41  | BH    | 7    | ASP  | CB-CG-OD1   | -6.37 | 112.57      | 118.30   |
| 50  | BQ    | 85   | ALA  | N-CA-CB     | 6.37  | 119.01      | 110.10   |
| 1   | AA    | 413  | G    | P-O3'-C3'   | 6.36  | 127.33      | 119.70   |
| 1   | AA    | 767  | A    | N3-C4-C5    | -6.36 | 122.35      | 126.80   |
| 1   | AA    | 1375 | A    | C6-C5-N7    | -6.36 | 127.84      | 132.30   |
| 1   | AA    | 1401 | G    | N3-C2-N2    | 6.36  | 124.35      | 119.90   |
| 3   | AC    | 92   | ASP  | CB-CG-OD2   | 6.36  | 124.03      | 118.30   |
| 35  | BB    | 21   | A    | N1-C2-N3    | -6.36 | 126.12      | 129.30   |
| 35  | BB    | 189  | G    | O5'-P-OP2   | -6.36 | 99.97       | 105.70   |
| 35  | BB    | 507  | A    | N3-C4-C5    | -6.36 | 122.34      | 126.80   |
| 35  | BB    | 1522 | A    | P-O3'-C3'   | 6.36  | 127.34      | 119.70   |
| 35  | BB    | 1869 | G    | C6-N1-C2    | 6.36  | 128.92      | 125.10   |
| 1   | AA    | 32   | A    | C5-N7-C8    | 6.36  | 107.08      | 103.90   |
| 1   | AA    | 539  | A    | C5-C6-N1    | -6.36 | 114.52      | 117.70   |
| 2   | AB    | 212  | TYR  | CG-CD2-CE2  | 6.36  | 126.39      | 121.30   |
| 35  | BB    | 262  | A    | C5-N7-C8    | 6.36  | 107.08      | 103.90   |
| 35  | BB    | 1084 | A    | P-O5'-C5'   | 6.36  | 131.08      | 120.90   |
| 35  | BB    | 1148 | U    | C1'-O4'-C4' | 6.36  | 114.99      | 109.90   |
| 52  | BS    | 54   | ALA  | N-CA-CB     | 6.36  | 119.01      | 110.10   |
| 1   | AA    | 345  | C    | C4-C5-C6    | 6.36  | 120.58      | 117.40   |
| 1   | AA    | 1196 | A    | C5-C6-N1    | -6.36 | 114.52      | 117.70   |
| 1   | AA    | 1310 | G    | C2-N3-C4    | 6.36  | 115.08      | 111.90   |
| 1   | AA    | 1482 | G    | C1'-O4'-C4' | -6.36 | 104.81      | 109.90   |
| 22  | AV    | 39   | G    | N7-C8-N9    | 6.36  | 116.28      | 113.10   |
| 35  | BB    | 81   | G    | N1-C2-N3    | 6.36  | 127.72      | 123.90   |
| 35  | BB    | 1278 | C    | OP1-P-OP2   | -6.36 | 110.06      | 119.60   |
| 35  | BB    | 1767 | G    | C6-C5-N7    | -6.36 | 126.58      | 130.40   |
| 35  | BB    | 2280 | G    | C6-N1-C2    | 6.36  | 128.92      | 125.10   |
| 35  | BB    | 2790 | U    | P-O5'-C5'   | 6.36  | 131.08      | 120.90   |
| 1   | AA    | 1231 | G    | O4'-C1'-N9  | 6.36  | 113.29      | 108.20   |
| 22  | AV    | 18   | G    | C5-C6-O6    | -6.36 | 124.78      | 128.60   |
| 35  | BB    | 1232 | G    | C2-N3-C4    | 6.36  | 115.08      | 111.90   |
| 35  | BB    | 1572 | A    | C4-C5-C6    | 6.36  | 120.18      | 117.00   |
| 35  | BB    | 1817 | G    | C5-C6-O6    | -6.36 | 124.78      | 128.60   |
| 35  | BB    | 2261 | C    | C2-N1-C1'   | 6.36  | 125.80      | 118.80   |
| 35  | BB    | 2606 | C    | N3-C4-C5    | -6.36 | 119.36      | 121.90   |
| 35  | BB    | 2673 | G    | C6-C5-N7    | -6.36 | 126.58      | 130.40   |
| 35  | BB    | 2780 | G    | C5-C6-N1    | -6.36 | 108.32      | 111.50   |
| 1   | AA    | 1153 | G    | N7-C8-N9    | 6.36  | 116.28      | 113.10   |
| 1   | AA    | 1166 | G    | C4-C5-C6    | 6.36  | 122.61      | 118.80   |
| 1   | AA    | 1525 | G    | C6-N1-C2    | 6.36  | 128.91      | 125.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 359  | G    | C1'-O4'-C4' | 6.36  | 114.99      | 109.90   |
| 35  | BB    | 544  | C    | C2-N3-C4    | 6.36  | 123.08      | 119.90   |
| 35  | BB    | 554  | U    | P-O3'-C3'   | 6.36  | 127.33      | 119.70   |
| 35  | BB    | 810  | U    | N3-C4-O4    | 6.36  | 123.85      | 119.40   |
| 35  | BB    | 827  | U    | C5-C4-O4    | -6.36 | 122.09      | 125.90   |
| 35  | BB    | 1137 | G    | N1-C6-O6    | 6.36  | 123.71      | 119.90   |
| 35  | BB    | 2219 | U    | C5-C4-O4    | -6.36 | 122.09      | 125.90   |
| 35  | BB    | 2419 | U    | P-O3'-C3'   | -6.36 | 112.07      | 119.70   |
| 35  | BB    | 2485 | G    | N1-C2-N2    | -6.36 | 110.48      | 116.20   |
| 35  | BB    | 2667 | C    | N3-C4-N4    | 6.36  | 122.45      | 118.00   |
| 1   | AA    | 1021 | A    | C2-N3-C4    | -6.36 | 107.42      | 110.60   |
| 1   | AA    | 1191 | A    | C4-C5-N7    | -6.36 | 107.52      | 110.70   |
| 1   | AA    | 1393 | U    | N3-C2-O2    | 6.36  | 126.65      | 122.20   |
| 30  | B5    | 53   | ARG  | NE-CZ-NH2   | -6.36 | 117.12      | 120.30   |
| 34  | BA    | 58   | A    | C4-C5-C6    | 6.36  | 120.18      | 117.00   |
| 35  | BB    | 8    | C    | C6-N1-C2    | -6.36 | 117.76      | 120.30   |
| 35  | BB    | 658  | U    | C2-N3-C4    | -6.36 | 123.19      | 127.00   |
| 35  | BB    | 799  | G    | C4-N9-C1'   | 6.36  | 134.76      | 126.50   |
| 35  | BB    | 1017 | G    | C4'-C3'-C2' | -6.36 | 96.24       | 102.60   |
| 35  | BB    | 1317 | G    | C4-C5-C6    | 6.36  | 122.61      | 118.80   |
| 35  | BB    | 2401 | U    | O4'-C1'-N1  | 6.36  | 113.28      | 108.20   |
| 35  | BB    | 2418 | A    | C4-C5-C6    | 6.36  | 120.18      | 117.00   |
| 1   | AA    | 177  | G    | O4'-C1'-N9  | 6.35  | 113.28      | 108.20   |
| 1   | AA    | 246  | A    | N7-C8-N9    | -6.35 | 110.62      | 113.80   |
| 1   | AA    | 537  | G    | O4'-C1'-N9  | 6.35  | 113.28      | 108.20   |
| 35  | BB    | 1128 | G    | N1-C6-O6    | 6.35  | 123.71      | 119.90   |
| 35  | BB    | 1457 | U    | C4-C5-C6    | -6.35 | 115.89      | 119.70   |
| 1   | AA    | 631  | C    | O4'-C1'-N1  | 6.35  | 113.28      | 108.20   |
| 35  | BB    | 27   | G    | C2-N3-C4    | -6.35 | 108.72      | 111.90   |
| 35  | BB    | 359  | G    | N3-C2-N2    | 6.35  | 124.35      | 119.90   |
| 35  | BB    | 482  | A    | C6-C5-N7    | -6.35 | 127.85      | 132.30   |
| 35  | BB    | 1040 | A    | N7-C8-N9    | -6.35 | 110.62      | 113.80   |
| 35  | BB    | 1291 | C    | C2-N1-C1'   | 6.35  | 125.79      | 118.80   |
| 35  | BB    | 1965 | C    | C3'-C2'-C1' | -6.35 | 96.42       | 101.50   |
| 35  | BB    | 2060 | A    | C5-C6-N1    | -6.35 | 114.52      | 117.70   |
| 35  | BB    | 2631 | G    | C6-C5-N7    | -6.35 | 126.59      | 130.40   |
| 35  | BB    | 2654 | A    | C1'-O4'-C4' | 6.35  | 114.98      | 109.90   |
| 35  | BB    | 2714 | G    | N7-C8-N9    | -6.35 | 109.92      | 113.10   |
| 1   | AA    | 69   | G    | C5'-C4'-O4' | 6.35  | 116.72      | 109.10   |
| 1   | AA    | 385  | C    | N3-C4-C5    | -6.35 | 119.36      | 121.90   |
| 1   | AA    | 934  | C    | C5-C6-N1    | -6.35 | 117.83      | 121.00   |
| 1   | AA    | 1343 | G    | N1-C2-N3    | -6.35 | 120.09      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 151  | C    | C6-N1-C2    | -6.35 | 117.76      | 120.30   |
| 35  | BB    | 910  | A    | O4'-C1'-N9  | 6.35  | 113.28      | 108.20   |
| 35  | BB    | 1076 | C    | C2-N3-C4    | 6.35  | 123.08      | 119.90   |
| 35  | BB    | 1238 | G    | C1'-O4'-C4' | 6.35  | 114.98      | 109.90   |
| 1   | AA    | 331  | G    | N9-C1'-C2'  | -6.35 | 105.02      | 112.00   |
| 1   | AA    | 566  | G    | C8-N9-C4    | -6.35 | 103.86      | 106.40   |
| 1   | AA    | 914  | A    | C5-C6-N1    | -6.35 | 114.53      | 117.70   |
| 1   | AA    | 1092 | A    | O4'-C1'-N9  | 6.35  | 113.28      | 108.20   |
| 1   | AA    | 1430 | A    | P-O3'-C3'   | -6.35 | 112.08      | 119.70   |
| 35  | BB    | 923  | G    | C5-C6-O6    | -6.35 | 124.79      | 128.60   |
| 35  | BB    | 1036 | G    | C8-N9-C4    | -6.35 | 103.86      | 106.40   |
| 35  | BB    | 1177 | G    | O4'-C1'-N9  | 6.35  | 113.28      | 108.20   |
| 35  | BB    | 2019 | A    | C4-C5-C6    | 6.35  | 120.17      | 117.00   |
| 35  | BB    | 2099 | U    | P-O3'-C3'   | -6.35 | 112.08      | 119.70   |
| 35  | BB    | 2217 | G    | C5-N7-C8    | 6.35  | 107.47      | 104.30   |
| 35  | BB    | 2264 | C    | N3-C4-C5    | -6.35 | 119.36      | 121.90   |
| 35  | BB    | 2737 | G    | N3-C2-N2    | 6.35  | 124.34      | 119.90   |
| 1   | AA    | 293  | G    | C6-N1-C2    | 6.35  | 128.91      | 125.10   |
| 1   | AA    | 1383 | C    | P-O3'-C3'   | -6.35 | 112.08      | 119.70   |
| 16  | AP    | 14   | ARG  | N-CA-CB     | 6.35  | 122.03      | 110.60   |
| 35  | BB    | 818  | G    | N7-C8-N9    | 6.35  | 116.27      | 113.10   |
| 35  | BB    | 941  | A    | C5-C6-N1    | -6.35 | 114.53      | 117.70   |
| 35  | BB    | 1143 | A    | C5-N7-C8    | 6.35  | 107.07      | 103.90   |
| 35  | BB    | 1171 | G    | N3-C4-C5    | -6.35 | 125.43      | 128.60   |
| 35  | BB    | 1332 | G    | N3-C2-N2    | 6.35  | 124.34      | 119.90   |
| 35  | BB    | 1750 | G    | N1-C2-N3    | -6.35 | 120.09      | 123.90   |
| 35  | BB    | 1841 | U    | C5-C4-O4    | 6.35  | 129.71      | 125.90   |
| 35  | BB    | 2061 | G    | C8-N9-C1'   | -6.35 | 118.75      | 127.00   |
| 35  | BB    | 869  | G    | C2-N3-C4    | 6.35  | 115.07      | 111.90   |
| 35  | BB    | 1368 | G    | C6-C5-N7    | -6.35 | 126.59      | 130.40   |
| 35  | BB    | 1388 | G    | O5'-C5'-C4' | -6.35 | 99.64       | 111.70   |
| 35  | BB    | 2126 | A    | OP1-P-OP2   | -6.35 | 110.08      | 119.60   |
| 1   | AA    | 56   | U    | C6-N1-C2    | 6.34  | 124.81      | 121.00   |
| 1   | AA    | 649  | A    | C4-C5-N7    | -6.34 | 107.53      | 110.70   |
| 1   | AA    | 1482 | G    | P-O5'-C5'   | -6.34 | 110.75      | 120.90   |
| 35  | BB    | 135  | U    | N1-C2-N3    | -6.34 | 111.09      | 114.90   |
| 35  | BB    | 783  | A    | C2-N3-C4    | -6.34 | 107.43      | 110.60   |
| 35  | BB    | 993  | G    | C6-N1-C2    | 6.34  | 128.91      | 125.10   |
| 35  | BB    | 1081 | U    | C5'-C4'-O4' | -6.34 | 101.49      | 109.10   |
| 35  | BB    | 1830 | C    | C5-C4-N4    | -6.34 | 115.76      | 120.20   |
| 35  | BB    | 2270 | A    | N7-C8-N9    | 6.34  | 116.97      | 113.80   |
| 35  | BB    | 2515 | C    | C4-C5-C6    | 6.34  | 120.57      | 117.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2535 | G    | C5-C6-O6    | -6.34 | 124.79      | 128.60   |
| 1   | AA    | 1297 | G    | C5-C6-N1    | -6.34 | 108.33      | 111.50   |
| 1   | AA    | 1411 | C    | N3-C4-C5    | -6.34 | 119.36      | 121.90   |
| 1   | AA    | 1486 | G    | C4-C5-C6    | 6.34  | 122.61      | 118.80   |
| 35  | BB    | 244  | A    | N7-C8-N9    | -6.34 | 110.63      | 113.80   |
| 35  | BB    | 1378 | A    | N7-C8-N9    | -6.34 | 110.63      | 113.80   |
| 35  | BB    | 1825 | U    | N3-C2-O2    | 6.34  | 126.64      | 122.20   |
| 1   | AA    | 72   | A    | N1-C6-N6    | 6.34  | 122.41      | 118.60   |
| 1   | AA    | 587  | G    | N1-C6-O6    | 6.34  | 123.70      | 119.90   |
| 1   | AA    | 1014 | A    | O4'-C1'-N9  | 6.34  | 113.27      | 108.20   |
| 1   | AA    | 1223 | C    | C5-C4-N4    | -6.34 | 115.76      | 120.20   |
| 1   | AA    | 1397 | C    | N3-C4-C5    | -6.34 | 119.36      | 121.90   |
| 35  | BB    | 154  | U    | C6-N1-C2    | -6.34 | 117.19      | 121.00   |
| 35  | BB    | 946  | C    | C5-C4-N4    | -6.34 | 115.76      | 120.20   |
| 35  | BB    | 1004 | U    | C4'-C3'-C2' | -6.34 | 96.26       | 102.60   |
| 35  | BB    | 1226 | A    | C8-N9-C4    | -6.34 | 103.26      | 105.80   |
| 35  | BB    | 2004 | G    | C3'-C2'-C1' | 6.34  | 106.57      | 101.50   |
| 35  | BB    | 2167 | U    | P-O3'-C3'   | 6.34  | 127.31      | 119.70   |
| 35  | BB    | 2177 | C    | C2-N3-C4    | 6.34  | 123.07      | 119.90   |
| 35  | BB    | 2773 | C    | C5-C4-N4    | -6.34 | 115.76      | 120.20   |
| 1   | AA    | 503  | C    | N3-C4-N4    | 6.34  | 122.44      | 118.00   |
| 1   | AA    | 959  | A    | C4-C5-C6    | 6.34  | 120.17      | 117.00   |
| 35  | BB    | 88   | G    | N1-C6-O6    | 6.34  | 123.70      | 119.90   |
| 35  | BB    | 420  | C    | N3-C4-N4    | 6.34  | 122.44      | 118.00   |
| 35  | BB    | 472  | A    | N7-C8-N9    | -6.34 | 110.63      | 113.80   |
| 35  | BB    | 1481 | U    | O4'-C1'-N1  | 6.34  | 113.27      | 108.20   |
| 35  | BB    | 2040 | G    | C6-C5-N7    | -6.34 | 126.60      | 130.40   |
| 35  | BB    | 2047 | C    | O4'-C1'-N1  | 6.34  | 113.27      | 108.20   |
| 35  | BB    | 2163 | A    | C4-C5-N7    | -6.34 | 107.53      | 110.70   |
| 1   | AA    | 167  | A    | P-O3'-C3'   | -6.34 | 112.09      | 119.70   |
| 1   | AA    | 386  | C    | N1-C2-O2    | -6.34 | 115.10      | 118.90   |
| 1   | AA    | 845  | A    | O4'-C1'-N9  | 6.34  | 113.27      | 108.20   |
| 1   | AA    | 1497 | G    | C6-N1-C2    | 6.34  | 128.90      | 125.10   |
| 35  | BB    | 73   | A    | C8-N9-C4    | -6.34 | 103.27      | 105.80   |
| 35  | BB    | 1142 | A    | C5'-C4'-O4' | 6.34  | 116.70      | 109.10   |
| 35  | BB    | 1509 | A    | C4-C5-N7    | -6.34 | 107.53      | 110.70   |
| 35  | BB    | 1532 | A    | N3-C4-N9    | 6.34  | 132.47      | 127.40   |
| 35  | BB    | 2798 | U    | N1-C2-N3    | 6.34  | 118.70      | 114.90   |
| 1   | AA    | 943  | U    | C5-C4-O4    | -6.34 | 122.10      | 125.90   |
| 1   | AA    | 1182 | G    | N7-C8-N9    | 6.34  | 116.27      | 113.10   |
| 35  | BB    | 173  | A    | N9-C1'-C2'  | -6.34 | 105.03      | 112.00   |
| 35  | BB    | 578  | G    | N7-C8-N9    | 6.34  | 116.27      | 113.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1252 | G    | N1-C2-N3    | -6.34 | 120.10      | 123.90   |
| 35  | BB    | 1470 | A    | C5-C6-N6    | -6.34 | 118.63      | 123.70   |
| 35  | BB    | 1614 | A    | C6-C5-N7    | -6.34 | 127.86      | 132.30   |
| 35  | BB    | 1701 | A    | C2-N3-C4    | -6.34 | 107.43      | 110.60   |
| 35  | BB    | 1949 | G    | C5-C6-N1    | -6.34 | 108.33      | 111.50   |
| 35  | BB    | 2402 | U    | N3-C4-O4    | 6.34  | 123.83      | 119.40   |
| 35  | BB    | 2502 | G    | N7-C8-N9    | -6.34 | 109.93      | 113.10   |
| 1   | AA    | 98   | A    | C5-N7-C8    | 6.33  | 107.07      | 103.90   |
| 1   | AA    | 139  | A    | O4'-C1'-N9  | 6.33  | 113.27      | 108.20   |
| 1   | AA    | 731  | G    | C5-C6-O6    | -6.33 | 124.80      | 128.60   |
| 35  | BB    | 10   | A    | N7-C8-N9    | -6.33 | 110.63      | 113.80   |
| 35  | BB    | 1393 | A    | OP1-P-OP2   | -6.33 | 110.10      | 119.60   |
| 35  | BB    | 1577 | C    | C5-C4-N4    | -6.33 | 115.77      | 120.20   |
| 35  | BB    | 2139 | U    | O4'-C1'-N1  | 6.33  | 113.27      | 108.20   |
| 35  | BB    | 2472 | G    | O4'-C1'-N9  | 6.33  | 113.27      | 108.20   |
| 35  | BB    | 2813 | A    | C3'-C2'-C1' | 6.33  | 106.57      | 101.50   |
| 35  | BB    | 2889 | C    | N3-C4-C5    | -6.33 | 119.37      | 121.90   |
| 1   | AA    | 668  | G    | C6-C5-N7    | -6.33 | 126.60      | 130.40   |
| 1   | AA    | 1023 | U    | N3-C4-O4    | -6.33 | 114.97      | 119.40   |
| 1   | AA    | 1181 | G    | O4'-C1'-N9  | 6.33  | 113.27      | 108.20   |
| 35  | BB    | 391  | A    | O4'-C1'-N9  | 6.33  | 113.27      | 108.20   |
| 35  | BB    | 773  | U    | O4'-C1'-N1  | 6.33  | 113.27      | 108.20   |
| 46  | BM    | 40   | ARG  | NE-CZ-NH2   | 6.33  | 123.47      | 120.30   |
| 1   | AA    | 227  | G    | O4'-C1'-N9  | 6.33  | 113.27      | 108.20   |
| 1   | AA    | 550  | G    | N1-C2-N3    | -6.33 | 120.10      | 123.90   |
| 1   | AA    | 791  | G    | C5-C6-O6    | -6.33 | 124.80      | 128.60   |
| 3   | AC    | 164  | THR  | CA-CB-CG2   | -6.33 | 103.53      | 112.40   |
| 5   | AE    | 19   | ARG  | NE-CZ-NH2   | -6.33 | 117.13      | 120.30   |
| 35  | BB    | 264  | C    | C6-N1-C2    | -6.33 | 117.77      | 120.30   |
| 35  | BB    | 808  | G    | O4'-C1'-N9  | 6.33  | 113.27      | 108.20   |
| 35  | BB    | 1496 | A    | N7-C8-N9    | 6.33  | 116.97      | 113.80   |
| 35  | BB    | 2530 | A    | O4'-C4'-C3' | -6.33 | 97.67       | 104.00   |
| 1   | AA    | 1099 | G    | C3'-C2'-C1' | 6.33  | 106.56      | 101.50   |
| 34  | BA    | 115  | A    | C8-N9-C4    | -6.33 | 103.27      | 105.80   |
| 35  | BB    | 1298 | C    | N3-C4-C5    | -6.33 | 119.37      | 121.90   |
| 35  | BB    | 1811 | G    | N3-C4-N9    | -6.33 | 122.20      | 126.00   |
| 35  | BB    | 1951 | U    | N1-C2-N3    | -6.33 | 111.10      | 114.90   |
| 35  | BB    | 2556 | C    | O4'-C1'-N1  | 6.33  | 113.26      | 108.20   |
| 37  | BD    | 43   | ASP  | CB-CG-OD1   | -6.33 | 112.60      | 118.30   |
| 1   | AA    | 57   | G    | C8-N9-C4    | -6.33 | 103.87      | 106.40   |
| 1   | AA    | 548  | G    | O4'-C1'-N9  | 6.33  | 113.26      | 108.20   |
| 34  | BA    | 47   | C    | O4'-C1'-N1  | 6.33  | 113.26      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 481  | G    | C3'-C2'-C1' | -6.33 | 96.44       | 101.50   |
| 35  | BB    | 577  | G    | O4'-C1'-N9  | 6.33  | 113.26      | 108.20   |
| 35  | BB    | 707  | G    | N3-C4-N9    | 6.33  | 129.80      | 126.00   |
| 35  | BB    | 805  | G    | C6-C5-N7    | -6.33 | 126.60      | 130.40   |
| 35  | BB    | 1010 | A    | C4-C5-N7    | -6.33 | 107.54      | 110.70   |
| 35  | BB    | 1464 | G    | O4'-C4'-C3' | -6.33 | 97.67       | 104.00   |
| 35  | BB    | 2079 | U    | C5-C6-N1    | 6.33  | 125.86      | 122.70   |
| 35  | BB    | 2149 | U    | C6-N1-C2    | -6.33 | 117.20      | 121.00   |
| 35  | BB    | 2166 | U    | N1-C2-N3    | -6.33 | 111.10      | 114.90   |
| 1   | AA    | 163  | C    | N3-C4-C5    | -6.33 | 119.37      | 121.90   |
| 1   | AA    | 500  | G    | N3-C2-N2    | 6.33  | 124.33      | 119.90   |
| 1   | AA    | 1505 | G    | N3-C4-N9    | 6.33  | 129.80      | 126.00   |
| 22  | AV    | 69   | G    | C5-N7-C8    | 6.33  | 107.46      | 104.30   |
| 35  | BB    | 396  | G    | N3-C2-N2    | 6.33  | 124.33      | 119.90   |
| 35  | BB    | 496  | G    | N9-C4-C5    | -6.33 | 102.87      | 105.40   |
| 35  | BB    | 956  | G    | N3-C2-N2    | 6.33  | 124.33      | 119.90   |
| 35  | BB    | 1166 | G    | N1-C6-O6    | 6.33  | 123.70      | 119.90   |
| 1   | AA    | 334  | C    | N1-C2-O2    | -6.33 | 115.11      | 118.90   |
| 1   | AA    | 440  | C    | N3-C4-N4    | 6.33  | 122.43      | 118.00   |
| 1   | AA    | 734  | G    | N1-C6-O6    | 6.33  | 123.70      | 119.90   |
| 1   | AA    | 771  | G    | N1-C2-N2    | -6.33 | 110.51      | 116.20   |
| 1   | AA    | 1000 | A    | C2-N3-C4    | -6.33 | 107.44      | 110.60   |
| 1   | AA    | 1332 | A    | N1-C2-N3    | 6.33  | 132.46      | 129.30   |
| 1   | AA    | 1422 | G    | C4'-C3'-C2' | -6.33 | 96.28       | 102.60   |
| 35  | BB    | 151  | C    | C4-C5-C6    | 6.33  | 120.56      | 117.40   |
| 35  | BB    | 177  | G    | O4'-C1'-N9  | 6.33  | 113.26      | 108.20   |
| 35  | BB    | 247  | G    | N1-C2-N3    | -6.33 | 120.11      | 123.90   |
| 35  | BB    | 906  | U    | C3'-C2'-C1' | 6.33  | 106.56      | 101.50   |
| 35  | BB    | 1276 | A    | C5'-C4'-O4' | 6.33  | 116.69      | 109.10   |
| 35  | BB    | 1382 | G    | O5'-P-OP1   | -6.33 | 100.01      | 105.70   |
| 35  | BB    | 1555 | G    | O4'-C1'-N9  | 6.33  | 113.26      | 108.20   |
| 35  | BB    | 2353 | G    | N9-C4-C5    | -6.33 | 102.87      | 105.40   |
| 35  | BB    | 2452 | C    | C6-N1-C2    | 6.33  | 122.83      | 120.30   |
| 35  | BB    | 2882 | A    | O4'-C1'-N9  | 6.33  | 113.26      | 108.20   |
| 35  | BB    | 825  | A    | C4'-C3'-C2' | -6.32 | 96.28       | 102.60   |
| 35  | BB    | 1021 | A    | N7-C8-N9    | 6.32  | 116.96      | 113.80   |
| 35  | BB    | 1216 | G    | C5-C6-O6    | -6.32 | 124.81      | 128.60   |
| 35  | BB    | 2094 | A    | P-O5'-C5'   | 6.32  | 131.02      | 120.90   |
| 35  | BB    | 2492 | U    | P-O3'-C3'   | -6.32 | 112.11      | 119.70   |
| 35  | BB    | 2660 | A    | O4'-C1'-N9  | 6.32  | 113.26      | 108.20   |
| 1   | AA    | 1028 | C    | N3-C4-N4    | 6.32  | 122.42      | 118.00   |
| 34  | BA    | 51   | G    | N1-C6-O6    | 6.32  | 123.69      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1928 | A    | O4'-C1'-N9  | 6.32  | 113.26      | 108.20   |
| 35  | BB    | 2397 | G    | N3-C4-C5    | 6.32  | 131.76      | 128.60   |
| 1   | AA    | 35   | G    | C4-C5-N7    | 6.32  | 113.33      | 110.80   |
| 1   | AA    | 1340 | A    | O4'-C4'-C3' | -6.32 | 97.68       | 104.00   |
| 22  | AV    | 5    | A    | C5'-C4'-C3' | 6.32  | 126.11      | 116.00   |
| 30  | B5    | 92   | ALA  | N-CA-CB     | 6.32  | 118.95      | 110.10   |
| 35  | BB    | 677  | A    | N3-C4-C5    | -6.32 | 122.38      | 126.80   |
| 35  | BB    | 1033 | U    | C2-N1-C1'   | -6.32 | 110.11      | 117.70   |
| 35  | BB    | 1524 | G    | N1-C6-O6    | 6.32  | 123.69      | 119.90   |
| 35  | BB    | 1651 | G    | C5-N7-C8    | 6.32  | 107.46      | 104.30   |
| 35  | BB    | 1733 | G    | C8-N9-C4    | -6.32 | 103.87      | 106.40   |
| 35  | BB    | 2626 | C    | O4'-C1'-N1  | 6.32  | 113.26      | 108.20   |
| 1   | AA    | 569  | C    | P-O3'-C3'   | -6.32 | 112.12      | 119.70   |
| 1   | AA    | 726  | C    | N3-C4-C5    | -6.32 | 119.37      | 121.90   |
| 1   | AA    | 502  | A    | O4'-C4'-C3' | -6.32 | 97.68       | 104.00   |
| 1   | AA    | 591  | U    | C4'-C3'-C2' | -6.32 | 96.28       | 102.60   |
| 1   | AA    | 685  | G    | C8-N9-C4    | 6.32  | 108.93      | 106.40   |
| 1   | AA    | 964  | A    | N3-C4-C5    | -6.32 | 122.38      | 126.80   |
| 1   | AA    | 1532 | U    | P-O5'-C5'   | 6.32  | 131.01      | 120.90   |
| 10  | AJ    | 37   | ARG  | N-CA-CB     | 6.32  | 121.97      | 110.60   |
| 35  | BB    | 500  | G    | C5-N7-C8    | 6.32  | 107.46      | 104.30   |
| 35  | BB    | 691  | C    | C2-N3-C4    | 6.32  | 123.06      | 119.90   |
| 35  | BB    | 1371 | G    | C4-C5-N7    | 6.32  | 113.33      | 110.80   |
| 35  | BB    | 1636 | U    | N1-C2-O2    | -6.32 | 118.38      | 122.80   |
| 1   | AA    | 200  | G    | N7-C8-N9    | -6.32 | 109.94      | 113.10   |
| 1   | AA    | 350  | G    | O4'-C1'-N9  | 6.32  | 113.25      | 108.20   |
| 1   | AA    | 1262 | C    | OP1-P-OP2   | -6.32 | 110.13      | 119.60   |
| 1   | AA    | 1349 | A    | C8-N9-C4    | -6.32 | 103.27      | 105.80   |
| 9   | AI    | 83   | THR  | CA-CB-CG2   | -6.32 | 103.56      | 112.40   |
| 22  | AV    | 6    | C    | O4'-C1'-N1  | 6.32  | 113.25      | 108.20   |
| 22  | AV    | 9    | A    | C4-C5-C6    | 6.32  | 120.16      | 117.00   |
| 35  | BB    | 58   | G    | O4'-C1'-N9  | 6.32  | 113.25      | 108.20   |
| 35  | BB    | 221  | A    | N3-C4-C5    | -6.32 | 122.38      | 126.80   |
| 35  | BB    | 1244 | A    | P-O3'-C3'   | -6.32 | 112.12      | 119.70   |
| 35  | BB    | 1441 | G    | N1-C6-O6    | 6.32  | 123.69      | 119.90   |
| 35  | BB    | 1587 | G    | N9-C4-C5    | 6.32  | 107.93      | 105.40   |
| 35  | BB    | 1785 | A    | C8-N9-C4    | 6.32  | 108.33      | 105.80   |
| 35  | BB    | 2101 | A    | C1'-O4'-C4' | 6.32  | 114.95      | 109.90   |
| 35  | BB    | 2172 | U    | P-O3'-C3'   | -6.32 | 112.12      | 119.70   |
| 35  | BB    | 2228 | G    | C6-C5-N7    | -6.32 | 126.61      | 130.40   |
| 35  | BB    | 2545 | G    | C8-N9-C4    | 6.32  | 108.93      | 106.40   |
| 1   | AA    | 324  | G    | C4-C5-N7    | 6.31  | 113.33      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 343  | U    | N3-C4-O4    | 6.31  | 123.82      | 119.40   |
| 1   | AA    | 1495 | U    | O4'-C1'-N1  | 6.31  | 113.25      | 108.20   |
| 35  | BB    | 474  | G    | C6-C5-N7    | -6.31 | 126.61      | 130.40   |
| 35  | BB    | 1009 | A    | C6-N1-C2    | 6.31  | 122.39      | 118.60   |
| 35  | BB    | 1156 | A    | N9-C4-C5    | -6.31 | 103.27      | 105.80   |
| 35  | BB    | 2747 | G    | C5-C6-O6    | -6.31 | 124.81      | 128.60   |
| 1   | AA    | 612  | C    | O4'-C1'-N1  | 6.31  | 113.25      | 108.20   |
| 1   | AA    | 1265 | C    | C4-C5-C6    | 6.31  | 120.56      | 117.40   |
| 35  | BB    | 2633 | G    | C5-C6-O6    | -6.31 | 124.81      | 128.60   |
| 1   | AA    | 101  | A    | O4'-C1'-N9  | 6.31  | 113.25      | 108.20   |
| 1   | AA    | 1061 | G    | O4'-C1'-N9  | 6.31  | 113.25      | 108.20   |
| 34  | BA    | 51   | G    | P-O5'-C5'   | -6.31 | 110.80      | 120.90   |
| 35  | BB    | 360  | U    | C4'-C3'-C2' | -6.31 | 96.29       | 102.60   |
| 35  | BB    | 974  | G    | C5-C6-N1    | -6.31 | 108.34      | 111.50   |
| 35  | BB    | 2253 | G    | N7-C8-N9    | 6.31  | 116.25      | 113.10   |
| 1   | AA    | 411  | A    | C2-N3-C4    | -6.31 | 107.45      | 110.60   |
| 1   | AA    | 778  | G    | C6-N1-C2    | 6.31  | 128.89      | 125.10   |
| 35  | BB    | 75   | G    | O4'-C1'-N9  | 6.31  | 113.25      | 108.20   |
| 35  | BB    | 503  | A    | N3-C4-C5    | -6.31 | 122.38      | 126.80   |
| 35  | BB    | 724  | U    | N1-C2-O2    | -6.31 | 118.38      | 122.80   |
| 35  | BB    | 728  | G    | C2-N3-C4    | 6.31  | 115.06      | 111.90   |
| 35  | BB    | 826  | U    | C4-C5-C6    | 6.31  | 123.49      | 119.70   |
| 35  | BB    | 883  | G    | C2-N3-C4    | -6.31 | 108.75      | 111.90   |
| 35  | BB    | 1725 | U    | N3-C4-O4    | 6.31  | 123.82      | 119.40   |
| 35  | BB    | 1847 | A    | C3'-C2'-C1' | 6.31  | 106.55      | 101.50   |
| 35  | BB    | 2122 | U    | C5-C4-O4    | -6.31 | 122.11      | 125.90   |
| 35  | BB    | 2325 | G    | C4-C5-N7    | 6.31  | 113.32      | 110.80   |
| 35  | BB    | 2344 | U    | N1-C2-N3    | 6.31  | 118.69      | 114.90   |
| 35  | BB    | 2735 | G    | C8-N9-C4    | -6.31 | 103.88      | 106.40   |
| 35  | BB    | 108  | G    | C6-C5-N7    | -6.31 | 126.62      | 130.40   |
| 35  | BB    | 1340 | U    | C4'-C3'-C2' | -6.31 | 96.29       | 102.60   |
| 35  | BB    | 1460 | U    | N3-C4-C5    | -6.31 | 110.82      | 114.60   |
| 35  | BB    | 2045 | C    | O4'-C1'-N1  | 6.31  | 113.25      | 108.20   |
| 35  | BB    | 2095 | A    | N1-C2-N3    | 6.31  | 132.45      | 129.30   |
| 35  | BB    | 2206 | C    | O4'-C1'-N1  | 6.31  | 113.25      | 108.20   |
| 35  | BB    | 2276 | G    | N1-C6-O6    | 6.31  | 123.68      | 119.90   |
| 35  | BB    | 2630 | G    | N3-C2-N2    | 6.31  | 124.32      | 119.90   |
| 35  | BB    | 2895 | G    | N3-C2-N2    | 6.31  | 124.31      | 119.90   |
| 1   | AA    | 1274 | A    | O4'-C1'-N9  | 6.31  | 113.25      | 108.20   |
| 30  | B5    | 130  | VAL  | CA-CB-CG2   | 6.31  | 120.36      | 110.90   |
| 35  | BB    | 805  | G    | C6-N1-C2    | 6.31  | 128.88      | 125.10   |
| 35  | BB    | 1600 | C    | C5'-C4'-C3' | -6.31 | 105.91      | 116.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2212 | A    | N3-C4-C5    | -6.31 | 122.39      | 126.80   |
| 1   | AA    | 226  | G    | O4'-C1'-N9  | 6.30  | 113.24      | 108.20   |
| 1   | AA    | 699  | C    | C6-N1-C2    | 6.30  | 122.82      | 120.30   |
| 1   | AA    | 818  | G    | C5'-C4'-O4' | 6.30  | 116.67      | 109.10   |
| 1   | AA    | 1058 | G    | C5-C6-O6    | -6.30 | 124.82      | 128.60   |
| 35  | BB    | 671  | C    | C4'-C3'-C2' | 6.30  | 108.91      | 102.60   |
| 35  | BB    | 1675 | C    | N1-C2-O2    | 6.30  | 122.68      | 118.90   |
| 35  | BB    | 1804 | C    | N3-C4-N4    | 6.30  | 122.41      | 118.00   |
| 35  | BB    | 1835 | G    | C4-C5-C6    | 6.30  | 122.58      | 118.80   |
| 35  | BB    | 1872 | A    | O4'-C1'-N9  | 6.30  | 113.24      | 108.20   |
| 35  | BB    | 2436 | G    | C6-C5-N7    | -6.30 | 126.62      | 130.40   |
| 35  | BB    | 2635 | A    | C8-N9-C4    | -6.30 | 103.28      | 105.80   |
| 35  | BB    | 2770 | G    | C4-C5-N7    | 6.30  | 113.32      | 110.80   |
| 35  | BB    | 2850 | A    | C8-N9-C4    | 6.30  | 108.32      | 105.80   |
| 46  | BM    | 55   | ARG  | NE-CZ-NH1   | -6.30 | 117.15      | 120.30   |
| 34  | BA    | 76   | G    | C6-N1-C2    | 6.30  | 128.88      | 125.10   |
| 35  | BB    | 472  | A    | C4-C5-C6    | 6.30  | 120.15      | 117.00   |
| 35  | BB    | 1564 | C    | O4'-C1'-N1  | 6.30  | 113.24      | 108.20   |
| 35  | BB    | 2345 | G    | N7-C8-N9    | -6.30 | 109.95      | 113.10   |
| 35  | BB    | 2489 | U    | C4'-C3'-C2' | 6.30  | 108.90      | 102.60   |
| 35  | BB    | 2774 | C    | C6-N1-C2    | 6.30  | 122.82      | 120.30   |
| 36  | BC    | 156  | SER  | N-CA-CB     | 6.30  | 119.95      | 110.50   |
| 1   | AA    | 15   | G    | N3-C4-C5    | -6.30 | 125.45      | 128.60   |
| 1   | AA    | 1449 | C    | C6-N1-C2    | -6.30 | 117.78      | 120.30   |
| 34  | BA    | 15   | A    | N1-C2-N3    | 6.30  | 132.45      | 129.30   |
| 35  | BB    | 493  | G    | O4'-C1'-N9  | 6.30  | 113.24      | 108.20   |
| 35  | BB    | 577  | G    | P-O5'-C5'   | -6.30 | 110.82      | 120.90   |
| 35  | BB    | 863  | A    | C4-C5-C6    | 6.30  | 120.15      | 117.00   |
| 35  | BB    | 908  | C    | N1-C2-O2    | -6.30 | 115.12      | 118.90   |
| 35  | BB    | 989  | G    | C4-C5-C6    | 6.30  | 122.58      | 118.80   |
| 35  | BB    | 1252 | G    | N9-C4-C5    | 6.30  | 107.92      | 105.40   |
| 35  | BB    | 1362 | C    | N1-C2-N3    | -6.30 | 114.79      | 119.20   |
| 35  | BB    | 1753 | G    | C8-N9-C4    | -6.30 | 103.88      | 106.40   |
| 35  | BB    | 2128 | G    | N1-C2-N3    | -6.30 | 120.12      | 123.90   |
| 35  | BB    | 2193 | G    | N1-C2-N3    | -6.30 | 120.12      | 123.90   |
| 1   | AA    | 112  | G    | N3-C4-C5    | -6.30 | 125.45      | 128.60   |
| 1   | AA    | 267  | C    | N3-C4-N4    | 6.30  | 122.41      | 118.00   |
| 1   | AA    | 482  | A    | C4-C5-C6    | 6.30  | 120.15      | 117.00   |
| 1   | AA    | 1113 | C    | O4'-C1'-N1  | 6.30  | 113.24      | 108.20   |
| 1   | AA    | 1458 | G    | O4'-C1'-N9  | 6.30  | 113.24      | 108.20   |
| 1   | AA    | 1511 | G    | C4-C5-N7    | -6.30 | 108.28      | 110.80   |
| 2   | AB    | 158  | ASP  | CB-CG-OD1   | 6.30  | 123.97      | 118.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | AV    | 66   | C    | P-O3'-C3'   | 6.30  | 127.26      | 119.70   |
| 35  | BB    | 245  | G    | C4'-C3'-C2' | -6.30 | 96.30       | 102.60   |
| 35  | BB    | 1060 | U    | C5-C6-N1    | 6.30  | 125.85      | 122.70   |
| 35  | BB    | 1092 | C    | C4'-C3'-C2' | -6.30 | 96.30       | 102.60   |
| 35  | BB    | 1789 | A    | C4-C5-C6    | 6.30  | 120.15      | 117.00   |
| 35  | BB    | 1934 | C    | N3-C4-C5    | -6.30 | 119.38      | 121.90   |
| 35  | BB    | 2597 | G    | N9-C4-C5    | -6.30 | 102.88      | 105.40   |
| 35  | BB    | 2613 | U    | C2-N1-C1'   | -6.30 | 110.14      | 117.70   |
| 1   | AA    | 1148 | U    | C3'-C2'-C1' | 6.30  | 106.54      | 101.50   |
| 35  | BB    | 2624 | G    | C5-C6-O6    | -6.30 | 124.82      | 128.60   |
| 1   | AA    | 1007 | U    | O4'-C1'-N1  | 6.30  | 113.24      | 108.20   |
| 1   | AA    | 1324 | A    | C5-C6-N6    | -6.30 | 118.66      | 123.70   |
| 1   | AA    | 1412 | C    | O4'-C1'-N1  | 6.30  | 113.24      | 108.20   |
| 35  | BB    | 87   | U    | O4'-C1'-N1  | 6.30  | 113.24      | 108.20   |
| 35  | BB    | 388  | G    | N1-C6-O6    | 6.30  | 123.68      | 119.90   |
| 35  | BB    | 597  | G    | C3'-C2'-C1' | 6.30  | 106.54      | 101.50   |
| 35  | BB    | 1228 | G    | N1-C6-O6    | 6.30  | 123.68      | 119.90   |
| 35  | BB    | 1589 | U    | C5-C6-N1    | 6.30  | 125.85      | 122.70   |
| 35  | BB    | 2521 | C    | N3-C4-N4    | 6.30  | 122.41      | 118.00   |
| 52  | BS    | 25   | ARG  | CD-NE-CZ    | -6.30 | 114.78      | 123.60   |
| 35  | BB    | 223  | A    | P-O3'-C3'   | 6.29  | 127.25      | 119.70   |
| 35  | BB    | 427  | U    | N3-C4-O4    | 6.29  | 123.81      | 119.40   |
| 35  | BB    | 1860 | G    | C6-C5-N7    | -6.29 | 126.62      | 130.40   |
| 35  | BB    | 2491 | U    | C3'-C2'-C1' | 6.29  | 106.54      | 101.50   |
| 1   | AA    | 216  | U    | O4'-C1'-N1  | 6.29  | 113.23      | 108.20   |
| 1   | AA    | 349  | A    | N1-C2-N3    | 6.29  | 132.45      | 129.30   |
| 1   | AA    | 723  | U    | C3'-C2'-C1' | 6.29  | 106.53      | 101.50   |
| 1   | AA    | 837  | U    | C3'-C2'-C1' | 6.29  | 106.53      | 101.50   |
| 1   | AA    | 837  | U    | C4'-C3'-C2' | -6.29 | 96.31       | 102.60   |
| 1   | AA    | 914  | A    | P-O3'-C3'   | -6.29 | 112.15      | 119.70   |
| 1   | AA    | 1323 | G    | N1-C6-O6    | 6.29  | 123.68      | 119.90   |
| 22  | AV    | 2    | G    | N1-C2-N3    | -6.29 | 120.12      | 123.90   |
| 35  | BB    | 581  | C    | C5-C4-N4    | -6.29 | 115.80      | 120.20   |
| 35  | BB    | 676  | A    | C6-C5-N7    | -6.29 | 127.89      | 132.30   |
| 35  | BB    | 1448 | G    | C4-C5-N7    | -6.29 | 108.28      | 110.80   |
| 35  | BB    | 2063 | C    | C3'-C2'-C1' | -6.29 | 96.47       | 101.50   |
| 35  | BB    | 2357 | G    | C5'-C4'-O4' | 6.29  | 116.65      | 109.10   |
| 35  | BB    | 2749 | A    | C1'-O4'-C4' | 6.29  | 114.94      | 109.90   |
| 1   | AA    | 240  | G    | O4'-C1'-N9  | 6.29  | 113.23      | 108.20   |
| 1   | AA    | 368  | U    | OP1-P-O3'   | 6.29  | 119.04      | 105.20   |
| 1   | AA    | 547  | A    | C5-C6-N1    | -6.29 | 114.55      | 117.70   |
| 1   | AA    | 1082 | A    | N9-C4-C5    | 6.29  | 108.32      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | BA    | 83   | G    | C4'-C3'-C2' | -6.29 | 96.31       | 102.60   |
| 35  | BB    | 152  | A    | P-O3'-C3'   | -6.29 | 112.15      | 119.70   |
| 35  | BB    | 1083 | U    | C6-N1-C2    | 6.29  | 124.78      | 121.00   |
| 35  | BB    | 1809 | A    | C8-N9-C4    | -6.29 | 103.28      | 105.80   |
| 35  | BB    | 2478 | A    | C6-N1-C2    | 6.29  | 122.38      | 118.60   |
| 35  | BB    | 2485 | G    | C5-C6-N1    | -6.29 | 108.35      | 111.50   |
| 35  | BB    | 2537 | U    | O4'-C4'-C3' | -6.29 | 97.71       | 104.00   |
| 35  | BB    | 2764 | A    | C5-N7-C8    | 6.29  | 107.05      | 103.90   |
| 38  | BE    | 91   | ASP  | CB-CG-OD1   | 6.29  | 123.96      | 118.30   |
| 39  | BF    | 31   | GLU  | N-CA-CB     | 6.29  | 121.93      | 110.60   |
| 35  | BB    | 45   | G    | O4'-C1'-N9  | 6.29  | 113.23      | 108.20   |
| 35  | BB    | 1536 | C    | C6-N1-C1'   | 6.29  | 128.35      | 120.80   |
| 1   | AA    | 445  | G    | C2-N3-C4    | -6.29 | 108.76      | 111.90   |
| 1   | AA    | 465  | A    | P-O3'-C3'   | 6.29  | 127.25      | 119.70   |
| 1   | AA    | 1257 | A    | P-O3'-C3'   | 6.29  | 127.25      | 119.70   |
| 3   | AC    | 153  | SER  | N-CA-CB     | -6.29 | 101.07      | 110.50   |
| 22  | AV    | 39   | G    | C2'-C3'-O3' | 6.29  | 123.76      | 113.70   |
| 35  | BB    | 223  | A    | N1-C6-N6    | 6.29  | 122.37      | 118.60   |
| 35  | BB    | 1178 | C    | C6-N1-C2    | -6.29 | 117.78      | 120.30   |
| 35  | BB    | 1518 | C    | C2-N3-C4    | 6.29  | 123.04      | 119.90   |
| 35  | BB    | 1783 | A    | C5-C6-N1    | -6.29 | 114.56      | 117.70   |
| 35  | BB    | 1794 | A    | N1-C6-N6    | 6.29  | 122.37      | 118.60   |
| 35  | BB    | 1921 | G    | N1-C2-N3    | -6.29 | 120.13      | 123.90   |
| 35  | BB    | 2885 | G    | C1'-O4'-C4' | -6.29 | 104.87      | 109.90   |
| 35  | BB    | 2854 | G    | C2-N3-C4    | 6.29  | 115.04      | 111.90   |
| 1   | AA    | 7    | A    | P-O5'-C5'   | -6.29 | 110.84      | 120.90   |
| 1   | AA    | 71   | A    | C4-N9-C1'   | -6.29 | 114.98      | 126.30   |
| 1   | AA    | 354  | G    | C4-C5-C6    | 6.29  | 122.57      | 118.80   |
| 1   | AA    | 354  | G    | C5'-C4'-O4' | 6.29  | 116.64      | 109.10   |
| 1   | AA    | 966  | G    | C5-N7-C8    | 6.29  | 107.44      | 104.30   |
| 34  | BA    | 46   | A    | O4'-C1'-N9  | 6.29  | 113.23      | 108.20   |
| 35  | BB    | 762  | U    | C5-C6-N1    | 6.29  | 125.84      | 122.70   |
| 35  | BB    | 1363 | C    | N3-C4-C5    | -6.29 | 119.39      | 121.90   |
| 35  | BB    | 1671 | U    | C5-C6-N1    | 6.29  | 125.84      | 122.70   |
| 35  | BB    | 1737 | G    | C5-N7-C8    | -6.29 | 101.16      | 104.30   |
| 35  | BB    | 2628 | C    | P-O3'-C3'   | 6.29  | 127.24      | 119.70   |
| 35  | BB    | 2659 | G    | N9-C4-C5    | 6.29  | 107.91      | 105.40   |
| 35  | BB    | 2802 | G    | N7-C8-N9    | 6.29  | 116.24      | 113.10   |
| 1   | AA    | 666  | G    | O4'-C1'-N9  | 6.28  | 113.23      | 108.20   |
| 1   | AA    | 1053 | G    | C8-N9-C4    | -6.28 | 103.89      | 106.40   |
| 1   | AA    | 1263 | C    | O4'-C1'-N1  | 6.28  | 113.23      | 108.20   |
| 1   | AA    | 1297 | G    | C2-N3-C4    | -6.28 | 108.76      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1451 | U    | N3-C4-C5    | -6.28 | 110.83      | 114.60   |
| 35  | BB    | 838  | C    | O4'-C4'-C3' | -6.28 | 97.72       | 104.00   |
| 35  | BB    | 887  | U    | OP2-P-O3'   | 6.28  | 119.02      | 105.20   |
| 35  | BB    | 1371 | G    | P-O3'-C3'   | 6.28  | 127.24      | 119.70   |
| 35  | BB    | 1532 | A    | C6-C5-N7    | -6.28 | 127.90      | 132.30   |
| 35  | BB    | 1589 | U    | O4'-C4'-C3' | -6.28 | 97.72       | 104.00   |
| 35  | BB    | 2023 | C    | O4'-C1'-N1  | 6.28  | 113.23      | 108.20   |
| 35  | BB    | 2738 | A    | C8-N9-C4    | 6.28  | 108.31      | 105.80   |
| 35  | BB    | 2899 | A    | C4'-C3'-C2' | -6.28 | 96.32       | 102.60   |
| 22  | AV    | 49   | G    | C5-C6-O6    | -6.28 | 124.83      | 128.60   |
| 35  | BB    | 975  | A    | C2-N3-C4    | -6.28 | 107.46      | 110.60   |
| 35  | BB    | 997  | G    | N9-C4-C5    | -6.28 | 102.89      | 105.40   |
| 35  | BB    | 1260 | A    | N7-C8-N9    | 6.28  | 116.94      | 113.80   |
| 35  | BB    | 1421 | G    | N9-C4-C5    | -6.28 | 102.89      | 105.40   |
| 35  | BB    | 2090 | A    | C5-C6-N6    | -6.28 | 118.67      | 123.70   |
| 1   | AA    | 327  | A    | C8-N9-C4    | -6.28 | 103.29      | 105.80   |
| 1   | AA    | 1305 | G    | C6-N1-C2    | 6.28  | 128.87      | 125.10   |
| 35  | BB    | 49   | A    | C5-C6-N6    | -6.28 | 118.67      | 123.70   |
| 35  | BB    | 98   | G    | C6-C5-N7    | -6.28 | 126.63      | 130.40   |
| 35  | BB    | 396  | G    | C5-C6-O6    | -6.28 | 124.83      | 128.60   |
| 35  | BB    | 1067 | A    | N3-C4-C5    | -6.28 | 122.40      | 126.80   |
| 35  | BB    | 1806 | C    | C2-N3-C4    | 6.28  | 123.04      | 119.90   |
| 56  | BY    | 25   | PHE  | CB-CG-CD2   | -6.28 | 116.40      | 120.80   |
| 1   | AA    | 785  | G    | N1-C6-O6    | 6.28  | 123.67      | 119.90   |
| 19  | AS    | 11   | ASP  | N-CA-CB     | 6.28  | 121.90      | 110.60   |
| 35  | BB    | 466  | A    | C5-N7-C8    | 6.28  | 107.04      | 103.90   |
| 35  | BB    | 1422 | G    | C5-C6-N1    | -6.28 | 108.36      | 111.50   |
| 35  | BB    | 1697 | G    | C6-N1-C2    | 6.28  | 128.87      | 125.10   |
| 35  | BB    | 2758 | A    | O4'-C1'-N9  | 6.28  | 113.22      | 108.20   |
| 1   | AA    | 160  | A    | C4-C5-N7    | -6.28 | 107.56      | 110.70   |
| 1   | AA    | 241  | G    | C2-N3-C4    | -6.28 | 108.76      | 111.90   |
| 1   | AA    | 255  | G    | C4-C5-N7    | -6.28 | 108.29      | 110.80   |
| 1   | AA    | 328  | C    | O4'-C1'-C2' | -6.28 | 99.52       | 105.80   |
| 5   | AE    | 74   | ALA  | N-CA-CB     | 6.28  | 118.89      | 110.10   |
| 35  | BB    | 295  | G    | C5-N7-C8    | -6.28 | 101.16      | 104.30   |
| 35  | BB    | 470  | A    | C6-N1-C2    | -6.28 | 114.83      | 118.60   |
| 35  | BB    | 682  | G    | P-O3'-C3'   | -6.28 | 112.17      | 119.70   |
| 35  | BB    | 940  | G    | N7-C8-N9    | 6.28  | 116.24      | 113.10   |
| 35  | BB    | 1114 | C    | C4-C5-C6    | 6.28  | 120.54      | 117.40   |
| 35  | BB    | 1214 | A    | N9-C4-C5    | -6.28 | 103.29      | 105.80   |
| 35  | BB    | 1247 | A    | O4'-C1'-N9  | 6.28  | 113.22      | 108.20   |
| 35  | BB    | 2413 | G    | N3-C4-N9    | 6.28  | 129.77      | 126.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 552  | U    | N3-C4-C5    | -6.28 | 110.83      | 114.60   |
| 1   | AA    | 702  | A    | O4'-C1'-N9  | 6.28  | 113.22      | 108.20   |
| 1   | AA    | 1158 | C    | N3-C4-N4    | 6.28  | 122.39      | 118.00   |
| 1   | AA    | 1171 | A    | C5-C6-N1    | -6.28 | 114.56      | 117.70   |
| 1   | AA    | 1341 | U    | N3-C2-O2    | 6.28  | 126.59      | 122.20   |
| 1   | AA    | 1385 | G    | C5-C6-O6    | -6.28 | 124.83      | 128.60   |
| 1   | AA    | 1434 | A    | C6-C5-N7    | -6.28 | 127.91      | 132.30   |
| 35  | BB    | 908  | C    | N3-C4-C5    | -6.28 | 119.39      | 121.90   |
| 35  | BB    | 1206 | G    | C6-N1-C2    | 6.28  | 128.87      | 125.10   |
| 35  | BB    | 1362 | C    | N3-C2-O2    | 6.28  | 126.29      | 121.90   |
| 35  | BB    | 1644 | C    | C5-C6-N1    | 6.28  | 124.14      | 121.00   |
| 35  | BB    | 2027 | G    | N1-C2-N3    | -6.28 | 120.14      | 123.90   |
| 35  | BB    | 2415 | G    | O4'-C1'-N9  | 6.28  | 113.22      | 108.20   |
| 50  | BQ    | 75   | TYR  | CZ-CE2-CD2  | -6.28 | 114.15      | 119.80   |
| 1   | AA    | 171  | A    | C4-C5-C6    | 6.27  | 120.14      | 117.00   |
| 1   | AA    | 389  | A    | N7-C8-N9    | 6.27  | 116.94      | 113.80   |
| 1   | AA    | 623  | C    | C4-C5-C6    | 6.27  | 120.54      | 117.40   |
| 1   | AA    | 1394 | A    | N1-C2-N3    | 6.27  | 132.44      | 129.30   |
| 16  | AP    | 23   | ASP  | CB-CG-OD1   | -6.27 | 112.65      | 118.30   |
| 34  | BA    | 7    | G    | C5-C6-O6    | -6.27 | 124.83      | 128.60   |
| 35  | BB    | 1969 | A    | O3'-P-O5'   | -6.27 | 92.08       | 104.00   |
| 35  | BB    | 2163 | A    | C2-N3-C4    | 6.27  | 113.74      | 110.60   |
| 35  | BB    | 2556 | C    | C5-C4-N4    | -6.27 | 115.81      | 120.20   |
| 1   | AA    | 1386 | G    | C2-N3-C4    | 6.27  | 115.04      | 111.90   |
| 1   | AA    | 1410 | A    | C8-N9-C4    | -6.27 | 103.29      | 105.80   |
| 1   | AA    | 1519 | A    | C5-N7-C8    | -6.27 | 100.76      | 103.90   |
| 11  | AK    | 104  | PHE  | CB-CG-CD2   | 6.27  | 125.19      | 120.80   |
| 35  | BB    | 901  | C    | OP1-P-OP2   | -6.27 | 110.19      | 119.60   |
| 35  | BB    | 955  | U    | C5-C6-N1    | 6.27  | 125.84      | 122.70   |
| 35  | BB    | 1144 | A    | C6-C5-N7    | -6.27 | 127.91      | 132.30   |
| 35  | BB    | 1267 | U    | N3-C4-C5    | -6.27 | 110.84      | 114.60   |
| 35  | BB    | 1281 | G    | N9-C4-C5    | 6.27  | 107.91      | 105.40   |
| 35  | BB    | 2439 | A    | N7-C8-N9    | 6.27  | 116.94      | 113.80   |
| 35  | BB    | 2674 | G    | C5-C6-O6    | -6.27 | 124.84      | 128.60   |
| 35  | BB    | 2765 | A    | C2-N3-C4    | -6.27 | 107.46      | 110.60   |
| 35  | BB    | 2799 | A    | C5-C6-N6    | -6.27 | 118.68      | 123.70   |
| 1   | AA    | 1145 | A    | C8-N9-C4    | -6.27 | 103.29      | 105.80   |
| 1   | AA    | 1191 | A    | C1'-O4'-C4' | 6.27  | 114.92      | 109.90   |
| 35  | BB    | 141  | G    | C6-C5-N7    | -6.27 | 126.64      | 130.40   |
| 1   | AA    | 357  | G    | C5'-C4'-C3' | -6.27 | 105.97      | 116.00   |
| 1   | AA    | 484  | G    | C8-N9-C1'   | -6.27 | 118.85      | 127.00   |
| 1   | AA    | 1083 | U    | C4'-C3'-C2' | 6.27  | 108.87      | 102.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1410 | A    | C1'-O4'-C4' | -6.27 | 104.89      | 109.90   |
| 8   | AH    | 114  | ALA  | N-CA-CB     | 6.27  | 118.88      | 110.10   |
| 35  | BB    | 309  | A    | C6-N1-C2    | -6.27 | 114.84      | 118.60   |
| 35  | BB    | 519  | U    | C5-C4-O4    | -6.27 | 122.14      | 125.90   |
| 35  | BB    | 632  | A    | N1-C6-N6    | 6.27  | 122.36      | 118.60   |
| 35  | BB    | 1148 | U    | N3-C4-C5    | -6.27 | 110.84      | 114.60   |
| 35  | BB    | 1277 | G    | C6-C5-N7    | -6.27 | 126.64      | 130.40   |
| 35  | BB    | 1924 | C    | C4-C5-C6    | -6.27 | 114.27      | 117.40   |
| 35  | BB    | 1927 | A    | C4-C5-C6    | 6.27  | 120.14      | 117.00   |
| 35  | BB    | 2388 | A    | N1-C2-N3    | 6.27  | 132.44      | 129.30   |
| 35  | BB    | 2727 | A    | N9-C4-C5    | 6.27  | 108.31      | 105.80   |
| 1   | AA    | 443  | C    | N3-C4-C5    | -6.27 | 119.39      | 121.90   |
| 1   | AA    | 645  | G    | N7-C8-N9    | -6.27 | 109.97      | 113.10   |
| 1   | AA    | 1505 | G    | O4'-C1'-C2' | 6.27  | 113.24      | 107.60   |
| 4   | AD    | 3    | TYR  | CD1-CE1-CZ  | -6.27 | 114.16      | 119.80   |
| 22  | AV    | 26   | A    | C4-C5-C6    | 6.27  | 120.13      | 117.00   |
| 35  | BB    | 427  | U    | C5-C4-O4    | -6.27 | 122.14      | 125.90   |
| 35  | BB    | 508  | A    | N3-C4-C5    | -6.27 | 122.41      | 126.80   |
| 35  | BB    | 535  | G    | N3-C2-N2    | 6.27  | 124.29      | 119.90   |
| 35  | BB    | 553  | G    | C2-N3-C4    | -6.27 | 108.77      | 111.90   |
| 35  | BB    | 1241 | A    | C5-N7-C8    | 6.27  | 107.03      | 103.90   |
| 35  | BB    | 1695 | G    | C4-C5-C6    | 6.27  | 122.56      | 118.80   |
| 35  | BB    | 2043 | C    | N1-C2-N3    | 6.27  | 123.59      | 119.20   |
| 35  | BB    | 2316 | G    | C5-C6-O6    | -6.27 | 124.84      | 128.60   |
| 35  | BB    | 2861 | U    | N1-C2-N3    | 6.27  | 118.66      | 114.90   |
| 35  | BB    | 108  | G    | N1-C2-N3    | -6.27 | 120.14      | 123.90   |
| 35  | BB    | 269  | C    | C2-N3-C4    | 6.27  | 123.03      | 119.90   |
| 35  | BB    | 460  | A    | N7-C8-N9    | -6.27 | 110.67      | 113.80   |
| 35  | BB    | 628  | G    | N9-C1'-C2'  | -6.27 | 105.11      | 112.00   |
| 35  | BB    | 1558 | C    | C1'-O4'-C4' | 6.27  | 114.91      | 109.90   |
| 35  | BB    | 1703 | G    | N9-C4-C5    | 6.27  | 107.91      | 105.40   |
| 1   | AA    | 341  | C    | P-O3'-C3'   | -6.26 | 112.18      | 119.70   |
| 1   | AA    | 474  | G    | C8-N9-C4    | 6.26  | 108.91      | 106.40   |
| 1   | AA    | 619  | U    | N3-C2-O2    | 6.26  | 126.59      | 122.20   |
| 1   | AA    | 1366 | C    | N3-C4-N4    | 6.26  | 122.39      | 118.00   |
| 1   | AA    | 1515 | G    | C8-N9-C1'   | 6.26  | 135.14      | 127.00   |
| 34  | BA    | 38   | C    | N3-C4-N4    | 6.26  | 122.39      | 118.00   |
| 35  | BB    | 1067 | A    | C5-C6-N6    | -6.26 | 118.69      | 123.70   |
| 35  | BB    | 1184 | U    | N1-C2-O2    | 6.26  | 127.19      | 122.80   |
| 35  | BB    | 2193 | G    | C4-C5-N7    | -6.26 | 108.29      | 110.80   |
| 41  | BH    | 31   | VAL  | N-CA-C      | -6.26 | 94.08       | 111.00   |
| 1   | AA    | 606  | G    | N9-C4-C5    | -6.26 | 102.89      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 507  | A    | N1-C2-N3    | -6.26 | 126.17      | 129.30   |
| 1   | AA    | 413  | G    | N1-C6-O6    | 6.26  | 123.66      | 119.90   |
| 1   | AA    | 851  | G    | C6-C5-N7    | -6.26 | 126.64      | 130.40   |
| 1   | AA    | 1038 | C    | N3-C4-N4    | 6.26  | 122.38      | 118.00   |
| 1   | AA    | 1155 | A    | O4'-C1'-N9  | 6.26  | 113.21      | 108.20   |
| 1   | AA    | 1346 | A    | C2-N3-C4    | -6.26 | 107.47      | 110.60   |
| 4   | AD    | 19   | PHE  | CB-CG-CD2   | 6.26  | 125.18      | 120.80   |
| 22  | AV    | 70   | C    | P-O5'-C5'   | 6.26  | 130.92      | 120.90   |
| 35  | BB    | 356  | G    | C8-N9-C4    | -6.26 | 103.89      | 106.40   |
| 35  | BB    | 648  | G    | N3-C2-N2    | 6.26  | 124.28      | 119.90   |
| 35  | BB    | 778  | G    | C5-N7-C8    | -6.26 | 101.17      | 104.30   |
| 35  | BB    | 843  | G    | C8-N9-C4    | 6.26  | 108.90      | 106.40   |
| 35  | BB    | 1140 | C    | O4'-C4'-C3' | -6.26 | 97.74       | 104.00   |
| 35  | BB    | 1799 | G    | O4'-C1'-N9  | 6.26  | 113.21      | 108.20   |
| 35  | BB    | 2439 | A    | C4-C5-C6    | 6.26  | 120.13      | 117.00   |
| 1   | AA    | 72   | A    | C8-N9-C4    | -6.26 | 103.30      | 105.80   |
| 1   | AA    | 162  | A    | N7-C8-N9    | -6.26 | 110.67      | 113.80   |
| 1   | AA    | 780  | A    | C5-N7-C8    | 6.26  | 107.03      | 103.90   |
| 14  | AN    | 67   | GLY  | C-N-CA      | 6.26  | 137.35      | 121.70   |
| 19  | AS    | 12   | LEU  | CB-CG-CD2   | 6.26  | 121.64      | 111.00   |
| 35  | BB    | 12   | U    | C5-C4-O4    | -6.26 | 122.14      | 125.90   |
| 35  | BB    | 195  | A    | C4'-C3'-C2' | -6.26 | 96.34       | 102.60   |
| 35  | BB    | 455  | C    | C3'-C2'-C1' | 6.26  | 106.51      | 101.50   |
| 35  | BB    | 532  | A    | C4-C5-C6    | 6.26  | 120.13      | 117.00   |
| 35  | BB    | 756  | A    | C1'-O4'-C4' | 6.26  | 114.91      | 109.90   |
| 35  | BB    | 1711 | A    | C5-C6-N6    | -6.26 | 118.69      | 123.70   |
| 35  | BB    | 2592 | G    | C1'-O4'-C4' | 6.26  | 114.91      | 109.90   |
| 52  | BS    | 110  | ARG  | NE-CZ-NH1   | 6.26  | 123.43      | 120.30   |
| 1   | AA    | 802  | A    | C8-N9-C4    | -6.26 | 103.30      | 105.80   |
| 35  | BB    | 248  | G    | N3-C2-N2    | 6.26  | 124.28      | 119.90   |
| 35  | BB    | 790  | U    | N3-C4-O4    | 6.26  | 123.78      | 119.40   |
| 35  | BB    | 846  | U    | C4'-C3'-C2' | -6.26 | 96.34       | 102.60   |
| 35  | BB    | 1952 | A    | N9-C4-C5    | -6.26 | 103.30      | 105.80   |
| 1   | AA    | 175  | C    | C5-C6-N1    | 6.26  | 124.13      | 121.00   |
| 1   | AA    | 251  | G    | O4'-C1'-N9  | 6.26  | 113.20      | 108.20   |
| 34  | BA    | 42   | C    | C4-C5-C6    | 6.26  | 120.53      | 117.40   |
| 35  | BB    | 267  | C    | N3-C4-N4    | 6.26  | 122.38      | 118.00   |
| 35  | BB    | 656  | G    | C3'-C2'-C1' | 6.26  | 106.50      | 101.50   |
| 35  | BB    | 914  | G    | C3'-C2'-C1' | -6.26 | 96.49       | 101.50   |
| 35  | BB    | 1868 | C    | C6-N1-C2    | 6.26  | 122.80      | 120.30   |
| 35  | BB    | 1944 | U    | C4'-C3'-C2' | 6.26  | 108.86      | 102.60   |
| 35  | BB    | 2076 | U    | C2-N1-C1'   | 6.26  | 125.21      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2670 | A    | C5-C6-N6    | -6.26 | 118.69      | 123.70   |
| 1   | AA    | 1001 | C    | C6-N1-C2    | -6.25 | 117.80      | 120.30   |
| 1   | AA    | 1267 | C    | N3-C4-N4    | 6.25  | 122.38      | 118.00   |
| 1   | AA    | 1377 | A    | C4-C5-C6    | 6.25  | 120.13      | 117.00   |
| 35  | BB    | 91   | A    | N7-C8-N9    | -6.25 | 110.67      | 113.80   |
| 35  | BB    | 1424 | G    | C8-N9-C4    | -6.25 | 103.90      | 106.40   |
| 35  | BB    | 1495 | A    | O4'-C1'-N9  | 6.25  | 113.20      | 108.20   |
| 35  | BB    | 2290 | G    | O4'-C1'-N9  | 6.25  | 113.20      | 108.20   |
| 38  | BE    | 49   | ARG  | NE-CZ-NH1   | -6.25 | 117.17      | 120.30   |
| 1   | AA    | 1142 | G    | C8-N9-C4    | -6.25 | 103.90      | 106.40   |
| 1   | AA    | 1143 | G    | N1-C6-O6    | 6.25  | 123.65      | 119.90   |
| 35  | BB    | 81   | G    | N7-C8-N9    | 6.25  | 116.23      | 113.10   |
| 35  | BB    | 139  | U    | N3-C2-O2    | 6.25  | 126.58      | 122.20   |
| 35  | BB    | 328  | U    | C2-N3-C4    | 6.25  | 130.75      | 127.00   |
| 35  | BB    | 510  | C    | C6-N1-C1'   | -6.25 | 113.30      | 120.80   |
| 35  | BB    | 660  | C    | N3-C4-N4    | 6.25  | 122.38      | 118.00   |
| 35  | BB    | 1312 | U    | O4'-C1'-N1  | 6.25  | 113.20      | 108.20   |
| 35  | BB    | 1744 | A    | C5-N7-C8    | 6.25  | 107.03      | 103.90   |
| 35  | BB    | 2020 | A    | P-O5'-C5'   | 6.25  | 130.90      | 120.90   |
| 35  | BB    | 2819 | G    | N1-C6-O6    | 6.25  | 123.65      | 119.90   |
| 1   | AA    | 195  | A    | C5-C6-N6    | -6.25 | 118.70      | 123.70   |
| 1   | AA    | 879  | C    | N3-C4-C5    | -6.25 | 119.40      | 121.90   |
| 1   | AA    | 1377 | A    | N3-C4-C5    | -6.25 | 122.42      | 126.80   |
| 4   | AD    | 36   | ALA  | N-CA-CB     | 6.25  | 118.85      | 110.10   |
| 35  | BB    | 1    | G    | O4'-C1'-N9  | 6.25  | 113.20      | 108.20   |
| 35  | BB    | 85   | G    | C5-C6-N1    | -6.25 | 108.37      | 111.50   |
| 35  | BB    | 868  | U    | N3-C4-C5    | -6.25 | 110.85      | 114.60   |
| 35  | BB    | 952  | G    | OP1-P-OP2   | -6.25 | 110.22      | 119.60   |
| 35  | BB    | 1276 | A    | C6-C5-N7    | -6.25 | 127.92      | 132.30   |
| 35  | BB    | 1826 | G    | O4'-C1'-N9  | 6.25  | 113.20      | 108.20   |
| 35  | BB    | 1993 | U    | O5'-P-OP2   | 6.25  | 118.20      | 110.70   |
| 35  | BB    | 2656 | U    | C1'-O4'-C4' | 6.25  | 114.90      | 109.90   |
| 1   | AA    | 352  | C    | N1-C2-N3    | -6.25 | 114.83      | 119.20   |
| 1   | AA    | 443  | C    | P-O3'-C3'   | -6.25 | 112.20      | 119.70   |
| 1   | AA    | 456  | A    | C5-C6-N6    | -6.25 | 118.70      | 123.70   |
| 1   | AA    | 657  | U    | N3-C4-C5    | -6.25 | 110.85      | 114.60   |
| 35  | BB    | 781  | A    | C6-N1-C2    | 6.25  | 122.35      | 118.60   |
| 35  | BB    | 893  | C    | C5'-C4'-O4' | 6.25  | 116.60      | 109.10   |
| 35  | BB    | 1537 | G    | N9-C1'-C2'  | -6.25 | 105.12      | 112.00   |
| 35  | BB    | 2776 | A    | C6-N1-C2    | 6.25  | 122.35      | 118.60   |
| 1   | AA    | 136  | C    | C3'-C2'-C1' | 6.25  | 106.50      | 101.50   |
| 1   | AA    | 183  | C    | N3-C2-O2    | 6.25  | 126.27      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 626  | G    | N3-C2-N2    | 6.25  | 124.27      | 119.90   |
| 1   | AA    | 1129 | C    | C5-C6-N1    | 6.25  | 124.12      | 121.00   |
| 1   | AA    | 1308 | U    | O4'-C1'-N1  | 6.25  | 113.20      | 108.20   |
| 1   | AA    | 1461 | G    | N9-C4-C5    | -6.25 | 102.90      | 105.40   |
| 11  | AK    | 126  | ARG  | NE-CZ-NH2   | -6.25 | 117.17      | 120.30   |
| 34  | BA    | 99   | A    | C4-C5-N7    | -6.25 | 107.58      | 110.70   |
| 35  | BB    | 554  | U    | C1'-O4'-C4' | 6.25  | 114.90      | 109.90   |
| 35  | BB    | 649  | G    | C1'-O4'-C4' | -6.25 | 104.90      | 109.90   |
| 35  | BB    | 784  | G    | C4-C5-C6    | 6.25  | 122.55      | 118.80   |
| 35  | BB    | 1460 | U    | C6-N1-C2    | 6.25  | 124.75      | 121.00   |
| 35  | BB    | 1901 | A    | O4'-C1'-N9  | 6.25  | 113.20      | 108.20   |
| 35  | BB    | 2134 | A    | O4'-C4'-C3' | -6.25 | 97.75       | 104.00   |
| 35  | BB    | 2207 | C    | C5-C4-N4    | 6.25  | 124.57      | 120.20   |
| 35  | BB    | 2207 | C    | C2-N1-C1'   | 6.25  | 125.67      | 118.80   |
| 1   | AA    | 41   | G    | C5-C6-O6    | -6.25 | 124.85      | 128.60   |
| 1   | AA    | 50   | A    | C5-C6-N6    | -6.25 | 118.70      | 123.70   |
| 1   | AA    | 158  | G    | C5-C6-O6    | 6.25  | 132.35      | 128.60   |
| 1   | AA    | 297  | G    | C4-N9-C1'   | -6.25 | 118.38      | 126.50   |
| 1   | AA    | 322  | C    | N3-C4-C5    | -6.25 | 119.40      | 121.90   |
| 1   | AA    | 357  | G    | C2-N3-C4    | 6.25  | 115.02      | 111.90   |
| 1   | AA    | 664  | G    | O4'-C1'-N9  | 6.25  | 113.20      | 108.20   |
| 1   | AA    | 862  | C    | C4-C5-C6    | 6.25  | 120.52      | 117.40   |
| 1   | AA    | 902  | G    | C2-N3-C4    | 6.25  | 115.02      | 111.90   |
| 1   | AA    | 920  | U    | N1-C2-O2    | -6.25 | 118.43      | 122.80   |
| 35  | BB    | 59   | U    | C2-N3-C4    | 6.25  | 130.75      | 127.00   |
| 35  | BB    | 377  | G    | C4-C5-C6    | 6.25  | 122.55      | 118.80   |
| 35  | BB    | 605  | G    | C6-N1-C2    | 6.25  | 128.85      | 125.10   |
| 35  | BB    | 1363 | C    | C5'-C4'-C3' | -6.25 | 106.01      | 116.00   |
| 35  | BB    | 2800 | A    | C5-C6-N1    | -6.25 | 114.58      | 117.70   |
| 1   | AA    | 76   | G    | C6-C5-N7    | -6.25 | 126.65      | 130.40   |
| 1   | AA    | 285  | C    | C2-N1-C1'   | 6.25  | 125.67      | 118.80   |
| 1   | AA    | 763  | G    | C4'-C3'-C2' | -6.25 | 96.36       | 102.60   |
| 1   | AA    | 949  | A    | N9-C4-C5    | 6.25  | 108.30      | 105.80   |
| 35  | BB    | 724  | U    | N3-C2-O2    | 6.25  | 126.57      | 122.20   |
| 35  | BB    | 1465 | G    | P-O5'-C5'   | 6.25  | 130.89      | 120.90   |
| 35  | BB    | 1866 | A    | C8-N9-C4    | -6.25 | 103.30      | 105.80   |
| 35  | BB    | 1963 | U    | C1'-O4'-C4' | 6.25  | 114.90      | 109.90   |
| 35  | BB    | 2484 | G    | P-O3'-C3'   | -6.25 | 112.21      | 119.70   |
| 1   | AA    | 1117 | A    | C2-N3-C4    | -6.24 | 107.48      | 110.60   |
| 34  | BA    | 30   | C    | C2-N1-C1'   | 6.24  | 125.67      | 118.80   |
| 35  | BB    | 1016 | G    | C5-C6-O6    | -6.24 | 124.85      | 128.60   |
| 35  | BB    | 1089 | A    | N9-C1'-C2'  | -6.24 | 105.13      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1404 | C    | N3-C4-C5    | -6.24 | 119.40      | 121.90   |
| 35  | BB    | 1552 | A    | C5'-C4'-O4' | -6.24 | 101.61      | 109.10   |
| 35  | BB    | 1661 | G    | C5-N7-C8    | 6.24  | 107.42      | 104.30   |
| 35  | BB    | 2674 | G    | C5-C6-N1    | -6.24 | 108.38      | 111.50   |
| 1   | AA    | 21   | G    | N9-C4-C5    | 6.24  | 107.90      | 105.40   |
| 1   | AA    | 207  | C    | C6-N1-C2    | -6.24 | 117.80      | 120.30   |
| 1   | AA    | 693  | G    | N1-C2-N2    | -6.24 | 110.58      | 116.20   |
| 1   | AA    | 881  | G    | N3-C4-N9    | -6.24 | 122.25      | 126.00   |
| 1   | AA    | 985  | C    | C4-C5-C6    | 6.24  | 120.52      | 117.40   |
| 1   | AA    | 1444 | U    | N1-C2-N3    | -6.24 | 111.16      | 114.90   |
| 35  | BB    | 551  | G    | C2-N3-C4    | 6.24  | 115.02      | 111.90   |
| 35  | BB    | 801  | G    | C5-C6-O6    | -6.24 | 124.86      | 128.60   |
| 35  | BB    | 1674 | G    | C8-N9-C4    | -6.24 | 103.90      | 106.40   |
| 35  | BB    | 1722 | A    | C8-N9-C4    | -6.24 | 103.30      | 105.80   |
| 35  | BB    | 1822 | C    | C2-N3-C4    | 6.24  | 123.02      | 119.90   |
| 1   | AA    | 1126 | U    | C4-C5-C6    | 6.24  | 123.44      | 119.70   |
| 4   | AD    | 118  | SER  | N-CA-CB     | 6.24  | 119.86      | 110.50   |
| 35  | BB    | 367  | G    | C4-C5-C6    | 6.24  | 122.55      | 118.80   |
| 35  | BB    | 554  | U    | C3'-C2'-C1' | 6.24  | 106.49      | 101.50   |
| 35  | BB    | 684  | G    | N1-C6-O6    | 6.24  | 123.64      | 119.90   |
| 35  | BB    | 1419 | A    | N7-C8-N9    | 6.24  | 116.92      | 113.80   |
| 35  | BB    | 2277 | G    | C6-C5-N7    | -6.24 | 126.66      | 130.40   |
| 35  | BB    | 2365 | G    | N3-C2-N2    | 6.24  | 124.27      | 119.90   |
| 35  | BB    | 2867 | G    | N1-C6-O6    | 6.24  | 123.64      | 119.90   |
| 1   | AA    | 263  | A    | C5-N7-C8    | -6.24 | 100.78      | 103.90   |
| 1   | AA    | 663  | A    | N1-C2-N3    | 6.24  | 132.42      | 129.30   |
| 35  | BB    | 240  | C    | N3-C4-C5    | -6.24 | 119.40      | 121.90   |
| 35  | BB    | 244  | A    | N1-C6-N6    | 6.24  | 122.34      | 118.60   |
| 35  | BB    | 1368 | G    | C3'-C2'-C1' | 6.24  | 106.49      | 101.50   |
| 35  | BB    | 2087 | G    | N1-C2-N3    | -6.24 | 120.16      | 123.90   |
| 35  | BB    | 2317 | A    | C6-C5-N7    | -6.24 | 127.93      | 132.30   |
| 35  | BB    | 2600 | A    | C2-N3-C4    | -6.24 | 107.48      | 110.60   |
| 35  | BB    | 2802 | G    | C6-C5-N7    | -6.24 | 126.66      | 130.40   |
| 44  | BK    | 30   | ARG  | NE-CZ-NH1   | 6.24  | 123.42      | 120.30   |
| 1   | AA    | 323  | U    | O4'-C1'-N1  | 6.24  | 113.19      | 108.20   |
| 1   | AA    | 474  | G    | N1-C2-N3    | -6.24 | 120.16      | 123.90   |
| 1   | AA    | 992  | U    | C5'-C4'-O4' | 6.24  | 116.58      | 109.10   |
| 1   | AA    | 1086 | U    | C6-N1-C2    | -6.24 | 117.26      | 121.00   |
| 1   | AA    | 1365 | G    | C2-N3-C4    | 6.24  | 115.02      | 111.90   |
| 35  | BB    | 96   | C    | C6-N1-C2    | 6.24  | 122.80      | 120.30   |
| 35  | BB    | 155  | A    | N3-C4-C5    | -6.24 | 122.43      | 126.80   |
| 35  | BB    | 1078 | U    | P-O3'-C3'   | -6.24 | 112.22      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2085 | U    | C1'-O4'-C4' | 6.24  | 114.89      | 109.90   |
| 35  | BB    | 2824 | C    | C6-N1-C2    | -6.24 | 117.81      | 120.30   |
| 1   | AA    | 100  | G    | C6-C5-N7    | -6.24 | 126.66      | 130.40   |
| 1   | AA    | 238  | A    | C4-C5-C6    | -6.24 | 113.88      | 117.00   |
| 1   | AA    | 867  | G    | C6-C5-N7    | -6.24 | 126.66      | 130.40   |
| 1   | AA    | 1290 | G    | C4-C5-C6    | 6.24  | 122.54      | 118.80   |
| 34  | BA    | 42   | C    | O4'-C1'-N1  | 6.24  | 113.19      | 108.20   |
| 35  | BB    | 830  | G    | O4'-C1'-N9  | 6.24  | 113.19      | 108.20   |
| 35  | BB    | 1666 | G    | O4'-C1'-N9  | 6.24  | 113.19      | 108.20   |
| 35  | BB    | 1836 | C    | C2-N3-C4    | 6.24  | 123.02      | 119.90   |
| 35  | BB    | 2008 | C    | N3-C4-C5    | -6.24 | 119.41      | 121.90   |
| 35  | BB    | 2861 | U    | P-O5'-C5'   | 6.24  | 130.88      | 120.90   |
| 1   | AA    | 475  | C    | C4-C5-C6    | 6.23  | 120.52      | 117.40   |
| 1   | AA    | 1408 | A    | C2-N3-C4    | -6.23 | 107.48      | 110.60   |
| 35  | BB    | 680  | C    | N1-C2-O2    | -6.23 | 115.16      | 118.90   |
| 35  | BB    | 981  | A    | N3-C4-N9    | 6.23  | 132.39      | 127.40   |
| 35  | BB    | 1008 | A    | N1-C2-N3    | 6.23  | 132.42      | 129.30   |
| 35  | BB    | 1025 | G    | C4-C5-C6    | 6.23  | 122.54      | 118.80   |
| 35  | BB    | 2532 | G    | C8-N9-C4    | -6.23 | 103.91      | 106.40   |
| 35  | BB    | 2573 | C    | O4'-C1'-N1  | 6.23  | 113.19      | 108.20   |
| 51  | BR    | 1    | MET  | CG-SD-CE    | 6.23  | 110.17      | 100.20   |
| 1   | AA    | 573  | A    | N1-C6-N6    | 6.23  | 122.34      | 118.60   |
| 1   | AA    | 639  | G    | C2-N3-C4    | 6.23  | 115.02      | 111.90   |
| 1   | AA    | 1020 | G    | C8-N9-C4    | -6.23 | 103.91      | 106.40   |
| 1   | AA    | 1046 | A    | O4'-C1'-N9  | 6.23  | 113.19      | 108.20   |
| 35  | BB    | 15   | G    | C5-N7-C8    | -6.23 | 101.18      | 104.30   |
| 35  | BB    | 624  | C    | O4'-C1'-N1  | 6.23  | 113.19      | 108.20   |
| 35  | BB    | 802  | A    | C5-C6-N6    | -6.23 | 118.71      | 123.70   |
| 35  | BB    | 1067 | A    | C3'-C2'-C1' | -6.23 | 96.51       | 101.50   |
| 35  | BB    | 1099 | G    | C6-C5-N7    | -6.23 | 126.66      | 130.40   |
| 35  | BB    | 1144 | A    | N3-C4-C5    | -6.23 | 122.44      | 126.80   |
| 35  | BB    | 1371 | G    | C5-C6-N1    | -6.23 | 108.38      | 111.50   |
| 35  | BB    | 2115 | G    | N1-C2-N2    | -6.23 | 110.59      | 116.20   |
| 35  | BB    | 2149 | U    | N3-C4-C5    | 6.23  | 118.34      | 114.60   |
| 35  | BB    | 2407 | A    | N3-C4-C5    | -6.23 | 122.44      | 126.80   |
| 47  | BN    | 108  | ALA  | N-CA-CB     | 6.23  | 118.83      | 110.10   |
| 1   | AA    | 182  | A    | C4-C5-C6    | 6.23  | 120.11      | 117.00   |
| 1   | AA    | 626  | G    | O4'-C1'-N9  | 6.23  | 113.18      | 108.20   |
| 1   | AA    | 838  | G    | N1-C2-N3    | -6.23 | 120.16      | 123.90   |
| 1   | AA    | 919  | A    | C4'-C3'-C2' | -6.23 | 96.37       | 102.60   |
| 1   | AA    | 1028 | C    | C4'-C3'-C2' | -6.23 | 96.37       | 102.60   |
| 1   | AA    | 1131 | G    | C5-C6-O6    | -6.23 | 124.86      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | AV    | 66   | C    | O4'-C1'-N1  | 6.23  | 113.18      | 108.20   |
| 34  | BA    | 20   | G    | C5'-C4'-O4' | 6.23  | 116.58      | 109.10   |
| 35  | BB    | 478  | A    | C4-C5-N7    | 6.23  | 113.81      | 110.70   |
| 35  | BB    | 529  | A    | N9-C4-C5    | 6.23  | 108.29      | 105.80   |
| 35  | BB    | 1052 | C    | O4'-C1'-N1  | 6.23  | 113.18      | 108.20   |
| 35  | BB    | 1120 | G    | C8-N9-C4    | -6.23 | 103.91      | 106.40   |
| 35  | BB    | 1775 | U    | N1-C2-N3    | -6.23 | 111.16      | 114.90   |
| 35  | BB    | 2902 | C    | C6-N1-C2    | 6.23  | 122.79      | 120.30   |
| 1   | AA    | 841  | C    | O4'-C1'-N1  | 6.23  | 113.18      | 108.20   |
| 1   | AA    | 932  | C    | C4-C5-C6    | -6.23 | 114.29      | 117.40   |
| 35  | BB    | 59   | U    | N3-C2-O2    | 6.23  | 126.56      | 122.20   |
| 35  | BB    | 440  | C    | N3-C4-N4    | 6.23  | 122.36      | 118.00   |
| 35  | BB    | 1628 | G    | C6-C5-N7    | -6.23 | 126.66      | 130.40   |
| 1   | AA    | 567  | G    | N1-C2-N3    | -6.23 | 120.16      | 123.90   |
| 35  | BB    | 251  | A    | C5-C6-N6    | -6.23 | 118.72      | 123.70   |
| 35  | BB    | 433  | C    | O4'-C1'-N1  | 6.23  | 113.18      | 108.20   |
| 35  | BB    | 1566 | A    | C2-N3-C4    | -6.23 | 107.49      | 110.60   |
| 35  | BB    | 1677 | A    | C6-N1-C2    | 6.23  | 122.34      | 118.60   |
| 35  | BB    | 1692 | U    | C4-C5-C6    | 6.23  | 123.44      | 119.70   |
| 35  | BB    | 1829 | A    | C4-C5-N7    | 6.23  | 113.81      | 110.70   |
| 35  | BB    | 2142 | A    | O4'-C4'-C3' | -6.23 | 97.77       | 104.00   |
| 35  | BB    | 2552 | U    | C6-N1-C2    | 6.23  | 124.74      | 121.00   |
| 35  | BB    | 2629 | U    | O4'-C1'-N1  | 6.23  | 113.18      | 108.20   |
| 35  | BB    | 2754 | U    | C2-N3-C4    | -6.23 | 123.26      | 127.00   |
| 1   | AA    | 811  | C    | C4'-C3'-C2' | 6.23  | 108.83      | 102.60   |
| 1   | AA    | 1152 | A    | C5-C6-N6    | -6.23 | 118.72      | 123.70   |
| 9   | AI    | 89   | TYR  | CB-CG-CD2   | 6.23  | 124.73      | 121.00   |
| 1   | AA    | 70   | U    | N3-C4-C5    | -6.22 | 110.86      | 114.60   |
| 1   | AA    | 300  | A    | N7-C8-N9    | -6.22 | 110.69      | 113.80   |
| 1   | AA    | 616  | G    | N1-C6-O6    | 6.22  | 123.63      | 119.90   |
| 35  | BB    | 177  | G    | C8-N9-C4    | 6.22  | 108.89      | 106.40   |
| 35  | BB    | 721  | A    | O4'-C4'-C3' | -6.22 | 97.78       | 104.00   |
| 35  | BB    | 991  | C    | N1-C2-N3    | -6.22 | 114.84      | 119.20   |
| 35  | BB    | 1281 | G    | P-O5'-C5'   | -6.22 | 110.94      | 120.90   |
| 35  | BB    | 2252 | G    | C4-C5-C6    | 6.22  | 122.53      | 118.80   |
| 1   | AA    | 675  | A    | O4'-C4'-C3' | -6.22 | 97.78       | 104.00   |
| 1   | AA    | 987  | G    | C8-N9-C4    | -6.22 | 103.91      | 106.40   |
| 22  | AV    | 38   | U    | C6-N1-C2    | -6.22 | 117.27      | 121.00   |
| 34  | BA    | 23   | G    | C5-C6-N1    | -6.22 | 108.39      | 111.50   |
| 34  | BA    | 73   | A    | C4-C5-C6    | 6.22  | 120.11      | 117.00   |
| 35  | BB    | 1    | G    | C4-C5-C6    | 6.22  | 122.53      | 118.80   |
| 35  | BB    | 215  | G    | C4-C5-C6    | 6.22  | 122.53      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 923  | G    | N7-C8-N9    | -6.22 | 109.99      | 113.10   |
| 35  | BB    | 1031 | G    | N1-C6-O6    | 6.22  | 123.63      | 119.90   |
| 35  | BB    | 1073 | A    | C4-C5-C6    | 6.22  | 120.11      | 117.00   |
| 35  | BB    | 1415 | U    | N1-C2-O2    | 6.22  | 127.16      | 122.80   |
| 35  | BB    | 1620 | G    | N1-C2-N3    | -6.22 | 120.17      | 123.90   |
| 45  | BL    | 117  | THR  | N-CA-CB     | 6.22  | 122.12      | 110.30   |
| 1   | AA    | 18   | C    | C1'-O4'-C4' | 6.22  | 114.88      | 109.90   |
| 1   | AA    | 868  | C    | C5-C4-N4    | -6.22 | 115.84      | 120.20   |
| 35  | BB    | 783  | A    | C4-C5-C6    | 6.22  | 120.11      | 117.00   |
| 1   | AA    | 120  | A    | C3'-C2'-C1' | 6.22  | 106.48      | 101.50   |
| 1   | AA    | 125  | U    | N3-C2-O2    | 6.22  | 126.55      | 122.20   |
| 1   | AA    | 919  | A    | C6-C5-N7    | -6.22 | 127.95      | 132.30   |
| 1   | AA    | 1089 | G    | C4-C5-C6    | 6.22  | 122.53      | 118.80   |
| 1   | AA    | 1280 | A    | O4'-C1'-N9  | 6.22  | 113.17      | 108.20   |
| 1   | AA    | 1444 | U    | N3-C4-C5    | -6.22 | 110.87      | 114.60   |
| 1   | AA    | 1516 | G    | C1'-O4'-C4' | -6.22 | 104.92      | 109.90   |
| 22  | AV    | 37   | G    | N9-C4-C5    | 6.22  | 107.89      | 105.40   |
| 35  | BB    | 1387 | A    | N3-C4-N9    | -6.22 | 122.42      | 127.40   |
| 35  | BB    | 1788 | C    | N3-C4-C5    | -6.22 | 119.41      | 121.90   |
| 35  | BB    | 2377 | A    | C4-C5-C6    | 6.22  | 120.11      | 117.00   |
| 1   | AA    | 1172 | C    | O4'-C1'-N1  | 6.22  | 113.17      | 108.20   |
| 1   | AA    | 1291 | U    | C5-C4-O4    | 6.22  | 129.63      | 125.90   |
| 35  | BB    | 879  | G    | N1-C2-N3    | -6.22 | 120.17      | 123.90   |
| 35  | BB    | 2141 | G    | C4-C5-C6    | 6.22  | 122.53      | 118.80   |
| 1   | AA    | 121  | U    | C2-N1-C1'   | 6.22  | 125.16      | 117.70   |
| 1   | AA    | 213  | G    | O4'-C1'-N9  | 6.22  | 113.17      | 108.20   |
| 1   | AA    | 239  | U    | N3-C4-O4    | 6.22  | 123.75      | 119.40   |
| 3   | AC    | 127  | VAL  | C-N-CA      | 6.22  | 137.24      | 121.70   |
| 8   | AH    | 8    | ASP  | CB-CG-OD1   | 6.22  | 123.89      | 118.30   |
| 35  | BB    | 5    | A    | N9-C4-C5    | 6.22  | 108.29      | 105.80   |
| 35  | BB    | 124  | G    | N7-C8-N9    | -6.22 | 109.99      | 113.10   |
| 35  | BB    | 972  | A    | N1-C6-N6    | 6.22  | 122.33      | 118.60   |
| 35  | BB    | 1389 | G    | O4'-C1'-N9  | 6.22  | 113.17      | 108.20   |
| 35  | BB    | 2195 | U    | O4'-C1'-N1  | 6.22  | 113.17      | 108.20   |
| 35  | BB    | 2397 | G    | N9-C4-C5    | -6.22 | 102.91      | 105.40   |
| 35  | BB    | 2536 | G    | N1-C2-N3    | -6.22 | 120.17      | 123.90   |
| 35  | BB    | 2639 | A    | N1-C2-N3    | 6.22  | 132.41      | 129.30   |
| 35  | BB    | 2659 | G    | P-O3'-C3'   | -6.22 | 112.24      | 119.70   |
| 35  | BB    | 2776 | A    | O4'-C1'-N9  | 6.22  | 113.17      | 108.20   |
| 35  | BB    | 2877 | G    | N7-C8-N9    | -6.22 | 109.99      | 113.10   |
| 35  | BB    | 2900 | A    | C5-C6-N1    | -6.22 | 114.59      | 117.70   |
| 1   | AA    | 42   | G    | C4-C5-N7    | -6.21 | 108.31      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1015 | G    | C4-C5-C6    | 6.21  | 122.53      | 118.80   |
| 1   | AA    | 1023 | U    | C6-N1-C2    | -6.21 | 117.27      | 121.00   |
| 1   | AA    | 1258 | G    | C6-C5-N7    | -6.21 | 126.67      | 130.40   |
| 1   | AA    | 1350 | A    | C4-C5-N7    | 6.21  | 113.81      | 110.70   |
| 1   | AA    | 1398 | A    | C4'-C3'-C2' | -6.21 | 96.39       | 102.60   |
| 34  | BA    | 24   | G    | N1-C2-N3    | -6.21 | 120.17      | 123.90   |
| 34  | BA    | 110  | C    | C5-C4-N4    | -6.21 | 115.85      | 120.20   |
| 35  | BB    | 10   | A    | N9-C4-C5    | 6.21  | 108.29      | 105.80   |
| 35  | BB    | 313  | G    | N9-C4-C5    | 6.21  | 107.89      | 105.40   |
| 35  | BB    | 405  | U    | C3'-C2'-C1' | -6.21 | 96.53       | 101.50   |
| 35  | BB    | 1606 | C    | O4'-C1'-C2' | 6.21  | 113.19      | 107.60   |
| 35  | BB    | 2148 | G    | C5-N7-C8    | 6.21  | 107.41      | 104.30   |
| 1   | AA    | 179  | A    | C4'-C3'-C2' | -6.21 | 96.39       | 102.60   |
| 1   | AA    | 635  | A    | C4'-C3'-C2' | -6.21 | 96.39       | 102.60   |
| 1   | AA    | 1208 | C    | O4'-C1'-N1  | 6.21  | 113.17      | 108.20   |
| 1   | AA    | 1214 | C    | N3-C4-C5    | -6.21 | 119.42      | 121.90   |
| 35  | BB    | 341  | C    | O4'-C1'-N1  | 6.21  | 113.17      | 108.20   |
| 35  | BB    | 1537 | G    | C8-N9-C4    | -6.21 | 103.92      | 106.40   |
| 35  | BB    | 2895 | G    | C4'-C3'-C2' | -6.21 | 96.39       | 102.60   |
| 1   | AA    | 533  | A    | N3-C4-C5    | -6.21 | 122.45      | 126.80   |
| 1   | AA    | 712  | A    | N1-C6-N6    | 6.21  | 122.33      | 118.60   |
| 1   | AA    | 859  | G    | N3-C2-N2    | 6.21  | 124.25      | 119.90   |
| 1   | AA    | 887  | G    | C4'-C3'-C2' | -6.21 | 96.39       | 102.60   |
| 1   | AA    | 1110 | A    | C2-N3-C4    | -6.21 | 107.50      | 110.60   |
| 1   | AA    | 1163 | A    | C2-N3-C4    | 6.21  | 113.70      | 110.60   |
| 1   | AA    | 1496 | C    | N3-C4-C5    | -6.21 | 119.42      | 121.90   |
| 13  | AM    | 112  | ARG  | NE-CZ-NH1   | 6.21  | 123.41      | 120.30   |
| 35  | BB    | 97   | C    | C5'-C4'-O4' | -6.21 | 101.65      | 109.10   |
| 35  | BB    | 414  | C    | C6-N1-C2    | -6.21 | 117.81      | 120.30   |
| 35  | BB    | 1244 | A    | P-O5'-C5'   | -6.21 | 110.96      | 120.90   |
| 35  | BB    | 1267 | U    | O4'-C4'-C3' | -6.21 | 97.79       | 104.00   |
| 35  | BB    | 2367 | G    | N1-C6-O6    | 6.21  | 123.63      | 119.90   |
| 1   | AA    | 1482 | G    | N3-C2-N2    | 6.21  | 124.25      | 119.90   |
| 35  | BB    | 556  | A    | C8-N9-C4    | -6.21 | 103.32      | 105.80   |
| 35  | BB    | 583  | G    | N1-C2-N3    | -6.21 | 120.17      | 123.90   |
| 35  | BB    | 799  | G    | N1-C6-O6    | 6.21  | 123.63      | 119.90   |
| 35  | BB    | 1954 | G    | N1-C2-N3    | -6.21 | 120.17      | 123.90   |
| 35  | BB    | 2050 | C    | C5-C6-N1    | -6.21 | 117.89      | 121.00   |
| 35  | BB    | 2067 | G    | N7-C8-N9    | 6.21  | 116.20      | 113.10   |
| 35  | BB    | 2791 | G    | N3-C4-N9    | -6.21 | 122.27      | 126.00   |
| 1   | AA    | 214  | C    | C5-C6-N1    | 6.21  | 124.10      | 121.00   |
| 1   | AA    | 387  | U    | O4'-C1'-N1  | 6.21  | 113.17      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 394  | G    | N1-C6-O6    | 6.21  | 123.62      | 119.90   |
| 1   | AA    | 615  | G    | C8-N9-C4    | -6.21 | 103.92      | 106.40   |
| 1   | AA    | 745  | G    | C8-N9-C4    | -6.21 | 103.92      | 106.40   |
| 1   | AA    | 918  | A    | C6-C5-N7    | -6.21 | 127.95      | 132.30   |
| 1   | AA    | 992  | U    | C5-C6-N1    | 6.21  | 125.80      | 122.70   |
| 35  | BB    | 147  | C    | N3-C4-N4    | 6.21  | 122.34      | 118.00   |
| 35  | BB    | 309  | A    | C8-N9-C4    | -6.21 | 103.32      | 105.80   |
| 35  | BB    | 739  | A    | C6-C5-N7    | -6.21 | 127.95      | 132.30   |
| 35  | BB    | 757  | G    | C6-C5-N7    | 6.21  | 134.12      | 130.40   |
| 35  | BB    | 1145 | C    | N3-C2-O2    | 6.21  | 126.25      | 121.90   |
| 35  | BB    | 1414 | C    | C2-N3-C4    | 6.21  | 123.00      | 119.90   |
| 35  | BB    | 2811 | G    | C8-N9-C4    | -6.21 | 103.92      | 106.40   |
| 35  | BB    | 2834 | G    | OP1-P-OP2   | -6.21 | 110.29      | 119.60   |
| 1   | AA    | 298  | A    | C5-C6-N1    | -6.21 | 114.60      | 117.70   |
| 1   | AA    | 306  | A    | OP1-P-OP2   | -6.21 | 110.29      | 119.60   |
| 1   | AA    | 351  | G    | N7-C8-N9    | -6.21 | 110.00      | 113.10   |
| 1   | AA    | 579  | A    | C5-N7-C8    | -6.21 | 100.80      | 103.90   |
| 1   | AA    | 1056 | U    | O4'-C1'-N1  | 6.21  | 113.16      | 108.20   |
| 34  | BA    | 71   | C    | C2-N3-C4    | -6.21 | 116.80      | 119.90   |
| 35  | BB    | 692  | C    | C5-C4-N4    | -6.21 | 115.86      | 120.20   |
| 35  | BB    | 729  | G    | N7-C8-N9    | -6.21 | 110.00      | 113.10   |
| 35  | BB    | 825  | A    | C8-N9-C4    | -6.21 | 103.32      | 105.80   |
| 35  | BB    | 1005 | C    | C4'-C3'-C2' | 6.21  | 108.81      | 102.60   |
| 35  | BB    | 1742 | U    | O4'-C1'-N1  | 6.21  | 113.17      | 108.20   |
| 35  | BB    | 2007 | U    | C5-C4-O4    | -6.21 | 122.18      | 125.90   |
| 35  | BB    | 2222 | C    | C5-C4-N4    | -6.21 | 115.86      | 120.20   |
| 35  | BB    | 2653 | U    | N3-C4-O4    | 6.21  | 123.74      | 119.40   |
| 1   | AA    | 360  | G    | N3-C4-C5    | -6.21 | 125.50      | 128.60   |
| 1   | AA    | 1387 | G    | N1-C2-N3    | -6.21 | 120.18      | 123.90   |
| 1   | AA    | 1432 | G    | N1-C2-N3    | -6.21 | 120.18      | 123.90   |
| 1   | AA    | 257  | G    | N3-C2-N2    | 6.20  | 124.24      | 119.90   |
| 1   | AA    | 734  | G    | C4-N9-C1'   | 6.20  | 134.56      | 126.50   |
| 1   | AA    | 1296 | C    | N1-C2-O2    | 6.20  | 122.62      | 118.90   |
| 35  | BB    | 283  | G    | N7-C8-N9    | -6.20 | 110.00      | 113.10   |
| 35  | BB    | 309  | A    | C5-N7-C8    | 6.20  | 107.00      | 103.90   |
| 35  | BB    | 498  | G    | N1-C6-O6    | 6.20  | 123.62      | 119.90   |
| 35  | BB    | 508  | A    | N9-C4-C5    | 6.20  | 108.28      | 105.80   |
| 35  | BB    | 2413 | G    | N1-C2-N2    | -6.20 | 110.62      | 116.20   |
| 35  | BB    | 2477 | U    | O4'-C1'-N1  | 6.20  | 113.16      | 108.20   |
| 50  | BQ    | 31   | TYR  | CB-CG-CD2   | 6.20  | 124.72      | 121.00   |
| 1   | AA    | 960  | U    | C5-C4-O4    | -6.20 | 122.18      | 125.90   |
| 1   | AA    | 1270 | G    | C2-N3-C4    | 6.20  | 115.00      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 26   | G    | N9-C4-C5    | -6.20 | 102.92      | 105.40   |
| 35  | BB    | 708  | G    | C4-C5-N7    | 6.20  | 113.28      | 110.80   |
| 35  | BB    | 1073 | A    | C5-C6-N6    | -6.20 | 118.74      | 123.70   |
| 35  | BB    | 1601 | G    | N1-C6-O6    | 6.20  | 123.62      | 119.90   |
| 35  | BB    | 1835 | G    | C4-C5-N7    | -6.20 | 108.32      | 110.80   |
| 35  | BB    | 2126 | A    | C4-C5-N7    | -6.20 | 107.60      | 110.70   |
| 1   | AA    | 249  | U    | O4'-C1'-N1  | 6.20  | 113.16      | 108.20   |
| 1   | AA    | 596  | A    | N9-C4-C5    | -6.20 | 103.32      | 105.80   |
| 1   | AA    | 664  | G    | C4-C5-N7    | 6.20  | 113.28      | 110.80   |
| 1   | AA    | 671  | G    | C5'-C4'-C3' | -6.20 | 106.08      | 116.00   |
| 1   | AA    | 1049 | U    | P-O3'-C3'   | 6.20  | 127.14      | 119.70   |
| 1   | AA    | 1074 | G    | N1-C6-O6    | 6.20  | 123.62      | 119.90   |
| 1   | AA    | 1154 | G    | C4-C5-C6    | 6.20  | 122.52      | 118.80   |
| 1   | AA    | 1453 | G    | C5-N7-C8    | 6.20  | 107.40      | 104.30   |
| 20  | AT    | 59   | ARG  | CD-NE-CZ    | 6.20  | 132.28      | 123.60   |
| 35  | BB    | 582  | A    | C5-C6-N1    | -6.20 | 114.60      | 117.70   |
| 35  | BB    | 2092 | U    | N3-C4-O4    | 6.20  | 123.74      | 119.40   |
| 35  | BB    | 2477 | U    | N3-C2-O2    | 6.20  | 126.54      | 122.20   |
| 35  | BB    | 2718 | G    | N9-C4-C5    | 6.20  | 107.88      | 105.40   |
| 1   | AA    | 52   | C    | C5-C4-N4    | -6.20 | 115.86      | 120.20   |
| 1   | AA    | 563  | A    | N3-C4-N9    | 6.20  | 132.36      | 127.40   |
| 1   | AA    | 674  | G    | N1-C2-N3    | -6.20 | 120.18      | 123.90   |
| 35  | BB    | 41   | C    | N3-C4-C5    | -6.20 | 119.42      | 121.90   |
| 35  | BB    | 989  | G    | N9-C4-C5    | 6.20  | 107.88      | 105.40   |
| 35  | BB    | 1950 | G    | N7-C8-N9    | -6.20 | 110.00      | 113.10   |
| 35  | BB    | 2790 | U    | C6-N1-C2    | -6.20 | 117.28      | 121.00   |
| 35  | BB    | 27   | G    | N3-C2-N2    | 6.20  | 124.24      | 119.90   |
| 35  | BB    | 205  | G    | C8-N9-C4    | 6.20  | 108.88      | 106.40   |
| 35  | BB    | 247  | G    | C8-N9-C4    | 6.20  | 108.88      | 106.40   |
| 35  | BB    | 1930 | G    | C4-C5-N7    | 6.20  | 113.28      | 110.80   |
| 35  | BB    | 2151 | U    | N3-C4-C5    | 6.20  | 118.32      | 114.60   |
| 1   | AA    | 872  | A    | C4-C5-C6    | 6.20  | 120.10      | 117.00   |
| 12  | AL    | 64   | SER  | N-CA-CB     | 6.20  | 119.79      | 110.50   |
| 34  | BA    | 56   | G    | C5-C6-O6    | -6.20 | 124.88      | 128.60   |
| 34  | BA    | 62   | C    | C4'-C3'-C2' | -6.20 | 96.41       | 102.60   |
| 35  | BB    | 1210 | G    | C5'-C4'-C3' | -6.20 | 106.09      | 116.00   |
| 35  | BB    | 1402 | U    | O4'-C1'-N1  | 6.20  | 113.16      | 108.20   |
| 35  | BB    | 1583 | A    | C5-C6-N6    | -6.20 | 118.74      | 123.70   |
| 35  | BB    | 1863 | G    | N3-C2-N2    | 6.20  | 124.24      | 119.90   |
| 35  | BB    | 2019 | A    | N9-C4-C5    | -6.20 | 103.32      | 105.80   |
| 35  | BB    | 2122 | U    | N3-C4-O4    | 6.20  | 123.74      | 119.40   |
| 35  | BB    | 2588 | G    | N9-C1'-C2'  | -6.20 | 105.19      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2856 | A    | OP1-P-OP2   | -6.20 | 110.31      | 119.60   |
| 1   | AA    | 616  | G    | C4-C5-C6    | 6.19  | 122.52      | 118.80   |
| 35  | BB    | 646  | U    | O4'-C1'-N1  | 6.19  | 113.16      | 108.20   |
| 35  | BB    | 1213 | A    | N9-C4-C5    | -6.19 | 103.32      | 105.80   |
| 35  | BB    | 1353 | A    | N7-C8-N9    | 6.19  | 116.90      | 113.80   |
| 35  | BB    | 2763 | G    | C6-C5-N7    | -6.19 | 126.68      | 130.40   |
| 1   | AA    | 141  | G    | C2-N3-C4    | 6.19  | 115.00      | 111.90   |
| 1   | AA    | 146  | G    | C6-C5-N7    | -6.19 | 126.69      | 130.40   |
| 1   | AA    | 180  | U    | P-O3'-C3'   | -6.19 | 112.27      | 119.70   |
| 1   | AA    | 416  | G    | C6-C5-N7    | -6.19 | 126.68      | 130.40   |
| 1   | AA    | 481  | G    | N3-C4-N9    | 6.19  | 129.72      | 126.00   |
| 1   | AA    | 723  | U    | O4'-C1'-N1  | 6.19  | 113.15      | 108.20   |
| 1   | AA    | 1334 | G    | C8-N9-C4    | -6.19 | 103.92      | 106.40   |
| 22  | AV    | 2    | G    | C5-C6-N1    | -6.19 | 108.40      | 111.50   |
| 35  | BB    | 705  | A    | C8-N9-C4    | -6.19 | 103.32      | 105.80   |
| 35  | BB    | 799  | G    | C2-N3-C4    | -6.19 | 108.80      | 111.90   |
| 35  | BB    | 821  | A    | C8-N9-C4    | -6.19 | 103.32      | 105.80   |
| 35  | BB    | 1266 | G    | P-O3'-C3'   | 6.19  | 127.13      | 119.70   |
| 35  | BB    | 1306 | C    | O4'-C4'-C3' | -6.19 | 97.81       | 104.00   |
| 1   | AA    | 91   | U    | N3-C4-C5    | -6.19 | 110.89      | 114.60   |
| 1   | AA    | 128  | G    | N7-C8-N9    | -6.19 | 110.00      | 113.10   |
| 1   | AA    | 512  | U    | P-O5'-C5'   | 6.19  | 130.81      | 120.90   |
| 1   | AA    | 653  | U    | C3'-C2'-C1' | -6.19 | 96.55       | 101.50   |
| 1   | AA    | 1436 | U    | P-O3'-C3'   | -6.19 | 112.27      | 119.70   |
| 11  | AK    | 84   | MET  | CG-SD-CE    | -6.19 | 90.29       | 100.20   |
| 35  | BB    | 530  | G    | N1-C6-O6    | 6.19  | 123.61      | 119.90   |
| 35  | BB    | 1172 | C    | P-O3'-C3'   | 6.19  | 127.13      | 119.70   |
| 35  | BB    | 1201 | U    | C5-C4-O4    | -6.19 | 122.19      | 125.90   |
| 35  | BB    | 1337 | G    | C5'-C4'-C3' | -6.19 | 106.09      | 116.00   |
| 35  | BB    | 1529 | G    | N1-C2-N3    | -6.19 | 120.19      | 123.90   |
| 35  | BB    | 2215 | C    | N3-C4-N4    | 6.19  | 122.33      | 118.00   |
| 35  | BB    | 2445 | G    | N3-C4-C5    | 6.19  | 131.69      | 128.60   |
| 1   | AA    | 144  | G    | C6-N1-C2    | 6.19  | 128.81      | 125.10   |
| 1   | AA    | 812  | G    | C4-C5-C6    | 6.19  | 122.51      | 118.80   |
| 35  | BB    | 415  | A    | N1-C2-N3    | 6.19  | 132.40      | 129.30   |
| 35  | BB    | 1757 | A    | P-O5'-C5'   | -6.19 | 111.00      | 120.90   |
| 35  | BB    | 1817 | G    | N3-C2-N2    | 6.19  | 124.23      | 119.90   |
| 35  | BB    | 2639 | A    | C4-C5-N7    | -6.19 | 107.61      | 110.70   |
| 1   | AA    | 329  | A    | C5-C6-N1    | -6.19 | 114.61      | 117.70   |
| 1   | AA    | 552  | U    | C1'-O4'-C4' | -6.19 | 104.95      | 109.90   |
| 1   | AA    | 816  | A    | C5-N7-C8    | 6.19  | 106.99      | 103.90   |
| 1   | AA    | 935  | A    | O4'-C1'-N9  | 6.19  | 113.15      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 30  | B5    | 74   | ARG  | NE-CZ-NH2   | -6.19 | 117.21      | 120.30   |
| 35  | BB    | 946  | C    | C4'-C3'-C2' | -6.19 | 96.41       | 102.60   |
| 35  | BB    | 1232 | G    | P-O3'-C3'   | -6.19 | 112.28      | 119.70   |
| 35  | BB    | 2010 | G    | C4-C5-C6    | 6.19  | 122.51      | 118.80   |
| 35  | BB    | 2640 | G    | C5-C6-N1    | 6.19  | 114.59      | 111.50   |
| 1   | AA    | 305  | G    | N1-C2-N3    | -6.19 | 120.19      | 123.90   |
| 35  | BB    | 1854 | A    | C2-N3-C4    | 6.19  | 113.69      | 110.60   |
| 1   | AA    | 492  | C    | C1'-O4'-C4' | 6.18  | 114.85      | 109.90   |
| 1   | AA    | 1378 | C    | C6-N1-C2    | -6.18 | 117.83      | 120.30   |
| 35  | BB    | 361  | G    | C8-N9-C4    | -6.18 | 103.93      | 106.40   |
| 35  | BB    | 1095 | A    | C4-C5-N7    | -6.18 | 107.61      | 110.70   |
| 35  | BB    | 1706 | C    | C6-N1-C2    | -6.18 | 117.83      | 120.30   |
| 35  | BB    | 1891 | G    | C3'-C2'-C1' | -6.18 | 96.55       | 101.50   |
| 35  | BB    | 2616 | C    | N3-C4-N4    | 6.18  | 122.33      | 118.00   |
| 35  | BB    | 2688 | G    | C5-N7-C8    | 6.18  | 107.39      | 104.30   |
| 37  | BD    | 2    | ILE  | CA-CB-CG1   | 6.18  | 122.75      | 111.00   |
| 1   | AA    | 355  | C    | C5-C4-N4    | -6.18 | 115.87      | 120.20   |
| 1   | AA    | 712  | A    | N1-C2-N3    | -6.18 | 126.21      | 129.30   |
| 1   | AA    | 725  | G    | C4-C5-C6    | 6.18  | 122.51      | 118.80   |
| 35  | BB    | 353  | C    | N3-C4-C5    | -6.18 | 119.43      | 121.90   |
| 35  | BB    | 1442 | U    | C4-C5-C6    | -6.18 | 115.99      | 119.70   |
| 35  | BB    | 1558 | C    | C6-N1-C1'   | -6.18 | 113.38      | 120.80   |
| 35  | BB    | 1689 | A    | C4-C5-C6    | 6.18  | 120.09      | 117.00   |
| 35  | BB    | 2337 | G    | C4-C5-C6    | 6.18  | 122.51      | 118.80   |
| 35  | BB    | 2393 | U    | C5-C6-N1    | 6.18  | 125.79      | 122.70   |
| 1   | AA    | 340  | U    | C5-C4-O4    | -6.18 | 122.19      | 125.90   |
| 1   | AA    | 1054 | C    | OP2-P-O3'   | 6.18  | 118.80      | 105.20   |
| 1   | AA    | 1424 | U    | N3-C4-O4    | 6.18  | 123.73      | 119.40   |
| 23  | AX    | 22   | A    | N1-C6-N6    | -6.18 | 114.89      | 118.60   |
| 35  | BB    | 14   | A    | N1-C6-N6    | 6.18  | 122.31      | 118.60   |
| 35  | BB    | 1660 | G    | C2-N3-C4    | 6.18  | 114.99      | 111.90   |
| 35  | BB    | 1669 | A    | C4-C5-N7    | -6.18 | 107.61      | 110.70   |
| 35  | BB    | 2620 | C    | C6-N1-C2    | 6.18  | 122.77      | 120.30   |
| 1   | AA    | 460  | A    | N1-C2-N3    | -6.18 | 126.21      | 129.30   |
| 1   | AA    | 823  | C    | N3-C4-N4    | 6.18  | 122.33      | 118.00   |
| 1   | AA    | 892  | A    | C5-C6-N1    | -6.18 | 114.61      | 117.70   |
| 35  | BB    | 508  | A    | C1'-O4'-C4' | -6.18 | 104.96      | 109.90   |
| 35  | BB    | 618  | G    | N1-C6-O6    | 6.18  | 123.61      | 119.90   |
| 35  | BB    | 1166 | G    | C5-C6-O6    | -6.18 | 124.89      | 128.60   |
| 35  | BB    | 1175 | A    | O4'-C1'-N9  | 6.18  | 113.14      | 108.20   |
| 35  | BB    | 1783 | A    | O4'-C1'-N9  | 6.18  | 113.14      | 108.20   |
| 35  | BB    | 2058 | A    | N1-C6-N6    | 6.18  | 122.31      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2089 | C    | P-O3'-C3'   | -6.18 | 112.28      | 119.70   |
| 35  | BB    | 2175 | C    | P-O3'-C3'   | 6.18  | 127.12      | 119.70   |
| 35  | BB    | 2511 | U    | N1-C2-N3    | -6.18 | 111.19      | 114.90   |
| 35  | BB    | 2534 | A    | C5-C6-N1    | -6.18 | 114.61      | 117.70   |
| 1   | AA    | 118  | U    | C5-C6-N1    | 6.18  | 125.79      | 122.70   |
| 1   | AA    | 454  | G    | N1-C6-O6    | 6.18  | 123.61      | 119.90   |
| 1   | AA    | 1214 | C    | C4-C5-C6    | 6.18  | 120.49      | 117.40   |
| 3   | AC    | 111  | ASP  | N-CA-CB     | 6.18  | 121.72      | 110.60   |
| 35  | BB    | 1907 | G    | N1-C6-O6    | 6.18  | 123.61      | 119.90   |
| 35  | BB    | 2576 | G    | C8-N9-C1'   | -6.18 | 118.97      | 127.00   |
| 1   | AA    | 834  | U    | C4-C5-C6    | 6.18  | 123.41      | 119.70   |
| 35  | BB    | 370  | G    | P-O3'-C3'   | 6.18  | 127.11      | 119.70   |
| 35  | BB    | 420  | C    | C5-C6-N1    | 6.18  | 124.09      | 121.00   |
| 35  | BB    | 496  | G    | N3-C4-N9    | 6.18  | 129.71      | 126.00   |
| 35  | BB    | 763  | G    | C4-N9-C1'   | -6.18 | 118.47      | 126.50   |
| 35  | BB    | 857  | G    | C6-C5-N7    | -6.18 | 126.69      | 130.40   |
| 35  | BB    | 2271 | G    | C5-C6-N1    | -6.18 | 108.41      | 111.50   |
| 35  | BB    | 2376 | A    | C5-C6-N6    | -6.18 | 118.76      | 123.70   |
| 35  | BB    | 2615 | U    | P-O3'-C3'   | -6.18 | 112.29      | 119.70   |
| 44  | BK    | 71   | ARG  | CD-NE-CZ    | -6.18 | 114.95      | 123.60   |
| 49  | BP    | 75   | THR  | CA-CB-CG2   | -6.18 | 103.75      | 112.40   |
| 1   | AA    | 103  | U    | O4'-C1'-N1  | 6.17  | 113.14      | 108.20   |
| 1   | AA    | 229  | U    | C5-C6-N1    | 6.17  | 125.79      | 122.70   |
| 1   | AA    | 951  | G    | N7-C8-N9    | 6.17  | 116.19      | 113.10   |
| 1   | AA    | 997  | U    | C1'-O4'-C4' | 6.17  | 114.84      | 109.90   |
| 35  | BB    | 37   | C    | C4'-C3'-C2' | -6.17 | 96.43       | 102.60   |
| 35  | BB    | 1338 | G    | N1-C6-O6    | 6.17  | 123.60      | 119.90   |
| 35  | BB    | 2314 | A    | N9-C1'-C2'  | -6.17 | 105.21      | 112.00   |
| 1   | AA    | 41   | G    | O4'-C1'-N9  | 6.17  | 113.14      | 108.20   |
| 1   | AA    | 300  | A    | C6-N1-C2    | -6.17 | 114.90      | 118.60   |
| 1   | AA    | 438  | U    | N1-C2-O2    | -6.17 | 118.48      | 122.80   |
| 1   | AA    | 669  | G    | N3-C4-N9    | 6.17  | 129.70      | 126.00   |
| 1   | AA    | 775  | G    | C6-C5-N7    | -6.17 | 126.70      | 130.40   |
| 35  | BB    | 950  | G    | N3-C4-N9    | -6.17 | 122.30      | 126.00   |
| 35  | BB    | 1426 | G    | C4-C5-C6    | 6.17  | 122.50      | 118.80   |
| 35  | BB    | 2188 | U    | C6-N1-C2    | -6.17 | 117.30      | 121.00   |
| 35  | BB    | 2248 | C    | C5-C6-N1    | 6.17  | 124.09      | 121.00   |
| 35  | BB    | 2290 | G    | C4-C5-N7    | -6.17 | 108.33      | 110.80   |
| 1   | AA    | 312  | C    | C5-C6-N1    | 6.17  | 124.09      | 121.00   |
| 1   | AA    | 902  | G    | C4-C5-N7    | 6.17  | 113.27      | 110.80   |
| 1   | AA    | 1454 | G    | C4-C5-N7    | -6.17 | 108.33      | 110.80   |
| 35  | BB    | 54   | G    | N1-C2-N3    | -6.17 | 120.20      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 285  | G    | N7-C8-N9    | 6.17  | 116.19      | 113.10   |
| 35  | BB    | 390  | U    | N3-C4-C5    | -6.17 | 110.90      | 114.60   |
| 35  | BB    | 985  | C    | C2-N3-C4    | 6.17  | 122.99      | 119.90   |
| 35  | BB    | 1580 | A    | C6-C5-N7    | -6.17 | 127.98      | 132.30   |
| 35  | BB    | 2044 | C    | C6-N1-C2    | -6.17 | 117.83      | 120.30   |
| 11  | AK    | 126  | ARG  | NE-CZ-NH1   | 6.17  | 123.39      | 120.30   |
| 12  | AL    | 109  | ARG  | NE-CZ-NH2   | -6.17 | 117.22      | 120.30   |
| 22  | AV    | 57   | A    | C4-C5-C6    | 6.17  | 120.08      | 117.00   |
| 35  | BB    | 406  | G    | C4-C5-N7    | -6.17 | 108.33      | 110.80   |
| 35  | BB    | 875  | G    | N1-C6-O6    | 6.17  | 123.60      | 119.90   |
| 35  | BB    | 2151 | U    | P-O5'-C5'   | 6.17  | 130.77      | 120.90   |
| 35  | BB    | 2569 | G    | O4'-C1'-N9  | 6.17  | 113.14      | 108.20   |
| 35  | BB    | 2718 | G    | P-O5'-C5'   | -6.17 | 111.03      | 120.90   |
| 1   | AA    | 35   | G    | C5-C6-O6    | -6.17 | 124.90      | 128.60   |
| 1   | AA    | 249  | U    | N3-C2-O2    | 6.17  | 126.52      | 122.20   |
| 1   | AA    | 503  | C    | C5-C4-N4    | -6.17 | 115.88      | 120.20   |
| 1   | AA    | 630  | A    | C5-C6-N1    | -6.17 | 114.62      | 117.70   |
| 1   | AA    | 962  | C    | N3-C2-O2    | 6.17  | 126.22      | 121.90   |
| 1   | AA    | 1093 | A    | C4-C5-N7    | 6.17  | 113.78      | 110.70   |
| 1   | AA    | 1349 | A    | N1-C6-N6    | 6.17  | 122.30      | 118.60   |
| 9   | AI    | 129  | ARG  | NE-CZ-NH2   | -6.17 | 117.22      | 120.30   |
| 11  | AK    | 122  | PRO  | N-CA-CB     | -6.17 | 95.81       | 102.60   |
| 15  | AO    | 53   | ARG  | NE-CZ-NH1   | 6.17  | 123.38      | 120.30   |
| 35  | BB    | 277  | G    | N7-C8-N9    | -6.17 | 110.02      | 113.10   |
| 35  | BB    | 405  | U    | C6-N1-C2    | 6.17  | 124.70      | 121.00   |
| 35  | BB    | 1164 | C    | C1'-O4'-C4' | -6.17 | 104.97      | 109.90   |
| 35  | BB    | 1951 | U    | C2-N3-C4    | 6.17  | 130.70      | 127.00   |
| 35  | BB    | 2148 | G    | P-O3'-C3'   | 6.17  | 127.10      | 119.70   |
| 35  | BB    | 2688 | G    | P-O3'-C3'   | -6.17 | 112.30      | 119.70   |
| 1   | AA    | 1093 | A    | C2-N3-C4    | 6.17  | 113.68      | 110.60   |
| 34  | BA    | 101  | A    | N9-C4-C5    | -6.17 | 103.33      | 105.80   |
| 35  | BB    | 249  | C    | C4-C5-C6    | -6.17 | 114.32      | 117.40   |
| 35  | BB    | 423  | A    | C8-N9-C4    | -6.17 | 103.33      | 105.80   |
| 35  | BB    | 523  | C    | C6-N1-C2    | 6.17  | 122.77      | 120.30   |
| 1   | AA    | 129  | A    | C4-C5-N7    | -6.17 | 107.62      | 110.70   |
| 1   | AA    | 213  | G    | C1'-O4'-C4' | -6.17 | 104.97      | 109.90   |
| 1   | AA    | 272  | C    | C2-N3-C4    | 6.17  | 122.98      | 119.90   |
| 1   | AA    | 799  | G    | C2-N3-C4    | 6.17  | 114.98      | 111.90   |
| 35  | BB    | 375  | G    | C5-N7-C8    | 6.17  | 107.38      | 104.30   |
| 35  | BB    | 2046 | G    | N3-C2-N2    | 6.17  | 124.22      | 119.90   |
| 1   | AA    | 295  | C    | C2-N3-C4    | 6.16  | 122.98      | 119.90   |
| 1   | AA    | 404  | G    | N1-C2-N3    | -6.16 | 120.20      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 604  | G    | N1-C2-N2    | -6.16 | 110.65      | 116.20   |
| 1   | AA    | 615  | G    | O4'-C1'-N9  | 6.16  | 113.13      | 108.20   |
| 1   | AA    | 1236 | A    | C6-C5-N7    | -6.16 | 127.99      | 132.30   |
| 3   | AC    | 182  | ASP  | CB-CG-OD2   | -6.16 | 112.75      | 118.30   |
| 35  | BB    | 534  | U    | N3-C4-O4    | 6.16  | 123.71      | 119.40   |
| 35  | BB    | 614  | A    | C5'-C4'-C3' | -6.16 | 106.14      | 116.00   |
| 35  | BB    | 641  | U    | N3-C2-O2    | 6.16  | 126.52      | 122.20   |
| 35  | BB    | 875  | G    | O4'-C1'-N9  | 6.16  | 113.13      | 108.20   |
| 35  | BB    | 1142 | A    | N1-C2-N3    | -6.16 | 126.22      | 129.30   |
| 35  | BB    | 1246 | A    | C6-N1-C2    | 6.16  | 122.30      | 118.60   |
| 35  | BB    | 1567 | G    | O4'-C1'-N9  | 6.16  | 113.13      | 108.20   |
| 35  | BB    | 1778 | U    | C6-N1-C2    | -6.16 | 117.30      | 121.00   |
| 35  | BB    | 2108 | A    | N1-C6-N6    | 6.16  | 122.30      | 118.60   |
| 1   | AA    | 84   | U    | C3'-C2'-C1' | -6.16 | 96.57       | 101.50   |
| 1   | AA    | 728  | A    | C1'-O4'-C4' | 6.16  | 114.83      | 109.90   |
| 35  | BB    | 194  | G    | N3-C4-C5    | 6.16  | 131.68      | 128.60   |
| 35  | BB    | 294  | A    | N1-C2-N3    | 6.16  | 132.38      | 129.30   |
| 35  | BB    | 1354 | A    | C2-N3-C4    | -6.16 | 107.52      | 110.60   |
| 35  | BB    | 1523 | U    | OP1-P-OP2   | -6.16 | 110.36      | 119.60   |
| 35  | BB    | 2416 | C    | C3'-C2'-C1' | -6.16 | 96.57       | 101.50   |
| 35  | BB    | 2717 | C    | C2-N1-C1'   | 6.16  | 125.58      | 118.80   |
| 40  | BG    | 29   | ASN  | N-CA-CB     | 6.16  | 121.69      | 110.60   |
| 1   | AA    | 48   | C    | C6-N1-C2    | -6.16 | 117.84      | 120.30   |
| 1   | AA    | 452  | A    | C4-C5-C6    | 6.16  | 120.08      | 117.00   |
| 1   | AA    | 1092 | A    | C1'-O4'-C4' | -6.16 | 104.97      | 109.90   |
| 1   | AA    | 1492 | A    | N3-C4-C5    | -6.16 | 122.49      | 126.80   |
| 35  | BB    | 621  | A    | C5-N7-C8    | -6.16 | 100.82      | 103.90   |
| 35  | BB    | 1008 | A    | C2-N3-C4    | -6.16 | 107.52      | 110.60   |
| 35  | BB    | 1709 | U    | N3-C2-O2    | 6.16  | 126.51      | 122.20   |
| 35  | BB    | 2087 | G    | O4'-C1'-N9  | 6.16  | 113.13      | 108.20   |
| 35  | BB    | 2445 | G    | C2'-C3'-O3' | 6.16  | 123.56      | 113.70   |
| 35  | BB    | 2470 | G    | O4'-C1'-N9  | 6.16  | 113.13      | 108.20   |
| 35  | BB    | 2523 | G    | C6-C5-N7    | -6.16 | 126.70      | 130.40   |
| 1   | AA    | 1268 | G    | N3-C4-C5    | -6.16 | 125.52      | 128.60   |
| 1   | AA    | 1427 | C    | P-O3'-C3'   | -6.16 | 112.31      | 119.70   |
| 1   | AA    | 1503 | A    | O5'-P-OP1   | -6.16 | 100.16      | 105.70   |
| 7   | AG    | 118  | ARG  | NE-CZ-NH1   | 6.16  | 123.38      | 120.30   |
| 35  | BB    | 231  | A    | C5-C6-N6    | -6.16 | 118.77      | 123.70   |
| 35  | BB    | 1255 | U    | P-O3'-C3'   | -6.16 | 112.31      | 119.70   |
| 35  | BB    | 1586 | A    | C5-C6-N6    | -6.16 | 118.77      | 123.70   |
| 35  | BB    | 1605 | C    | O4'-C1'-N1  | 6.16  | 113.13      | 108.20   |
| 35  | BB    | 1720 | U    | N3-C4-O4    | 6.16  | 123.71      | 119.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1899 | A    | N1-C2-N3    | 6.16  | 132.38      | 129.30   |
| 35  | BB    | 1953 | A    | C4-C5-C6    | 6.16  | 120.08      | 117.00   |
| 35  | BB    | 2602 | A    | N1-C2-N3    | 6.16  | 132.38      | 129.30   |
| 1   | AA    | 1229 | A    | C4'-C3'-C2' | -6.16 | 96.44       | 102.60   |
| 35  | BB    | 794  | A    | C5-C6-N6    | -6.16 | 118.78      | 123.70   |
| 35  | BB    | 2395 | C    | N1-C2-O2    | 6.16  | 122.59      | 118.90   |
| 1   | AA    | 259  | G    | C3'-C2'-C1' | 6.16  | 106.42      | 101.50   |
| 1   | AA    | 517  | G    | C5'-C4'-O4' | 6.16  | 116.49      | 109.10   |
| 1   | AA    | 1086 | U    | N3-C4-O4    | 6.16  | 123.71      | 119.40   |
| 1   | AA    | 1156 | G    | C4-C5-N7    | -6.16 | 108.34      | 110.80   |
| 35  | BB    | 118  | A    | O4'-C1'-N9  | 6.16  | 113.12      | 108.20   |
| 35  | BB    | 141  | G    | N3-C4-C5    | 6.16  | 131.68      | 128.60   |
| 35  | BB    | 487  | C    | N1-C2-O2    | 6.16  | 122.59      | 118.90   |
| 35  | BB    | 496  | G    | C4-C5-N7    | 6.16  | 113.26      | 110.80   |
| 35  | BB    | 734  | A    | N1-C2-N3    | 6.16  | 132.38      | 129.30   |
| 35  | BB    | 830  | G    | N9-C4-C5    | 6.16  | 107.86      | 105.40   |
| 35  | BB    | 1028 | A    | C6-C5-N7    | -6.16 | 127.99      | 132.30   |
| 35  | BB    | 1059 | G    | C1'-O4'-C4' | -6.16 | 104.98      | 109.90   |
| 35  | BB    | 2477 | U    | N3-C4-O4    | 6.16  | 123.71      | 119.40   |
| 35  | BB    | 1926 | U    | C5-C6-N1    | 6.15  | 125.78      | 122.70   |
| 35  | BB    | 2231 | U    | C3'-C2'-C1' | -6.15 | 96.58       | 101.50   |
| 1   | AA    | 383  | A    | C4-C5-C6    | 6.15  | 120.08      | 117.00   |
| 1   | AA    | 758  | C    | C6-N1-C2    | -6.15 | 117.84      | 120.30   |
| 1   | AA    | 1148 | U    | C5-C4-O4    | -6.15 | 122.21      | 125.90   |
| 35  | BB    | 799  | G    | C5-N7-C8    | -6.15 | 101.22      | 104.30   |
| 35  | BB    | 852  | U    | C5-C6-N1    | 6.15  | 125.78      | 122.70   |
| 35  | BB    | 1068 | G    | C4-C5-N7    | -6.15 | 108.34      | 110.80   |
| 35  | BB    | 1099 | G    | C6-N1-C2    | -6.15 | 121.41      | 125.10   |
| 35  | BB    | 1177 | G    | C8-N9-C4    | 6.15  | 108.86      | 106.40   |
| 35  | BB    | 1206 | G    | N1-C2-N3    | -6.15 | 120.21      | 123.90   |
| 35  | BB    | 2718 | G    | N1-C2-N3    | -6.15 | 120.21      | 123.90   |
| 1   | AA    | 322  | C    | C5-C4-N4    | 6.15  | 124.50      | 120.20   |
| 1   | AA    | 577  | G    | N1-C2-N3    | -6.15 | 120.21      | 123.90   |
| 1   | AA    | 1087 | G    | C6-N1-C2    | 6.15  | 128.79      | 125.10   |
| 16  | AP    | 23   | ASP  | CB-CG-OD2   | 6.15  | 123.83      | 118.30   |
| 35  | BB    | 117  | G    | C4-C5-N7    | 6.15  | 113.26      | 110.80   |
| 35  | BB    | 483  | A    | N9-C4-C5    | 6.15  | 108.26      | 105.80   |
| 35  | BB    | 1546 | G    | C5'-C4'-C3' | -6.15 | 106.16      | 116.00   |
| 35  | BB    | 2099 | U    | O4'-C1'-N1  | 6.15  | 113.12      | 108.20   |
| 35  | BB    | 2279 | G    | N7-C8-N9    | 6.15  | 116.18      | 113.10   |
| 35  | BB    | 2577 | A    | P-O3'-C3'   | 6.15  | 127.08      | 119.70   |
| 36  | BC    | 59   | GLN  | N-CA-CB     | 6.15  | 121.67      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1187 | G    | N3-C2-N2    | 6.15  | 124.20      | 119.90   |
| 1   | AA    | 1393 | U    | C5-C4-O4    | -6.15 | 122.21      | 125.90   |
| 1   | AA    | 1402 | C    | C2-N3-C4    | 6.15  | 122.97      | 119.90   |
| 1   | AA    | 1405 | G    | C5-C6-N1    | -6.15 | 108.43      | 111.50   |
| 3   | AC    | 116  | ALA  | CB-CA-C     | 6.15  | 119.32      | 110.10   |
| 35  | BB    | 258  | G    | N3-C2-N2    | 6.15  | 124.20      | 119.90   |
| 35  | BB    | 867  | C    | N1-C2-N3    | -6.15 | 114.90      | 119.20   |
| 35  | BB    | 1167 | C    | C1'-O4'-C4' | 6.15  | 114.82      | 109.90   |
| 35  | BB    | 1276 | A    | N7-C8-N9    | 6.15  | 116.88      | 113.80   |
| 35  | BB    | 1914 | C    | N3-C4-N4    | 6.15  | 122.30      | 118.00   |
| 1   | AA    | 119  | A    | N1-C6-N6    | 6.15  | 122.29      | 118.60   |
| 1   | AA    | 720  | C    | C4-C5-C6    | -6.15 | 114.33      | 117.40   |
| 1   | AA    | 1012 | A    | C5-N7-C8    | 6.15  | 106.97      | 103.90   |
| 1   | AA    | 1266 | G    | N1-C6-O6    | 6.15  | 123.59      | 119.90   |
| 20  | AT    | 69   | ASN  | CB-CA-C     | -6.15 | 98.10       | 110.40   |
| 35  | BB    | 1275 | A    | C3'-C2'-C1' | 6.15  | 106.42      | 101.50   |
| 35  | BB    | 1425 | G    | P-O3'-C3'   | -6.15 | 112.32      | 119.70   |
| 1   | AA    | 1522 | U    | N1-C2-O2    | 6.15  | 127.10      | 122.80   |
| 13  | AM    | 107  | THR  | CA-CB-CG2   | -6.15 | 103.80      | 112.40   |
| 35  | BB    | 57   | C    | N3-C4-C5    | -6.15 | 119.44      | 121.90   |
| 35  | BB    | 287  | G    | N7-C8-N9    | 6.15  | 116.17      | 113.10   |
| 35  | BB    | 449  | A    | C2-N3-C4    | 6.15  | 113.67      | 110.60   |
| 35  | BB    | 1197 | G    | N7-C8-N9    | 6.15  | 116.17      | 113.10   |
| 35  | BB    | 1858 | A    | OP1-P-OP2   | -6.15 | 110.38      | 119.60   |
| 35  | BB    | 2200 | C    | C6-N1-C1'   | -6.15 | 113.42      | 120.80   |
| 1   | AA    | 36   | C    | N1-C1'-C2'  | -6.14 | 105.24      | 112.00   |
| 1   | AA    | 227  | G    | C6-C5-N7    | -6.14 | 126.71      | 130.40   |
| 1   | AA    | 881  | G    | C4'-C3'-C2' | -6.14 | 96.45       | 102.60   |
| 1   | AA    | 1070 | U    | C5-C4-O4    | -6.14 | 122.21      | 125.90   |
| 1   | AA    | 1096 | C    | C6-N1-C2    | 6.14  | 122.76      | 120.30   |
| 1   | AA    | 1357 | A    | C2-N3-C4    | -6.14 | 107.53      | 110.60   |
| 3   | AC    | 176  | THR  | CA-CB-CG2   | -6.14 | 103.80      | 112.40   |
| 19  | AS    | 80   | ARG  | NE-CZ-NH2   | -6.14 | 117.23      | 120.30   |
| 34  | BA    | 36   | C    | N3-C4-C5    | -6.14 | 119.44      | 121.90   |
| 35  | BB    | 109  | C    | N3-C4-C5    | -6.14 | 119.44      | 121.90   |
| 35  | BB    | 217  | A    | N3-C4-N9    | 6.14  | 132.31      | 127.40   |
| 35  | BB    | 419  | U    | N1-C2-O2    | -6.14 | 118.50      | 122.80   |
| 35  | BB    | 602  | A    | C5-N7-C8    | 6.14  | 106.97      | 103.90   |
| 35  | BB    | 1042 | G    | P-O3'-C3'   | -6.14 | 112.33      | 119.70   |
| 35  | BB    | 1212 | G    | C4'-C3'-C2' | -6.14 | 96.46       | 102.60   |
| 35  | BB    | 1274 | A    | C1'-O4'-C4' | -6.14 | 104.98      | 109.90   |
| 1   | AA    | 404  | G    | C6-C5-N7    | -6.14 | 126.72      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 781  | A    | C5-N7-C8    | 6.14  | 106.97      | 103.90   |
| 1   | AA    | 1185 | G    | O4'-C1'-C2' | -6.14 | 99.66       | 105.80   |
| 5   | AE    | 68   | ARG  | NE-CZ-NH2   | -6.14 | 117.23      | 120.30   |
| 35  | BB    | 5    | A    | C4'-C3'-C2' | -6.14 | 96.46       | 102.60   |
| 35  | BB    | 303  | G    | C6-C5-N7    | -6.14 | 126.72      | 130.40   |
| 35  | BB    | 307  | G    | C5-C6-N1    | -6.14 | 108.43      | 111.50   |
| 35  | BB    | 618  | G    | C6-C5-N7    | -6.14 | 126.72      | 130.40   |
| 35  | BB    | 934  | U    | C2-N3-C4    | 6.14  | 130.69      | 127.00   |
| 35  | BB    | 1163 | G    | N7-C8-N9    | -6.14 | 110.03      | 113.10   |
| 35  | BB    | 1836 | C    | N3-C4-N4    | 6.14  | 122.30      | 118.00   |
| 35  | BB    | 2107 | G    | O3'-P-O5'   | -6.14 | 92.33       | 104.00   |
| 35  | BB    | 2213 | U    | C1'-O4'-C4' | -6.14 | 104.99      | 109.90   |
| 35  | BB    | 2659 | G    | N7-C8-N9    | 6.14  | 116.17      | 113.10   |
| 1   | AA    | 289  | G    | O4'-C1'-N9  | 6.14  | 113.11      | 108.20   |
| 1   | AA    | 523  | A    | N9-C4-C5    | 6.14  | 108.26      | 105.80   |
| 1   | AA    | 1122 | U    | N1-C2-O2    | -6.14 | 118.50      | 122.80   |
| 1   | AA    | 1487 | G    | C4-C5-N7    | -6.14 | 108.34      | 110.80   |
| 22  | AV    | 13   | C    | N3-C4-N4    | 6.14  | 122.30      | 118.00   |
| 35  | BB    | 309  | A    | N3-C4-N9    | -6.14 | 122.49      | 127.40   |
| 35  | BB    | 1487 | U    | C4'-C3'-C2' | -6.14 | 96.46       | 102.60   |
| 1   | AA    | 829  | G    | N7-C8-N9    | 6.14  | 116.17      | 113.10   |
| 1   | AA    | 1198 | G    | N1-C6-O6    | 6.14  | 123.58      | 119.90   |
| 21  | AU    | 37   | TYR  | CB-CG-CD2   | -6.14 | 117.32      | 121.00   |
| 34  | BA    | 62   | C    | C5-C4-N4    | -6.14 | 115.90      | 120.20   |
| 35  | BB    | 702  | U    | C5-C6-N1    | 6.14  | 125.77      | 122.70   |
| 35  | BB    | 895  | U    | N1-C2-O2    | -6.14 | 118.50      | 122.80   |
| 35  | BB    | 1075 | C    | C2-N1-C1'   | -6.14 | 112.05      | 118.80   |
| 35  | BB    | 1322 | A    | C4-C5-C6    | 6.14  | 120.07      | 117.00   |
| 35  | BB    | 1527 | G    | O4'-C1'-N9  | 6.14  | 113.11      | 108.20   |
| 35  | BB    | 1529 | G    | C8-N9-C4    | -6.14 | 103.94      | 106.40   |
| 35  | BB    | 2278 | A    | C4-C5-C6    | 6.14  | 120.07      | 117.00   |
| 1   | AA    | 128  | G    | N1-C2-N2    | -6.14 | 110.68      | 116.20   |
| 1   | AA    | 1531 | A    | N3-C4-C5    | -6.14 | 122.50      | 126.80   |
| 34  | BA    | 57   | A    | C1'-O4'-C4' | -6.14 | 104.99      | 109.90   |
| 35  | BB    | 698  | C    | C6-N1-C1'   | 6.14  | 128.16      | 120.80   |
| 35  | BB    | 1535 | A    | C4-C5-N7    | 6.14  | 113.77      | 110.70   |
| 35  | BB    | 1653 | G    | N9-C4-C5    | -6.14 | 102.94      | 105.40   |
| 1   | AA    | 860  | A    | C4-C5-C6    | 6.14  | 120.07      | 117.00   |
| 1   | AA    | 1403 | C    | N3-C4-N4    | 6.14  | 122.30      | 118.00   |
| 35  | BB    | 52   | A    | C4'-C3'-C2' | -6.14 | 96.46       | 102.60   |
| 35  | BB    | 218  | A    | N3-C4-N9    | -6.14 | 122.49      | 127.40   |
| 35  | BB    | 604  | G    | C5-C6-N1    | -6.14 | 108.43      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 715  | A    | N1-C2-N3    | 6.14  | 132.37      | 129.30   |
| 35  | BB    | 808  | G    | N1-C6-O6    | 6.14  | 123.58      | 119.90   |
| 35  | BB    | 1638 | C    | N3-C4-N4    | 6.14  | 122.30      | 118.00   |
| 35  | BB    | 2371 | G    | C4-C5-C6    | 6.14  | 122.48      | 118.80   |
| 35  | BB    | 2590 | A    | C1'-O4'-C4' | 6.14  | 114.81      | 109.90   |
| 41  | BH    | 149  | GLU  | N-CA-CB     | 6.14  | 121.65      | 110.60   |
| 56  | BY    | 14   | ASP  | CB-CG-OD2   | 6.14  | 123.82      | 118.30   |
| 1   | AA    | 1142 | G    | N9-C4-C5    | 6.13  | 107.85      | 105.40   |
| 1   | AA    | 1173 | U    | C5-C4-O4    | -6.13 | 122.22      | 125.90   |
| 1   | AA    | 1220 | G    | C2-N3-C4    | 6.13  | 114.97      | 111.90   |
| 1   | AA    | 1310 | G    | C5-N7-C8    | -6.13 | 101.23      | 104.30   |
| 34  | BA    | 106  | G    | N1-C6-O6    | 6.13  | 123.58      | 119.90   |
| 35  | BB    | 48   | G    | C8-N9-C4    | 6.13  | 108.85      | 106.40   |
| 35  | BB    | 103  | A    | C4-C5-N7    | -6.13 | 107.63      | 110.70   |
| 35  | BB    | 355  | U    | P-O3'-C3'   | -6.13 | 112.34      | 119.70   |
| 35  | BB    | 496  | G    | C5'-C4'-C3' | -6.13 | 106.19      | 116.00   |
| 35  | BB    | 806  | C    | N3-C4-N4    | 6.13  | 122.29      | 118.00   |
| 35  | BB    | 833  | A    | O4'-C1'-N9  | 6.13  | 113.11      | 108.20   |
| 35  | BB    | 886  | A    | C5-C6-N6    | -6.13 | 118.79      | 123.70   |
| 35  | BB    | 899  | A    | N9-C4-C5    | -6.13 | 103.35      | 105.80   |
| 35  | BB    | 1066 | U    | O4'-C1'-N1  | 6.13  | 113.11      | 108.20   |
| 35  | BB    | 1189 | A    | N3-C4-N9    | -6.13 | 122.49      | 127.40   |
| 35  | BB    | 1203 | U    | C4-C5-C6    | 6.13  | 123.38      | 119.70   |
| 35  | BB    | 2565 | A    | C5-C6-N6    | -6.13 | 118.79      | 123.70   |
| 35  | BB    | 2625 | G    | C6-C5-N7    | -6.13 | 126.72      | 130.40   |
| 1   | AA    | 400  | C    | P-O3'-C3'   | -6.13 | 112.34      | 119.70   |
| 1   | AA    | 410  | G    | N1-C2-N3    | -6.13 | 120.22      | 123.90   |
| 1   | AA    | 669  | G    | N1-C6-O6    | 6.13  | 123.58      | 119.90   |
| 2   | AB    | 112  | ARG  | NE-CZ-NH1   | 6.13  | 123.37      | 120.30   |
| 35  | BB    | 187  | G    | O4'-C1'-N9  | 6.13  | 113.11      | 108.20   |
| 35  | BB    | 1423 | G    | C5-C6-O6    | -6.13 | 124.92      | 128.60   |
| 35  | BB    | 2645 | G    | C6-C5-N7    | -6.13 | 126.72      | 130.40   |
| 1   | AA    | 111  | G    | C5-N7-C8    | 6.13  | 107.37      | 104.30   |
| 1   | AA    | 185  | U    | C5-C6-N1    | 6.13  | 125.77      | 122.70   |
| 1   | AA    | 561  | U    | N3-C4-O4    | -6.13 | 115.11      | 119.40   |
| 35  | BB    | 767  | U    | N1-C2-O2    | -6.13 | 118.51      | 122.80   |
| 35  | BB    | 1233 | C    | N1-C1'-C2'  | -6.13 | 105.25      | 112.00   |
| 35  | BB    | 1359 | A    | C8-N9-C4    | -6.13 | 103.35      | 105.80   |
| 35  | BB    | 1941 | C    | C5-C4-N4    | -6.13 | 115.91      | 120.20   |
| 35  | BB    | 2057 | G    | C5-C6-N1    | -6.13 | 108.43      | 111.50   |
| 35  | BB    | 2144 | G    | C4-C5-C6    | 6.13  | 122.48      | 118.80   |
| 35  | BB    | 2223 | G    | O4'-C1'-N9  | 6.13  | 113.11      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2502 | G    | C6-C5-N7    | -6.13 | 126.72      | 130.40   |
| 35  | BB    | 2689 | U    | N1-C2-O2    | 6.13  | 127.09      | 122.80   |
| 35  | BB    | 2763 | G    | N7-C8-N9    | 6.13  | 116.17      | 113.10   |
| 35  | BB    | 2843 | G    | N3-C4-C5    | -6.13 | 125.53      | 128.60   |
| 52  | BS    | 34   | ASP  | CB-CA-C     | -6.13 | 98.14       | 110.40   |
| 34  | BA    | 37   | C    | C1'-O4'-C4' | 6.13  | 114.80      | 109.90   |
| 35  | BB    | 162  | U    | O4'-C1'-N1  | 6.13  | 113.10      | 108.20   |
| 35  | BB    | 205  | G    | C6-C5-N7    | -6.13 | 126.72      | 130.40   |
| 35  | BB    | 743  | A    | P-O3'-C3'   | -6.13 | 112.34      | 119.70   |
| 1   | AA    | 189  | A    | C5-C6-N1    | -6.13 | 114.64      | 117.70   |
| 35  | BB    | 119  | A    | O4'-C1'-N9  | 6.13  | 113.10      | 108.20   |
| 35  | BB    | 571  | U    | O4'-C1'-N1  | 6.13  | 113.10      | 108.20   |
| 35  | BB    | 769  | U    | C5-C4-O4    | -6.13 | 122.22      | 125.90   |
| 35  | BB    | 912  | C    | P-O5'-C5'   | 6.13  | 130.71      | 120.90   |
| 35  | BB    | 981  | A    | N3-C4-C5    | -6.13 | 122.51      | 126.80   |
| 35  | BB    | 1207 | C    | N3-C4-C5    | -6.13 | 119.45      | 121.90   |
| 35  | BB    | 2382 | G    | N9-C4-C5    | -6.13 | 102.95      | 105.40   |
| 35  | BB    | 2399 | G    | P-O3'-C3'   | -6.13 | 112.35      | 119.70   |
| 35  | BB    | 43   | G    | N1-C2-N3    | -6.13 | 120.22      | 123.90   |
| 35  | BB    | 51   | G    | C5-C6-O6    | -6.13 | 124.92      | 128.60   |
| 35  | BB    | 723  | C    | C5-C4-N4    | -6.13 | 115.91      | 120.20   |
| 35  | BB    | 756  | A    | O4'-C1'-N9  | 6.13  | 113.10      | 108.20   |
| 35  | BB    | 808  | G    | C2-N3-C4    | -6.13 | 108.84      | 111.90   |
| 35  | BB    | 1036 | G    | N3-C2-N2    | 6.13  | 124.19      | 119.90   |
| 35  | BB    | 1394 | U    | C4'-C3'-C2' | -6.13 | 96.47       | 102.60   |
| 35  | BB    | 1475 | G    | C2-N3-C4    | 6.13  | 114.96      | 111.90   |
| 35  | BB    | 1604 | C    | O4'-C1'-N1  | 6.13  | 113.10      | 108.20   |
| 35  | BB    | 1910 | G    | C6-C5-N7    | -6.13 | 126.72      | 130.40   |
| 35  | BB    | 2100 | G    | C8-N9-C4    | -6.13 | 103.95      | 106.40   |
| 35  | BB    | 2172 | U    | N1-C2-N3    | -6.13 | 111.22      | 114.90   |
| 35  | BB    | 2563 | U    | C2-N3-C4    | 6.13  | 130.68      | 127.00   |
| 35  | BB    | 2902 | C    | C1'-O4'-C4' | -6.13 | 105.00      | 109.90   |
| 1   | AA    | 280  | C    | C4'-C3'-C2' | 6.12  | 108.72      | 102.60   |
| 1   | AA    | 756  | C    | C5-C4-N4    | -6.12 | 115.91      | 120.20   |
| 1   | AA    | 817  | C    | C5'-C4'-C3' | -6.12 | 106.20      | 116.00   |
| 1   | AA    | 838  | G    | C4-C5-N7    | 6.12  | 113.25      | 110.80   |
| 13  | AM    | 91   | ARG  | NE-CZ-NH1   | 6.12  | 123.36      | 120.30   |
| 35  | BB    | 328  | U    | O4'-C1'-N1  | 6.12  | 113.10      | 108.20   |
| 35  | BB    | 366  | C    | C2-N3-C4    | 6.12  | 122.96      | 119.90   |
| 35  | BB    | 570  | G    | N9-C4-C5    | 6.12  | 107.85      | 105.40   |
| 35  | BB    | 1372 | U    | C5-C6-N1    | -6.12 | 119.64      | 122.70   |
| 35  | BB    | 1429 | G    | C4-C5-C6    | 6.12  | 122.47      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2065 | C    | O4'-C1'-C2' | 6.12  | 113.11      | 107.60   |
| 35  | BB    | 2455 | G    | N1-C2-N2    | -6.12 | 110.69      | 116.20   |
| 1   | AA    | 660  | C    | N3-C4-N4    | 6.12  | 122.29      | 118.00   |
| 1   | AA    | 742  | G    | O4'-C1'-N9  | 6.12  | 113.10      | 108.20   |
| 1   | AA    | 1002 | G    | C2-N3-C4    | 6.12  | 114.96      | 111.90   |
| 11  | AK    | 76   | TYR  | CB-CG-CD1   | -6.12 | 117.33      | 121.00   |
| 35  | BB    | 638  | G    | C8-N9-C1'   | 6.12  | 134.96      | 127.00   |
| 35  | BB    | 1266 | G    | O4'-C1'-C2' | -6.12 | 99.68       | 105.80   |
| 35  | BB    | 1563 | U    | N1-C2-N3    | -6.12 | 111.23      | 114.90   |
| 35  | BB    | 2127 | G    | C5'-C4'-O4' | -6.12 | 101.75      | 109.10   |
| 1   | AA    | 140  | U    | C1'-O4'-C4' | -6.12 | 105.00      | 109.90   |
| 1   | AA    | 407  | U    | O4'-C1'-N1  | 6.12  | 113.10      | 108.20   |
| 1   | AA    | 437  | U    | N3-C4-C5    | -6.12 | 110.93      | 114.60   |
| 1   | AA    | 728  | A    | N3-C4-C5    | -6.12 | 122.52      | 126.80   |
| 1   | AA    | 955  | U    | N3-C4-O4    | 6.12  | 123.69      | 119.40   |
| 19  | AS    | 79   | TYR  | CB-CG-CD1   | -6.12 | 117.33      | 121.00   |
| 35  | BB    | 1160 | G    | C5'-C4'-C3' | 6.12  | 125.79      | 116.00   |
| 35  | BB    | 1594 | U    | N1-C2-O2    | -6.12 | 118.52      | 122.80   |
| 35  | BB    | 1625 | C    | N3-C4-C5    | -6.12 | 119.45      | 121.90   |
| 35  | BB    | 1928 | A    | C5-C6-N6    | -6.12 | 118.80      | 123.70   |
| 35  | BB    | 2493 | U    | C4-C5-C6    | 6.12  | 123.37      | 119.70   |
| 36  | BC    | 82   | TYR  | CB-CG-CD1   | -6.12 | 117.33      | 121.00   |
| 1   | AA    | 304  | U    | N3-C4-C5    | -6.12 | 110.93      | 114.60   |
| 1   | AA    | 951  | G    | C5-C6-N1    | -6.12 | 108.44      | 111.50   |
| 1   | AA    | 1092 | A    | C5-C6-N1    | -6.12 | 114.64      | 117.70   |
| 35  | BB    | 727  | A    | C3'-C2'-C1' | 6.12  | 106.40      | 101.50   |
| 35  | BB    | 1880 | U    | C5-C6-N1    | 6.12  | 125.76      | 122.70   |
| 1   | AA    | 31   | G    | C5'-C4'-C3' | -6.12 | 106.21      | 116.00   |
| 1   | AA    | 69   | G    | N3-C4-C5    | 6.12  | 131.66      | 128.60   |
| 1   | AA    | 627  | G    | C6-C5-N7    | -6.12 | 126.73      | 130.40   |
| 1   | AA    | 916  | U    | O4'-C1'-N1  | 6.12  | 113.10      | 108.20   |
| 1   | AA    | 962  | C    | C1'-O4'-C4' | 6.12  | 114.80      | 109.90   |
| 35  | BB    | 407  | G    | N3-C4-C5    | -6.12 | 125.54      | 128.60   |
| 35  | BB    | 468  | G    | N1-C2-N3    | -6.12 | 120.23      | 123.90   |
| 35  | BB    | 1366 | A    | O4'-C1'-N9  | 6.12  | 113.09      | 108.20   |
| 35  | BB    | 1369 | G    | N1-C2-N3    | -6.12 | 120.23      | 123.90   |
| 35  | BB    | 1663 | G    | P-O3'-C3'   | 6.12  | 127.04      | 119.70   |
| 35  | BB    | 1664 | A    | C5-C6-N1    | -6.12 | 114.64      | 117.70   |
| 35  | BB    | 2829 | A    | C4-C5-N7    | 6.12  | 113.76      | 110.70   |
| 35  | BB    | 2860 | A    | C4-C5-C6    | 6.12  | 120.06      | 117.00   |
| 1   | AA    | 474  | G    | C4-C5-C6    | 6.12  | 122.47      | 118.80   |
| 1   | AA    | 511  | C    | C5'-C4'-O4' | 6.12  | 116.44      | 109.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | BA    | 7    | G    | N3-C2-N2    | 6.12  | 124.18      | 119.90   |
| 35  | BB    | 2788 | C    | C5-C6-N1    | 6.12  | 124.06      | 121.00   |
| 1   | AA    | 377  | G    | C8-N9-C4    | -6.12 | 103.95      | 106.40   |
| 1   | AA    | 418  | C    | C2-N1-C1'   | 6.12  | 125.53      | 118.80   |
| 1   | AA    | 964  | A    | O4'-C1'-N9  | 6.12  | 113.09      | 108.20   |
| 1   | AA    | 1043 | G    | C4'-C3'-C2' | 6.12  | 108.72      | 102.60   |
| 34  | BA    | 118  | C    | N1-C2-O2    | -6.12 | 115.23      | 118.90   |
| 35  | BB    | 366  | C    | P-O3'-C3'   | -6.12 | 112.36      | 119.70   |
| 35  | BB    | 500  | G    | C4-C5-C6    | 6.12  | 122.47      | 118.80   |
| 35  | BB    | 623  | C    | C4'-C3'-C2' | -6.12 | 96.48       | 102.60   |
| 35  | BB    | 805  | G    | C5-C6-O6    | -6.12 | 124.93      | 128.60   |
| 35  | BB    | 912  | C    | C6-N1-C2    | -6.12 | 117.85      | 120.30   |
| 35  | BB    | 1029 | A    | C6-C5-N7    | -6.12 | 128.02      | 132.30   |
| 35  | BB    | 1072 | C    | C6-N1-C2    | -6.12 | 117.85      | 120.30   |
| 35  | BB    | 1567 | G    | C5-C6-O6    | -6.12 | 124.93      | 128.60   |
| 35  | BB    | 1929 | G    | N1-C6-O6    | 6.12  | 123.57      | 119.90   |
| 35  | BB    | 2095 | A    | C5'-C4'-O4' | 6.12  | 116.44      | 109.10   |
| 35  | BB    | 2748 | A    | N9-C4-C5    | -6.12 | 103.35      | 105.80   |
| 35  | BB    | 2846 | G    | O4'-C1'-N9  | 6.12  | 113.09      | 108.20   |
| 1   | AA    | 203  | G    | P-O3'-C3'   | -6.11 | 112.36      | 119.70   |
| 1   | AA    | 805  | C    | C6-N1-C2    | -6.11 | 117.85      | 120.30   |
| 1   | AA    | 973  | G    | N7-C8-N9    | 6.11  | 116.16      | 113.10   |
| 1   | AA    | 1063 | C    | N3-C4-N4    | 6.11  | 122.28      | 118.00   |
| 1   | AA    | 1072 | G    | OP1-P-OP2   | -6.11 | 110.43      | 119.60   |
| 1   | AA    | 1483 | A    | C5-C6-N6    | -6.11 | 118.81      | 123.70   |
| 35  | BB    | 930  | G    | C5-C6-O6    | -6.11 | 124.93      | 128.60   |
| 35  | BB    | 1527 | G    | C5-C6-N1    | -6.11 | 108.44      | 111.50   |
| 35  | BB    | 1861 | G    | C1'-O4'-C4' | -6.11 | 105.01      | 109.90   |
| 35  | BB    | 1870 | C    | O4'-C1'-N1  | 6.11  | 113.09      | 108.20   |
| 35  | BB    | 2405 | G    | C5-N7-C8    | 6.11  | 107.36      | 104.30   |
| 1   | AA    | 92   | U    | O4'-C1'-N1  | 6.11  | 113.09      | 108.20   |
| 35  | BB    | 26   | G    | N1-C2-N3    | -6.11 | 120.23      | 123.90   |
| 35  | BB    | 507  | A    | O4'-C1'-N9  | 6.11  | 113.09      | 108.20   |
| 35  | BB    | 1232 | G    | O4'-C1'-N9  | 6.11  | 113.09      | 108.20   |
| 46  | BM    | 75   | GLU  | N-CA-C      | -6.11 | 94.50       | 111.00   |
| 1   | AA    | 1041 | G    | O4'-C1'-N9  | 6.11  | 113.09      | 108.20   |
| 4   | AD    | 18   | LEU  | N-CA-CB     | 6.11  | 122.62      | 110.40   |
| 35  | BB    | 459  | U    | N1-C2-O2    | -6.11 | 118.52      | 122.80   |
| 35  | BB    | 606  | U    | P-O3'-C3'   | 6.11  | 127.03      | 119.70   |
| 35  | BB    | 1027 | A    | C5-C6-N6    | -6.11 | 118.81      | 123.70   |
| 35  | BB    | 1525 | A    | C5-C6-N1    | -6.11 | 114.64      | 117.70   |
| 35  | BB    | 2147 | A    | N1-C2-N3    | 6.11  | 132.35      | 129.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2533 | U    | N3-C2-O2    | -6.11 | 117.92      | 122.20   |
| 40  | BG    | 51   | PHE  | CB-CG-CD1   | -6.11 | 116.52      | 120.80   |
| 1   | AA    | 488  | C    | N1-C2-O2    | -6.11 | 115.23      | 118.90   |
| 1   | AA    | 1300 | G    | C5-N7-C8    | 6.11  | 107.36      | 104.30   |
| 35  | BB    | 711  | G    | C8-N9-C4    | -6.11 | 103.96      | 106.40   |
| 35  | BB    | 830  | G    | C4-C5-N7    | -6.11 | 108.36      | 110.80   |
| 43  | BJ    | 6    | ALA  | CB-CA-C     | -6.11 | 100.94      | 110.10   |
| 1   | AA    | 149  | A    | O4'-C1'-N9  | 6.11  | 113.08      | 108.20   |
| 1   | AA    | 353  | A    | C4-C5-N7    | -6.11 | 107.65      | 110.70   |
| 1   | AA    | 592  | G    | C5-C6-N1    | -6.11 | 108.45      | 111.50   |
| 1   | AA    | 725  | G    | C8-N9-C4    | 6.11  | 108.84      | 106.40   |
| 35  | BB    | 262  | A    | C6-N1-C2    | 6.11  | 122.26      | 118.60   |
| 35  | BB    | 313  | G    | C5-C6-N1    | -6.11 | 108.45      | 111.50   |
| 35  | BB    | 527  | C    | C6-N1-C1'   | -6.11 | 113.47      | 120.80   |
| 35  | BB    | 594  | U    | N3-C4-C5    | -6.11 | 110.94      | 114.60   |
| 35  | BB    | 898  | C    | N3-C4-C5    | -6.11 | 119.46      | 121.90   |
| 35  | BB    | 1161 | C    | N3-C4-C5    | -6.11 | 119.46      | 121.90   |
| 35  | BB    | 1452 | G    | N1-C2-N3    | -6.11 | 120.24      | 123.90   |
| 35  | BB    | 2119 | A    | N7-C8-N9    | -6.11 | 110.75      | 113.80   |
| 1   | AA    | 202  | G    | N3-C2-N2    | 6.11  | 124.17      | 119.90   |
| 1   | AA    | 239  | U    | N3-C2-O2    | 6.11  | 126.47      | 122.20   |
| 1   | AA    | 449  | G    | C4-C5-N7    | 6.11  | 113.24      | 110.80   |
| 1   | AA    | 1185 | G    | O4'-C4'-C3' | -6.11 | 97.89       | 104.00   |
| 1   | AA    | 1436 | U    | C2-N3-C4    | 6.11  | 130.66      | 127.00   |
| 16  | AP    | 17   | TYR  | CZ-CE2-CD2  | 6.11  | 125.30      | 119.80   |
| 35  | BB    | 500  | G    | C1'-O4'-C4' | 6.11  | 114.78      | 109.90   |
| 35  | BB    | 1354 | A    | N1-C2-N3    | 6.11  | 132.35      | 129.30   |
| 35  | BB    | 1661 | G    | N1-C2-N2    | 6.11  | 121.69      | 116.20   |
| 35  | BB    | 2055 | C    | C5'-C4'-O4' | 6.11  | 116.42      | 109.10   |
| 35  | BB    | 2171 | A    | C2-N3-C4    | -6.11 | 107.55      | 110.60   |
| 35  | BB    | 2197 | U    | C6-N1-C2    | 6.11  | 124.66      | 121.00   |
| 35  | BB    | 2493 | U    | O4'-C1'-N1  | 6.11  | 113.08      | 108.20   |
| 35  | BB    | 2666 | C    | N1-C2-N3    | -6.11 | 114.93      | 119.20   |
| 1   | AA    | 292  | G    | C5-C6-O6    | -6.10 | 124.94      | 128.60   |
| 1   | AA    | 374  | A    | C5-N7-C8    | 6.10  | 106.95      | 103.90   |
| 1   | AA    | 1158 | C    | C6-N1-C2    | -6.10 | 117.86      | 120.30   |
| 1   | AA    | 1310 | G    | C6-C5-N7    | -6.10 | 126.74      | 130.40   |
| 35  | BB    | 750  | A    | C5-C6-N6    | -6.10 | 118.82      | 123.70   |
| 35  | BB    | 1131 | G    | N1-C2-N3    | -6.10 | 120.24      | 123.90   |
| 35  | BB    | 1504 | A    | O4'-C1'-N9  | 6.10  | 113.08      | 108.20   |
| 35  | BB    | 1635 | A    | O4'-C1'-N9  | 6.10  | 113.08      | 108.20   |
| 35  | BB    | 1829 | A    | C6-C5-N7    | -6.10 | 128.03      | 132.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2872 | A    | C4-C5-C6    | 6.10  | 120.05      | 117.00   |
| 1   | AA    | 86   | G    | N1-C2-N2    | -6.10 | 110.71      | 116.20   |
| 1   | AA    | 156  | C    | O5'-C5'-C4' | -6.10 | 100.11      | 111.70   |
| 1   | AA    | 862  | C    | P-O3'-C3'   | 6.10  | 127.02      | 119.70   |
| 1   | AA    | 1443 | C    | C6-N1-C2    | 6.10  | 122.74      | 120.30   |
| 1   | AA    | 1447 | A    | O4'-C1'-N9  | 6.10  | 113.08      | 108.20   |
| 35  | BB    | 254  | G    | N3-C4-C5    | -6.10 | 125.55      | 128.60   |
| 35  | BB    | 1248 | G    | C6-C5-N7    | -6.10 | 126.74      | 130.40   |
| 35  | BB    | 1801 | A    | C5-C6-N1    | -6.10 | 114.65      | 117.70   |
| 35  | BB    | 38   | A    | OP1-P-OP2   | -6.10 | 110.45      | 119.60   |
| 35  | BB    | 432  | A    | C4-C5-N7    | -6.10 | 107.65      | 110.70   |
| 35  | BB    | 1374 | G    | C4-C5-N7    | 6.10  | 113.24      | 110.80   |
| 35  | BB    | 1790 | C    | N3-C4-C5    | -6.10 | 119.46      | 121.90   |
| 35  | BB    | 2531 | A    | C4-C5-N7    | -6.10 | 107.65      | 110.70   |
| 1   | AA    | 69   | G    | C5-C6-O6    | -6.10 | 124.94      | 128.60   |
| 1   | AA    | 1218 | C    | O4'-C1'-N1  | 6.10  | 113.08      | 108.20   |
| 1   | AA    | 1221 | G    | N1-C2-N3    | -6.10 | 120.24      | 123.90   |
| 35  | BB    | 1664 | A    | C5'-C4'-C3' | -6.10 | 106.24      | 116.00   |
| 35  | BB    | 1962 | C    | O4'-C1'-N1  | 6.10  | 113.08      | 108.20   |
| 35  | BB    | 1990 | C    | C5-C6-N1    | -6.10 | 117.95      | 121.00   |
| 35  | BB    | 2047 | C    | N3-C4-N4    | 6.10  | 122.27      | 118.00   |
| 35  | BB    | 2164 | C    | N3-C4-C5    | -6.10 | 119.46      | 121.90   |
| 35  | BB    | 2247 | A    | N9-C4-C5    | -6.10 | 103.36      | 105.80   |
| 35  | BB    | 2578 | G    | N3-C4-N9    | 6.10  | 129.66      | 126.00   |
| 35  | BB    | 2702 | G    | N1-C2-N3    | -6.10 | 120.24      | 123.90   |
| 1   | AA    | 142  | G    | C6-C5-N7    | -6.10 | 126.74      | 130.40   |
| 1   | AA    | 337  | G    | C4-C5-C6    | 6.10  | 122.46      | 118.80   |
| 1   | AA    | 748  | G    | N3-C2-N2    | 6.10  | 124.17      | 119.90   |
| 1   | AA    | 801  | U    | N3-C2-O2    | 6.10  | 126.47      | 122.20   |
| 1   | AA    | 1444 | U    | C5-C6-N1    | 6.10  | 125.75      | 122.70   |
| 1   | AA    | 1491 | G    | C6-C5-N7    | -6.10 | 126.74      | 130.40   |
| 34  | BA    | 60   | C    | C1'-O4'-C4' | 6.10  | 114.78      | 109.90   |
| 35  | BB    | 621  | A    | C4-C5-N7    | 6.10  | 113.75      | 110.70   |
| 35  | BB    | 706  | A    | C4-C5-C6    | 6.10  | 120.05      | 117.00   |
| 35  | BB    | 1730 | C    | C2-N1-C1'   | 6.10  | 125.51      | 118.80   |
| 35  | BB    | 1744 | A    | O4'-C1'-N9  | 6.10  | 113.08      | 108.20   |
| 35  | BB    | 1766 | G    | C4-C5-C6    | 6.10  | 122.46      | 118.80   |
| 35  | BB    | 1936 | A    | C6-C5-N7    | -6.10 | 128.03      | 132.30   |
| 35  | BB    | 2219 | U    | C2-N3-C4    | -6.10 | 123.34      | 127.00   |
| 35  | BB    | 2499 | C    | N3-C4-N4    | 6.10  | 122.27      | 118.00   |
| 35  | BB    | 2756 | U    | C5-C6-N1    | 6.10  | 125.75      | 122.70   |
| 35  | BB    | 2856 | A    | C5-N7-C8    | 6.10  | 106.95      | 103.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 39  | BF    | 124  | ARG  | NE-CZ-NH1   | 6.10  | 123.35      | 120.30   |
| 16  | AP    | 68   | SER  | O-C-N       | -6.10 | 112.95      | 122.70   |
| 22  | AV    | 26   | A    | C5-C6-N6    | -6.10 | 118.82      | 123.70   |
| 35  | BB    | 1186 | G    | N1-C6-O6    | 6.10  | 123.56      | 119.90   |
| 35  | BB    | 1444 | G    | N1-C2-N3    | 6.10  | 127.56      | 123.90   |
| 35  | BB    | 1770 | G    | C5-N7-C8    | -6.10 | 101.25      | 104.30   |
| 1   | AA    | 21   | G    | C2-N3-C4    | 6.09  | 114.95      | 111.90   |
| 1   | AA    | 582  | C    | O4'-C1'-N1  | 6.09  | 113.08      | 108.20   |
| 1   | AA    | 754  | C    | C2-N1-C1'   | 6.09  | 125.50      | 118.80   |
| 1   | AA    | 1032 | G    | C2-N3-C4    | 6.09  | 114.95      | 111.90   |
| 1   | AA    | 1134 | G    | N3-C4-C5    | -6.09 | 125.55      | 128.60   |
| 1   | AA    | 1271 | A    | O4'-C1'-N9  | 6.09  | 113.08      | 108.20   |
| 1   | AA    | 1515 | G    | C5-N7-C8    | 6.09  | 107.35      | 104.30   |
| 34  | BA    | 118  | C    | C5-C4-N4    | -6.09 | 115.93      | 120.20   |
| 35  | BB    | 562  | U    | N3-C2-O2    | 6.09  | 126.47      | 122.20   |
| 35  | BB    | 896  | A    | C4-C5-C6    | 6.09  | 120.05      | 117.00   |
| 35  | BB    | 993  | G    | N3-C2-N2    | 6.09  | 124.17      | 119.90   |
| 35  | BB    | 1417 | C    | C6-N1-C2    | 6.09  | 122.74      | 120.30   |
| 35  | BB    | 1528 | A    | C4-C5-C6    | 6.09  | 120.05      | 117.00   |
| 35  | BB    | 2447 | G    | C4-C5-C6    | -6.09 | 115.14      | 118.80   |
| 35  | BB    | 2827 | C    | C1'-O4'-C4' | -6.09 | 105.02      | 109.90   |
| 43  | BJ    | 27   | ARG  | NE-CZ-NH2   | -6.09 | 117.25      | 120.30   |
| 1   | AA    | 279  | A    | N1-C2-N3    | 6.09  | 132.35      | 129.30   |
| 1   | AA    | 522  | C    | C5-C6-N1    | 6.09  | 124.05      | 121.00   |
| 35  | BB    | 979  | A    | C2-N3-C4    | -6.09 | 107.55      | 110.60   |
| 35  | BB    | 2498 | C    | O4'-C1'-N1  | 6.09  | 113.08      | 108.20   |
| 1   | AA    | 77   | A    | C6-N1-C2    | 6.09  | 122.25      | 118.60   |
| 1   | AA    | 670  | G    | N3-C4-N9    | -6.09 | 122.34      | 126.00   |
| 1   | AA    | 1129 | C    | N3-C4-C5    | -6.09 | 119.46      | 121.90   |
| 1   | AA    | 1312 | G    | C6-N1-C2    | 6.09  | 128.75      | 125.10   |
| 34  | BA    | 97   | C    | P-O3'-C3'   | -6.09 | 112.39      | 119.70   |
| 35  | BB    | 1038 | G    | C4-C5-N7    | 6.09  | 113.24      | 110.80   |
| 35  | BB    | 1743 | G    | O4'-C1'-N9  | 6.09  | 113.07      | 108.20   |
| 35  | BB    | 2087 | G    | C3'-C2'-C1' | 6.09  | 106.37      | 101.50   |
| 1   | AA    | 141  | G    | O4'-C1'-N9  | 6.09  | 113.07      | 108.20   |
| 1   | AA    | 174  | A    | N7-C8-N9    | -6.09 | 110.76      | 113.80   |
| 1   | AA    | 402  | G    | C6-N1-C2    | -6.09 | 121.45      | 125.10   |
| 1   | AA    | 445  | G    | C3'-C2'-C1' | -6.09 | 96.63       | 101.50   |
| 1   | AA    | 969  | A    | C5-C6-N1    | -6.09 | 114.66      | 117.70   |
| 34  | BA    | 76   | G    | C2-N3-C4    | 6.09  | 114.94      | 111.90   |
| 35  | BB    | 501  | A    | C8-N9-C4    | -6.09 | 103.36      | 105.80   |
| 35  | BB    | 862  | G    | C4-C5-N7    | 6.09  | 113.24      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1111 | A    | C4-C5-N7    | 6.09  | 113.75      | 110.70   |
| 35  | BB    | 1159 | U    | OP1-P-OP2   | -6.09 | 110.47      | 119.60   |
| 35  | BB    | 1260 | A    | C5-C6-N6    | -6.09 | 118.83      | 123.70   |
| 35  | BB    | 1378 | A    | N1-C2-N3    | 6.09  | 132.34      | 129.30   |
| 35  | BB    | 2005 | A    | C5-C6-N1    | -6.09 | 114.66      | 117.70   |
| 35  | BB    | 2125 | G    | C4'-C3'-C2' | -6.09 | 96.51       | 102.60   |
| 35  | BB    | 2140 | G    | OP1-P-OP2   | -6.09 | 110.47      | 119.60   |
| 35  | BB    | 2280 | G    | C5-C6-N1    | -6.09 | 108.46      | 111.50   |
| 35  | BB    | 2590 | A    | O4'-C1'-N9  | 6.09  | 113.07      | 108.20   |
| 48  | BO    | 37   | ALA  | N-CA-CB     | 6.09  | 118.62      | 110.10   |
| 1   | AA    | 178  | C    | O4'-C1'-N1  | 6.09  | 113.07      | 108.20   |
| 1   | AA    | 514  | C    | C2-N3-C4    | 6.09  | 122.94      | 119.90   |
| 1   | AA    | 531  | U    | C5-C6-N1    | 6.09  | 125.74      | 122.70   |
| 1   | AA    | 821  | G    | N1-C2-N2    | -6.09 | 110.72      | 116.20   |
| 28  | B3    | 39   | ARG  | NE-CZ-NH1   | 6.09  | 123.34      | 120.30   |
| 35  | BB    | 91   | A    | C4-C5-N7    | -6.09 | 107.66      | 110.70   |
| 35  | BB    | 1129 | A    | N3-C4-N9    | 6.09  | 132.27      | 127.40   |
| 35  | BB    | 2173 | A    | O4'-C1'-N9  | 6.09  | 113.07      | 108.20   |
| 35  | BB    | 2528 | U    | O4'-C1'-N1  | 6.09  | 113.07      | 108.20   |
| 1   | AA    | 954  | G    | C4-C5-N7    | -6.09 | 108.36      | 110.80   |
| 3   | AC    | 92   | ASP  | CB-CG-OD1   | -6.09 | 112.82      | 118.30   |
| 35  | BB    | 963  | U    | N3-C4-C5    | -6.09 | 110.95      | 114.60   |
| 35  | BB    | 1668 | A    | C5-C6-N6    | -6.09 | 118.83      | 123.70   |
| 35  | BB    | 1770 | G    | C4-C5-C6    | 6.09  | 122.45      | 118.80   |
| 35  | BB    | 1830 | C    | C6-N1-C2    | 6.09  | 122.73      | 120.30   |
| 35  | BB    | 1884 | G    | N7-C8-N9    | -6.09 | 110.06      | 113.10   |
| 35  | BB    | 2480 | C    | C4'-C3'-C2' | -6.09 | 96.51       | 102.60   |
| 35  | BB    | 2581 | G    | C5'-C4'-O4' | 6.09  | 116.40      | 109.10   |
| 1   | AA    | 37   | U    | C6-N1-C2    | 6.08  | 124.65      | 121.00   |
| 35  | BB    | 876  | C    | C5'-C4'-C3' | -6.08 | 106.26      | 116.00   |
| 35  | BB    | 1139 | G    | N1-C6-O6    | 6.08  | 123.55      | 119.90   |
| 35  | BB    | 2353 | G    | C5-C6-O6    | -6.08 | 124.95      | 128.60   |
| 52  | BS    | 62   | ASP  | N-CA-CB     | 6.08  | 121.55      | 110.60   |
| 1   | AA    | 276  | G    | C6-C5-N7    | -6.08 | 126.75      | 130.40   |
| 1   | AA    | 901  | A    | N1-C2-N3    | 6.08  | 132.34      | 129.30   |
| 15  | AO    | 71   | ARG  | NE-CZ-NH1   | -6.08 | 117.26      | 120.30   |
| 35  | BB    | 347  | A    | N1-C2-N3    | -6.08 | 126.26      | 129.30   |
| 35  | BB    | 953  | G    | C4-C5-N7    | 6.08  | 113.23      | 110.80   |
| 35  | BB    | 1084 | A    | O4'-C1'-N9  | 6.08  | 113.07      | 108.20   |
| 35  | BB    | 1303 | G    | C5-C6-O6    | -6.08 | 124.95      | 128.60   |
| 35  | BB    | 1415 | U    | N3-C4-C5    | -6.08 | 110.95      | 114.60   |
| 35  | BB    | 1434 | A    | C5'-C4'-O4' | -6.08 | 101.80      | 109.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2223 | G    | C4-C5-C6    | 6.08  | 122.45      | 118.80   |
| 35  | BB    | 2642 | G    | N3-C4-N9    | -6.08 | 122.35      | 126.00   |
| 35  | BB    | 2778 | A    | C8-N9-C4    | 6.08  | 108.23      | 105.80   |
| 35  | BB    | 2870 | C    | C5-C4-N4    | -6.08 | 115.94      | 120.20   |
| 56  | BY    | 59   | PHE  | CB-CG-CD2   | -6.08 | 116.54      | 120.80   |
| 1   | AA    | 816  | A    | O4'-C1'-C2' | 6.08  | 113.07      | 107.60   |
| 1   | AA    | 1376 | U    | N1-C2-N3    | -6.08 | 111.25      | 114.90   |
| 35  | BB    | 279  | A    | C5-C6-N6    | -6.08 | 118.83      | 123.70   |
| 35  | BB    | 444  | C    | N1-C2-O2    | -6.08 | 115.25      | 118.90   |
| 35  | BB    | 508  | A    | C5-C6-N6    | -6.08 | 118.83      | 123.70   |
| 35  | BB    | 543  | G    | C2-N3-C4    | 6.08  | 114.94      | 111.90   |
| 35  | BB    | 1201 | U    | O4'-C4'-C3' | -6.08 | 97.92       | 104.00   |
| 35  | BB    | 1454 | C    | P-O5'-C5'   | -6.08 | 111.17      | 120.90   |
| 35  | BB    | 1985 | C    | OP1-P-OP2   | -6.08 | 110.48      | 119.60   |
| 35  | BB    | 2521 | C    | N3-C2-O2    | 6.08  | 126.16      | 121.90   |
| 35  | BB    | 2665 | A    | C5-N7-C8    | 6.08  | 106.94      | 103.90   |
| 45  | BL    | 107  | PHE  | CB-CG-CD1   | 6.08  | 125.06      | 120.80   |
| 1   | AA    | 886  | G    | N1-C6-O6    | 6.08  | 123.55      | 119.90   |
| 34  | BA    | 55   | U    | O4'-C1'-N1  | 6.08  | 113.06      | 108.20   |
| 35  | BB    | 1756 | G    | C5-C6-N1    | -6.08 | 108.46      | 111.50   |
| 1   | AA    | 514  | C    | O4'-C1'-N1  | 6.08  | 113.06      | 108.20   |
| 1   | AA    | 928  | G    | C2-N3-C4    | -6.08 | 108.86      | 111.90   |
| 34  | BA    | 116  | G    | N3-C2-N2    | 6.08  | 124.16      | 119.90   |
| 35  | BB    | 144  | A    | N7-C8-N9    | 6.08  | 116.84      | 113.80   |
| 35  | BB    | 311  | A    | C4-C5-N7    | -6.08 | 107.66      | 110.70   |
| 35  | BB    | 581  | C    | N3-C4-N4    | 6.08  | 122.25      | 118.00   |
| 35  | BB    | 701  | G    | P-O3'-C3'   | -6.08 | 112.41      | 119.70   |
| 35  | BB    | 936  | A    | C5-C6-N6    | -6.08 | 118.84      | 123.70   |
| 35  | BB    | 1519 | G    | C4-C5-N7    | -6.08 | 108.37      | 110.80   |
| 35  | BB    | 2329 | U    | C5-C6-N1    | 6.08  | 125.74      | 122.70   |
| 35  | BB    | 2425 | A    | P-O3'-C3'   | 6.08  | 127.00      | 119.70   |
| 1   | AA    | 894  | G    | O4'-C1'-N9  | 6.08  | 113.06      | 108.20   |
| 1   | AA    | 1042 | A    | N3-C4-C5    | 6.08  | 131.05      | 126.80   |
| 1   | AA    | 1082 | A    | N3-C4-N9    | -6.08 | 122.54      | 127.40   |
| 1   | AA    | 1325 | C    | C4-C5-C6    | 6.08  | 120.44      | 117.40   |
| 35  | BB    | 980  | A    | C2-N3-C4    | -6.08 | 107.56      | 110.60   |
| 35  | BB    | 1243 | C    | C5-C6-N1    | 6.08  | 124.04      | 121.00   |
| 35  | BB    | 1296 | G    | C5-C6-N1    | -6.08 | 108.46      | 111.50   |
| 35  | BB    | 1298 | C    | C6-N1-C2    | 6.08  | 122.73      | 120.30   |
| 35  | BB    | 1546 | G    | N1-C6-O6    | 6.08  | 123.55      | 119.90   |
| 35  | BB    | 1786 | A    | C4-C5-C6    | 6.08  | 120.04      | 117.00   |
| 35  | BB    | 1892 | C    | O4'-C1'-N1  | 6.08  | 113.06      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2260 | C    | N3-C4-N4    | 6.08  | 122.25      | 118.00   |
| 1   | AA    | 163  | C    | N3-C4-N4    | 6.08  | 122.25      | 118.00   |
| 1   | AA    | 172  | A    | P-O3'-C3'   | -6.08 | 112.41      | 119.70   |
| 1   | AA    | 552  | U    | C5-C6-N1    | 6.08  | 125.74      | 122.70   |
| 1   | AA    | 693  | G    | P-O5'-C5'   | 6.08  | 130.62      | 120.90   |
| 1   | AA    | 726  | C    | P-O5'-C5'   | 6.08  | 130.62      | 120.90   |
| 1   | AA    | 1282 | C    | N3-C4-N4    | 6.08  | 122.25      | 118.00   |
| 1   | AA    | 1344 | C    | OP1-P-OP2   | -6.08 | 110.49      | 119.60   |
| 1   | AA    | 1530 | G    | N3-C2-N2    | 6.08  | 124.15      | 119.90   |
| 35  | BB    | 102  | U    | C5-C6-N1    | 6.08  | 125.74      | 122.70   |
| 35  | BB    | 245  | G    | C8-N9-C4    | -6.08 | 103.97      | 106.40   |
| 35  | BB    | 332  | A    | N3-C4-C5    | -6.08 | 122.55      | 126.80   |
| 35  | BB    | 599  | A    | C5-C6-N6    | -6.08 | 118.84      | 123.70   |
| 35  | BB    | 671  | C    | C1'-O4'-C4' | -6.08 | 105.04      | 109.90   |
| 35  | BB    | 727  | A    | C5-C6-N1    | -6.08 | 114.66      | 117.70   |
| 35  | BB    | 792  | A    | C6-C5-N7    | -6.08 | 128.05      | 132.30   |
| 35  | BB    | 964  | C    | C3'-C2'-C1' | 6.08  | 106.36      | 101.50   |
| 35  | BB    | 1109 | C    | C6-N1-C1'   | -6.08 | 113.51      | 120.80   |
| 35  | BB    | 1699 | G    | N3-C4-N9    | -6.08 | 122.36      | 126.00   |
| 35  | BB    | 2451 | A    | N1-C2-N3    | -6.08 | 126.26      | 129.30   |
| 35  | BB    | 2682 | A    | C5-C6-N1    | -6.08 | 114.66      | 117.70   |
| 43  | BJ    | 48   | VAL  | CA-CB-CG1   | -6.08 | 101.79      | 110.90   |
| 1   | AA    | 586  | C    | C2-N3-C4    | 6.07  | 122.94      | 119.90   |
| 1   | AA    | 777  | A    | N3-C4-C5    | 6.07  | 131.05      | 126.80   |
| 1   | AA    | 878  | A    | N1-C6-N6    | 6.07  | 122.24      | 118.60   |
| 1   | AA    | 1268 | G    | N3-C4-N9    | 6.07  | 129.64      | 126.00   |
| 1   | AA    | 1422 | G    | P-O3'-C3'   | -6.07 | 112.41      | 119.70   |
| 34  | BA    | 19   | C    | C6-N1-C2    | -6.07 | 117.87      | 120.30   |
| 35  | BB    | 110  | G    | C6-N1-C2    | 6.07  | 128.75      | 125.10   |
| 35  | BB    | 270  | A    | N1-C6-N6    | 6.07  | 122.24      | 118.60   |
| 35  | BB    | 949  | G    | N9-C4-C5    | -6.07 | 102.97      | 105.40   |
| 35  | BB    | 1392 | A    | O4'-C4'-C3' | -6.07 | 97.93       | 104.00   |
| 35  | BB    | 1957 | C    | C5-C4-N4    | -6.07 | 115.95      | 120.20   |
| 35  | BB    | 2269 | G    | C5-C6-O6    | -6.07 | 124.96      | 128.60   |
| 35  | BB    | 2286 | G    | N7-C8-N9    | 6.07  | 116.14      | 113.10   |
| 35  | BB    | 2386 | A    | C5-C6-N6    | -6.07 | 118.84      | 123.70   |
| 35  | BB    | 2801 | G    | N3-C4-N9    | 6.07  | 129.64      | 126.00   |
| 50  | BQ    | 47   | ARG  | NE-CZ-NH2   | 6.07  | 123.34      | 120.30   |
| 1   | AA    | 898  | G    | N9-C4-C5    | -6.07 | 102.97      | 105.40   |
| 1   | AA    | 1088 | G    | C1'-O4'-C4' | 6.07  | 114.76      | 109.90   |
| 1   | AA    | 1195 | C    | O4'-C1'-N1  | 6.07  | 113.06      | 108.20   |
| 1   | AA    | 1402 | C    | O5'-P-OP2   | -6.07 | 100.23      | 105.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 125  | A    | C4-C5-N7    | -6.07 | 107.66      | 110.70   |
| 35  | BB    | 907  | G    | P-O5'-C5'   | 6.07  | 130.62      | 120.90   |
| 35  | BB    | 1133 | A    | C5-N7-C8    | 6.07  | 106.94      | 103.90   |
| 35  | BB    | 1521 | G    | C5-C6-N1    | -6.07 | 108.46      | 111.50   |
| 35  | BB    | 2144 | G    | N3-C4-N9    | 6.07  | 129.64      | 126.00   |
| 35  | BB    | 2337 | G    | C1'-O4'-C4' | 6.07  | 114.76      | 109.90   |
| 1   | AA    | 544  | G    | O4'-C1'-N9  | 6.07  | 113.06      | 108.20   |
| 1   | AA    | 688  | G    | N7-C8-N9    | -6.07 | 110.06      | 113.10   |
| 1   | AA    | 1491 | G    | C8-N9-C1'   | 6.07  | 134.89      | 127.00   |
| 35  | BB    | 18   | U    | N1-C2-N3    | -6.07 | 111.26      | 114.90   |
| 35  | BB    | 1069 | A    | N3-C4-N9    | 6.07  | 132.26      | 127.40   |
| 35  | BB    | 1133 | A    | C5-C6-N6    | -6.07 | 118.84      | 123.70   |
| 35  | BB    | 1655 | A    | N1-C6-N6    | 6.07  | 122.24      | 118.60   |
| 43  | BJ    | 52   | ASP  | N-CA-CB     | 6.07  | 121.53      | 110.60   |
| 22  | AV    | 21   | A    | C5-C6-N6    | -6.07 | 118.84      | 123.70   |
| 22  | AV    | 37   | G    | C5-N7-C8    | 6.07  | 107.33      | 104.30   |
| 34  | BA    | 114  | C    | C4-C5-C6    | -6.07 | 114.37      | 117.40   |
| 35  | BB    | 1228 | G    | C2-N3-C4    | 6.07  | 114.94      | 111.90   |
| 35  | BB    | 1359 | A    | N1-C2-N3    | 6.07  | 132.33      | 129.30   |
| 35  | BB    | 1668 | A    | C4-C5-N7    | -6.07 | 107.67      | 110.70   |
| 35  | BB    | 1992 | G    | N9-C4-C5    | 6.07  | 107.83      | 105.40   |
| 35  | BB    | 2692 | G    | N3-C2-N2    | 6.07  | 124.15      | 119.90   |
| 36  | BC    | 246  | PRO  | N-CA-CB     | 6.07  | 110.58      | 103.30   |
| 1   | AA    | 617  | G    | P-O3'-C3'   | -6.07 | 112.42      | 119.70   |
| 17  | AQ    | 76   | ARG  | N-CA-CB     | 6.07  | 121.52      | 110.60   |
| 22  | AV    | 52   | G    | O4'-C1'-N9  | 6.07  | 113.05      | 108.20   |
| 35  | BB    | 222  | A    | P-O3'-C3'   | -6.07 | 112.42      | 119.70   |
| 35  | BB    | 447  | A    | C6-N1-C2    | -6.07 | 114.96      | 118.60   |
| 35  | BB    | 809  | G    | C2-N3-C4    | 6.07  | 114.93      | 111.90   |
| 35  | BB    | 1196 | C    | N3-C2-O2    | 6.07  | 126.15      | 121.90   |
| 35  | BB    | 1413 | A    | C1'-O4'-C4' | 6.07  | 114.75      | 109.90   |
| 35  | BB    | 1437 | C    | N3-C4-N4    | 6.07  | 122.25      | 118.00   |
| 35  | BB    | 2280 | G    | N1-C6-O6    | 6.07  | 123.54      | 119.90   |
| 35  | BB    | 2335 | A    | N1-C2-N3    | -6.07 | 126.27      | 129.30   |
| 35  | BB    | 2488 | G    | C4-N9-C1'   | 6.07  | 134.39      | 126.50   |
| 35  | BB    | 2654 | A    | C2-N3-C4    | -6.07 | 107.57      | 110.60   |
| 1   | AA    | 412  | A    | C5'-C4'-O4' | 6.07  | 116.38      | 109.10   |
| 1   | AA    | 600  | A    | O4'-C1'-N9  | 6.07  | 113.05      | 108.20   |
| 1   | AA    | 1079 | G    | P-O3'-C3'   | 6.07  | 126.98      | 119.70   |
| 1   | AA    | 1099 | G    | O4'-C1'-N9  | 6.07  | 113.05      | 108.20   |
| 1   | AA    | 1235 | U    | C5-C6-N1    | -6.07 | 119.67      | 122.70   |
| 35  | BB    | 376  | G    | C2-N3-C4    | 6.07  | 114.93      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 693  | A    | C5-N7-C8    | 6.07  | 106.93      | 103.90   |
| 35  | BB    | 985  | C    | C4-C5-C6    | 6.07  | 120.43      | 117.40   |
| 35  | BB    | 1252 | G    | C8-N9-C4    | -6.07 | 103.97      | 106.40   |
| 35  | BB    | 1664 | A    | C4-C5-C6    | 6.07  | 120.03      | 117.00   |
| 35  | BB    | 1980 | G    | N3-C2-N2    | 6.07  | 124.15      | 119.90   |
| 35  | BB    | 2803 | G    | O4'-C1'-N9  | 6.07  | 113.05      | 108.20   |
| 22  | AV    | 44   | G    | O4'-C1'-N9  | 6.06  | 113.05      | 108.20   |
| 35  | BB    | 244  | A    | O4'-C1'-N9  | 6.06  | 113.05      | 108.20   |
| 35  | BB    | 698  | C    | N1-C2-N3    | 6.06  | 123.44      | 119.20   |
| 35  | BB    | 954  | G    | O4'-C4'-C3' | -6.06 | 97.94       | 104.00   |
| 35  | BB    | 1307 | A    | N7-C8-N9    | -6.06 | 110.77      | 113.80   |
| 35  | BB    | 1666 | G    | N1-C6-O6    | 6.06  | 123.54      | 119.90   |
| 35  | BB    | 1757 | A    | N3-C4-N9    | 6.06  | 132.25      | 127.40   |
| 35  | BB    | 2207 | C    | N3-C4-N4    | -6.06 | 113.75      | 118.00   |
| 1   | AA    | 750  | C    | N3-C4-N4    | 6.06  | 122.24      | 118.00   |
| 3   | AC    | 167  | TYR  | CB-CG-CD2   | 6.06  | 124.64      | 121.00   |
| 35  | BB    | 891  | G    | C1'-O4'-C4' | -6.06 | 105.05      | 109.90   |
| 35  | BB    | 1187 | G    | N9-C4-C5    | 6.06  | 107.83      | 105.40   |
| 35  | BB    | 1367 | A    | N7-C8-N9    | -6.06 | 110.77      | 113.80   |
| 35  | BB    | 1710 | G    | O5'-P-OP2   | 6.06  | 117.97      | 110.70   |
| 35  | BB    | 2061 | G    | C5-C6-N1    | -6.06 | 108.47      | 111.50   |
| 35  | BB    | 2898 | U    | C5-C4-O4    | 6.06  | 129.54      | 125.90   |
| 1   | AA    | 348  | G    | N3-C4-C5    | -6.06 | 125.57      | 128.60   |
| 1   | AA    | 1266 | G    | C5-C6-O6    | -6.06 | 124.96      | 128.60   |
| 34  | BA    | 94   | A    | C5-C6-N1    | -6.06 | 114.67      | 117.70   |
| 35  | BB    | 1991 | U    | O4'-C1'-N1  | 6.06  | 113.05      | 108.20   |
| 1   | AA    | 79   | G    | C4-C5-C6    | 6.06  | 122.44      | 118.80   |
| 1   | AA    | 376  | G    | C4-C5-N7    | 6.06  | 113.22      | 110.80   |
| 1   | AA    | 554  | A    | C8-N9-C4    | -6.06 | 103.38      | 105.80   |
| 1   | AA    | 1055 | A    | O4'-C1'-N9  | 6.06  | 113.05      | 108.20   |
| 1   | AA    | 1347 | G    | C8-N9-C1'   | 6.06  | 134.88      | 127.00   |
| 1   | AA    | 1429 | A    | C6-C5-N7    | -6.06 | 128.06      | 132.30   |
| 2   | AB    | 204  | ASP  | CB-CG-OD2   | -6.06 | 112.85      | 118.30   |
| 22  | AV    | 74   | C    | C3'-C2'-C1' | -6.06 | 96.65       | 101.50   |
| 35  | BB    | 451  | U    | N1-C2-O2    | 6.06  | 127.04      | 122.80   |
| 35  | BB    | 858  | G    | C8-N9-C4    | -6.06 | 103.98      | 106.40   |
| 35  | BB    | 895  | U    | N1-C2-N3    | 6.06  | 118.54      | 114.90   |
| 35  | BB    | 1020 | A    | C6-C5-N7    | -6.06 | 128.06      | 132.30   |
| 35  | BB    | 1108 | U    | N3-C2-O2    | 6.06  | 126.44      | 122.20   |
| 35  | BB    | 1252 | G    | C5-C6-O6    | -6.06 | 124.96      | 128.60   |
| 35  | BB    | 2128 | G    | O4'-C1'-N9  | 6.06  | 113.05      | 108.20   |
| 35  | BB    | 2273 | A    | O4'-C1'-C2' | 6.06  | 113.05      | 107.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2288 | A    | O4'-C1'-N9  | 6.06  | 113.05      | 108.20   |
| 35  | BB    | 2412 | A    | C2-N3-C4    | -6.06 | 107.57      | 110.60   |
| 1   | AA    | 729  | A    | C4'-C3'-C2' | -6.06 | 96.54       | 102.60   |
| 1   | AA    | 938  | A    | C5-C6-N1    | -6.06 | 114.67      | 117.70   |
| 1   | AA    | 972  | C    | O4'-C1'-N1  | 6.06  | 113.05      | 108.20   |
| 1   | AA    | 1000 | A    | C3'-C2'-C1' | -6.06 | 96.65       | 101.50   |
| 1   | AA    | 1484 | C    | C5-C4-N4    | 6.06  | 124.44      | 120.20   |
| 35  | BB    | 652  | U    | C5-C4-O4    | -6.06 | 122.27      | 125.90   |
| 35  | BB    | 770  | G    | C6-C5-N7    | -6.06 | 126.77      | 130.40   |
| 35  | BB    | 816  | C    | N3-C4-C5    | -6.06 | 119.48      | 121.90   |
| 35  | BB    | 2857 | G    | C4-C5-C6    | 6.06  | 122.44      | 118.80   |
| 36  | BC    | 62   | ARG  | N-CA-C      | -6.06 | 94.64       | 111.00   |
| 1   | AA    | 1150 | A    | C5-C6-N6    | -6.06 | 118.86      | 123.70   |
| 22  | AV    | 1    | C    | C5-C4-N4    | -6.06 | 115.96      | 120.20   |
| 35  | BB    | 2146 | C    | C5-C4-N4    | 6.06  | 124.44      | 120.20   |
| 41  | BH    | 113  | SER  | N-CA-CB     | 6.06  | 119.58      | 110.50   |
| 1   | AA    | 359  | G    | N1-C6-O6    | 6.05  | 123.53      | 119.90   |
| 1   | AA    | 572  | A    | N1-C2-N3    | 6.05  | 132.33      | 129.30   |
| 1   | AA    | 916  | U    | C4-C5-C6    | -6.05 | 116.07      | 119.70   |
| 1   | AA    | 1101 | A    | O4'-C1'-C2' | -6.05 | 99.75       | 105.80   |
| 34  | BA    | 20   | G    | C5-C6-O6    | -6.05 | 124.97      | 128.60   |
| 35  | BB    | 345  | A    | N1-C6-N6    | 6.05  | 122.23      | 118.60   |
| 35  | BB    | 960  | A    | N9-C4-C5    | 6.05  | 108.22      | 105.80   |
| 35  | BB    | 1555 | G    | C6-C5-N7    | -6.05 | 126.77      | 130.40   |
| 35  | BB    | 2015 | A    | N1-C6-N6    | 6.05  | 122.23      | 118.60   |
| 35  | BB    | 2177 | C    | N3-C2-O2    | 6.05  | 126.14      | 121.90   |
| 35  | BB    | 2877 | G    | N1-C2-N3    | -6.05 | 120.27      | 123.90   |
| 40  | BG    | 2    | ARG  | NH1-CZ-NH2  | -6.05 | 112.74      | 119.40   |
| 1   | AA    | 37   | U    | C5-C4-O4    | -6.05 | 122.27      | 125.90   |
| 1   | AA    | 195  | A    | C6-N1-C2    | -6.05 | 114.97      | 118.60   |
| 1   | AA    | 228  | A    | N7-C8-N9    | 6.05  | 116.83      | 113.80   |
| 1   | AA    | 1519 | A    | OP1-P-OP2   | -6.05 | 110.52      | 119.60   |
| 35  | BB    | 762  | U    | N1-C2-O2    | -6.05 | 118.56      | 122.80   |
| 35  | BB    | 1111 | A    | N9-C4-C5    | -6.05 | 103.38      | 105.80   |
| 35  | BB    | 1839 | G    | N9-C4-C5    | -6.05 | 102.98      | 105.40   |
| 35  | BB    | 1906 | G    | C5-C6-O6    | -6.05 | 124.97      | 128.60   |
| 35  | BB    | 2386 | A    | C2-N3-C4    | -6.05 | 107.57      | 110.60   |
| 35  | BB    | 2410 | G    | C5-C6-N1    | -6.05 | 108.47      | 111.50   |
| 35  | BB    | 2749 | A    | C5-C6-N1    | -6.05 | 114.67      | 117.70   |
| 1   | AA    | 65   | A    | C6-C5-N7    | -6.05 | 128.06      | 132.30   |
| 1   | AA    | 751  | U    | P-O5'-C5'   | 6.05  | 130.58      | 120.90   |
| 1   | AA    | 945  | G    | N1-C2-N3    | -6.05 | 120.27      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 994  | A    | C4-C5-N7    | -6.05 | 107.67      | 110.70   |
| 1   | AA    | 1388 | C    | O4'-C1'-N1  | 6.05  | 113.04      | 108.20   |
| 35  | BB    | 164  | C    | C4-C5-C6    | 6.05  | 120.43      | 117.40   |
| 35  | BB    | 241  | A    | C5-N7-C8    | 6.05  | 106.93      | 103.90   |
| 35  | BB    | 448  | U    | C6-N1-C2    | -6.05 | 117.37      | 121.00   |
| 35  | BB    | 682  | G    | N3-C4-C5    | -6.05 | 125.57      | 128.60   |
| 35  | BB    | 840  | C    | C3'-C2'-C1' | -6.05 | 96.66       | 101.50   |
| 35  | BB    | 1416 | G    | C3'-C2'-C1' | 6.05  | 106.34      | 101.50   |
| 35  | BB    | 1550 | C    | C4'-C3'-C2' | -6.05 | 96.55       | 102.60   |
| 35  | BB    | 1587 | G    | C1'-O4'-C4' | 6.05  | 114.74      | 109.90   |
| 35  | BB    | 2192 | U    | N3-C4-O4    | 6.05  | 123.64      | 119.40   |
| 35  | BB    | 2221 | G    | N1-C6-O6    | 6.05  | 123.53      | 119.90   |
| 35  | BB    | 2336 | A    | N7-C8-N9    | 6.05  | 116.83      | 113.80   |
| 1   | AA    | 93   | U    | P-O3'-C3'   | -6.05 | 112.44      | 119.70   |
| 1   | AA    | 591  | U    | C1'-O4'-C4' | -6.05 | 105.06      | 109.90   |
| 1   | AA    | 678  | U    | C2-N3-C4    | -6.05 | 123.37      | 127.00   |
| 1   | AA    | 1399 | C    | O4'-C1'-N1  | 6.05  | 113.04      | 108.20   |
| 35  | BB    | 1119 | U    | P-O3'-C3'   | -6.05 | 112.44      | 119.70   |
| 35  | BB    | 1171 | G    | C2-N3-C4    | 6.05  | 114.92      | 111.90   |
| 35  | BB    | 1489 | C    | C2-N1-C1'   | 6.05  | 125.45      | 118.80   |
| 35  | BB    | 1797 | G    | N3-C2-N2    | 6.05  | 124.14      | 119.90   |
| 35  | BB    | 2123 | G    | N1-C2-N2    | -6.05 | 110.75      | 116.20   |
| 35  | BB    | 2210 | U    | N1-C2-N3    | -6.05 | 111.27      | 114.90   |
| 35  | BB    | 2328 | A    | O4'-C1'-N9  | 6.05  | 113.04      | 108.20   |
| 35  | BB    | 2408 | U    | O4'-C1'-N1  | 6.05  | 113.04      | 108.20   |
| 35  | BB    | 2532 | G    | N3-C4-N9    | -6.05 | 122.37      | 126.00   |
| 35  | BB    | 2623 | G    | C8-N9-C4    | -6.05 | 103.98      | 106.40   |
| 35  | BB    | 2781 | A    | C4-C5-C6    | 6.05  | 120.03      | 117.00   |
| 1   | AA    | 860  | A    | C2-N3-C4    | -6.05 | 107.58      | 110.60   |
| 22  | AV    | 59   | A    | O4'-C1'-N9  | 6.05  | 113.04      | 108.20   |
| 22  | AV    | 75   | C    | C2-N3-C4    | 6.05  | 122.92      | 119.90   |
| 35  | BB    | 1222 | U    | N3-C4-O4    | 6.05  | 123.63      | 119.40   |
| 35  | BB    | 1806 | C    | C4-C5-C6    | 6.05  | 120.42      | 117.40   |
| 1   | AA    | 713  | G    | N3-C2-N2    | 6.05  | 124.13      | 119.90   |
| 35  | BB    | 113  | U    | N1-C2-O2    | -6.05 | 118.57      | 122.80   |
| 35  | BB    | 138  | U    | C2-N3-C4    | -6.05 | 123.37      | 127.00   |
| 35  | BB    | 1480 | C    | C5-C6-N1    | -6.05 | 117.98      | 121.00   |
| 35  | BB    | 1531 | C    | N3-C4-N4    | 6.05  | 122.23      | 118.00   |
| 35  | BB    | 1587 | G    | C5-C6-O6    | -6.05 | 124.97      | 128.60   |
| 35  | BB    | 1603 | A    | C5-C6-N1    | -6.05 | 114.68      | 117.70   |
| 35  | BB    | 1704 | C    | C1'-O4'-C4' | -6.05 | 105.06      | 109.90   |
| 35  | BB    | 1860 | G    | C5-C6-N1    | -6.05 | 108.48      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2436 | G    | O4'-C1'-N9  | 6.05  | 113.04      | 108.20   |
| 35  | BB    | 2628 | C    | N1-C2-N3    | -6.05 | 114.97      | 119.20   |
| 35  | BB    | 2634 | A    | C5-C6-N6    | -6.05 | 118.86      | 123.70   |
| 1   | AA    | 278  | G    | N3-C4-N9    | 6.04  | 129.63      | 126.00   |
| 34  | BA    | 20   | G    | N3-C4-N9    | -6.04 | 122.37      | 126.00   |
| 35  | BB    | 6    | A    | C6-C5-N7    | -6.04 | 128.07      | 132.30   |
| 35  | BB    | 300  | A    | N1-C2-N3    | 6.04  | 132.32      | 129.30   |
| 35  | BB    | 565  | C    | C4'-C3'-C2' | -6.04 | 96.56       | 102.60   |
| 35  | BB    | 2314 | A    | N9-C4-C5    | 6.04  | 108.22      | 105.80   |
| 35  | BB    | 2611 | C    | N3-C4-N4    | 6.04  | 122.23      | 118.00   |
| 35  | BB    | 2876 | G    | C4-N9-C1'   | -6.04 | 118.64      | 126.50   |
| 1   | AA    | 406  | G    | C5-N7-C8    | 6.04  | 107.32      | 104.30   |
| 1   | AA    | 1029 | U    | C5'-C4'-C3' | 6.04  | 125.67      | 116.00   |
| 1   | AA    | 1056 | U    | C5-C6-N1    | -6.04 | 119.68      | 122.70   |
| 1   | AA    | 1179 | A    | N9-C4-C5    | 6.04  | 108.22      | 105.80   |
| 34  | BA    | 99   | A    | C5'-C4'-O4' | -6.04 | 101.85      | 109.10   |
| 35  | BB    | 80   | G    | N1-C2-N3    | -6.04 | 120.27      | 123.90   |
| 35  | BB    | 861  | A    | C2-N3-C4    | -6.04 | 107.58      | 110.60   |
| 35  | BB    | 1557 | C    | N3-C4-C5    | -6.04 | 119.48      | 121.90   |
| 35  | BB    | 2255 | G    | C2-N3-C4    | 6.04  | 114.92      | 111.90   |
| 47  | BN    | 38   | LEU  | CB-CG-CD2   | 6.04  | 121.28      | 111.00   |
| 1   | AA    | 64   | G    | C5'-C4'-O4' | 6.04  | 116.35      | 109.10   |
| 1   | AA    | 190  | A    | C5-C6-N6    | -6.04 | 118.87      | 123.70   |
| 1   | AA    | 547  | A    | N7-C8-N9    | -6.04 | 110.78      | 113.80   |
| 1   | AA    | 700  | G    | C3'-C2'-C1' | 6.04  | 106.33      | 101.50   |
| 1   | AA    | 919  | A    | C5-C6-N6    | -6.04 | 118.87      | 123.70   |
| 1   | AA    | 1105 | A    | C5-C6-N6    | -6.04 | 118.87      | 123.70   |
| 34  | BA    | 107  | G    | C5-N7-C8    | -6.04 | 101.28      | 104.30   |
| 35  | BB    | 50   | U    | C6-N1-C1'   | -6.04 | 112.74      | 121.20   |
| 35  | BB    | 990  | A    | C5-N7-C8    | 6.04  | 106.92      | 103.90   |
| 35  | BB    | 1199 | U    | N3-C2-O2    | 6.04  | 126.43      | 122.20   |
| 35  | BB    | 1407 | G    | C6-C5-N7    | -6.04 | 126.78      | 130.40   |
| 35  | BB    | 1521 | G    | C6-N1-C2    | 6.04  | 128.72      | 125.10   |
| 35  | BB    | 1701 | A    | P-O5'-C5'   | -6.04 | 111.23      | 120.90   |
| 35  | BB    | 1880 | U    | C1'-O4'-C4' | 6.04  | 114.73      | 109.90   |
| 35  | BB    | 1969 | A    | C8-N9-C4    | -6.04 | 103.38      | 105.80   |
| 35  | BB    | 2081 | U    | C5-C6-N1    | 6.04  | 125.72      | 122.70   |
| 35  | BB    | 2601 | C    | N3-C4-N4    | 6.04  | 122.23      | 118.00   |
| 35  | BB    | 930  | G    | C6-C5-N7    | -6.04 | 126.78      | 130.40   |
| 35  | BB    | 1011 | G    | C4-N9-C1'   | -6.04 | 118.65      | 126.50   |
| 35  | BB    | 2513 | A    | C5-C6-N6    | -6.04 | 118.87      | 123.70   |
| 35  | BB    | 2626 | C    | N1-C1'-C2'  | -6.04 | 105.36      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 50  | BQ    | 99   | VAL  | CA-CB-CG1   | -6.04 | 101.84      | 110.90   |
| 1   | AA    | 806  | C    | C6-N1-C2    | 6.04  | 122.72      | 120.30   |
| 35  | BB    | 501  | A    | C5-C6-N1    | -6.04 | 114.68      | 117.70   |
| 35  | BB    | 1076 | C    | N1-C2-N3    | -6.04 | 114.97      | 119.20   |
| 35  | BB    | 1869 | G    | P-O3'-C3'   | 6.04  | 126.95      | 119.70   |
| 35  | BB    | 2599 | G    | C4'-C3'-C2' | -6.04 | 96.56       | 102.60   |
| 35  | BB    | 2731 | G    | C5-C6-N1    | -6.04 | 108.48      | 111.50   |
| 35  | BB    | 2900 | A    | O4'-C1'-N9  | 6.04  | 113.03      | 108.20   |
| 34  | BA    | 10   | G    | N3-C4-C5    | 6.04  | 131.62      | 128.60   |
| 35  | BB    | 1037 | G    | C6-C5-N7    | -6.04 | 126.78      | 130.40   |
| 35  | BB    | 1540 | G    | C6-C5-N7    | -6.04 | 126.78      | 130.40   |
| 35  | BB    | 2127 | G    | C5-N7-C8    | 6.04  | 107.32      | 104.30   |
| 35  | BB    | 2218 | G    | C8-N9-C4    | 6.04  | 108.81      | 106.40   |
| 35  | BB    | 2341 | G    | C5-C6-O6    | -6.04 | 124.98      | 128.60   |
| 1   | AA    | 61   | G    | P-O3'-C3'   | -6.04 | 112.46      | 119.70   |
| 1   | AA    | 553  | A    | N1-C6-N6    | 6.04  | 122.22      | 118.60   |
| 1   | AA    | 929  | G    | N1-C2-N2    | -6.04 | 110.77      | 116.20   |
| 1   | AA    | 986  | U    | P-O3'-C3'   | -6.04 | 112.46      | 119.70   |
| 1   | AA    | 1528 | U    | C5-C6-N1    | -6.04 | 119.68      | 122.70   |
| 35  | BB    | 21   | A    | O4'-C1'-N9  | 6.04  | 113.03      | 108.20   |
| 35  | BB    | 27   | G    | C6-C5-N7    | -6.04 | 126.78      | 130.40   |
| 35  | BB    | 819  | A    | C6-N1-C2    | -6.04 | 114.98      | 118.60   |
| 35  | BB    | 851  | C    | N3-C4-N4    | 6.04  | 122.22      | 118.00   |
| 35  | BB    | 1603 | A    | OP2-P-O3'   | 6.04  | 118.48      | 105.20   |
| 35  | BB    | 1997 | C    | C4-C5-C6    | 6.04  | 120.42      | 117.40   |
| 35  | BB    | 2212 | A    | N3-C4-N9    | 6.04  | 132.23      | 127.40   |
| 35  | BB    | 2252 | G    | N3-C2-N2    | -6.04 | 115.67      | 119.90   |
| 1   | AA    | 86   | G    | N9-C4-C5    | 6.03  | 107.81      | 105.40   |
| 1   | AA    | 567  | G    | C6-N1-C2    | 6.03  | 128.72      | 125.10   |
| 1   | AA    | 954  | G    | N1-C6-O6    | 6.03  | 123.52      | 119.90   |
| 1   | AA    | 1193 | G    | O4'-C1'-N9  | 6.03  | 113.03      | 108.20   |
| 1   | AA    | 1324 | A    | C8-N9-C4    | -6.03 | 103.39      | 105.80   |
| 1   | AA    | 1387 | G    | N3-C4-N9    | -6.03 | 122.38      | 126.00   |
| 35  | BB    | 301  | G    | C8-N9-C1'   | 6.03  | 134.84      | 127.00   |
| 35  | BB    | 340  | A    | C4'-C3'-C2' | -6.03 | 96.57       | 102.60   |
| 35  | BB    | 472  | A    | O4'-C1'-N9  | 6.03  | 113.03      | 108.20   |
| 35  | BB    | 479  | A    | O4'-C1'-N9  | 6.03  | 113.03      | 108.20   |
| 35  | BB    | 569  | U    | C5-C6-N1    | 6.03  | 125.72      | 122.70   |
| 35  | BB    | 664  | G    | O5'-P-OP2   | -6.03 | 100.27      | 105.70   |
| 35  | BB    | 728  | G    | C8-N9-C4    | 6.03  | 108.81      | 106.40   |
| 35  | BB    | 914  | G    | O4'-C1'-C2' | 6.03  | 113.03      | 107.60   |
| 35  | BB    | 1226 | A    | C5-C6-N1    | -6.03 | 114.68      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1581 | G    | C2-N3-C4    | 6.03  | 114.92      | 111.90   |
| 48  | BO    | 36   | TYR  | CB-CG-CD1   | -6.03 | 117.38      | 121.00   |
| 1   | AA    | 427  | U    | N3-C4-C5    | -6.03 | 110.98      | 114.60   |
| 1   | AA    | 537  | G    | C8-N9-C4    | -6.03 | 103.99      | 106.40   |
| 35  | BB    | 474  | G    | N9-C1'-C2'  | -6.03 | 105.36      | 112.00   |
| 35  | BB    | 539  | G    | N1-C2-N3    | -6.03 | 120.28      | 123.90   |
| 35  | BB    | 1494 | A    | N1-C2-N3    | -6.03 | 126.28      | 129.30   |
| 35  | BB    | 2222 | C    | N3-C4-C5    | -6.03 | 119.49      | 121.90   |
| 51  | BR    | 21   | ARG  | NE-CZ-NH2   | 6.03  | 123.32      | 120.30   |
| 1   | AA    | 452  | A    | OP1-P-OP2   | -6.03 | 110.56      | 119.60   |
| 1   | AA    | 538  | G    | C2-N3-C4    | 6.03  | 114.92      | 111.90   |
| 1   | AA    | 573  | A    | C4-C5-C6    | 6.03  | 120.02      | 117.00   |
| 1   | AA    | 728  | A    | N3-C4-N9    | 6.03  | 132.22      | 127.40   |
| 1   | AA    | 734  | G    | P-O3'-C3'   | -6.03 | 112.46      | 119.70   |
| 1   | AA    | 1297 | G    | C4-C5-C6    | 6.03  | 122.42      | 118.80   |
| 35  | BB    | 111  | A    | C5-C6-N6    | -6.03 | 118.88      | 123.70   |
| 35  | BB    | 299  | A    | N3-C4-C5    | -6.03 | 122.58      | 126.80   |
| 35  | BB    | 481  | G    | N3-C4-C5    | 6.03  | 131.62      | 128.60   |
| 35  | BB    | 620  | G    | C2-N3-C4    | 6.03  | 114.92      | 111.90   |
| 35  | BB    | 1050 | A    | C6-C5-N7    | -6.03 | 128.08      | 132.30   |
| 35  | BB    | 1212 | G    | P-O3'-C3'   | 6.03  | 126.94      | 119.70   |
| 35  | BB    | 1446 | C    | N3-C4-C5    | -6.03 | 119.49      | 121.90   |
| 35  | BB    | 2132 | U    | N3-C4-C5    | -6.03 | 110.98      | 114.60   |
| 35  | BB    | 2633 | G    | C6-C5-N7    | -6.03 | 126.78      | 130.40   |
| 36  | BC    | 12   | ARG  | NE-CZ-NH1   | 6.03  | 123.31      | 120.30   |
| 1   | AA    | 450  | G    | C6-C5-N7    | -6.03 | 126.78      | 130.40   |
| 1   | AA    | 1074 | G    | N3-C4-C5    | -6.03 | 125.59      | 128.60   |
| 1   | AA    | 1283 | U    | C5'-C4'-C3' | -6.03 | 106.36      | 116.00   |
| 34  | BA    | 29   | A    | P-O3'-C3'   | 6.03  | 126.93      | 119.70   |
| 34  | BA    | 44   | G    | C3'-C2'-C1' | -6.03 | 96.68       | 101.50   |
| 35  | BB    | 5    | A    | N3-C4-C5    | -6.03 | 122.58      | 126.80   |
| 35  | BB    | 71   | A    | O4'-C1'-N9  | 6.03  | 113.02      | 108.20   |
| 35  | BB    | 167  | A    | C5-N7-C8    | 6.03  | 106.91      | 103.90   |
| 35  | BB    | 407  | G    | C2-N3-C4    | 6.03  | 114.91      | 111.90   |
| 35  | BB    | 1262 | A    | C5-C6-N6    | -6.03 | 118.88      | 123.70   |
| 35  | BB    | 1328 | A    | N7-C8-N9    | -6.03 | 110.79      | 113.80   |
| 35  | BB    | 1459 | G    | C5'-C4'-O4' | 6.03  | 116.33      | 109.10   |
| 35  | BB    | 1567 | G    | C6-N1-C2    | -6.03 | 121.48      | 125.10   |
| 35  | BB    | 2101 | A    | N1-C2-N3    | -6.03 | 126.29      | 129.30   |
| 35  | BB    | 2598 | A    | N1-C6-N6    | 6.03  | 122.22      | 118.60   |
| 35  | BB    | 2624 | G    | N1-C2-N3    | -6.03 | 120.28      | 123.90   |
| 35  | BB    | 2846 | G    | C2-N3-C4    | -6.03 | 108.89      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 113  | G    | C5-C6-O6    | -6.03 | 124.98      | 128.60   |
| 1   | AA    | 158  | G    | O4'-C1'-N9  | 6.03  | 113.02      | 108.20   |
| 1   | AA    | 454  | G    | C2-N3-C4    | 6.03  | 114.91      | 111.90   |
| 35  | BB    | 159  | G    | C5-N7-C8    | 6.03  | 107.31      | 104.30   |
| 35  | BB    | 856  | G    | C5'-C4'-O4' | 6.03  | 116.33      | 109.10   |
| 35  | BB    | 2171 | A    | C3'-C2'-C1' | -6.03 | 96.68       | 101.50   |
| 35  | BB    | 2307 | G    | C4-N9-C1'   | 6.03  | 134.33      | 126.50   |
| 35  | BB    | 2339 | C    | C4-C5-C6    | 6.03  | 120.41      | 117.40   |
| 35  | BB    | 2444 | G    | N3-C2-N2    | 6.03  | 124.12      | 119.90   |
| 1   | AA    | 384  | G    | C2-N3-C4    | 6.02  | 114.91      | 111.90   |
| 11  | AK    | 92   | ARG  | CB-CA-C     | -6.02 | 98.35       | 110.40   |
| 35  | BB    | 354  | A    | N9-C4-C5    | 6.02  | 108.21      | 105.80   |
| 35  | BB    | 1566 | A    | N1-C2-N3    | -6.02 | 126.29      | 129.30   |
| 35  | BB    | 1897 | G    | N3-C4-C5    | 6.02  | 131.61      | 128.60   |
| 35  | BB    | 2304 | G    | C6-N1-C2    | 6.02  | 128.72      | 125.10   |
| 1   | AA    | 402  | G    | N7-C8-N9    | -6.02 | 110.09      | 113.10   |
| 1   | AA    | 802  | A    | N9-C4-C5    | 6.02  | 108.21      | 105.80   |
| 35  | BB    | 662  | G    | C5-C6-N1    | -6.02 | 108.49      | 111.50   |
| 35  | BB    | 821  | A    | C5'-C4'-O4' | 6.02  | 116.33      | 109.10   |
| 35  | BB    | 929  | U    | C5-C4-O4    | -6.02 | 122.29      | 125.90   |
| 35  | BB    | 1137 | G    | P-O3'-C3'   | -6.02 | 112.47      | 119.70   |
| 35  | BB    | 1194 | A    | C5-C6-N1    | -6.02 | 114.69      | 117.70   |
| 35  | BB    | 1959 | G    | O4'-C1'-N9  | 6.02  | 113.02      | 108.20   |
| 35  | BB    | 2409 | G    | N1-C6-O6    | 6.02  | 123.51      | 119.90   |
| 1   | AA    | 203  | G    | C5-C6-O6    | -6.02 | 124.99      | 128.60   |
| 1   | AA    | 277  | C    | P-O3'-C3'   | -6.02 | 112.47      | 119.70   |
| 1   | AA    | 904  | U    | N1-C2-N3    | -6.02 | 111.29      | 114.90   |
| 34  | BA    | 39   | A    | C5-N7-C8    | 6.02  | 106.91      | 103.90   |
| 35  | BB    | 361  | G    | O4'-C1'-N9  | 6.02  | 113.02      | 108.20   |
| 35  | BB    | 2465 | C    | N3-C4-C5    | -6.02 | 119.49      | 121.90   |
| 35  | BB    | 2751 | G    | C4-N9-C1'   | 6.02  | 134.33      | 126.50   |
| 35  | BB    | 2896 | C    | O5'-P-OP2   | -6.02 | 100.28      | 105.70   |
| 1   | AA    | 904  | U    | O4'-C4'-C3' | -6.02 | 97.98       | 104.00   |
| 4   | AD    | 48   | SER  | N-CA-CB     | 6.02  | 119.53      | 110.50   |
| 35  | BB    | 56   | A    | C4-C5-C6    | 6.02  | 120.01      | 117.00   |
| 35  | BB    | 333  | G    | C5-C6-N1    | -6.02 | 108.49      | 111.50   |
| 35  | BB    | 561  | G    | P-O3'-C3'   | 6.02  | 126.92      | 119.70   |
| 35  | BB    | 567  | U    | N3-C4-O4    | 6.02  | 123.61      | 119.40   |
| 35  | BB    | 598  | U    | C5-C6-N1    | 6.02  | 125.71      | 122.70   |
| 35  | BB    | 731  | C    | N3-C4-N4    | 6.02  | 122.21      | 118.00   |
| 35  | BB    | 762  | U    | C4'-C3'-C2' | -6.02 | 96.58       | 102.60   |
| 35  | BB    | 831  | G    | C5-N7-C8    | 6.02  | 107.31      | 104.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1230 | A    | O4'-C1'-N9  | 6.02  | 113.02      | 108.20   |
| 35  | BB    | 1304 | A    | C8-N9-C4    | -6.02 | 103.39      | 105.80   |
| 35  | BB    | 1327 | A    | C5-N7-C8    | 6.02  | 106.91      | 103.90   |
| 35  | BB    | 1373 | A    | C5-C6-N1    | -6.02 | 114.69      | 117.70   |
| 35  | BB    | 1750 | G    | C5-C6-N1    | 6.02  | 114.51      | 111.50   |
| 35  | BB    | 2136 | G    | C8-N9-C4    | -6.02 | 103.99      | 106.40   |
| 35  | BB    | 2261 | C    | C2-N3-C4    | 6.02  | 122.91      | 119.90   |
| 35  | BB    | 2660 | A    | P-O3'-C3'   | 6.02  | 126.92      | 119.70   |
| 46  | BM    | 42   | THR  | CA-CB-CG2   | -6.02 | 103.97      | 112.40   |
| 52  | BS    | 110  | ARG  | NE-CZ-NH2   | -6.02 | 117.29      | 120.30   |
| 55  | BW    | 21   | ARG  | NE-CZ-NH1   | -6.02 | 117.29      | 120.30   |
| 1   | AA    | 313  | A    | C5-C6-N6    | -6.02 | 118.89      | 123.70   |
| 1   | AA    | 671  | G    | N3-C2-N2    | 6.02  | 124.11      | 119.90   |
| 1   | AA    | 724  | G    | N3-C2-N2    | 6.02  | 124.11      | 119.90   |
| 1   | AA    | 765  | G    | O4'-C4'-C3' | -6.02 | 97.98       | 104.00   |
| 1   | AA    | 1053 | G    | C4-N9-C1'   | -6.02 | 118.68      | 126.50   |
| 1   | AA    | 1399 | C    | C3'-C2'-C1' | -6.02 | 96.69       | 101.50   |
| 35  | BB    | 95   | A    | C8-N9-C4    | -6.02 | 103.39      | 105.80   |
| 35  | BB    | 212  | G    | O4'-C1'-N9  | 6.02  | 113.01      | 108.20   |
| 35  | BB    | 547  | A    | OP1-P-OP2   | -6.02 | 110.57      | 119.60   |
| 35  | BB    | 618  | G    | C2-N3-C4    | 6.02  | 114.91      | 111.90   |
| 35  | BB    | 621  | A    | N9-C4-C5    | -6.02 | 103.39      | 105.80   |
| 35  | BB    | 756  | A    | C5-N7-C8    | 6.02  | 106.91      | 103.90   |
| 35  | BB    | 842  | U    | N1-C2-O2    | -6.02 | 118.59      | 122.80   |
| 35  | BB    | 1397 | U    | P-O3'-C3'   | 6.02  | 126.92      | 119.70   |
| 35  | BB    | 1643 | G    | C6-N1-C2    | 6.02  | 128.71      | 125.10   |
| 35  | BB    | 2109 | U    | N1-C2-O2    | -6.02 | 118.59      | 122.80   |
| 35  | BB    | 2534 | A    | C5-C6-N6    | -6.02 | 118.89      | 123.70   |
| 35  | BB    | 2608 | G    | C6-N1-C2    | 6.02  | 128.71      | 125.10   |
| 35  | BB    | 2844 | G    | N7-C8-N9    | 6.02  | 116.11      | 113.10   |
| 1   | AA    | 552  | U    | N3-C4-O4    | 6.02  | 123.61      | 119.40   |
| 35  | BB    | 267  | C    | C4-C5-C6    | 6.02  | 120.41      | 117.40   |
| 35  | BB    | 1021 | A    | C5-C6-N6    | -6.02 | 118.89      | 123.70   |
| 35  | BB    | 1213 | A    | C5-C6-N1    | -6.02 | 114.69      | 117.70   |
| 35  | BB    | 2398 | U    | N1-C2-N3    | -6.02 | 111.29      | 114.90   |
| 1   | AA    | 491  | G    | N3-C4-N9    | 6.01  | 129.61      | 126.00   |
| 1   | AA    | 1207 | G    | N7-C8-N9    | -6.01 | 110.09      | 113.10   |
| 2   | AB    | 199  | ILE  | N-CA-C      | -6.01 | 94.76       | 111.00   |
| 34  | BA    | 13   | G    | C6-C5-N7    | -6.01 | 126.79      | 130.40   |
| 34  | BA    | 25   | U    | C5-C4-O4    | -6.01 | 122.29      | 125.90   |
| 34  | BA    | 98   | G    | N1-C2-N3    | -6.01 | 120.29      | 123.90   |
| 35  | BB    | 356  | G    | C6-C5-N7    | -6.01 | 126.79      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 925  | A    | C4-C5-C6    | 6.01  | 120.01      | 117.00   |
| 35  | BB    | 1872 | A    | N3-C4-C5    | -6.01 | 122.59      | 126.80   |
| 1   | AA    | 62   | U    | N1-C2-N3    | -6.01 | 111.29      | 114.90   |
| 1   | AA    | 360  | G    | C5-N7-C8    | 6.01  | 107.31      | 104.30   |
| 35  | BB    | 1513 | U    | C1'-O4'-C4' | -6.01 | 105.09      | 109.90   |
| 1   | AA    | 809  | G    | O4'-C1'-N9  | 6.01  | 113.01      | 108.20   |
| 1   | AA    | 1252 | A    | P-O5'-C5'   | 6.01  | 130.52      | 120.90   |
| 1   | AA    | 1279 | G    | N1-C2-N3    | -6.01 | 120.29      | 123.90   |
| 1   | AA    | 1412 | C    | N3-C4-N4    | 6.01  | 122.21      | 118.00   |
| 35  | BB    | 11   | C    | N3-C4-C5    | -6.01 | 119.50      | 121.90   |
| 35  | BB    | 1117 | C    | C5-C4-N4    | -6.01 | 115.99      | 120.20   |
| 35  | BB    | 1471 | G    | O4'-C1'-N9  | 6.01  | 113.01      | 108.20   |
| 35  | BB    | 1772 | A    | N9-C4-C5    | 6.01  | 108.20      | 105.80   |
| 35  | BB    | 2145 | C    | N1-C2-O2    | 6.01  | 122.51      | 118.90   |
| 35  | BB    | 2155 | U    | N1-C2-N3    | 6.01  | 118.51      | 114.90   |
| 1   | AA    | 78   | A    | C6-C5-N7    | -6.01 | 128.09      | 132.30   |
| 1   | AA    | 383  | A    | P-O5'-C5'   | -6.01 | 111.28      | 120.90   |
| 1   | AA    | 766  | A    | C5-N7-C8    | 6.01  | 106.90      | 103.90   |
| 1   | AA    | 851  | G    | N9-C4-C5    | -6.01 | 103.00      | 105.40   |
| 1   | AA    | 1034 | G    | N1-C6-O6    | 6.01  | 123.50      | 119.90   |
| 1   | AA    | 1120 | C    | N3-C4-N4    | 6.01  | 122.21      | 118.00   |
| 1   | AA    | 1302 | C    | N3-C4-C5    | -6.01 | 119.50      | 121.90   |
| 10  | AJ    | 98   | VAL  | CG1-CB-CG2  | -6.01 | 101.29      | 110.90   |
| 35  | BB    | 125  | A    | C2-N3-C4    | -6.01 | 107.59      | 110.60   |
| 35  | BB    | 195  | A    | N7-C8-N9    | -6.01 | 110.80      | 113.80   |
| 35  | BB    | 669  | G    | N3-C4-N9    | -6.01 | 122.39      | 126.00   |
| 35  | BB    | 730  | A    | C1'-O4'-C4' | 6.01  | 114.71      | 109.90   |
| 35  | BB    | 786  | C    | O4'-C1'-N1  | 6.01  | 113.01      | 108.20   |
| 35  | BB    | 1228 | G    | O4'-C1'-N9  | 6.01  | 113.01      | 108.20   |
| 35  | BB    | 1979 | U    | N3-C4-O4    | 6.01  | 123.61      | 119.40   |
| 38  | BE    | 158  | PHE  | CB-CG-CD1   | 6.01  | 125.01      | 120.80   |
| 1   | AA    | 187  | G    | N1-C2-N3    | -6.01 | 120.30      | 123.90   |
| 1   | AA    | 233  | C    | N3-C4-C5    | -6.01 | 119.50      | 121.90   |
| 1   | AA    | 353  | A    | C4-C5-C6    | 6.01  | 120.00      | 117.00   |
| 1   | AA    | 518  | C    | C5-C4-N4    | -6.01 | 115.99      | 120.20   |
| 35  | BB    | 209  | C    | C2-N1-C1'   | 6.01  | 125.41      | 118.80   |
| 35  | BB    | 874  | G    | C8-N9-C4    | -6.01 | 104.00      | 106.40   |
| 35  | BB    | 1579 | A    | N9-C4-C5    | -6.01 | 103.40      | 105.80   |
| 35  | BB    | 2136 | G    | C5'-C4'-C3' | -6.01 | 106.39      | 116.00   |
| 35  | BB    | 2426 | A    | C4-C5-N7    | -6.01 | 107.70      | 110.70   |
| 35  | BB    | 2666 | C    | C5-C6-N1    | 6.01  | 124.00      | 121.00   |
| 35  | BB    | 2770 | G    | C6-N1-C2    | -6.01 | 121.50      | 125.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 897  | C    | N3-C2-O2    | 6.01  | 126.10      | 121.90   |
| 1   | AA    | 966  | G    | O4'-C1'-N9  | 6.01  | 113.00      | 108.20   |
| 1   | AA    | 1435 | G    | C8-N9-C4    | -6.01 | 104.00      | 106.40   |
| 1   | AA    | 1487 | G    | C4-N9-C1'   | -6.01 | 118.69      | 126.50   |
| 34  | BA    | 76   | G    | C5'-C4'-O4' | 6.01  | 116.31      | 109.10   |
| 35  | BB    | 201  | C    | N3-C4-N4    | 6.01  | 122.20      | 118.00   |
| 35  | BB    | 782  | A    | C3'-C2'-C1' | -6.01 | 96.69       | 101.50   |
| 35  | BB    | 1234 | U    | C5-C6-N1    | 6.01  | 125.70      | 122.70   |
| 35  | BB    | 2669 | G    | O4'-C1'-N9  | 6.01  | 113.01      | 108.20   |
| 35  | BB    | 2740 | A    | P-O5'-C5'   | -6.01 | 111.29      | 120.90   |
| 35  | BB    | 2742 | G    | C5-C6-N1    | -6.01 | 108.50      | 111.50   |
| 35  | BB    | 2781 | A    | C8-N9-C4    | -6.01 | 103.40      | 105.80   |
| 35  | BB    | 2870 | C    | N1-C2-O2    | -6.01 | 115.30      | 118.90   |
| 1   | AA    | 266  | G    | C3'-C2'-C1' | 6.00  | 106.30      | 101.50   |
| 1   | AA    | 303  | A    | C4-C5-N7    | 6.00  | 113.70      | 110.70   |
| 1   | AA    | 408  | A    | C4-C5-C6    | 6.00  | 120.00      | 117.00   |
| 35  | BB    | 678  | C    | O4'-C4'-C3' | -6.00 | 98.00       | 104.00   |
| 35  | BB    | 922  | C    | N3-C4-C5    | 6.00  | 124.30      | 121.90   |
| 35  | BB    | 1678 | A    | C3'-C2'-C1' | 6.00  | 106.30      | 101.50   |
| 35  | BB    | 1686 | C    | C6-N1-C2    | 6.00  | 122.70      | 120.30   |
| 35  | BB    | 2422 | C    | C5-C6-N1    | 6.00  | 124.00      | 121.00   |
| 1   | AA    | 250  | A    | C4-C5-C6    | 6.00  | 120.00      | 117.00   |
| 1   | AA    | 863  | U    | O4'-C1'-N1  | 6.00  | 113.00      | 108.20   |
| 1   | AA    | 1181 | G    | P-O3'-C3'   | 6.00  | 126.90      | 119.70   |
| 13  | AM    | 21   | ILE  | C-N-CA      | 6.00  | 136.71      | 121.70   |
| 35  | BB    | 554  | U    | N3-C4-C5    | -6.00 | 111.00      | 114.60   |
| 35  | BB    | 594  | U    | C2-N3-C4    | 6.00  | 130.60      | 127.00   |
| 35  | BB    | 933  | A    | C2-N3-C4    | -6.00 | 107.60      | 110.60   |
| 35  | BB    | 1698 | A    | P-O3'-C3'   | -6.00 | 112.50      | 119.70   |
| 35  | BB    | 1811 | G    | O4'-C4'-C3' | -6.00 | 98.00       | 104.00   |
| 35  | BB    | 2221 | G    | N3-C4-C5    | -6.00 | 125.60      | 128.60   |
| 35  | BB    | 2689 | U    | C1'-O4'-C4' | 6.00  | 114.70      | 109.90   |
| 34  | BA    | 50   | A    | N9-C4-C5    | 6.00  | 108.20      | 105.80   |
| 35  | BB    | 34   | U    | C4-C5-C6    | 6.00  | 123.30      | 119.70   |
| 35  | BB    | 250  | G    | N3-C4-N9    | 6.00  | 129.60      | 126.00   |
| 35  | BB    | 534  | U    | C5-C6-N1    | 6.00  | 125.70      | 122.70   |
| 35  | BB    | 1653 | G    | C5'-C4'-O4' | 6.00  | 116.30      | 109.10   |
| 35  | BB    | 1962 | C    | C5-C6-N1    | 6.00  | 124.00      | 121.00   |
| 1   | AA    | 430  | A    | C4-C5-N7    | -6.00 | 107.70      | 110.70   |
| 1   | AA    | 864  | A    | C2-N3-C4    | -6.00 | 107.60      | 110.60   |
| 1   | AA    | 932  | C    | C5'-C4'-C3' | -6.00 | 106.40      | 116.00   |
| 35  | BB    | 282  | A    | C4-C5-N7    | -6.00 | 107.70      | 110.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1102 | C    | N3-C2-O2    | 6.00  | 126.10      | 121.90   |
| 35  | BB    | 1527 | G    | C4-C5-C6    | 6.00  | 122.40      | 118.80   |
| 1   | AA    | 74   | A    | C4-C5-N7    | -6.00 | 107.70      | 110.70   |
| 1   | AA    | 833  | G    | N3-C4-C5    | -6.00 | 125.60      | 128.60   |
| 1   | AA    | 846  | G    | C2-N3-C4    | 6.00  | 114.90      | 111.90   |
| 1   | AA    | 849  | G    | P-O3'-C3'   | 6.00  | 126.90      | 119.70   |
| 1   | AA    | 1353 | G    | C4-C5-N7    | -6.00 | 108.40      | 110.80   |
| 1   | AA    | 1424 | U    | N1-C2-N3    | 6.00  | 118.50      | 114.90   |
| 8   | AH    | 26   | MET  | N-CA-CB     | 6.00  | 121.40      | 110.60   |
| 30  | B5    | 102  | ASP  | CB-CG-OD1   | 6.00  | 123.70      | 118.30   |
| 31  | B6    | 39   | ARG  | NE-CZ-NH2   | -6.00 | 117.30      | 120.30   |
| 35  | BB    | 1025 | G    | C8-N9-C4    | 6.00  | 108.80      | 106.40   |
| 35  | BB    | 1275 | A    | C4-C5-C6    | 6.00  | 120.00      | 117.00   |
| 35  | BB    | 1619 | G    | N1-C2-N2    | -6.00 | 110.80      | 116.20   |
| 35  | BB    | 1770 | G    | N9-C4-C5    | 6.00  | 107.80      | 105.40   |
| 35  | BB    | 1828 | G    | C5-N7-C8    | 6.00  | 107.30      | 104.30   |
| 46  | BM    | 82   | MET  | CG-SD-CE    | -6.00 | 90.60       | 100.20   |
| 54  | BU    | 94   | PHE  | CB-CG-CD2   | 6.00  | 125.00      | 120.80   |
| 1   | AA    | 190  | A    | C6-C5-N7    | -6.00 | 128.10      | 132.30   |
| 1   | AA    | 914  | A    | C5-C6-N6    | -6.00 | 118.90      | 123.70   |
| 1   | AA    | 1316 | G    | C5-N7-C8    | 6.00  | 107.30      | 104.30   |
| 1   | AA    | 1467 | C    | N3-C4-N4    | 6.00  | 122.20      | 118.00   |
| 29  | B4    | 5    | ARG  | NE-CZ-NH1   | 6.00  | 123.30      | 120.30   |
| 35  | BB    | 262  | A    | C4-C5-C6    | 6.00  | 120.00      | 117.00   |
| 35  | BB    | 512  | G    | N1-C2-N2    | -6.00 | 110.80      | 116.20   |
| 35  | BB    | 771  | G    | C4-N9-C1'   | -6.00 | 118.70      | 126.50   |
| 35  | BB    | 863  | A    | C5-N7-C8    | 6.00  | 106.90      | 103.90   |
| 35  | BB    | 1027 | A    | N7-C8-N9    | 6.00  | 116.80      | 113.80   |
| 35  | BB    | 2087 | G    | C5-C6-N1    | -6.00 | 108.50      | 111.50   |
| 35  | BB    | 2089 | C    | C3'-C2'-C1' | -6.00 | 96.70       | 101.50   |
| 54  | BU    | 92   | VAL  | N-CA-C      | -6.00 | 94.81       | 111.00   |
| 1   | AA    | 835  | U    | C4'-C3'-C2' | -6.00 | 96.61       | 102.60   |
| 1   | AA    | 1153 | G    | C6-C5-N7    | -6.00 | 126.80      | 130.40   |
| 35  | BB    | 1803 | A    | C2-N3-C4    | 6.00  | 113.60      | 110.60   |
| 35  | BB    | 1981 | A    | C5'-C4'-C3' | -6.00 | 106.41      | 116.00   |
| 35  | BB    | 2095 | A    | C2-N3-C4    | -6.00 | 107.60      | 110.60   |
| 35  | BB    | 2179 | C    | OP1-P-OP2   | -6.00 | 110.61      | 119.60   |
| 45  | BL    | 95   | LEU  | CB-CG-CD1   | -6.00 | 100.81      | 111.00   |
| 1   | AA    | 359  | G    | C4-C5-N7    | 5.99  | 113.20      | 110.80   |
| 1   | AA    | 506  | G    | C5-C6-N1    | 5.99  | 114.50      | 111.50   |
| 1   | AA    | 608  | A    | OP2-P-O3'   | 5.99  | 118.39      | 105.20   |
| 1   | AA    | 1061 | G    | C2-N3-C4    | 5.99  | 114.90      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1397 | C    | C2-N1-C1'   | 5.99  | 125.39      | 118.80   |
| 1   | AA    | 1479 | C    | C6-N1-C2    | -5.99 | 117.90      | 120.30   |
| 34  | BA    | 110  | C    | N1-C2-O2    | -5.99 | 115.30      | 118.90   |
| 35  | BB    | 253  | C    | O4'-C1'-N1  | 5.99  | 113.00      | 108.20   |
| 35  | BB    | 405  | U    | C6-N1-C1'   | -5.99 | 112.81      | 121.20   |
| 35  | BB    | 911  | A    | C5-C6-N1    | -5.99 | 114.70      | 117.70   |
| 35  | BB    | 1969 | A    | N9-C4-C5    | 5.99  | 108.20      | 105.80   |
| 35  | BB    | 2640 | G    | C5-C6-O6    | -5.99 | 125.00      | 128.60   |
| 35  | BB    | 2853 | C    | C5-C4-N4    | -5.99 | 116.00      | 120.20   |
| 1   | AA    | 95   | C    | C2-N1-C1'   | 5.99  | 125.39      | 118.80   |
| 34  | BA    | 109  | A    | C4-C5-N7    | 5.99  | 113.70      | 110.70   |
| 35  | BB    | 271  | G    | C2'-C3'-O3' | 5.99  | 123.29      | 113.70   |
| 35  | BB    | 1040 | A    | C8-N9-C4    | 5.99  | 108.20      | 105.80   |
| 35  | BB    | 1817 | G    | P-O3'-C3'   | 5.99  | 126.89      | 119.70   |
| 35  | BB    | 2067 | G    | C6-N1-C2    | 5.99  | 128.69      | 125.10   |
| 1   | AA    | 399  | G    | C6-C5-N7    | -5.99 | 126.81      | 130.40   |
| 1   | AA    | 1398 | A    | O4'-C1'-N9  | 5.99  | 112.99      | 108.20   |
| 1   | AA    | 1470 | U    | N1-C2-O2    | -5.99 | 118.61      | 122.80   |
| 35  | BB    | 372  | G    | C1'-O4'-C4' | -5.99 | 105.11      | 109.90   |
| 35  | BB    | 485  | C    | C4'-C3'-C2' | -5.99 | 96.61       | 102.60   |
| 35  | BB    | 797  | G    | C5'-C4'-O4' | 5.99  | 116.29      | 109.10   |
| 35  | BB    | 1343 | G    | P-O5'-C5'   | -5.99 | 111.31      | 120.90   |
| 35  | BB    | 1545 | A    | N9-C4-C5    | 5.99  | 108.20      | 105.80   |
| 35  | BB    | 2382 | G    | C3'-C2'-C1' | 5.99  | 106.29      | 101.50   |
| 35  | BB    | 2512 | C    | C5-C6-N1    | -5.99 | 118.00      | 121.00   |
| 35  | BB    | 2566 | A    | C6-C5-N7    | -5.99 | 128.11      | 132.30   |
| 1   | AA    | 223  | A    | N1-C2-N3    | 5.99  | 132.29      | 129.30   |
| 1   | AA    | 1218 | C    | C5'-C4'-C3' | 5.99  | 125.58      | 116.00   |
| 1   | AA    | 1275 | A    | P-O3'-C3'   | -5.99 | 112.52      | 119.70   |
| 22  | AV    | 76   | A    | C1'-O4'-C4' | 5.99  | 114.69      | 109.90   |
| 35  | BB    | 271  | G    | N9-C4-C5    | -5.99 | 103.00      | 105.40   |
| 35  | BB    | 492  | A    | C5'-C4'-O4' | -5.99 | 101.91      | 109.10   |
| 35  | BB    | 748  | G    | P-O3'-C3'   | -5.99 | 112.51      | 119.70   |
| 35  | BB    | 945  | A    | N3-C4-N9    | 5.99  | 132.19      | 127.40   |
| 35  | BB    | 1386 | C    | C4'-C3'-C2' | -5.99 | 96.61       | 102.60   |
| 35  | BB    | 2027 | G    | C5-N7-C8    | -5.99 | 101.31      | 104.30   |
| 35  | BB    | 2477 | U    | C4-C5-C6    | 5.99  | 123.29      | 119.70   |
| 35  | BB    | 2544 | G    | C4-C5-N7    | 5.99  | 113.20      | 110.80   |
| 53  | BT    | 3    | ARG  | NE-CZ-NH1   | -5.99 | 117.31      | 120.30   |
| 1   | AA    | 119  | A    | N9-C4-C5    | 5.99  | 108.19      | 105.80   |
| 1   | AA    | 1246 | A    | N3-C4-C5    | -5.99 | 122.61      | 126.80   |
| 35  | BB    | 1185 | G    | C5-C6-O6    | -5.99 | 125.01      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1890 | A    | C4-C5-C6    | 5.99  | 119.99      | 117.00   |
| 35  | BB    | 2124 | G    | OP1-P-OP2   | -5.99 | 110.62      | 119.60   |
| 1   | AA    | 831  | A    | C5-C6-N6    | -5.99 | 118.91      | 123.70   |
| 1   | AA    | 1026 | G    | C6-C5-N7    | -5.99 | 126.81      | 130.40   |
| 1   | AA    | 1096 | C    | P-O5'-C5'   | 5.99  | 130.48      | 120.90   |
| 1   | AA    | 1212 | U    | C2-N1-C1'   | 5.99  | 124.88      | 117.70   |
| 1   | AA    | 1511 | G    | C8-N9-C4    | 5.99  | 108.80      | 106.40   |
| 31  | B6    | 21   | ARG  | CD-NE-CZ    | -5.99 | 115.22      | 123.60   |
| 35  | BB    | 101  | A    | C5-C6-N1    | -5.99 | 114.71      | 117.70   |
| 35  | BB    | 249  | C    | C5'-C4'-O4' | 5.99  | 116.28      | 109.10   |
| 35  | BB    | 758  | C    | N3-C4-N4    | 5.99  | 122.19      | 118.00   |
| 35  | BB    | 1080 | A    | P-O5'-C5'   | -5.99 | 111.32      | 120.90   |
| 35  | BB    | 1091 | G    | C2-N3-C4    | 5.99  | 114.89      | 111.90   |
| 35  | BB    | 1334 | G    | C2-N3-C4    | 5.99  | 114.89      | 111.90   |
| 35  | BB    | 1803 | A    | N9-C4-C5    | 5.99  | 108.19      | 105.80   |
| 35  | BB    | 1941 | C    | N3-C4-N4    | 5.99  | 122.19      | 118.00   |
| 35  | BB    | 2001 | C    | C5-C6-N1    | 5.99  | 123.99      | 121.00   |
| 35  | BB    | 2559 | C    | C6-N1-C2    | -5.99 | 117.91      | 120.30   |
| 35  | BB    | 2620 | C    | N3-C2-O2    | 5.99  | 126.09      | 121.90   |
| 35  | BB    | 2760 | C    | N1-C2-O2    | 5.99  | 122.49      | 118.90   |
| 35  | BB    | 2803 | G    | C4-N9-C1'   | -5.99 | 118.72      | 126.50   |
| 37  | BD    | 69   | ALA  | CB-CA-C     | -5.99 | 101.12      | 110.10   |
| 35  | BB    | 45   | G    | N1-C2-N3    | -5.98 | 120.31      | 123.90   |
| 35  | BB    | 66   | C    | C6-N1-C2    | -5.98 | 117.91      | 120.30   |
| 35  | BB    | 1479 | G    | N3-C2-N2    | 5.98  | 124.09      | 119.90   |
| 35  | BB    | 2616 | C    | N1-C2-O2    | 5.98  | 122.49      | 118.90   |
| 35  | BB    | 2733 | A    | N9-C1'-C2'  | -5.98 | 105.42      | 112.00   |
| 39  | BF    | 31   | GLU  | OE1-CD-OE2  | 5.98  | 130.48      | 123.30   |
| 1   | AA    | 543  | U    | C6-N1-C2    | -5.98 | 117.41      | 121.00   |
| 1   | AA    | 609  | A    | O4'-C4'-C3' | -5.98 | 98.02       | 104.00   |
| 1   | AA    | 653  | U    | C5'-C4'-O4' | 5.98  | 116.28      | 109.10   |
| 1   | AA    | 675  | A    | C5'-C4'-C3' | 5.98  | 125.57      | 116.00   |
| 1   | AA    | 682  | G    | P-O3'-C3'   | -5.98 | 112.52      | 119.70   |
| 1   | AA    | 1008 | U    | N3-C4-O4    | 5.98  | 123.59      | 119.40   |
| 1   | AA    | 1512 | U    | C3'-C2'-C1' | -5.98 | 96.72       | 101.50   |
| 34  | BA    | 69   | G    | N3-C4-C5    | 5.98  | 131.59      | 128.60   |
| 35  | BB    | 128  | C    | C5-C4-N4    | -5.98 | 116.01      | 120.20   |
| 35  | BB    | 384  | A    | C4-C5-C6    | 5.98  | 119.99      | 117.00   |
| 35  | BB    | 511  | U    | O4'-C1'-N1  | 5.98  | 112.99      | 108.20   |
| 35  | BB    | 725  | G    | C5-C6-O6    | -5.98 | 125.01      | 128.60   |
| 35  | BB    | 1053 | C    | C6-N1-C2    | -5.98 | 117.91      | 120.30   |
| 35  | BB    | 1163 | G    | C2-N3-C4    | 5.98  | 114.89      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1295 | C    | N3-C4-C5    | -5.98 | 119.51      | 121.90   |
| 35  | BB    | 1792 | G    | OP1-P-OP2   | -5.98 | 110.63      | 119.60   |
| 1   | AA    | 308  | C    | N3-C4-N4    | 5.98  | 122.19      | 118.00   |
| 1   | AA    | 318  | G    | C4-N9-C1'   | -5.98 | 118.73      | 126.50   |
| 1   | AA    | 501  | C    | N3-C4-C5    | -5.98 | 119.51      | 121.90   |
| 1   | AA    | 1202 | U    | N3-C2-O2    | -5.98 | 118.01      | 122.20   |
| 1   | AA    | 1248 | A    | C5-C6-N1    | -5.98 | 114.71      | 117.70   |
| 1   | AA    | 1250 | A    | C5-C6-N6    | -5.98 | 118.92      | 123.70   |
| 1   | AA    | 1398 | A    | N7-C8-N9    | -5.98 | 110.81      | 113.80   |
| 1   | AA    | 1526 | G    | C6-C5-N7    | -5.98 | 126.81      | 130.40   |
| 34  | BA    | 62   | C    | C3'-C2'-C1' | 5.98  | 106.28      | 101.50   |
| 34  | BA    | 94   | A    | O4'-C4'-C3' | -5.98 | 98.02       | 104.00   |
| 35  | BB    | 614  | A    | C5-C6-N6    | -5.98 | 118.92      | 123.70   |
| 35  | BB    | 629  | G    | C8-N9-C1'   | 5.98  | 134.77      | 127.00   |
| 35  | BB    | 836  | G    | N1-C2-N3    | -5.98 | 120.31      | 123.90   |
| 35  | BB    | 937  | C    | C4'-C3'-C2' | -5.98 | 96.62       | 102.60   |
| 35  | BB    | 1200 | C    | C5-C4-N4    | -5.98 | 116.01      | 120.20   |
| 35  | BB    | 1384 | A    | C5-C6-N1    | -5.98 | 114.71      | 117.70   |
| 35  | BB    | 1448 | G    | N3-C2-N2    | 5.98  | 124.09      | 119.90   |
| 35  | BB    | 1695 | G    | C8-N9-C1'   | -5.98 | 119.22      | 127.00   |
| 35  | BB    | 1698 | A    | C4-C5-C6    | 5.98  | 119.99      | 117.00   |
| 35  | BB    | 2271 | G    | C5-C6-O6    | -5.98 | 125.01      | 128.60   |
| 35  | BB    | 2767 | C    | C5-C6-N1    | -5.98 | 118.01      | 121.00   |
| 1   | AA    | 51   | A    | N3-C4-N9    | 5.98  | 132.18      | 127.40   |
| 1   | AA    | 253  | A    | C6-C5-N7    | -5.98 | 128.11      | 132.30   |
| 1   | AA    | 453  | G    | O4'-C1'-N9  | 5.98  | 112.98      | 108.20   |
| 1   | AA    | 857  | C    | N3-C4-N4    | 5.98  | 122.19      | 118.00   |
| 35  | BB    | 1372 | U    | C2-N3-C4    | 5.98  | 130.59      | 127.00   |
| 35  | BB    | 2154 | A    | N1-C2-N3    | 5.98  | 132.29      | 129.30   |
| 35  | BB    | 2162 | G    | P-O3'-C3'   | -5.98 | 112.53      | 119.70   |
| 35  | BB    | 2733 | A    | C6-C5-N7    | -5.98 | 128.11      | 132.30   |
| 49  | BP    | 73   | PHE  | CB-CG-CD2   | -5.98 | 116.61      | 120.80   |
| 1   | AA    | 21   | G    | C1'-O4'-C4' | -5.98 | 105.12      | 109.90   |
| 1   | AA    | 88   | U    | N1-C2-N3    | -5.98 | 111.31      | 114.90   |
| 1   | AA    | 716  | A    | O4'-C1'-N9  | 5.98  | 112.98      | 108.20   |
| 1   | AA    | 834  | U    | C3'-C2'-C1' | -5.98 | 96.72       | 101.50   |
| 35  | BB    | 238  | C    | N3-C2-O2    | 5.98  | 126.08      | 121.90   |
| 35  | BB    | 374  | A    | C4-C5-C6    | 5.98  | 119.99      | 117.00   |
| 35  | BB    | 456  | C    | N3-C4-N4    | 5.98  | 122.18      | 118.00   |
| 35  | BB    | 718  | A    | N7-C8-N9    | -5.98 | 110.81      | 113.80   |
| 35  | BB    | 1112 | G    | C1'-O4'-C4' | 5.98  | 114.68      | 109.90   |
| 35  | BB    | 1144 | A    | N3-C4-N9    | 5.98  | 132.18      | 127.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1199 | U    | O4'-C1'-N1  | 5.98  | 112.98      | 108.20   |
| 35  | BB    | 1360 | G    | N3-C4-N9    | -5.98 | 122.41      | 126.00   |
| 35  | BB    | 1714 | U    | N3-C4-O4    | 5.98  | 123.58      | 119.40   |
| 35  | BB    | 2035 | G    | C6-N1-C2    | 5.98  | 128.69      | 125.10   |
| 35  | BB    | 2166 | U    | C3'-C2'-C1' | -5.98 | 96.72       | 101.50   |
| 35  | BB    | 2167 | U    | C6-N1-C2    | -5.98 | 117.41      | 121.00   |
| 35  | BB    | 2544 | G    | C5-C6-O6    | -5.98 | 125.01      | 128.60   |
| 1   | AA    | 1329 | A    | N7-C8-N9    | -5.98 | 110.81      | 113.80   |
| 35  | BB    | 2488 | G    | C5-C6-N1    | -5.98 | 108.51      | 111.50   |
| 35  | BB    | 2720 | U    | O4'-C4'-C3' | -5.98 | 98.02       | 104.00   |
| 1   | AA    | 616  | G    | N1-C2-N2    | 5.97  | 121.58      | 116.20   |
| 1   | AA    | 624  | C    | O4'-C1'-N1  | 5.97  | 112.98      | 108.20   |
| 1   | AA    | 855  | U    | O4'-C1'-N1  | 5.97  | 112.98      | 108.20   |
| 35  | BB    | 207  | A    | C6-C5-N7    | -5.97 | 128.12      | 132.30   |
| 35  | BB    | 298  | G    | N3-C2-N2    | 5.97  | 124.08      | 119.90   |
| 35  | BB    | 528  | A    | N7-C8-N9    | -5.97 | 110.81      | 113.80   |
| 35  | BB    | 1221 | C    | C4-C5-C6    | -5.97 | 114.41      | 117.40   |
| 35  | BB    | 1456 | G    | N1-C2-N2    | -5.97 | 110.82      | 116.20   |
| 35  | BB    | 1505 | A    | C2-N3-C4    | 5.97  | 113.59      | 110.60   |
| 35  | BB    | 1904 | G    | O4'-C1'-N9  | 5.97  | 112.98      | 108.20   |
| 35  | BB    | 2107 | G    | OP2-P-O3'   | 5.97  | 118.34      | 105.20   |
| 35  | BB    | 2116 | G    | C5-C6-N1    | -5.97 | 108.51      | 111.50   |
| 35  | BB    | 2393 | U    | C5-C4-O4    | -5.97 | 122.31      | 125.90   |
| 47  | BN    | 63   | ARG  | NE-CZ-NH2   | 5.97  | 123.29      | 120.30   |
| 1   | AA    | 349  | A    | N9-C4-C5    | 5.97  | 108.19      | 105.80   |
| 1   | AA    | 394  | G    | N1-C2-N3    | -5.97 | 120.32      | 123.90   |
| 1   | AA    | 945  | G    | N3-C2-N2    | 5.97  | 124.08      | 119.90   |
| 1   | AA    | 1139 | G    | N3-C2-N2    | 5.97  | 124.08      | 119.90   |
| 1   | AA    | 1142 | G    | C5'-C4'-C3' | 5.97  | 125.56      | 116.00   |
| 1   | AA    | 1239 | A    | C6-N1-C2    | 5.97  | 122.18      | 118.60   |
| 1   | AA    | 1366 | C    | N1-C2-O2    | -5.97 | 115.32      | 118.90   |
| 1   | AA    | 1369 | C    | N1-C2-N3    | -5.97 | 115.02      | 119.20   |
| 35  | BB    | 81   | G    | C4-C5-N7    | 5.97  | 113.19      | 110.80   |
| 35  | BB    | 86   | G    | N1-C2-N2    | -5.97 | 110.82      | 116.20   |
| 35  | BB    | 1098 | A    | C4-C5-C6    | 5.97  | 119.99      | 117.00   |
| 35  | BB    | 2181 | U    | N1-C2-O2    | -5.97 | 118.62      | 122.80   |
| 35  | BB    | 2224 | G    | N3-C2-N2    | 5.97  | 124.08      | 119.90   |
| 1   | AA    | 338  | A    | N7-C8-N9    | -5.97 | 110.81      | 113.80   |
| 1   | AA    | 1188 | A    | C6-C5-N7    | -5.97 | 128.12      | 132.30   |
| 35  | BB    | 1206 | G    | N3-C4-N9    | -5.97 | 122.42      | 126.00   |
| 1   | AA    | 9    | G    | C2-N3-C4    | 5.97  | 114.89      | 111.90   |
| 1   | AA    | 1252 | A    | C6-C5-N7    | -5.97 | 128.12      | 132.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1472 | U    | C5'-C4'-C3' | -5.97 | 106.45      | 116.00   |
| 35  | BB    | 1296 | G    | O4'-C1'-N9  | 5.97  | 112.98      | 108.20   |
| 35  | BB    | 1611 | C    | N3-C4-C5    | -5.97 | 119.51      | 121.90   |
| 35  | BB    | 1892 | C    | C5-C4-N4    | -5.97 | 116.02      | 120.20   |
| 35  | BB    | 1927 | A    | C5-N7-C8    | -5.97 | 100.92      | 103.90   |
| 35  | BB    | 1964 | G    | C8-N9-C4    | -5.97 | 104.01      | 106.40   |
| 35  | BB    | 2591 | C    | N3-C4-C5    | -5.97 | 119.51      | 121.90   |
| 35  | BB    | 2686 | G    | C4-C5-C6    | -5.97 | 115.22      | 118.80   |
| 41  | BH    | 123  | ARG  | NE-CZ-NH1   | -5.97 | 117.32      | 120.30   |
| 52  | BS    | 98   | LYS  | N-CA-CB     | 5.97  | 121.34      | 110.60   |
| 1   | AA    | 1458 | G    | O5'-P-OP1   | 5.97  | 117.86      | 110.70   |
| 35  | BB    | 91   | A    | N1-C2-N3    | -5.97 | 126.32      | 129.30   |
| 35  | BB    | 1221 | C    | C6-N1-C1'   | -5.97 | 113.64      | 120.80   |
| 35  | BB    | 1246 | A    | C5-C6-N6    | -5.97 | 118.92      | 123.70   |
| 35  | BB    | 2849 | U    | N3-C4-C5    | -5.97 | 111.02      | 114.60   |
| 1   | AA    | 7    | A    | C2-N3-C4    | -5.97 | 107.62      | 110.60   |
| 1   | AA    | 26   | A    | C4-C5-C6    | 5.97  | 119.98      | 117.00   |
| 1   | AA    | 705  | G    | C5-C6-O6    | -5.97 | 125.02      | 128.60   |
| 1   | AA    | 1074 | G    | N1-C2-N2    | -5.97 | 110.83      | 116.20   |
| 34  | BA    | 15   | A    | C5-C6-N6    | -5.97 | 118.93      | 123.70   |
| 35  | BB    | 144  | A    | C3'-C2'-C1' | -5.97 | 96.73       | 101.50   |
| 35  | BB    | 1369 | G    | O4'-C4'-C3' | -5.97 | 98.03       | 104.00   |
| 35  | BB    | 1524 | G    | C6-C5-N7    | -5.97 | 126.82      | 130.40   |
| 35  | BB    | 1721 | G    | N3-C4-C5    | -5.97 | 125.62      | 128.60   |
| 35  | BB    | 1921 | G    | C5-C6-N1    | -5.97 | 108.52      | 111.50   |
| 1   | AA    | 329  | A    | C6-C5-N7    | -5.96 | 128.12      | 132.30   |
| 1   | AA    | 329  | A    | N3-C4-N9    | 5.96  | 132.17      | 127.40   |
| 35  | BB    | 567  | U    | C2-N3-C4    | 5.96  | 130.58      | 127.00   |
| 35  | BB    | 1358 | G    | C4-C5-N7    | 5.96  | 113.19      | 110.80   |
| 35  | BB    | 1545 | A    | C4-C5-C6    | 5.96  | 119.98      | 117.00   |
| 35  | BB    | 2091 | C    | C6-N1-C2    | 5.96  | 122.69      | 120.30   |
| 35  | BB    | 2121 | G    | C5-C6-N1    | -5.96 | 108.52      | 111.50   |
| 35  | BB    | 2480 | C    | N1-C2-O2    | -5.96 | 115.32      | 118.90   |
| 41  | BH    | 93   | SER  | N-CA-CB     | 5.96  | 119.45      | 110.50   |
| 51  | BR    | 2    | TYR  | CA-CB-CG    | -5.96 | 102.07      | 113.40   |
| 1   | AA    | 868  | C    | C4'-C3'-C2' | -5.96 | 96.64       | 102.60   |
| 35  | BB    | 659  | G    | C6-C5-N7    | -5.96 | 126.82      | 130.40   |
| 35  | BB    | 1302 | A    | N1-C2-N3    | 5.96  | 132.28      | 129.30   |
| 35  | BB    | 1439 | A    | C2-N3-C4    | -5.96 | 107.62      | 110.60   |
| 35  | BB    | 1684 | G    | N7-C8-N9    | 5.96  | 116.08      | 113.10   |
| 35  | BB    | 2482 | A    | O4'-C1'-N9  | 5.96  | 112.97      | 108.20   |
| 51  | BR    | 2    | TYR  | CB-CG-CD2   | -5.96 | 117.42      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 431  | A    | C5-C6-N1    | -5.96 | 114.72      | 117.70   |
| 1   | AA    | 1006 | G    | N1-C2-N2    | -5.96 | 110.83      | 116.20   |
| 22  | AV    | 70   | C    | C5-C4-N4    | -5.96 | 116.03      | 120.20   |
| 35  | BB    | 188  | G    | O4'-C1'-N9  | 5.96  | 112.97      | 108.20   |
| 35  | BB    | 614  | A    | C2-N3-C4    | -5.96 | 107.62      | 110.60   |
| 35  | BB    | 819  | A    | O4'-C1'-N9  | 5.96  | 112.97      | 108.20   |
| 35  | BB    | 926  | G    | O5'-P-OP2   | -5.96 | 100.33      | 105.70   |
| 35  | BB    | 1745 | A    | C2-N3-C4    | -5.96 | 107.62      | 110.60   |
| 35  | BB    | 1917 | U    | O4'-C4'-C3' | -5.96 | 98.04       | 104.00   |
| 35  | BB    | 2752 | C    | O4'-C1'-N1  | 5.96  | 112.97      | 108.20   |
| 1   | AA    | 640  | A    | C2'-C3'-O3' | 5.96  | 123.24      | 113.70   |
| 35  | BB    | 488  | G    | C5-C6-N1    | -5.96 | 108.52      | 111.50   |
| 35  | BB    | 743  | A    | C5-C6-N1    | -5.96 | 114.72      | 117.70   |
| 35  | BB    | 788  | A    | N7-C8-N9    | -5.96 | 110.82      | 113.80   |
| 35  | BB    | 1386 | C    | N1-C2-N3    | -5.96 | 115.03      | 119.20   |
| 35  | BB    | 2413 | G    | C8-N9-C4    | 5.96  | 108.78      | 106.40   |
| 35  | BB    | 2641 | G    | N7-C8-N9    | -5.96 | 110.12      | 113.10   |
| 36  | BC    | 237  | ARG  | N-CA-CB     | 5.96  | 121.33      | 110.60   |
| 1   | AA    | 9    | G    | C4'-C3'-C2' | -5.96 | 96.64       | 102.60   |
| 1   | AA    | 667  | G    | C6-C5-N7    | -5.96 | 126.82      | 130.40   |
| 34  | BA    | 41   | G    | C6-C5-N7    | -5.96 | 126.82      | 130.40   |
| 35  | BB    | 169  | G    | N1-C6-O6    | 5.96  | 123.47      | 119.90   |
| 35  | BB    | 301  | G    | N3-C2-N2    | 5.96  | 124.07      | 119.90   |
| 35  | BB    | 1081 | U    | O4'-C1'-N1  | 5.96  | 112.97      | 108.20   |
| 35  | BB    | 1470 | A    | C6-C5-N7    | -5.96 | 128.13      | 132.30   |
| 35  | BB    | 1926 | U    | N1-C2-N3    | -5.96 | 111.33      | 114.90   |
| 35  | BB    | 1999 | C    | N1-C2-N3    | -5.96 | 115.03      | 119.20   |
| 49  | BP    | 97   | TYR  | CB-CG-CD1   | -5.96 | 117.42      | 121.00   |
| 1   | AA    | 22   | G    | C5-C6-O6    | -5.96 | 125.03      | 128.60   |
| 1   | AA    | 474  | G    | N3-C2-N2    | 5.96  | 124.07      | 119.90   |
| 1   | AA    | 474  | G    | C5-C6-N1    | -5.96 | 108.52      | 111.50   |
| 1   | AA    | 495  | A    | N3-C4-N9    | 5.96  | 132.17      | 127.40   |
| 1   | AA    | 1035 | A    | C6-C5-N7    | -5.96 | 128.13      | 132.30   |
| 1   | AA    | 1096 | C    | OP1-P-OP2   | -5.96 | 110.67      | 119.60   |
| 1   | AA    | 1294 | G    | P-O3'-C3'   | -5.96 | 112.55      | 119.70   |
| 1   | AA    | 1338 | G    | N3-C4-N9    | -5.96 | 122.43      | 126.00   |
| 2   | AB    | 122  | ASP  | N-CA-CB     | 5.96  | 121.32      | 110.60   |
| 35  | BB    | 105  | C    | O4'-C1'-N1  | 5.96  | 112.97      | 108.20   |
| 35  | BB    | 463  | G    | C2-N3-C4    | 5.96  | 114.88      | 111.90   |
| 35  | BB    | 530  | G    | C2-N3-C4    | 5.96  | 114.88      | 111.90   |
| 35  | BB    | 910  | A    | C8-N9-C4    | -5.96 | 103.42      | 105.80   |
| 35  | BB    | 1337 | G    | N3-C2-N2    | 5.96  | 124.07      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1802 | A    | N3-C4-C5    | -5.96 | 122.63      | 126.80   |
| 35  | BB    | 2245 | U    | O3'-P-O5'   | -5.96 | 92.68       | 104.00   |
| 35  | BB    | 2322 | A    | C5-C6-N1    | -5.96 | 114.72      | 117.70   |
| 35  | BB    | 2436 | G    | C2-N3-C4    | -5.96 | 108.92      | 111.90   |
| 35  | BB    | 2634 | A    | C6-C5-N7    | -5.96 | 128.13      | 132.30   |
| 1   | AA    | 158  | G    | C5-C6-N1    | -5.96 | 108.52      | 111.50   |
| 1   | AA    | 248  | C    | N1-C2-O2    | -5.96 | 115.33      | 118.90   |
| 1   | AA    | 488  | C    | C1'-O4'-C4' | 5.96  | 114.66      | 109.90   |
| 1   | AA    | 1059 | C    | N3-C4-C5    | 5.96  | 124.28      | 121.90   |
| 1   | AA    | 1082 | A    | N7-C8-N9    | 5.96  | 116.78      | 113.80   |
| 35  | BB    | 210  | C    | C5-C6-N1    | 5.96  | 123.98      | 121.00   |
| 35  | BB    | 1479 | G    | C4-C5-C6    | 5.96  | 122.37      | 118.80   |
| 47  | BN    | 96   | ARG  | NE-CZ-NH1   | 5.96  | 123.28      | 120.30   |
| 1   | AA    | 315  | A    | C4-C5-C6    | 5.95  | 119.98      | 117.00   |
| 35  | BB    | 406  | G    | N3-C2-N2    | 5.95  | 124.07      | 119.90   |
| 35  | BB    | 1134 | A    | C1'-O4'-C4' | 5.95  | 114.66      | 109.90   |
| 35  | BB    | 1457 | U    | N3-C4-C5    | 5.95  | 118.17      | 114.60   |
| 35  | BB    | 2225 | A    | N3-C4-C5    | -5.95 | 122.63      | 126.80   |
| 35  | BB    | 2352 | A    | C6-C5-N7    | -5.95 | 128.13      | 132.30   |
| 35  | BB    | 2813 | A    | C5-C6-N6    | -5.95 | 118.94      | 123.70   |
| 1   | AA    | 270  | A    | N3-C4-C5    | -5.95 | 122.63      | 126.80   |
| 1   | AA    | 1144 | G    | C4-C5-N7    | -5.95 | 108.42      | 110.80   |
| 34  | BA    | 44   | G    | OP1-P-O3'   | 5.95  | 118.29      | 105.20   |
| 35  | BB    | 760  | G    | OP1-P-OP2   | -5.95 | 110.67      | 119.60   |
| 35  | BB    | 1234 | U    | O4'-C1'-N1  | 5.95  | 112.96      | 108.20   |
| 35  | BB    | 2861 | U    | N3-C4-O4    | 5.95  | 123.57      | 119.40   |
| 1   | AA    | 1068 | G    | P-O5'-C5'   | -5.95 | 111.38      | 120.90   |
| 1   | AA    | 1385 | G    | C4-C5-N7    | -5.95 | 108.42      | 110.80   |
| 1   | AA    | 1393 | U    | C3'-C2'-C1' | 5.95  | 106.26      | 101.50   |
| 21  | AU    | 33   | ARG  | NE-CZ-NH1   | 5.95  | 123.28      | 120.30   |
| 34  | BA    | 56   | G    | C6-C5-N7    | -5.95 | 126.83      | 130.40   |
| 35  | BB    | 17   | G    | N7-C8-N9    | -5.95 | 110.12      | 113.10   |
| 35  | BB    | 140  | C    | C6-N1-C2    | -5.95 | 117.92      | 120.30   |
| 35  | BB    | 736  | C    | C5-C4-N4    | -5.95 | 116.03      | 120.20   |
| 35  | BB    | 831  | G    | C4-C5-C6    | 5.95  | 122.37      | 118.80   |
| 35  | BB    | 1458 | U    | N1-C2-N3    | -5.95 | 111.33      | 114.90   |
| 35  | BB    | 2619 | C    | C5-C4-N4    | -5.95 | 116.03      | 120.20   |
| 35  | BB    | 2724 | U    | N3-C4-O4    | 5.95  | 123.56      | 119.40   |
| 1   | AA    | 539  | A    | C5-N7-C8    | 5.95  | 106.87      | 103.90   |
| 1   | AA    | 543  | U    | N3-C4-O4    | 5.95  | 123.56      | 119.40   |
| 1   | AA    | 717  | U    | N1-C2-N3    | -5.95 | 111.33      | 114.90   |
| 1   | AA    | 1036 | A    | C5-C6-N1    | -5.95 | 114.73      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1244 | G    | C6-C5-N7   | -5.95 | 126.83      | 130.40   |
| 1   | AA    | 1475 | G    | C4-C5-C6   | 5.95  | 122.37      | 118.80   |
| 1   | AA    | 1501 | C    | N3-C4-N4   | 5.95  | 122.16      | 118.00   |
| 35  | BB    | 76   | C    | C5-C6-N1   | 5.95  | 123.97      | 121.00   |
| 35  | BB    | 173  | A    | C4-C5-N7   | -5.95 | 107.73      | 110.70   |
| 35  | BB    | 890  | C    | C6-N1-C2   | -5.95 | 117.92      | 120.30   |
| 35  | BB    | 1321 | A    | C4-C5-C6   | 5.95  | 119.97      | 117.00   |
| 35  | BB    | 1594 | U    | N3-C4-O4   | 5.95  | 123.56      | 119.40   |
| 35  | BB    | 1601 | G    | C6-N1-C2   | -5.95 | 121.53      | 125.10   |
| 35  | BB    | 1690 | A    | C8-N9-C4   | -5.95 | 103.42      | 105.80   |
| 35  | BB    | 1866 | A    | N1-C6-N6   | 5.95  | 122.17      | 118.60   |
| 35  | BB    | 2380 | C    | C2-N3-C4   | -5.95 | 116.93      | 119.90   |
| 35  | BB    | 2756 | U    | N3-C4-O4   | 5.95  | 123.56      | 119.40   |
| 35  | BB    | 2829 | A    | O4'-C1'-N9 | 5.95  | 112.96      | 108.20   |
| 1   | AA    | 311  | C    | C5-C6-N1   | 5.95  | 123.97      | 121.00   |
| 1   | AA    | 403  | C    | C5-C4-N4   | -5.95 | 116.04      | 120.20   |
| 1   | AA    | 1449 | C    | C2-N3-C4   | 5.95  | 122.87      | 119.90   |
| 1   | AA    | 524  | G    | C4-C5-N7   | 5.95  | 113.18      | 110.80   |
| 1   | AA    | 647  | C    | N3-C4-C5   | -5.95 | 119.52      | 121.90   |
| 1   | AA    | 778  | G    | P-O5'-C5'  | 5.95  | 130.41      | 120.90   |
| 1   | AA    | 788  | U    | C5-C6-N1   | 5.95  | 125.67      | 122.70   |
| 1   | AA    | 1230 | C    | N1-C2-O2   | 5.95  | 122.47      | 118.90   |
| 1   | AA    | 1447 | A    | C5-C6-N6   | -5.95 | 118.94      | 123.70   |
| 8   | AH    | 112  | ASP  | CB-CG-OD1  | 5.95  | 123.65      | 118.30   |
| 9   | AI    | 44   | ARG  | NE-CZ-NH2  | -5.95 | 117.33      | 120.30   |
| 29  | B4    | 42   | VAL  | C-N-CA     | 5.95  | 136.56      | 121.70   |
| 35  | BB    | 98   | G    | N9-C4-C5   | 5.95  | 107.78      | 105.40   |
| 35  | BB    | 296  | U    | C6-N1-C2   | -5.95 | 117.43      | 121.00   |
| 35  | BB    | 1021 | A    | P-O5'-C5'  | -5.95 | 111.39      | 120.90   |
| 35  | BB    | 1343 | G    | C5-C6-N1   | -5.95 | 108.53      | 111.50   |
| 35  | BB    | 2052 | A    | N7-C8-N9   | -5.95 | 110.83      | 113.80   |
| 35  | BB    | 2630 | G    | N1-C2-N3   | -5.95 | 120.33      | 123.90   |
| 35  | BB    | 2727 | A    | P-O5'-C5'  | -5.95 | 111.39      | 120.90   |
| 1   | AA    | 69   | G    | C2-N3-C4   | -5.94 | 108.93      | 111.90   |
| 1   | AA    | 123  | U    | P-O3'-C3'  | 5.94  | 126.83      | 119.70   |
| 1   | AA    | 1197 | A    | N7-C8-N9   | -5.94 | 110.83      | 113.80   |
| 34  | BA    | 70   | C    | N1-C2-N3   | -5.94 | 115.04      | 119.20   |
| 34  | BA    | 109  | A    | C5-C6-N1   | -5.94 | 114.73      | 117.70   |
| 35  | BB    | 269  | C    | C5-C6-N1   | 5.94  | 123.97      | 121.00   |
| 35  | BB    | 2329 | U    | N3-C2-O2   | -5.94 | 118.04      | 122.20   |
| 35  | BB    | 2411 | A    | N7-C8-N9   | -5.94 | 110.83      | 113.80   |
| 35  | BB    | 2572 | A    | C5-N7-C8   | 5.94  | 106.87      | 103.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 416  | G    | C4-C5-N7    | -5.94 | 108.42      | 110.80   |
| 1   | AA    | 695  | A    | C5-C6-N6    | -5.94 | 118.95      | 123.70   |
| 1   | AA    | 751  | U    | N3-C4-O4    | 5.94  | 123.56      | 119.40   |
| 1   | AA    | 846  | G    | C5-N7-C8    | 5.94  | 107.27      | 104.30   |
| 1   | AA    | 1423 | G    | N1-C6-O6    | 5.94  | 123.47      | 119.90   |
| 22  | AV    | 51   | A    | C5-C6-N6    | -5.94 | 118.94      | 123.70   |
| 35  | BB    | 199  | A    | N1-C2-N3    | 5.94  | 132.27      | 129.30   |
| 35  | BB    | 454  | A    | P-O3'-C3'   | 5.94  | 126.83      | 119.70   |
| 35  | BB    | 1038 | G    | N1-C6-O6    | 5.94  | 123.47      | 119.90   |
| 35  | BB    | 1411 | U    | C5-C4-O4    | 5.94  | 129.47      | 125.90   |
| 36  | BC    | 189  | ALA  | CB-CA-C     | -5.94 | 101.19      | 110.10   |
| 1   | AA    | 462  | G    | C1'-O4'-C4' | 5.94  | 114.65      | 109.90   |
| 1   | AA    | 561  | U    | P-O3'-C3'   | 5.94  | 126.83      | 119.70   |
| 1   | AA    | 605  | U    | N3-C4-C5    | -5.94 | 111.04      | 114.60   |
| 1   | AA    | 1488 | G    | N9-C4-C5    | 5.94  | 107.78      | 105.40   |
| 35  | BB    | 106  | C    | C3'-C2'-C1' | -5.94 | 96.75       | 101.50   |
| 35  | BB    | 406  | G    | C8-N9-C1'   | 5.94  | 134.72      | 127.00   |
| 35  | BB    | 1081 | U    | C1'-O4'-C4' | 5.94  | 114.65      | 109.90   |
| 35  | BB    | 1290 | C    | N3-C2-O2    | -5.94 | 117.74      | 121.90   |
| 35  | BB    | 1484 | U    | O4'-C1'-N1  | 5.94  | 112.95      | 108.20   |
| 35  | BB    | 2209 | G    | N9-C4-C5    | 5.94  | 107.78      | 105.40   |
| 35  | BB    | 2589 | A    | N9-C1'-C2'  | -5.94 | 105.47      | 112.00   |
| 35  | BB    | 2745 | C    | C6-N1-C2    | 5.94  | 122.68      | 120.30   |
| 1   | AA    | 378  | G    | C8-N9-C4    | -5.94 | 104.02      | 106.40   |
| 1   | AA    | 896  | C    | C5-C6-N1    | 5.94  | 123.97      | 121.00   |
| 1   | AA    | 1294 | G    | C4'-C3'-C2' | -5.94 | 96.66       | 102.60   |
| 4   | AD    | 62   | ARG  | NE-CZ-NH2   | 5.94  | 123.27      | 120.30   |
| 34  | BA    | 105  | G    | N3-C2-N2    | 5.94  | 124.06      | 119.90   |
| 35  | BB    | 1351 | C    | C1'-O4'-C4' | -5.94 | 105.15      | 109.90   |
| 35  | BB    | 1383 | A    | C5-C6-N6    | -5.94 | 118.95      | 123.70   |
| 35  | BB    | 1481 | U    | C6-N1-C2    | -5.94 | 117.44      | 121.00   |
| 35  | BB    | 1914 | C    | O4'-C1'-N1  | 5.94  | 112.95      | 108.20   |
| 35  | BB    | 2680 | U    | O4'-C1'-N1  | 5.94  | 112.95      | 108.20   |
| 38  | BE    | 162  | ARG  | NE-CZ-NH1   | -5.94 | 117.33      | 120.30   |
| 1   | AA    | 291  | U    | O4'-C1'-N1  | 5.94  | 112.95      | 108.20   |
| 1   | AA    | 1016 | A    | P-O3'-C3'   | -5.94 | 112.57      | 119.70   |
| 1   | AA    | 1200 | C    | O4'-C1'-C2' | 5.94  | 112.94      | 107.60   |
| 35  | BB    | 1257 | C    | N1-C2-N3    | -5.94 | 115.04      | 119.20   |
| 35  | BB    | 1314 | C    | C2-N3-C4    | -5.94 | 116.93      | 119.90   |
| 35  | BB    | 2895 | G    | C5'-C4'-C3' | -5.94 | 106.50      | 116.00   |
| 1   | AA    | 1074 | G    | N3-C4-N9    | 5.94  | 129.56      | 126.00   |
| 35  | BB    | 756  | A    | C4-C5-N7    | -5.94 | 107.73      | 110.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 762  | U    | N1-C1'-C2'  | -5.94 | 105.47      | 112.00   |
| 35  | BB    | 869  | G    | P-O5'-C5'   | 5.94  | 130.40      | 120.90   |
| 35  | BB    | 929  | U    | C5-C6-N1    | 5.94  | 125.67      | 122.70   |
| 35  | BB    | 1182 | G    | N3-C2-N2    | 5.94  | 124.06      | 119.90   |
| 35  | BB    | 1525 | A    | C4-C5-C6    | 5.94  | 119.97      | 117.00   |
| 35  | BB    | 1810 | A    | C4-C5-C6    | 5.94  | 119.97      | 117.00   |
| 35  | BB    | 2284 | A    | O4'-C1'-N9  | 5.94  | 112.95      | 108.20   |
| 35  | BB    | 2634 | A    | C1'-O4'-C4' | 5.94  | 114.65      | 109.90   |
| 35  | BB    | 2882 | A    | N1-C2-N3    | 5.94  | 132.27      | 129.30   |
| 1   | AA    | 342  | C    | N3-C2-O2    | 5.93  | 126.05      | 121.90   |
| 1   | AA    | 548  | G    | N3-C2-N2    | 5.93  | 124.05      | 119.90   |
| 1   | AA    | 936  | C    | N3-C4-N4    | 5.93  | 122.15      | 118.00   |
| 29  | B4    | 48   | TYR  | CB-CG-CD2   | -5.93 | 117.44      | 121.00   |
| 35  | BB    | 85   | G    | C4-C5-C6    | 5.93  | 122.36      | 118.80   |
| 35  | BB    | 676  | A    | C8-N9-C4    | 5.93  | 108.17      | 105.80   |
| 35  | BB    | 767  | U    | N3-C2-O2    | 5.93  | 126.35      | 122.20   |
| 35  | BB    | 1453 | A    | N1-C6-N6    | 5.93  | 122.16      | 118.60   |
| 35  | BB    | 1517 | G    | C5-N7-C8    | 5.93  | 107.27      | 104.30   |
| 35  | BB    | 1721 | G    | N1-C2-N3    | -5.93 | 120.34      | 123.90   |
| 35  | BB    | 1939 | U    | N3-C4-C5    | -5.93 | 111.04      | 114.60   |
| 35  | BB    | 2709 | G    | C1'-O4'-C4' | 5.93  | 114.65      | 109.90   |
| 35  | BB    | 2760 | C    | O4'-C1'-N1  | 5.93  | 112.95      | 108.20   |
| 35  | BB    | 2828 | G    | O4'-C1'-N9  | 5.93  | 112.95      | 108.20   |
| 35  | BB    | 2897 | U    | N1-C1'-C2'  | -5.93 | 105.47      | 112.00   |
| 1   | AA    | 161  | A    | N1-C2-N3    | 5.93  | 132.27      | 129.30   |
| 1   | AA    | 625  | U    | O4'-C1'-N1  | 5.93  | 112.95      | 108.20   |
| 1   | AA    | 765  | G    | C4-C5-C6    | 5.93  | 122.36      | 118.80   |
| 1   | AA    | 1096 | C    | C5-C4-N4    | -5.93 | 116.05      | 120.20   |
| 1   | AA    | 1187 | G    | N1-C6-O6    | 5.93  | 123.46      | 119.90   |
| 1   | AA    | 1354 | U    | O4'-C1'-N1  | 5.93  | 112.95      | 108.20   |
| 1   | AA    | 1361 | G    | C5-C6-N1    | 5.93  | 114.47      | 111.50   |
| 35  | BB    | 1095 | A    | C5-C6-N6    | -5.93 | 118.95      | 123.70   |
| 35  | BB    | 1275 | A    | N1-C6-N6    | 5.93  | 122.16      | 118.60   |
| 35  | BB    | 1302 | A    | O5'-C5'-C4' | 5.93  | 122.97      | 111.70   |
| 35  | BB    | 1891 | G    | C4-C5-N7    | -5.93 | 108.43      | 110.80   |
| 35  | BB    | 2062 | A    | C4-C5-N7    | 5.93  | 113.67      | 110.70   |
| 35  | BB    | 2461 | A    | O4'-C1'-C2' | -5.93 | 99.87       | 105.80   |
| 35  | BB    | 2712 | C    | C4-C5-C6    | 5.93  | 120.37      | 117.40   |
| 35  | BB    | 2770 | G    | C8-N9-C4    | 5.93  | 108.77      | 106.40   |
| 1   | AA    | 210  | C    | C5'-C4'-O4' | 5.93  | 116.22      | 109.10   |
| 35  | BB    | 915  | C    | N3-C4-N4    | 5.93  | 122.15      | 118.00   |
| 35  | BB    | 919  | U    | O4'-C1'-N1  | 5.93  | 112.94      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1154 | G    | O4'-C1'-N9  | 5.93  | 112.94      | 108.20   |
| 35  | BB    | 2010 | G    | C6-C5-N7    | -5.93 | 126.84      | 130.40   |
| 1   | AA    | 289  | G    | N1-C6-O6    | -5.93 | 116.34      | 119.90   |
| 1   | AA    | 292  | G    | N1-C6-O6    | 5.93  | 123.46      | 119.90   |
| 1   | AA    | 1108 | G    | C5-C6-O6    | -5.93 | 125.04      | 128.60   |
| 1   | AA    | 1300 | G    | N3-C4-C5    | 5.93  | 131.56      | 128.60   |
| 1   | AA    | 1430 | A    | C8-N9-C4    | 5.93  | 108.17      | 105.80   |
| 22  | AV    | 51   | A    | C4-C5-C6    | 5.93  | 119.96      | 117.00   |
| 35  | BB    | 26   | G    | P-O3'-C3'   | 5.93  | 126.82      | 119.70   |
| 35  | BB    | 491  | G    | N3-C4-C5    | -5.93 | 125.64      | 128.60   |
| 35  | BB    | 563  | A    | C6-N1-C2    | 5.93  | 122.16      | 118.60   |
| 35  | BB    | 891  | G    | C6-N1-C2    | 5.93  | 128.66      | 125.10   |
| 35  | BB    | 2120 | G    | N9-C4-C5    | -5.93 | 103.03      | 105.40   |
| 35  | BB    | 2151 | U    | P-O3'-C3'   | -5.93 | 112.58      | 119.70   |
| 35  | BB    | 2576 | G    | N1-C2-N3    | -5.93 | 120.34      | 123.90   |
| 35  | BB    | 2752 | C    | C5-C4-N4    | 5.93  | 124.35      | 120.20   |
| 35  | BB    | 2867 | G    | C4-C5-N7    | 5.93  | 113.17      | 110.80   |
| 1   | AA    | 262  | A    | C6-C5-N7    | -5.93 | 128.15      | 132.30   |
| 1   | AA    | 295  | C    | C1'-O4'-C4' | -5.93 | 105.16      | 109.90   |
| 18  | AR    | 71   | ASP  | CB-CA-C     | -5.93 | 98.54       | 110.40   |
| 35  | BB    | 942  | G    | N1-C2-N3    | -5.93 | 120.34      | 123.90   |
| 35  | BB    | 1017 | G    | C5-C6-N1    | -5.93 | 108.54      | 111.50   |
| 35  | BB    | 2859 | G    | C3'-C2'-C1' | -5.93 | 96.76       | 101.50   |
| 35  | BB    | 187  | G    | N1-C6-O6    | 5.93  | 123.46      | 119.90   |
| 35  | BB    | 539  | G    | O4'-C4'-C3' | -5.93 | 98.07       | 104.00   |
| 35  | BB    | 1381 | G    | C4'-C3'-C2' | -5.93 | 96.67       | 102.60   |
| 35  | BB    | 1398 | C    | C5-C4-N4    | -5.93 | 116.05      | 120.20   |
| 35  | BB    | 1888 | G    | C4-C5-C6    | 5.93  | 122.36      | 118.80   |
| 35  | BB    | 2175 | C    | N1-C2-O2    | 5.93  | 122.46      | 118.90   |
| 35  | BB    | 2288 | A    | C5-C6-N1    | -5.93 | 114.74      | 117.70   |
| 35  | BB    | 2383 | G    | C4-C5-N7    | -5.93 | 108.43      | 110.80   |
| 35  | BB    | 2436 | G    | C8-N9-C4    | 5.93  | 108.77      | 106.40   |
| 35  | BB    | 2634 | A    | C5-N7-C8    | 5.93  | 106.86      | 103.90   |
| 35  | BB    | 2796 | U    | N1-C2-O2    | -5.93 | 118.65      | 122.80   |
| 36  | BC    | 65   | ASP  | CB-CG-OD2   | -5.93 | 112.97      | 118.30   |
| 47  | BN    | 80   | PHE  | N-CA-CB     | 5.93  | 121.27      | 110.60   |
| 1   | AA    | 184  | G    | N9-C4-C5    | -5.92 | 103.03      | 105.40   |
| 1   | AA    | 631  | C    | N3-C4-C5    | 5.92  | 124.27      | 121.90   |
| 1   | AA    | 1135 | U    | C2-N3-C4    | -5.92 | 123.45      | 127.00   |
| 4   | AD    | 67   | LEU  | CB-CG-CD2   | 5.92  | 121.07      | 111.00   |
| 35  | BB    | 238  | C    | C2-N3-C4    | 5.92  | 122.86      | 119.90   |
| 35  | BB    | 307  | G    | N3-C4-C5    | -5.92 | 125.64      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 868  | U    | O4'-C1'-N1  | 5.92  | 112.94      | 108.20   |
| 35  | BB    | 1253 | A    | C5-C6-N1    | -5.92 | 114.74      | 117.70   |
| 35  | BB    | 1308 | A    | C8-N9-C4    | -5.92 | 103.43      | 105.80   |
| 35  | BB    | 1864 | U    | N3-C4-O4    | -5.92 | 115.25      | 119.40   |
| 35  | BB    | 2442 | C    | C5-C4-N4    | -5.92 | 116.05      | 120.20   |
| 35  | BB    | 2578 | G    | O4'-C1'-N9  | 5.92  | 112.94      | 108.20   |
| 35  | BB    | 2830 | C    | C2-N3-C4    | 5.92  | 122.86      | 119.90   |
| 35  | BB    | 2879 | A    | N7-C8-N9    | -5.92 | 110.84      | 113.80   |
| 1   | AA    | 866  | C    | C6-N1-C2    | -5.92 | 117.93      | 120.30   |
| 1   | AA    | 985  | C    | C5-C6-N1    | -5.92 | 118.04      | 121.00   |
| 1   | AA    | 1215 | G    | P-O3'-C3'   | -5.92 | 112.59      | 119.70   |
| 1   | AA    | 1229 | A    | C5-C6-N1    | -5.92 | 114.74      | 117.70   |
| 20  | AT    | 73   | ARG  | CD-NE-CZ    | 5.92  | 131.89      | 123.60   |
| 35  | BB    | 395  | U    | P-O5'-C5'   | 5.92  | 130.38      | 120.90   |
| 35  | BB    | 1471 | G    | N1-C6-O6    | 5.92  | 123.45      | 119.90   |
| 35  | BB    | 1493 | C    | N1-C1'-C2'  | -5.92 | 105.48      | 112.00   |
| 35  | BB    | 2093 | G    | N1-C2-N3    | -5.92 | 120.35      | 123.90   |
| 1   | AA    | 297  | G    | C5-C6-N1    | 5.92  | 114.46      | 111.50   |
| 1   | AA    | 619  | U    | C1'-O4'-C4' | -5.92 | 105.16      | 109.90   |
| 1   | AA    | 736  | C    | N1-C2-O2    | 5.92  | 122.45      | 118.90   |
| 1   | AA    | 952  | U    | C5'-C4'-C3' | 5.92  | 125.47      | 116.00   |
| 1   | AA    | 1458 | G    | N9-C4-C5    | -5.92 | 103.03      | 105.40   |
| 35  | BB    | 77   | G    | C6-C5-N7    | -5.92 | 126.85      | 130.40   |
| 35  | BB    | 526  | A    | C2-N3-C4    | -5.92 | 107.64      | 110.60   |
| 35  | BB    | 1268 | A    | C5-C6-N1    | -5.92 | 114.74      | 117.70   |
| 35  | BB    | 1308 | A    | N9-C4-C5    | 5.92  | 108.17      | 105.80   |
| 35  | BB    | 1521 | G    | C5-C6-O6    | -5.92 | 125.05      | 128.60   |
| 35  | BB    | 1659 | G    | O4'-C1'-N9  | 5.92  | 112.94      | 108.20   |
| 35  | BB    | 2075 | U    | C5-C6-N1    | 5.92  | 125.66      | 122.70   |
| 35  | BB    | 2549 | G    | C5'-C4'-C3' | -5.92 | 106.53      | 116.00   |
| 1   | AA    | 729  | A    | N7-C8-N9    | 5.92  | 116.76      | 113.80   |
| 1   | AA    | 1143 | G    | O4'-C1'-N9  | 5.92  | 112.94      | 108.20   |
| 1   | AA    | 1262 | C    | C6-N1-C2    | 5.92  | 122.67      | 120.30   |
| 35  | BB    | 69   | C    | C5'-C4'-O4' | -5.92 | 102.00      | 109.10   |
| 35  | BB    | 947  | A    | C5-N7-C8    | 5.92  | 106.86      | 103.90   |
| 35  | BB    | 1580 | A    | C6-N1-C2    | 5.92  | 122.15      | 118.60   |
| 50  | BQ    | 99   | VAL  | CG1-CB-CG2  | 5.92  | 120.37      | 110.90   |
| 1   | AA    | 170  | U    | C3'-C2'-C1' | -5.92 | 96.77       | 101.50   |
| 1   | AA    | 233  | C    | N3-C4-N4    | 5.92  | 122.14      | 118.00   |
| 1   | AA    | 297  | G    | O4'-C1'-N9  | 5.92  | 112.93      | 108.20   |
| 1   | AA    | 396  | C    | P-O3'-C3'   | -5.92 | 112.60      | 119.70   |
| 1   | AA    | 1175 | G    | C4'-C3'-C2' | -5.92 | 96.68       | 102.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1408 | A    | C4-C5-C6    | 5.92  | 119.96      | 117.00   |
| 1   | AA    | 1515 | G    | C5-C6-O6    | -5.92 | 125.05      | 128.60   |
| 35  | BB    | 2127 | G    | P-O3'-C3'   | 5.92  | 126.80      | 119.70   |
| 35  | BB    | 2266 | A    | C6-C5-N7    | -5.92 | 128.16      | 132.30   |
| 1   | AA    | 617  | G    | N9-C4-C5    | -5.92 | 103.03      | 105.40   |
| 1   | AA    | 989  | U    | N3-C4-O4    | 5.92  | 123.54      | 119.40   |
| 1   | AA    | 1092 | A    | N3-C4-C5    | -5.92 | 122.66      | 126.80   |
| 2   | AB    | 90   | PHE  | CB-CG-CD1   | -5.92 | 116.66      | 120.80   |
| 35  | BB    | 165  | A    | O4'-C1'-N9  | 5.92  | 112.93      | 108.20   |
| 35  | BB    | 1132 | U    | C4-C5-C6    | 5.92  | 123.25      | 119.70   |
| 35  | BB    | 1441 | G    | C8-N9-C1'   | 5.92  | 134.69      | 127.00   |
| 35  | BB    | 1809 | A    | C5-C6-N6    | -5.92 | 118.97      | 123.70   |
| 35  | BB    | 1925 | C    | C4-C5-C6    | 5.92  | 120.36      | 117.40   |
| 35  | BB    | 2413 | G    | C5-C6-N1    | -5.92 | 108.54      | 111.50   |
| 35  | BB    | 2534 | A    | C5'-C4'-O4' | 5.92  | 116.20      | 109.10   |
| 36  | BC    | 216  | ARG  | NE-CZ-NH2   | -5.92 | 117.34      | 120.30   |
| 37  | BD    | 127  | PHE  | CG-CD1-CE1  | 5.92  | 127.31      | 120.80   |
| 35  | BB    | 985  | C    | N1-C2-O2    | -5.92 | 115.35      | 118.90   |
| 35  | BB    | 1664 | A    | C8-N9-C1'   | -5.92 | 117.05      | 127.70   |
| 35  | BB    | 1730 | C    | O3'-P-O5'   | -5.92 | 92.76       | 104.00   |
| 35  | BB    | 1904 | G    | C5-N7-C8    | 5.92  | 107.26      | 104.30   |
| 35  | BB    | 2143 | C    | O4'-C1'-N1  | 5.92  | 112.93      | 108.20   |
| 35  | BB    | 2426 | A    | C8-N9-C4    | -5.92 | 103.43      | 105.80   |
| 35  | BB    | 2447 | G    | C5-C6-N1    | 5.92  | 114.46      | 111.50   |
| 1   | AA    | 292  | G    | N1-C2-N2    | -5.91 | 110.88      | 116.20   |
| 1   | AA    | 497  | G    | O4'-C1'-N9  | 5.91  | 112.93      | 108.20   |
| 1   | AA    | 559  | A    | N1-C2-N3    | -5.91 | 126.34      | 129.30   |
| 1   | AA    | 563  | A    | C5-C6-N6    | -5.91 | 118.97      | 123.70   |
| 1   | AA    | 1145 | A    | C4-C5-N7    | -5.91 | 107.74      | 110.70   |
| 5   | AE    | 137  | ARG  | N-CA-CB     | 5.91  | 121.24      | 110.60   |
| 17  | AQ    | 80   | LYS  | N-CA-CB     | 5.91  | 121.24      | 110.60   |
| 19  | AS    | 33   | TRP  | CD2-CE3-CZ3 | -5.91 | 111.11      | 118.80   |
| 35  | BB    | 618  | G    | C5-C6-O6    | -5.91 | 125.05      | 128.60   |
| 35  | BB    | 1001 | A    | C6-C5-N7    | -5.91 | 128.16      | 132.30   |
| 35  | BB    | 1330 | C    | C5-C6-N1    | 5.91  | 123.96      | 121.00   |
| 35  | BB    | 1730 | C    | C6-N1-C1'   | -5.91 | 113.70      | 120.80   |
| 35  | BB    | 1760 | C    | P-O5'-C5'   | -5.91 | 111.44      | 120.90   |
| 35  | BB    | 1849 | G    | N1-C2-N3    | -5.91 | 120.35      | 123.90   |
| 35  | BB    | 1912 | A    | C5'-C4'-O4' | -5.91 | 102.00      | 109.10   |
| 35  | BB    | 2282 | G    | C4'-C3'-C2' | 5.91  | 108.51      | 102.60   |
| 1   | AA    | 257  | G    | C2-N3-C4    | -5.91 | 108.94      | 111.90   |
| 1   | AA    | 1088 | G    | N9-C4-C5    | -5.91 | 103.03      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 20  | AT    | 9    | ARG  | NE-CZ-NH1   | 5.91  | 123.26      | 120.30   |
| 32  | B7    | 19   | GLY  | O-C-N       | -5.91 | 113.15      | 123.20   |
| 35  | BB    | 338  | G    | C4-C5-N7    | 5.91  | 113.17      | 110.80   |
| 35  | BB    | 368  | A    | N9-C4-C5    | 5.91  | 108.17      | 105.80   |
| 35  | BB    | 2355 | G    | N9-C4-C5    | -5.91 | 103.03      | 105.40   |
| 35  | BB    | 2688 | G    | C2-N3-C4    | -5.91 | 108.94      | 111.90   |
| 43  | BJ    | 48   | VAL  | N-CA-C      | -5.91 | 95.04       | 111.00   |
| 1   | AA    | 354  | G    | C6-C5-N7    | -5.91 | 126.85      | 130.40   |
| 1   | AA    | 442  | G    | C5-C6-O6    | -5.91 | 125.05      | 128.60   |
| 1   | AA    | 567  | G    | O4'-C1'-N9  | 5.91  | 112.93      | 108.20   |
| 1   | AA    | 715  | A    | C5-C6-N6    | -5.91 | 118.97      | 123.70   |
| 1   | AA    | 1216 | A    | N7-C8-N9    | -5.91 | 110.84      | 113.80   |
| 1   | AA    | 1301 | U    | C4-C5-C6    | -5.91 | 116.15      | 119.70   |
| 17  | AQ    | 27   | PHE  | CB-CG-CD2   | 5.91  | 124.94      | 120.80   |
| 22  | AV    | 68   | U    | C6-N1-C2    | -5.91 | 117.45      | 121.00   |
| 35  | BB    | 75   | G    | C2-N3-C4    | 5.91  | 114.86      | 111.90   |
| 35  | BB    | 347  | A    | C6-C5-N7    | -5.91 | 128.16      | 132.30   |
| 35  | BB    | 483  | A    | C5-C6-N6    | -5.91 | 118.97      | 123.70   |
| 1   | AA    | 152  | A    | C4'-C3'-C2' | -5.91 | 96.69       | 102.60   |
| 1   | AA    | 943  | U    | N1-C1'-C2'  | -5.91 | 105.50      | 112.00   |
| 1   | AA    | 1079 | G    | N1-C2-N3    | -5.91 | 120.36      | 123.90   |
| 1   | AA    | 1437 | A    | O4'-C1'-C2' | -5.91 | 99.89       | 105.80   |
| 2   | AB    | 138  | ARG  | NH1-CZ-NH2  | 5.91  | 125.90      | 119.40   |
| 22  | AV    | 49   | G    | O4'-C1'-N9  | 5.91  | 112.93      | 108.20   |
| 35  | BB    | 141  | G    | C2-N3-C4    | -5.91 | 108.95      | 111.90   |
| 35  | BB    | 199  | A    | O5'-P-OP2   | -5.91 | 100.38      | 105.70   |
| 35  | BB    | 268  | C    | C5-C6-N1    | 5.91  | 123.95      | 121.00   |
| 35  | BB    | 1366 | A    | C5-N7-C8    | 5.91  | 106.85      | 103.90   |
| 35  | BB    | 2152 | G    | C5-C6-N1    | -5.91 | 108.55      | 111.50   |
| 35  | BB    | 2464 | G    | P-O3'-C3'   | -5.91 | 112.61      | 119.70   |
| 1   | AA    | 829  | G    | C2-N3-C4    | 5.91  | 114.85      | 111.90   |
| 1   | AA    | 1003 | G    | C8-N9-C1'   | 5.91  | 134.68      | 127.00   |
| 35  | BB    | 274  | C    | C4-C5-C6    | 5.91  | 120.35      | 117.40   |
| 35  | BB    | 1104 | C    | C3'-C2'-C1' | 5.91  | 106.22      | 101.50   |
| 1   | AA    | 211  | G    | C8-N9-C1'   | -5.91 | 119.32      | 127.00   |
| 1   | AA    | 889  | A    | O4'-C1'-N9  | 5.91  | 112.92      | 108.20   |
| 1   | AA    | 1246 | A    | C4-C5-N7    | -5.91 | 107.75      | 110.70   |
| 31  | B6    | 21   | ARG  | NE-CZ-NH2   | 5.91  | 123.25      | 120.30   |
| 34  | BA    | 87   | U    | C3'-C2'-C1' | 5.91  | 106.22      | 101.50   |
| 35  | BB    | 686  | U    | N1-C2-O2    | 5.91  | 126.93      | 122.80   |
| 35  | BB    | 844  | A    | N1-C2-N3    | 5.91  | 132.25      | 129.30   |
| 35  | BB    | 1324 | G    | C5'-C4'-C3' | -5.91 | 106.55      | 116.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1522 | A    | C6-N1-C2    | 5.91  | 122.14      | 118.60   |
| 35  | BB    | 1731 | G    | O4'-C1'-N9  | 5.91  | 112.92      | 108.20   |
| 35  | BB    | 2101 | A    | C5-N7-C8    | 5.91  | 106.85      | 103.90   |
| 35  | BB    | 2518 | A    | P-O5'-C5'   | -5.91 | 111.45      | 120.90   |
| 36  | BC    | 120  | ASP  | CB-CG-OD2   | 5.91  | 123.61      | 118.30   |
| 50  | BQ    | 56   | PHE  | CB-CG-CD1   | -5.91 | 116.67      | 120.80   |
| 56  | BY    | 31   | LEU  | N-CA-C      | -5.91 | 95.06       | 111.00   |
| 1   | AA    | 169  | C    | C4'-C3'-C2' | -5.90 | 96.70       | 102.60   |
| 1   | AA    | 614  | C    | O4'-C1'-N1  | 5.90  | 112.92      | 108.20   |
| 35  | BB    | 967  | U    | O4'-C1'-N1  | 5.90  | 112.92      | 108.20   |
| 35  | BB    | 1860 | G    | N9-C1'-C2'  | -5.90 | 105.51      | 112.00   |
| 1   | AA    | 29   | U    | C1'-O4'-C4' | 5.90  | 114.62      | 109.90   |
| 1   | AA    | 426  | U    | P-O5'-C5'   | 5.90  | 130.34      | 120.90   |
| 1   | AA    | 1169 | A    | O5'-P-OP2   | -5.90 | 100.39      | 105.70   |
| 1   | AA    | 1301 | U    | N3-C4-O4    | -5.90 | 115.27      | 119.40   |
| 35  | BB    | 450  | G    | N3-C2-N2    | 5.90  | 124.03      | 119.90   |
| 35  | BB    | 763  | G    | C5-N7-C8    | 5.90  | 107.25      | 104.30   |
| 35  | BB    | 920  | A    | C5-C6-N6    | -5.90 | 118.98      | 123.70   |
| 35  | BB    | 997  | G    | N1-C6-O6    | -5.90 | 116.36      | 119.90   |
| 35  | BB    | 1659 | G    | P-O3'-C3'   | -5.90 | 112.62      | 119.70   |
| 35  | BB    | 2738 | A    | C4-C5-N7    | 5.90  | 113.65      | 110.70   |
| 35  | BB    | 2835 | A    | O4'-C1'-C2' | -5.90 | 99.90       | 105.80   |
| 35  | BB    | 2843 | G    | C6-C5-N7    | -5.90 | 126.86      | 130.40   |
| 1   | AA    | 705  | G    | O4'-C1'-N9  | 5.90  | 112.92      | 108.20   |
| 1   | AA    | 849  | G    | C4-C5-C6    | 5.90  | 122.34      | 118.80   |
| 35  | BB    | 23   | G    | N3-C4-N9    | 5.90  | 129.54      | 126.00   |
| 35  | BB    | 203  | A    | C8-N9-C4    | -5.90 | 103.44      | 105.80   |
| 35  | BB    | 244  | A    | C4-C5-C6    | 5.90  | 119.95      | 117.00   |
| 35  | BB    | 968  | C    | P-O3'-C3'   | -5.90 | 112.62      | 119.70   |
| 35  | BB    | 1136 | G    | P-O3'-C3'   | -5.90 | 112.62      | 119.70   |
| 35  | BB    | 1253 | A    | OP1-P-OP2   | -5.90 | 110.75      | 119.60   |
| 35  | BB    | 1605 | C    | N3-C4-N4    | 5.90  | 122.13      | 118.00   |
| 35  | BB    | 2069 | G    | C6-C5-N7    | -5.90 | 126.86      | 130.40   |
| 35  | BB    | 2655 | G    | N1-C2-N3    | -5.90 | 120.36      | 123.90   |
| 35  | BB    | 2868 | A    | C8-N9-C4    | 5.90  | 108.16      | 105.80   |
| 36  | BC    | 134  | ILE  | CA-CB-CG1   | 5.90  | 122.21      | 111.00   |
| 45  | BL    | 89   | VAL  | CA-CB-CG1   | -5.90 | 102.05      | 110.90   |
| 1   | AA    | 507  | C    | N1-C2-O2    | 5.90  | 122.44      | 118.90   |
| 1   | AA    | 873  | A    | N3-C4-C5    | -5.90 | 122.67      | 126.80   |
| 1   | AA    | 1134 | G    | N3-C4-N9    | 5.90  | 129.54      | 126.00   |
| 35  | BB    | 870  | U    | N1-C2-O2    | 5.90  | 126.93      | 122.80   |
| 35  | BB    | 2864 | G    | N3-C4-N9    | -5.90 | 122.46      | 126.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2891 | U    | N3-C2-O2    | 5.90  | 126.33      | 122.20   |
| 1   | AA    | 490  | C    | C4-C5-C6    | 5.90  | 120.35      | 117.40   |
| 1   | AA    | 934  | C    | C4-C5-C6    | 5.90  | 120.35      | 117.40   |
| 1   | AA    | 987  | G    | C4'-C3'-C2' | -5.90 | 96.70       | 102.60   |
| 1   | AA    | 1314 | C    | O4'-C4'-C3' | 5.90  | 110.82      | 106.10   |
| 35  | BB    | 358  | U    | C5-C4-O4    | -5.90 | 122.36      | 125.90   |
| 35  | BB    | 510  | C    | C5-C4-N4    | -5.90 | 116.07      | 120.20   |
| 35  | BB    | 1005 | C    | N1-C2-O2    | -5.90 | 115.36      | 118.90   |
| 35  | BB    | 1194 | A    | C5'-C4'-C3' | -5.90 | 106.56      | 116.00   |
| 35  | BB    | 1587 | G    | N3-C2-N2    | 5.90  | 124.03      | 119.90   |
| 35  | BB    | 1791 | A    | N9-C1'-C2'  | -5.90 | 105.51      | 112.00   |
| 35  | BB    | 1834 | U    | C1'-O4'-C4' | 5.90  | 114.62      | 109.90   |
| 35  | BB    | 2205 | A    | C6-C5-N7    | -5.90 | 128.17      | 132.30   |
| 35  | BB    | 2265 | U    | P-O3'-C3'   | 5.90  | 126.78      | 119.70   |
| 35  | BB    | 2267 | A    | C3'-C2'-C1' | -5.90 | 96.78       | 101.50   |
| 35  | BB    | 2297 | A    | OP2-P-O3'   | 5.90  | 118.17      | 105.20   |
| 35  | BB    | 2401 | U    | N1-C2-O2    | 5.90  | 126.93      | 122.80   |
| 35  | BB    | 2424 | C    | P-O3'-C3'   | -5.90 | 112.62      | 119.70   |
| 47  | BN    | 9    | GLN  | N-CA-CB     | 5.90  | 121.22      | 110.60   |
| 34  | BA    | 15   | A    | C5'-C4'-O4' | 5.90  | 116.18      | 109.10   |
| 35  | BB    | 690  | G    | C8-N9-C4    | -5.90 | 104.04      | 106.40   |
| 35  | BB    | 968  | C    | N3-C4-C5    | -5.90 | 119.54      | 121.90   |
| 35  | BB    | 1777 | U    | C5-C6-N1    | -5.90 | 119.75      | 122.70   |
| 35  | BB    | 1929 | G    | C5-C6-O6    | -5.90 | 125.06      | 128.60   |
| 35  | BB    | 2030 | A    | C6-C5-N7    | -5.90 | 128.17      | 132.30   |
| 35  | BB    | 2599 | G    | N1-C2-N2    | -5.90 | 110.89      | 116.20   |
| 1   | AA    | 547  | A    | C5-C6-N6    | -5.89 | 118.98      | 123.70   |
| 1   | AA    | 560  | A    | O4'-C1'-C2' | 5.89  | 112.91      | 107.60   |
| 1   | AA    | 878  | A    | C6-N1-C2    | -5.89 | 115.06      | 118.60   |
| 35  | BB    | 103  | A    | N3-C4-C5    | -5.89 | 122.67      | 126.80   |
| 35  | BB    | 218  | A    | C3'-C2'-C1' | 5.89  | 106.22      | 101.50   |
| 35  | BB    | 246  | C    | N1-C2-N3    | -5.89 | 115.07      | 119.20   |
| 35  | BB    | 294  | A    | C5-C6-N6    | -5.89 | 118.98      | 123.70   |
| 35  | BB    | 825  | A    | C2-N3-C4    | 5.89  | 113.55      | 110.60   |
| 35  | BB    | 1190 | G    | C2-N3-C4    | 5.89  | 114.85      | 111.90   |
| 35  | BB    | 1271 | G    | N3-C2-N2    | 5.89  | 124.03      | 119.90   |
| 35  | BB    | 1667 | G    | P-O5'-C5'   | 5.89  | 130.33      | 120.90   |
| 35  | BB    | 1734 | G    | C6-C5-N7    | -5.89 | 126.86      | 130.40   |
| 35  | BB    | 1743 | G    | N3-C2-N2    | 5.89  | 124.03      | 119.90   |
| 39  | BF    | 114  | ARG  | NH1-CZ-NH2  | 5.89  | 125.88      | 119.40   |
| 1   | AA    | 108  | G    | C6-N1-C2    | -5.89 | 121.56      | 125.10   |
| 1   | AA    | 113  | G    | O4'-C1'-N9  | 5.89  | 112.91      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 648  | A    | O4'-C1'-N9  | 5.89  | 112.91      | 108.20   |
| 1   | AA    | 1272 | G    | C6-C5-N7    | -5.89 | 126.86      | 130.40   |
| 7   | AG    | 143  | MET  | CG-SD-CE    | -5.89 | 90.77       | 100.20   |
| 25  | B0    | 67   | LEU  | CB-CG-CD2   | 5.89  | 121.02      | 111.00   |
| 34  | BA    | 71   | C    | N3-C2-O2    | -5.89 | 117.78      | 121.90   |
| 35  | BB    | 207  | A    | N1-C2-N3    | -5.89 | 126.35      | 129.30   |
| 35  | BB    | 504  | A    | C2-N3-C4    | -5.89 | 107.65      | 110.60   |
| 35  | BB    | 642  | U    | N1-C2-O2    | -5.89 | 118.68      | 122.80   |
| 35  | BB    | 1036 | G    | O4'-C1'-N9  | 5.89  | 112.92      | 108.20   |
| 35  | BB    | 2049 | G    | P-O3'-C3'   | -5.89 | 112.63      | 119.70   |
| 35  | BB    | 2741 | A    | C5-N7-C8    | 5.89  | 106.85      | 103.90   |
| 35  | BB    | 2878 | U    | P-O5'-C5'   | 5.89  | 130.33      | 120.90   |
| 1   | AA    | 408  | A    | C8-N9-C4    | -5.89 | 103.44      | 105.80   |
| 1   | AA    | 1492 | A    | C2-N3-C4    | 5.89  | 113.55      | 110.60   |
| 35  | BB    | 151  | C    | N3-C4-N4    | 5.89  | 122.12      | 118.00   |
| 1   | AA    | 1391 | U    | O5'-C5'-C4' | -5.89 | 100.51      | 111.70   |
| 1   | AA    | 1505 | G    | C2-N3-C4    | 5.89  | 114.84      | 111.90   |
| 35  | BB    | 321  | U    | N3-C4-C5    | -5.89 | 111.07      | 114.60   |
| 35  | BB    | 337  | C    | C2-N3-C4    | 5.89  | 122.84      | 119.90   |
| 35  | BB    | 644  | A    | N9-C4-C5    | -5.89 | 103.44      | 105.80   |
| 35  | BB    | 969  | G    | N3-C2-N2    | 5.89  | 124.02      | 119.90   |
| 35  | BB    | 1354 | A    | C4'-C3'-C2' | -5.89 | 96.71       | 102.60   |
| 35  | BB    | 1374 | G    | N1-C2-N2    | -5.89 | 110.90      | 116.20   |
| 35  | BB    | 2164 | C    | C2-N3-C4    | 5.89  | 122.84      | 119.90   |
| 35  | BB    | 2573 | C    | O4'-C4'-C3' | -5.89 | 98.11       | 104.00   |
| 35  | BB    | 2602 | A    | C1'-O4'-C4' | -5.89 | 105.19      | 109.90   |
| 35  | BB    | 2867 | G    | N9-C4-C5    | -5.89 | 103.04      | 105.40   |
| 35  | BB    | 2898 | U    | C5'-C4'-C3' | -5.89 | 106.58      | 116.00   |
| 1   | AA    | 112  | G    | C8-N9-C4    | -5.89 | 104.05      | 106.40   |
| 1   | AA    | 217  | C    | N1-C2-O2    | 5.89  | 122.43      | 118.90   |
| 1   | AA    | 448  | A    | C2-N3-C4    | -5.89 | 107.66      | 110.60   |
| 1   | AA    | 919  | A    | C3'-C2'-C1' | 5.89  | 106.21      | 101.50   |
| 1   | AA    | 1021 | A    | C4-C5-N7    | -5.89 | 107.76      | 110.70   |
| 1   | AA    | 1353 | G    | C4-C5-C6    | 5.89  | 122.33      | 118.80   |
| 1   | AA    | 1364 | U    | N3-C4-O4    | 5.89  | 123.52      | 119.40   |
| 35  | BB    | 924  | G    | C4-C5-N7    | 5.89  | 113.16      | 110.80   |
| 35  | BB    | 1156 | A    | N1-C2-N3    | 5.89  | 132.24      | 129.30   |
| 35  | BB    | 1410 | G    | N3-C4-C5    | 5.89  | 131.54      | 128.60   |
| 35  | BB    | 1463 | C    | P-O3'-C3'   | -5.89 | 112.63      | 119.70   |
| 1   | AA    | 622  | A    | P-O5'-C5'   | -5.89 | 111.48      | 120.90   |
| 1   | AA    | 697  | U    | C5-C4-O4    | 5.89  | 129.43      | 125.90   |
| 1   | AA    | 790  | A    | C8-N9-C4    | 5.89  | 108.16      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 844  | G    | O4'-C1'-N9  | 5.89  | 112.91      | 108.20   |
| 1   | AA    | 1021 | A    | C8-N9-C4    | -5.89 | 103.44      | 105.80   |
| 1   | AA    | 1428 | A    | N1-C2-N3    | 5.89  | 132.24      | 129.30   |
| 2   | AB    | 139  | GLU  | OE1-CD-OE2  | 5.89  | 130.36      | 123.30   |
| 34  | BA    | 78   | A    | N7-C8-N9    | -5.89 | 110.86      | 113.80   |
| 35  | BB    | 344  | A    | C6-C5-N7    | -5.89 | 128.18      | 132.30   |
| 35  | BB    | 384  | A    | N1-C2-N3    | -5.89 | 126.36      | 129.30   |
| 35  | BB    | 472  | A    | C5-C6-N6    | -5.89 | 118.99      | 123.70   |
| 35  | BB    | 771  | G    | N3-C4-C5    | -5.89 | 125.66      | 128.60   |
| 35  | BB    | 1542 | U    | N1-C2-O2    | -5.89 | 118.68      | 122.80   |
| 35  | BB    | 1667 | G    | C5'-C4'-O4' | 5.89  | 116.16      | 109.10   |
| 35  | BB    | 1852 | U    | C6-N1-C1'   | -5.89 | 112.96      | 121.20   |
| 35  | BB    | 1888 | G    | N1-C2-N2    | -5.89 | 110.90      | 116.20   |
| 35  | BB    | 1999 | C    | C4-C5-C6    | 5.89  | 120.34      | 117.40   |
| 35  | BB    | 2232 | C    | C4-C5-C6    | -5.89 | 114.46      | 117.40   |
| 1   | AA    | 297  | G    | C6-N1-C2    | -5.88 | 121.57      | 125.10   |
| 1   | AA    | 648  | A    | N1-C2-N3    | 5.88  | 132.24      | 129.30   |
| 1   | AA    | 1131 | G    | C2-N3-C4    | 5.88  | 114.84      | 111.90   |
| 35  | BB    | 68   | G    | P-O3'-C3'   | 5.88  | 126.76      | 119.70   |
| 35  | BB    | 1263 | U    | O4'-C1'-N1  | 5.88  | 112.91      | 108.20   |
| 35  | BB    | 1729 | U    | C6-N1-C1'   | -5.88 | 112.96      | 121.20   |
| 35  | BB    | 1981 | A    | O4'-C1'-N9  | 5.88  | 112.91      | 108.20   |
| 35  | BB    | 1992 | G    | O5'-P-OP1   | -5.88 | 100.41      | 105.70   |
| 35  | BB    | 2054 | A    | C4-C5-C6    | 5.88  | 119.94      | 117.00   |
| 35  | BB    | 2759 | G    | N3-C4-C5    | 5.88  | 131.54      | 128.60   |
| 35  | BB    | 2894 | G    | N3-C4-C5    | -5.88 | 125.66      | 128.60   |
| 1   | AA    | 553  | A    | N9-C4-C5    | 5.88  | 108.15      | 105.80   |
| 1   | AA    | 566  | G    | N1-C2-N3    | -5.88 | 120.37      | 123.90   |
| 1   | AA    | 700  | G    | C8-N9-C4    | 5.88  | 108.75      | 106.40   |
| 35  | BB    | 1650 | A    | C4-C5-N7    | -5.88 | 107.76      | 110.70   |
| 35  | BB    | 1730 | C    | C2'-C3'-O3' | 5.88  | 123.11      | 113.70   |
| 35  | BB    | 1966 | A    | N1-C6-N6    | 5.88  | 122.13      | 118.60   |
| 35  | BB    | 2459 | A    | N7-C8-N9    | 5.88  | 116.74      | 113.80   |
| 1   | AA    | 1243 | C    | P-O3'-C3'   | -5.88 | 112.64      | 119.70   |
| 1   | AA    | 1432 | G    | C5-N7-C8    | -5.88 | 101.36      | 104.30   |
| 35  | BB    | 380  | G    | N3-C4-N9    | -5.88 | 122.47      | 126.00   |
| 35  | BB    | 607  | U    | N1-C2-O2    | -5.88 | 118.68      | 122.80   |
| 35  | BB    | 745  | G    | C4-C5-C6    | 5.88  | 122.33      | 118.80   |
| 35  | BB    | 1379 | U    | N3-C4-O4    | 5.88  | 123.52      | 119.40   |
| 35  | BB    | 1524 | G    | C4-C5-C6    | 5.88  | 122.33      | 118.80   |
| 1   | AA    | 521  | G    | N3-C4-N9    | -5.88 | 122.47      | 126.00   |
| 1   | AA    | 637  | C    | O4'-C1'-N1  | 5.88  | 112.90      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1513 | A    | C8-N9-C4    | 5.88  | 108.15      | 105.80   |
| 35  | BB    | 249  | C    | P-O5'-C5'   | -5.88 | 111.49      | 120.90   |
| 35  | BB    | 1106 | G    | N3-C4-N9    | -5.88 | 122.47      | 126.00   |
| 1   | AA    | 296  | U    | C2-N3-C4    | -5.88 | 123.47      | 127.00   |
| 1   | AA    | 753  | A    | C6-C5-N7    | -5.88 | 128.19      | 132.30   |
| 1   | AA    | 873  | A    | P-O3'-C3'   | -5.88 | 112.64      | 119.70   |
| 1   | AA    | 1026 | G    | O5'-P-OP1   | 5.88  | 117.75      | 110.70   |
| 1   | AA    | 1181 | G    | N3-C2-N2    | 5.88  | 124.02      | 119.90   |
| 34  | BA    | 50   | A    | C4-C5-N7    | -5.88 | 107.76      | 110.70   |
| 35  | BB    | 416  | U    | C5-C4-O4    | -5.88 | 122.37      | 125.90   |
| 35  | BB    | 825  | A    | N9-C4-C5    | 5.88  | 108.15      | 105.80   |
| 35  | BB    | 1761 | C    | O4'-C1'-N1  | 5.88  | 112.90      | 108.20   |
| 35  | BB    | 2240 | U    | C5-C4-O4    | 5.88  | 129.43      | 125.90   |
| 35  | BB    | 2264 | C    | C1'-O4'-C4' | -5.88 | 105.20      | 109.90   |
| 35  | BB    | 2638 | G    | C6-N1-C2    | -5.88 | 121.57      | 125.10   |
| 43  | BJ    | 53   | TYR  | CZ-CE2-CD2  | 5.88  | 125.09      | 119.80   |
| 1   | AA    | 253  | A    | C5-C6-N6    | -5.88 | 119.00      | 123.70   |
| 1   | AA    | 877  | G    | C5-N7-C8    | -5.88 | 101.36      | 104.30   |
| 9   | AI    | 114  | LYS  | CA-CB-CG    | 5.88  | 126.33      | 113.40   |
| 35  | BB    | 820  | A    | C5-C6-N1    | -5.88 | 114.76      | 117.70   |
| 35  | BB    | 913  | U    | N1-C2-N3    | -5.88 | 111.37      | 114.90   |
| 35  | BB    | 928  | A    | C4-C5-N7    | -5.88 | 107.76      | 110.70   |
| 35  | BB    | 940  | G    | C8-N9-C4    | -5.88 | 104.05      | 106.40   |
| 35  | BB    | 997  | G    | C4-N9-C1'   | -5.88 | 118.86      | 126.50   |
| 35  | BB    | 1135 | C    | C6-N1-C1'   | -5.88 | 113.75      | 120.80   |
| 35  | BB    | 1566 | A    | N3-C4-C5    | 5.88  | 130.91      | 126.80   |
| 35  | BB    | 2589 | A    | C6-C5-N7    | -5.88 | 128.19      | 132.30   |
| 35  | BB    | 2820 | A    | N1-C6-N6    | 5.88  | 122.13      | 118.60   |
| 1   | AA    | 972  | C    | C5-C4-N4    | -5.88 | 116.09      | 120.20   |
| 35  | BB    | 32   | C    | C2-N3-C4    | 5.88  | 122.84      | 119.90   |
| 35  | BB    | 207  | A    | C5-C6-N1    | -5.88 | 114.76      | 117.70   |
| 35  | BB    | 2642 | G    | O4'-C1'-N9  | 5.88  | 112.90      | 108.20   |
| 35  | BB    | 2724 | U    | O4'-C1'-N1  | 5.88  | 112.90      | 108.20   |
| 37  | BD    | 84   | LEU  | CB-CG-CD1   | 5.88  | 120.99      | 111.00   |
| 1   | AA    | 1128 | C    | C5-C6-N1    | 5.87  | 123.94      | 121.00   |
| 35  | BB    | 39   | G    | C4-C5-N7    | -5.87 | 108.45      | 110.80   |
| 35  | BB    | 203  | A    | O4'-C1'-C2' | 5.87  | 112.89      | 107.60   |
| 35  | BB    | 460  | A    | C8-N9-C4    | 5.87  | 108.15      | 105.80   |
| 35  | BB    | 900  | A    | N9-C1'-C2'  | -5.87 | 105.54      | 112.00   |
| 35  | BB    | 1342 | A    | N9-C4-C5    | 5.87  | 108.15      | 105.80   |
| 35  | BB    | 1472 | C    | N1-C2-N3    | -5.87 | 115.09      | 119.20   |
| 35  | BB    | 1655 | A    | O4'-C1'-N9  | 5.87  | 112.90      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 226  | G    | N1-C2-N2    | -5.87 | 110.92      | 116.20   |
| 1   | AA    | 549  | C    | C4'-C3'-C2' | -5.87 | 96.73       | 102.60   |
| 1   | AA    | 927  | G    | N1-C2-N3    | -5.87 | 120.38      | 123.90   |
| 1   | AA    | 1242 | G    | O4'-C4'-C3' | -5.87 | 98.13       | 104.00   |
| 1   | AA    | 1274 | A    | C5-C6-N1    | -5.87 | 114.76      | 117.70   |
| 7   | AG    | 19   | SER  | N-CA-C      | -5.87 | 95.15       | 111.00   |
| 22  | AV    | 76   | A    | N7-C8-N9    | 5.87  | 116.74      | 113.80   |
| 34  | BA    | 16   | G    | C6-N1-C2    | -5.87 | 121.58      | 125.10   |
| 34  | BA    | 106  | G    | O4'-C1'-N9  | 5.87  | 112.90      | 108.20   |
| 35  | BB    | 157  | C    | C5-C6-N1    | 5.87  | 123.94      | 121.00   |
| 35  | BB    | 163  | C    | C6-N1-C2    | 5.87  | 122.65      | 120.30   |
| 35  | BB    | 592  | A    | O4'-C1'-N9  | 5.87  | 112.90      | 108.20   |
| 35  | BB    | 620  | G    | C8-N9-C4    | -5.87 | 104.05      | 106.40   |
| 35  | BB    | 1371 | G    | C4-N9-C1'   | -5.87 | 118.87      | 126.50   |
| 35  | BB    | 1430 | G    | C8-N9-C4    | 5.87  | 108.75      | 106.40   |
| 35  | BB    | 1857 | G    | C3'-C2'-C1' | -5.87 | 96.80       | 101.50   |
| 35  | BB    | 1928 | A    | C5-N7-C8    | 5.87  | 106.84      | 103.90   |
| 35  | BB    | 2439 | A    | C4-C5-N7    | 5.87  | 113.64      | 110.70   |
| 35  | BB    | 2871 | U    | N3-C4-O4    | 5.87  | 123.51      | 119.40   |
| 1   | AA    | 27   | G    | N3-C4-C5    | -5.87 | 125.67      | 128.60   |
| 1   | AA    | 302  | G    | C4-C5-C6    | 5.87  | 122.32      | 118.80   |
| 1   | AA    | 1225 | A    | N1-C2-N3    | -5.87 | 126.36      | 129.30   |
| 22  | AV    | 3    | G    | N3-C4-N9    | 5.87  | 129.52      | 126.00   |
| 35  | BB    | 326  | G    | C5-N7-C8    | -5.87 | 101.36      | 104.30   |
| 35  | BB    | 505  | A    | C5-C6-N1    | -5.87 | 114.77      | 117.70   |
| 35  | BB    | 914  | G    | C5-N7-C8    | -5.87 | 101.36      | 104.30   |
| 35  | BB    | 933  | A    | C5-C6-N6    | -5.87 | 119.00      | 123.70   |
| 35  | BB    | 1126 | A    | C8-N9-C4    | -5.87 | 103.45      | 105.80   |
| 35  | BB    | 1167 | C    | N3-C4-N4    | 5.87  | 122.11      | 118.00   |
| 35  | BB    | 1901 | A    | N1-C6-N6    | 5.87  | 122.12      | 118.60   |
| 1   | AA    | 149  | A    | C8-N9-C4    | -5.87 | 103.45      | 105.80   |
| 1   | AA    | 171  | A    | C5-C6-N6    | -5.87 | 119.00      | 123.70   |
| 1   | AA    | 341  | C    | C6-N1-C1'   | -5.87 | 113.76      | 120.80   |
| 1   | AA    | 511  | C    | N3-C4-N4    | 5.87  | 122.11      | 118.00   |
| 1   | AA    | 833  | G    | C6-C5-N7    | -5.87 | 126.88      | 130.40   |
| 1   | AA    | 1360 | A    | N3-C4-C5    | -5.87 | 122.69      | 126.80   |
| 34  | BA    | 4    | C    | O4'-C4'-C3' | -5.87 | 98.13       | 104.00   |
| 35  | BB    | 273  | G    | N9-C4-C5    | 5.87  | 107.75      | 105.40   |
| 35  | BB    | 759  | G    | N1-C2-N3    | -5.87 | 120.38      | 123.90   |
| 35  | BB    | 793  | A    | C6-C5-N7    | -5.87 | 128.19      | 132.30   |
| 35  | BB    | 872  | U    | O4'-C1'-N1  | 5.87  | 112.89      | 108.20   |
| 35  | BB    | 1064 | C    | O4'-C1'-N1  | 5.87  | 112.89      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1434 | A    | N3-C4-N9    | 5.87  | 132.09      | 127.40   |
| 35  | BB    | 1631 | G    | C8-N9-C4    | 5.87  | 108.75      | 106.40   |
| 35  | BB    | 1966 | A    | C5'-C4'-O4' | 5.87  | 116.14      | 109.10   |
| 35  | BB    | 1970 | A    | C6-C5-N7    | -5.87 | 128.19      | 132.30   |
| 35  | BB    | 1989 | G    | C6-C5-N7    | -5.87 | 126.88      | 130.40   |
| 35  | BB    | 2080 | A    | N1-C6-N6    | 5.87  | 122.12      | 118.60   |
| 35  | BB    | 2246 | G    | C5-C6-N1    | 5.87  | 114.44      | 111.50   |
| 35  | BB    | 2663 | G    | C5'-C4'-O4' | 5.87  | 116.14      | 109.10   |
| 35  | BB    | 36   | G    | C6-N1-C2    | 5.87  | 128.62      | 125.10   |
| 35  | BB    | 1727 | C    | N3-C4-N4    | 5.87  | 122.11      | 118.00   |
| 35  | BB    | 1950 | G    | C5-N7-C8    | 5.87  | 107.23      | 104.30   |
| 35  | BB    | 2074 | U    | C6-N1-C2    | 5.87  | 124.52      | 121.00   |
| 1   | AA    | 780  | A    | N3-C4-C5    | -5.87 | 122.69      | 126.80   |
| 1   | AA    | 1002 | G    | C5-C6-N1    | -5.87 | 108.57      | 111.50   |
| 35  | BB    | 268  | C    | N1-C2-O2    | 5.87  | 122.42      | 118.90   |
| 35  | BB    | 364  | C    | C6-N1-C2    | -5.87 | 117.95      | 120.30   |
| 35  | BB    | 553  | G    | C5-C6-O6    | -5.87 | 125.08      | 128.60   |
| 35  | BB    | 666  | A    | C6-C5-N7    | -5.87 | 128.19      | 132.30   |
| 35  | BB    | 734  | A    | C2-N3-C4    | -5.87 | 107.67      | 110.60   |
| 35  | BB    | 861  | A    | O4'-C1'-N9  | 5.87  | 112.89      | 108.20   |
| 35  | BB    | 906  | U    | C2-N3-C4    | 5.87  | 130.52      | 127.00   |
| 35  | BB    | 1028 | A    | C5'-C4'-O4' | 5.87  | 116.14      | 109.10   |
| 35  | BB    | 1352 | U    | C3'-C2'-C1' | 5.87  | 106.19      | 101.50   |
| 35  | BB    | 1779 | U    | O4'-C4'-C3' | -5.87 | 98.13       | 104.00   |
| 35  | BB    | 1801 | A    | N1-C2-N3    | -5.87 | 126.37      | 129.30   |
| 35  | BB    | 2239 | G    | C6-N1-C2    | -5.87 | 121.58      | 125.10   |
| 1   | AA    | 26   | A    | N3-C4-C5    | -5.86 | 122.70      | 126.80   |
| 1   | AA    | 148  | G    | C4'-C3'-C2' | -5.86 | 96.74       | 102.60   |
| 1   | AA    | 159  | G    | N3-C2-N2    | 5.86  | 124.00      | 119.90   |
| 1   | AA    | 198  | G    | N3-C4-N9    | 5.86  | 129.52      | 126.00   |
| 1   | AA    | 598  | U    | C2-N1-C1'   | 5.86  | 124.74      | 117.70   |
| 1   | AA    | 644  | U    | C5-C6-N1    | 5.86  | 125.63      | 122.70   |
| 1   | AA    | 1286 | U    | C5-C4-O4    | 5.86  | 129.42      | 125.90   |
| 1   | AA    | 1495 | U    | N3-C4-O4    | 5.86  | 123.50      | 119.40   |
| 13  | AM    | 94   | LEU  | CB-CG-CD2   | 5.86  | 120.97      | 111.00   |
| 23  | AX    | 20   | G    | P-O3'-C3'   | -5.86 | 112.66      | 119.70   |
| 34  | BA    | 116  | G    | C4-C5-C6    | 5.86  | 122.32      | 118.80   |
| 35  | BB    | 729  | G    | C8-N9-C1'   | -5.86 | 119.38      | 127.00   |
| 35  | BB    | 899  | A    | N1-C2-N3    | 5.86  | 132.23      | 129.30   |
| 35  | BB    | 1021 | A    | C2-N3-C4    | -5.86 | 107.67      | 110.60   |
| 35  | BB    | 1209 | U    | N1-C2-N3    | -5.86 | 111.38      | 114.90   |
| 35  | BB    | 1212 | G    | C4-N9-C1'   | 5.86  | 134.12      | 126.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1929 | G    | N9-C4-C5    | -5.86 | 103.06      | 105.40   |
| 35  | BB    | 1981 | A    | O5'-P-OP2   | -5.86 | 100.42      | 105.70   |
| 35  | BB    | 2444 | G    | C4-C5-C6    | 5.86  | 122.32      | 118.80   |
| 35  | BB    | 2700 | A    | N1-C6-N6    | 5.86  | 122.12      | 118.60   |
| 1   | AA    | 491  | G    | N3-C2-N2    | 5.86  | 124.00      | 119.90   |
| 1   | AA    | 1020 | G    | C5-N7-C8    | 5.86  | 107.23      | 104.30   |
| 1   | AA    | 1460 | C    | C4'-C3'-C2' | -5.86 | 96.74       | 102.60   |
| 35  | BB    | 1009 | A    | C6-C5-N7    | -5.86 | 128.20      | 132.30   |
| 35  | BB    | 1091 | G    | N1-C2-N3    | -5.86 | 120.38      | 123.90   |
| 35  | BB    | 1414 | C    | N3-C4-N4    | 5.86  | 122.10      | 118.00   |
| 35  | BB    | 1770 | G    | C8-N9-C4    | -5.86 | 104.06      | 106.40   |
| 1   | AA    | 82   | G    | C6-C5-N7    | -5.86 | 126.88      | 130.40   |
| 1   | AA    | 848  | C    | N3-C2-O2    | -5.86 | 117.80      | 121.90   |
| 1   | AA    | 1367 | C    | C4-C5-C6    | 5.86  | 120.33      | 117.40   |
| 19  | AS    | 9    | PHE  | CG-CD1-CE1  | 5.86  | 127.25      | 120.80   |
| 22  | AV    | 29   | G    | O4'-C1'-N9  | 5.86  | 112.89      | 108.20   |
| 35  | BB    | 201  | C    | C6-N1-C2    | -5.86 | 117.96      | 120.30   |
| 35  | BB    | 530  | G    | C8-N9-C4    | -5.86 | 104.06      | 106.40   |
| 35  | BB    | 663  | G    | O4'-C4'-C3' | -5.86 | 98.14       | 104.00   |
| 35  | BB    | 1210 | G    | C6-C5-N7    | -5.86 | 126.88      | 130.40   |
| 35  | BB    | 2062 | A    | C6-C5-N7    | -5.86 | 128.20      | 132.30   |
| 35  | BB    | 2152 | G    | C4-C5-N7    | -5.86 | 108.46      | 110.80   |
| 35  | BB    | 2279 | G    | C4-C5-N7    | 5.86  | 113.14      | 110.80   |
| 35  | BB    | 2317 | A    | N9-C4-C5    | 5.86  | 108.14      | 105.80   |
| 35  | BB    | 2461 | A    | N1-C6-N6    | 5.86  | 122.12      | 118.60   |
| 50  | BQ    | 38   | VAL  | CA-CB-CG2   | -5.86 | 102.11      | 110.90   |
| 1   | AA    | 74   | A    | N3-C4-C5    | -5.86 | 122.70      | 126.80   |
| 1   | AA    | 86   | G    | C6-N1-C2    | -5.86 | 121.58      | 125.10   |
| 1   | AA    | 1347 | G    | P-O5'-C5'   | 5.86  | 130.27      | 120.90   |
| 17  | AQ    | 30   | HIS  | CA-CB-CG    | -5.86 | 103.64      | 113.60   |
| 35  | BB    | 33   | C    | P-O3'-C3'   | 5.86  | 126.73      | 119.70   |
| 35  | BB    | 182  | A    | OP1-P-OP2   | -5.86 | 110.81      | 119.60   |
| 35  | BB    | 291  | G    | C4-C5-C6    | 5.86  | 122.31      | 118.80   |
| 35  | BB    | 294  | A    | C4-C5-N7    | -5.86 | 107.77      | 110.70   |
| 35  | BB    | 1256 | G    | C2-N3-C4    | 5.86  | 114.83      | 111.90   |
| 35  | BB    | 1844 | C    | OP1-P-OP2   | -5.86 | 110.81      | 119.60   |
| 35  | BB    | 1874 | C    | N1-C2-O2    | -5.86 | 115.38      | 118.90   |
| 1   | AA    | 406  | G    | C4-C5-C6    | 5.86  | 122.31      | 118.80   |
| 1   | AA    | 1397 | C    | C5-C4-N4    | -5.86 | 116.10      | 120.20   |
| 30  | B5    | 224  | VAL  | CG1-CB-CG2  | -5.86 | 101.53      | 110.90   |
| 35  | BB    | 230  | G    | N3-C4-N9    | 5.86  | 129.51      | 126.00   |
| 35  | BB    | 357  | C    | O4'-C1'-N1  | 5.86  | 112.89      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 662  | G    | N3-C2-N2    | 5.86  | 124.00      | 119.90   |
| 35  | BB    | 784  | G    | O3'-P-O5'   | -5.86 | 92.87       | 104.00   |
| 35  | BB    | 910  | A    | C5-C6-N1    | -5.86 | 114.77      | 117.70   |
| 35  | BB    | 1128 | G    | O4'-C1'-N9  | 5.86  | 112.89      | 108.20   |
| 35  | BB    | 1356 | G    | C2-N3-C4    | 5.86  | 114.83      | 111.90   |
| 35  | BB    | 2107 | G    | N1-C2-N2    | -5.86 | 110.93      | 116.20   |
| 35  | BB    | 2189 | U    | N1-C1'-C2'  | -5.86 | 105.56      | 112.00   |
| 35  | BB    | 2358 | A    | C5-C6-N1    | -5.86 | 114.77      | 117.70   |
| 35  | BB    | 2539 | C    | C4-C5-C6    | 5.86  | 120.33      | 117.40   |
| 35  | BB    | 2725 | A    | N7-C8-N9    | -5.86 | 110.87      | 113.80   |
| 1   | AA    | 124  | C    | C5-C4-N4    | -5.86 | 116.10      | 120.20   |
| 1   | AA    | 410  | G    | C5-N7-C8    | -5.86 | 101.37      | 104.30   |
| 1   | AA    | 693  | G    | C5-C6-O6    | -5.86 | 125.09      | 128.60   |
| 1   | AA    | 880  | C    | N3-C4-N4    | 5.86  | 122.10      | 118.00   |
| 1   | AA    | 1036 | A    | C4-C5-C6    | 5.86  | 119.93      | 117.00   |
| 1   | AA    | 1260 | G    | P-O3'-C3'   | 5.86  | 126.73      | 119.70   |
| 1   | AA    | 1392 | G    | C4-C5-C6    | 5.86  | 122.31      | 118.80   |
| 1   | AA    | 1457 | G    | C5-C6-N1    | -5.86 | 108.57      | 111.50   |
| 35  | BB    | 370  | G    | P-O5'-C5'   | 5.86  | 130.27      | 120.90   |
| 35  | BB    | 446  | G    | N1-C2-N3    | -5.86 | 120.39      | 123.90   |
| 35  | BB    | 537  | G    | C5-C6-O6    | -5.86 | 125.09      | 128.60   |
| 35  | BB    | 918  | A    | N9-C4-C5    | 5.86  | 108.14      | 105.80   |
| 35  | BB    | 1122 | G    | N1-C2-N2    | -5.86 | 110.93      | 116.20   |
| 35  | BB    | 2357 | G    | N3-C4-C5    | -5.86 | 125.67      | 128.60   |
| 1   | AA    | 57   | G    | C6-N1-C2    | -5.85 | 121.59      | 125.10   |
| 1   | AA    | 177  | G    | N1-C2-N3    | -5.85 | 120.39      | 123.90   |
| 26  | B1    | 23   | ARG  | N-CA-CB     | 5.85  | 121.14      | 110.60   |
| 35  | BB    | 1149 | G    | C5-C6-O6    | -5.85 | 125.09      | 128.60   |
| 35  | BB    | 1710 | G    | C4-C5-C6    | 5.85  | 122.31      | 118.80   |
| 35  | BB    | 1730 | C    | O4'-C1'-N1  | 5.85  | 112.88      | 108.20   |
| 35  | BB    | 1833 | C    | N3-C4-C5    | -5.85 | 119.56      | 121.90   |
| 48  | BO    | 99   | TYR  | CZ-CE2-CD2  | -5.85 | 114.53      | 119.80   |
| 1   | AA    | 162  | A    | C6-N1-C2    | 5.85  | 122.11      | 118.60   |
| 1   | AA    | 193  | C    | C6-N1-C2    | -5.85 | 117.96      | 120.30   |
| 1   | AA    | 648  | A    | C2-N3-C4    | -5.85 | 107.67      | 110.60   |
| 1   | AA    | 925  | G    | C6-C5-N7    | -5.85 | 126.89      | 130.40   |
| 1   | AA    | 1278 | G    | N9-C4-C5    | -5.85 | 103.06      | 105.40   |
| 1   | AA    | 1278 | G    | N3-C4-N9    | 5.85  | 129.51      | 126.00   |
| 35  | BB    | 469  | G    | C4'-C3'-C2' | -5.85 | 96.75       | 102.60   |
| 35  | BB    | 1469 | A    | C5-C6-N6    | 5.85  | 128.38      | 123.70   |
| 35  | BB    | 1540 | G    | C8-N9-C4    | 5.85  | 108.74      | 106.40   |
| 35  | BB    | 1553 | A    | N1-C6-N6    | 5.85  | 122.11      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2159 | G    | C5-C6-N1    | -5.85 | 108.57      | 111.50   |
| 35  | BB    | 2639 | A    | N7-C8-N9    | -5.85 | 110.87      | 113.80   |
| 1   | AA    | 492  | C    | C2-N3-C4    | -5.85 | 116.97      | 119.90   |
| 1   | AA    | 525  | C    | N1-C1'-C2'  | -5.85 | 105.56      | 112.00   |
| 1   | AA    | 777  | A    | N1-C2-N3    | 5.85  | 132.22      | 129.30   |
| 1   | AA    | 988  | G    | C8-N9-C4    | -5.85 | 104.06      | 106.40   |
| 22  | AV    | 9    | A    | C5-C6-N6    | -5.85 | 119.02      | 123.70   |
| 35  | BB    | 133  | U    | N3-C4-C5    | -5.85 | 111.09      | 114.60   |
| 35  | BB    | 558  | U    | N3-C2-O2    | 5.85  | 126.30      | 122.20   |
| 35  | BB    | 979  | A    | C5-N7-C8    | 5.85  | 106.83      | 103.90   |
| 35  | BB    | 1841 | U    | N1-C2-O2    | -5.85 | 118.70      | 122.80   |
| 35  | BB    | 2378 | A    | C8-N9-C4    | -5.85 | 103.46      | 105.80   |
| 1   | AA    | 15   | G    | C8-N9-C4    | -5.85 | 104.06      | 106.40   |
| 1   | AA    | 87   | C    | C6-N1-C1'   | -5.85 | 113.78      | 120.80   |
| 1   | AA    | 914  | A    | N7-C8-N9    | -5.85 | 110.88      | 113.80   |
| 1   | AA    | 1069 | C    | C4-C5-C6    | 5.85  | 120.33      | 117.40   |
| 1   | AA    | 1278 | G    | N1-C6-O6    | 5.85  | 123.41      | 119.90   |
| 1   | AA    | 1310 | G    | N7-C8-N9    | 5.85  | 116.03      | 113.10   |
| 34  | BA    | 63   | C    | C6-N1-C2    | 5.85  | 122.64      | 120.30   |
| 35  | BB    | 194  | G    | N3-C4-N9    | -5.85 | 122.49      | 126.00   |
| 35  | BB    | 252  | G    | N3-C2-N2    | 5.85  | 124.00      | 119.90   |
| 35  | BB    | 357  | C    | C2-N3-C4    | 5.85  | 122.83      | 119.90   |
| 35  | BB    | 381  | G    | P-O3'-C3'   | -5.85 | 112.68      | 119.70   |
| 35  | BB    | 801  | G    | C5-N7-C8    | 5.85  | 107.22      | 104.30   |
| 35  | BB    | 1004 | U    | C1'-O4'-C4' | -5.85 | 105.22      | 109.90   |
| 35  | BB    | 1020 | A    | C5-C6-N6    | -5.85 | 119.02      | 123.70   |
| 35  | BB    | 1382 | G    | O5'-P-OP2   | 5.85  | 117.72      | 110.70   |
| 35  | BB    | 2679 | A    | C5-C6-N6    | -5.85 | 119.02      | 123.70   |
| 1   | AA    | 83   | C    | N3-C4-C5    | -5.85 | 119.56      | 121.90   |
| 1   | AA    | 306  | A    | C8-N9-C4    | -5.85 | 103.46      | 105.80   |
| 1   | AA    | 1093 | A    | C5-C6-N6    | -5.85 | 119.02      | 123.70   |
| 1   | AA    | 1348 | U    | O4'-C1'-C2' | -5.85 | 99.95       | 105.80   |
| 2   | AB    | 68   | PHE  | CB-CG-CD2   | -5.85 | 116.71      | 120.80   |
| 34  | BA    | 31   | C    | C6-N1-C2    | -5.85 | 117.96      | 120.30   |
| 34  | BA    | 51   | G    | N9-C4-C5    | -5.85 | 103.06      | 105.40   |
| 35  | BB    | 489  | G    | N3-C2-N2    | 5.85  | 123.99      | 119.90   |
| 35  | BB    | 659  | G    | N1-C2-N2    | -5.85 | 110.94      | 116.20   |
| 35  | BB    | 773  | U    | C3'-C2'-C1' | 5.85  | 106.18      | 101.50   |
| 35  | BB    | 785  | G    | O4'-C1'-N9  | 5.85  | 112.88      | 108.20   |
| 35  | BB    | 1057 | A    | C5-C6-N1    | -5.85 | 114.78      | 117.70   |
| 35  | BB    | 1128 | G    | C2-N3-C4    | 5.85  | 114.82      | 111.90   |
| 35  | BB    | 1336 | A    | C2-N3-C4    | -5.85 | 107.68      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1490 | A    | C5-C6-N1    | -5.85 | 114.78      | 117.70   |
| 35  | BB    | 1873 | G    | C4-N9-C1'   | 5.85  | 134.10      | 126.50   |
| 35  | BB    | 1936 | A    | N1-C2-N3    | 5.85  | 132.22      | 129.30   |
| 35  | BB    | 1967 | C    | C4-C5-C6    | 5.85  | 120.32      | 117.40   |
| 35  | BB    | 2035 | G    | C4-C5-C6    | 5.85  | 122.31      | 118.80   |
| 35  | BB    | 2258 | C    | C1'-O4'-C4' | 5.85  | 114.58      | 109.90   |
| 35  | BB    | 2379 | G    | O4'-C1'-N9  | 5.85  | 112.88      | 108.20   |
| 35  | BB    | 2599 | G    | C4-N9-C1'   | -5.85 | 118.90      | 126.50   |
| 35  | BB    | 2701 | U    | C2-N3-C4    | -5.85 | 123.49      | 127.00   |
| 53  | BT    | 3    | ARG  | N-CA-CB     | 5.85  | 121.12      | 110.60   |
| 1   | AA    | 39   | G    | N1-C6-O6    | 5.85  | 123.41      | 119.90   |
| 1   | AA    | 41   | G    | N3-C4-C5    | 5.85  | 131.52      | 128.60   |
| 1   | AA    | 128  | G    | C3'-C2'-C1' | 5.85  | 106.18      | 101.50   |
| 22  | AV    | 36   | G    | O5'-C5'-C4' | 5.85  | 122.81      | 111.70   |
| 35  | BB    | 2048 | G    | N1-C6-O6    | 5.85  | 123.41      | 119.90   |
| 35  | BB    | 2233 | U    | OP1-P-OP2   | -5.85 | 110.83      | 119.60   |
| 1   | AA    | 128  | G    | C6-C5-N7    | -5.84 | 126.89      | 130.40   |
| 1   | AA    | 238  | A    | O4'-C1'-N9  | 5.84  | 112.88      | 108.20   |
| 1   | AA    | 657  | U    | C5-C4-O4    | -5.84 | 122.39      | 125.90   |
| 1   | AA    | 1323 | G    | O3'-P-O5'   | -5.84 | 92.90       | 104.00   |
| 1   | AA    | 1331 | G    | C6-N1-C2    | 5.84  | 128.61      | 125.10   |
| 34  | BA    | 89   | U    | C5-C4-O4    | 5.84  | 129.41      | 125.90   |
| 35  | BB    | 457  | A    | C8-N9-C4    | -5.84 | 103.46      | 105.80   |
| 35  | BB    | 458  | G    | N3-C4-C5    | -5.84 | 125.68      | 128.60   |
| 35  | BB    | 654  | A    | N9-C4-C5    | 5.84  | 108.14      | 105.80   |
| 35  | BB    | 961  | C    | O4'-C1'-C2' | -5.84 | 99.96       | 105.80   |
| 35  | BB    | 1508 | A    | O5'-P-OP2   | -5.84 | 100.44      | 105.70   |
| 35  | BB    | 1865 | U    | O4'-C1'-N1  | 5.84  | 112.88      | 108.20   |
| 35  | BB    | 1921 | G    | C8-N9-C4    | -5.84 | 104.06      | 106.40   |
| 35  | BB    | 2199 | A    | C4-C5-N7    | -5.84 | 107.78      | 110.70   |
| 35  | BB    | 2316 | G    | C5-N7-C8    | 5.84  | 107.22      | 104.30   |
| 35  | BB    | 2608 | G    | N1-C2-N3    | -5.84 | 120.39      | 123.90   |
| 43  | BJ    | 135  | GLN  | CB-CA-C     | 5.84  | 122.09      | 110.40   |
| 1   | AA    | 1055 | A    | C5'-C4'-O4' | 5.84  | 116.11      | 109.10   |
| 1   | AA    | 1191 | A    | C6-C5-N7    | -5.84 | 128.21      | 132.30   |
| 1   | AA    | 1343 | G    | C6-C5-N7    | -5.84 | 126.89      | 130.40   |
| 1   | AA    | 1486 | G    | N9-C4-C5    | 5.84  | 107.74      | 105.40   |
| 35  | BB    | 69   | C    | N3-C4-C5    | -5.84 | 119.56      | 121.90   |
| 35  | BB    | 704  | G    | C5-C6-O6    | -5.84 | 125.09      | 128.60   |
| 35  | BB    | 1230 | A    | C1'-O4'-C4' | -5.84 | 105.22      | 109.90   |
| 35  | BB    | 1466 | U    | C5-C6-N1    | 5.84  | 125.62      | 122.70   |
| 35  | BB    | 1734 | G    | N3-C4-C5    | -5.84 | 125.68      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1876 | A    | C2-N3-C4    | -5.84 | 107.68      | 110.60   |
| 1   | AA    | 224  | U    | O5'-P-OP2   | -5.84 | 100.44      | 105.70   |
| 1   | AA    | 640  | A    | C4-C5-C6    | 5.84  | 119.92      | 117.00   |
| 1   | AA    | 959  | A    | N3-C4-C5    | -5.84 | 122.71      | 126.80   |
| 26  | B1    | 26   | PHE  | CB-CG-CD2   | 5.84  | 124.89      | 120.80   |
| 35  | BB    | 116  | C    | C5-C4-N4    | -5.84 | 116.11      | 120.20   |
| 35  | BB    | 678  | C    | P-O3'-C3'   | -5.84 | 112.69      | 119.70   |
| 35  | BB    | 906  | U    | C6-N1-C2    | -5.84 | 117.50      | 121.00   |
| 35  | BB    | 1187 | G    | C8-N9-C1'   | 5.84  | 134.59      | 127.00   |
| 35  | BB    | 1240 | U    | O4'-C1'-C2' | -5.84 | 99.96       | 105.80   |
| 35  | BB    | 1435 | G    | N9-C4-C5    | 5.84  | 107.74      | 105.40   |
| 35  | BB    | 1713 | A    | P-O3'-C3'   | 5.84  | 126.71      | 119.70   |
| 35  | BB    | 1793 | C    | C4'-C3'-C2' | -5.84 | 96.76       | 102.60   |
| 35  | BB    | 2056 | G    | P-O3'-C3'   | -5.84 | 112.69      | 119.70   |
| 36  | BC    | 12   | ARG  | NE-CZ-NH2   | -5.84 | 117.38      | 120.30   |
| 47  | BN    | 72   | ASP  | CB-CG-OD2   | 5.84  | 123.56      | 118.30   |
| 1   | AA    | 201  | G    | N9-C4-C5    | 5.84  | 107.73      | 105.40   |
| 1   | AA    | 672  | U    | N3-C2-O2    | 5.84  | 126.29      | 122.20   |
| 35  | BB    | 551  | G    | N7-C8-N9    | 5.84  | 116.02      | 113.10   |
| 35  | BB    | 809  | G    | C8-N9-C4    | -5.84 | 104.06      | 106.40   |
| 35  | BB    | 1386 | C    | N3-C2-O2    | 5.84  | 125.99      | 121.90   |
| 35  | BB    | 2794 | C    | C5-C4-N4    | -5.84 | 116.11      | 120.20   |
| 1   | AA    | 582  | C    | N3-C4-C5    | -5.84 | 119.56      | 121.90   |
| 35  | BB    | 669  | G    | C4-N9-C1'   | 5.84  | 134.09      | 126.50   |
| 35  | BB    | 2126 | A    | O4'-C1'-C2' | -5.84 | 99.96       | 105.80   |
| 35  | BB    | 2737 | G    | N1-C2-N3    | -5.84 | 120.40      | 123.90   |
| 38  | BE    | 78   | TRP  | CB-CG-CD1   | 5.84  | 134.59      | 127.00   |
| 1   | AA    | 212  | G    | C4-C5-C6    | 5.84  | 122.30      | 118.80   |
| 1   | AA    | 560  | A    | C5-C6-N1    | -5.84 | 114.78      | 117.70   |
| 1   | AA    | 897  | C    | C6-N1-C2    | -5.84 | 117.97      | 120.30   |
| 1   | AA    | 1398 | A    | C2'-C3'-O3' | 5.84  | 123.04      | 113.70   |
| 35  | BB    | 163  | C    | C5-C4-N4    | -5.84 | 116.11      | 120.20   |
| 35  | BB    | 334  | C    | C1'-O4'-C4' | -5.84 | 105.23      | 109.90   |
| 35  | BB    | 351  | C    | N1-C2-O2    | -5.84 | 115.40      | 118.90   |
| 35  | BB    | 457  | A    | C4-C5-C6    | 5.84  | 119.92      | 117.00   |
| 35  | BB    | 895  | U    | P-O5'-C5'   | 5.84  | 130.24      | 120.90   |
| 35  | BB    | 1094 | U    | P-O3'-C3'   | 5.84  | 126.70      | 119.70   |
| 35  | BB    | 1260 | A    | C4-C5-C6    | 5.84  | 119.92      | 117.00   |
| 35  | BB    | 1309 | G    | C6-N1-C2    | -5.84 | 121.60      | 125.10   |
| 35  | BB    | 1430 | G    | C6-N1-C2    | 5.84  | 128.60      | 125.10   |
| 35  | BB    | 2380 | C    | C5-C6-N1    | -5.84 | 118.08      | 121.00   |
| 35  | BB    | 2899 | A    | C5-C6-N6    | -5.84 | 119.03      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 336  | A    | C5-C6-N1    | -5.83 | 114.78      | 117.70   |
| 34  | BA    | 44   | G    | P-O3'-C3'   | -5.83 | 112.70      | 119.70   |
| 35  | BB    | 178  | G    | N3-C4-N9    | 5.83  | 129.50      | 126.00   |
| 35  | BB    | 1149 | G    | C6-C5-N7    | -5.83 | 126.90      | 130.40   |
| 35  | BB    | 1290 | C    | N1-C2-O2    | 5.83  | 122.40      | 118.90   |
| 35  | BB    | 1323 | C    | N3-C4-N4    | 5.83  | 122.08      | 118.00   |
| 1   | AA    | 696  | A    | N1-C6-N6    | 5.83  | 122.10      | 118.60   |
| 1   | AA    | 725  | G    | N3-C4-C5    | -5.83 | 125.68      | 128.60   |
| 1   | AA    | 1031 | C    | C2-N3-C4    | 5.83  | 122.82      | 119.90   |
| 1   | AA    | 1091 | U    | N3-C4-C5    | -5.83 | 111.10      | 114.60   |
| 1   | AA    | 1105 | A    | N9-C4-C5    | -5.83 | 103.47      | 105.80   |
| 1   | AA    | 1117 | A    | O4'-C1'-N9  | 5.83  | 112.87      | 108.20   |
| 1   | AA    | 1152 | A    | C6-C5-N7    | -5.83 | 128.22      | 132.30   |
| 1   | AA    | 1218 | C    | N3-C4-N4    | 5.83  | 122.08      | 118.00   |
| 1   | AA    | 1353 | G    | C1'-O4'-C4' | 5.83  | 114.57      | 109.90   |
| 1   | AA    | 1389 | C    | C5-C6-N1    | 5.83  | 123.92      | 121.00   |
| 1   | AA    | 1525 | G    | N3-C2-N2    | 5.83  | 123.98      | 119.90   |
| 35  | BB    | 562  | U    | N1-C2-N3    | -5.83 | 111.40      | 114.90   |
| 35  | BB    | 619  | G    | C4-C5-N7    | 5.83  | 113.13      | 110.80   |
| 35  | BB    | 1210 | G    | N1-C2-N3    | -5.83 | 120.40      | 123.90   |
| 35  | BB    | 1285 | A    | C5-N7-C8    | 5.83  | 106.82      | 103.90   |
| 35  | BB    | 1716 | U    | N3-C4-C5    | -5.83 | 111.10      | 114.60   |
| 35  | BB    | 1944 | U    | C4-C5-C6    | 5.83  | 123.20      | 119.70   |
| 35  | BB    | 2349 | G    | C2-N3-C4    | -5.83 | 108.98      | 111.90   |
| 35  | BB    | 2361 | G    | O4'-C1'-N9  | 5.83  | 112.87      | 108.20   |
| 51  | BR    | 13   | ARG  | N-CA-CB     | 5.83  | 121.10      | 110.60   |
| 1   | AA    | 16   | A    | N1-C2-N3    | -5.83 | 126.38      | 129.30   |
| 1   | AA    | 17   | U    | C5-C4-O4    | -5.83 | 122.40      | 125.90   |
| 1   | AA    | 213  | G    | C5-C6-N1    | 5.83  | 114.42      | 111.50   |
| 1   | AA    | 225  | C    | N3-C2-O2    | -5.83 | 117.82      | 121.90   |
| 1   | AA    | 838  | G    | C6-C5-N7    | -5.83 | 126.90      | 130.40   |
| 22  | AV    | 16   | C    | N3-C4-N4    | 5.83  | 122.08      | 118.00   |
| 35  | BB    | 558  | U    | C1'-O4'-C4' | 5.83  | 114.57      | 109.90   |
| 35  | BB    | 1044 | C    | C6-N1-C2    | -5.83 | 117.97      | 120.30   |
| 35  | BB    | 1144 | A    | C2-N3-C4    | 5.83  | 113.52      | 110.60   |
| 35  | BB    | 1917 | U    | N1-C2-N3    | -5.83 | 111.40      | 114.90   |
| 35  | BB    | 1985 | C    | C6-N1-C2    | -5.83 | 117.97      | 120.30   |
| 35  | BB    | 2093 | G    | O4'-C1'-N9  | 5.83  | 112.86      | 108.20   |
| 35  | BB    | 2567 | G    | C4-C5-N7    | 5.83  | 113.13      | 110.80   |
| 44  | BK    | 56   | ASP  | CB-CG-OD1   | -5.83 | 113.05      | 118.30   |
| 1   | AA    | 411  | A    | N7-C8-N9    | -5.83 | 110.89      | 113.80   |
| 1   | AA    | 897  | C    | O4'-C1'-N1  | 5.83  | 112.86      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1243 | C    | C4-C5-C6    | 5.83  | 120.31      | 117.40   |
| 35  | BB    | 340  | A    | C5-C6-N1    | -5.83 | 114.78      | 117.70   |
| 35  | BB    | 1252 | G    | C2-N3-C4    | 5.83  | 114.81      | 111.90   |
| 35  | BB    | 1624 | U    | C4-C5-C6    | 5.83  | 123.20      | 119.70   |
| 35  | BB    | 1786 | A    | N7-C8-N9    | -5.83 | 110.89      | 113.80   |
| 35  | BB    | 1885 | A    | C5-C6-N1    | -5.83 | 114.78      | 117.70   |
| 35  | BB    | 2278 | A    | C5-N7-C8    | 5.83  | 106.81      | 103.90   |
| 35  | BB    | 2558 | C    | N3-C4-C5    | -5.83 | 119.57      | 121.90   |
| 35  | BB    | 2823 | A    | C5-C6-N6    | -5.83 | 119.04      | 123.70   |
| 35  | BB    | 2837 | A    | O4'-C1'-N9  | 5.83  | 112.86      | 108.20   |
| 1   | AA    | 208  | U    | C5-C4-O4    | -5.83 | 122.40      | 125.90   |
| 1   | AA    | 614  | C    | C1'-O4'-C4' | 5.83  | 114.56      | 109.90   |
| 1   | AA    | 667  | G    | C4-C5-C6    | 5.83  | 122.30      | 118.80   |
| 1   | AA    | 1019 | A    | O5'-P-OP1   | -5.83 | 100.45      | 105.70   |
| 1   | AA    | 1150 | A    | O3'-P-O5'   | -5.83 | 92.93       | 104.00   |
| 34  | BA    | 78   | A    | C5-C6-N1    | -5.83 | 114.79      | 117.70   |
| 35  | BB    | 1031 | G    | O4'-C1'-N9  | 5.83  | 112.86      | 108.20   |
| 35  | BB    | 1084 | A    | N7-C8-N9    | -5.83 | 110.89      | 113.80   |
| 35  | BB    | 1389 | G    | C4-C5-N7    | -5.83 | 108.47      | 110.80   |
| 35  | BB    | 1539 | U    | P-O3'-C3'   | -5.83 | 112.70      | 119.70   |
| 35  | BB    | 1827 | U    | N3-C4-O4    | 5.83  | 123.48      | 119.40   |
| 35  | BB    | 2367 | G    | N1-C2-N3    | -5.83 | 120.40      | 123.90   |
| 35  | BB    | 2413 | G    | O4'-C1'-N9  | 5.83  | 112.86      | 108.20   |
| 35  | BB    | 2613 | U    | C5'-C4'-O4' | 5.83  | 116.09      | 109.10   |
| 1   | AA    | 904  | U    | OP1-P-OP2   | -5.83 | 110.86      | 119.60   |
| 1   | AA    | 989  | U    | C5-C6-N1    | 5.83  | 125.61      | 122.70   |
| 1   | AA    | 1373 | G    | C1'-O4'-C4' | 5.83  | 114.56      | 109.90   |
| 15  | AO    | 88   | ARG  | NE-CZ-NH1   | 5.83  | 123.21      | 120.30   |
| 35  | BB    | 118  | A    | C5-N7-C8    | 5.83  | 106.81      | 103.90   |
| 35  | BB    | 1388 | G    | C4-C5-N7    | 5.83  | 113.13      | 110.80   |
| 35  | BB    | 1494 | A    | N1-C6-N6    | 5.83  | 122.10      | 118.60   |
| 35  | BB    | 1587 | G    | C4-N9-C1'   | 5.83  | 134.07      | 126.50   |
| 35  | BB    | 2122 | U    | O4'-C1'-N1  | 5.83  | 112.86      | 108.20   |
| 1   | AA    | 133  | U    | C4'-C3'-C2' | -5.83 | 96.77       | 102.60   |
| 1   | AA    | 287  | U    | O4'-C1'-N1  | 5.83  | 112.86      | 108.20   |
| 1   | AA    | 316  | C    | N1-C2-N3    | -5.83 | 115.12      | 119.20   |
| 1   | AA    | 425  | G    | C4-C5-N7    | 5.83  | 113.13      | 110.80   |
| 1   | AA    | 758  | C    | P-O3'-C3'   | 5.83  | 126.69      | 119.70   |
| 1   | AA    | 1253 | G    | O4'-C1'-C2' | -5.83 | 99.97       | 105.80   |
| 1   | AA    | 1278 | G    | C4-C5-N7    | 5.83  | 113.13      | 110.80   |
| 34  | BA    | 23   | G    | P-O5'-C5'   | 5.83  | 130.22      | 120.90   |
| 34  | BA    | 81   | G    | N9-C4-C5    | -5.83 | 103.07      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | BA    | 112  | G    | C6-C5-N7    | -5.83 | 126.90      | 130.40   |
| 35  | BB    | 312  | G    | C6-C5-N7    | -5.83 | 126.90      | 130.40   |
| 35  | BB    | 548  | G    | N7-C8-N9    | -5.83 | 110.19      | 113.10   |
| 35  | BB    | 1015 | U    | N3-C4-C5    | -5.83 | 111.11      | 114.60   |
| 35  | BB    | 1311 | G    | C6-C5-N7    | -5.83 | 126.91      | 130.40   |
| 35  | BB    | 1420 | A    | C1'-O4'-C4' | 5.83  | 114.56      | 109.90   |
| 35  | BB    | 1513 | U    | N1-C2-O2    | -5.83 | 118.72      | 122.80   |
| 35  | BB    | 1713 | A    | C2-N3-C4    | 5.83  | 113.51      | 110.60   |
| 35  | BB    | 1969 | A    | C5-N7-C8    | 5.83  | 106.81      | 103.90   |
| 35  | BB    | 2058 | A    | N9-C4-C5    | 5.83  | 108.13      | 105.80   |
| 35  | BB    | 2074 | U    | C4-C5-C6    | -5.83 | 116.20      | 119.70   |
| 35  | BB    | 2661 | G    | P-O3'-C3'   | 5.83  | 126.69      | 119.70   |
| 35  | BB    | 2838 | G    | C5-C6-N1    | 5.83  | 114.41      | 111.50   |
| 1   | AA    | 965  | U    | O4'-C1'-N1  | 5.82  | 112.86      | 108.20   |
| 1   | AA    | 1322 | C    | C5-C4-N4    | -5.82 | 116.12      | 120.20   |
| 1   | AA    | 1415 | G    | N3-C4-C5    | -5.82 | 125.69      | 128.60   |
| 12  | AL    | 28   | GLN  | O-C-N       | 5.82  | 132.02      | 122.70   |
| 19  | AS    | 79   | TYR  | CB-CG-CD2   | -5.82 | 117.51      | 121.00   |
| 35  | BB    | 664  | G    | C4'-C3'-C2' | -5.82 | 96.78       | 102.60   |
| 35  | BB    | 731  | C    | C5-C4-N4    | -5.82 | 116.12      | 120.20   |
| 35  | BB    | 735  | A    | C6-C5-N7    | -5.82 | 128.22      | 132.30   |
| 35  | BB    | 778  | G    | N3-C4-C5    | 5.82  | 131.51      | 128.60   |
| 35  | BB    | 804  | A    | N7-C8-N9    | -5.82 | 110.89      | 113.80   |
| 35  | BB    | 868  | U    | N1-C2-O2    | -5.82 | 118.72      | 122.80   |
| 35  | BB    | 871  | U    | C5'-C4'-C3' | -5.82 | 106.68      | 116.00   |
| 35  | BB    | 1095 | A    | C8-N9-C4    | -5.82 | 103.47      | 105.80   |
| 35  | BB    | 2115 | G    | C2-N3-C4    | -5.82 | 108.99      | 111.90   |
| 35  | BB    | 2291 | U    | C4-C5-C6    | 5.82  | 123.19      | 119.70   |
| 35  | BB    | 2575 | C    | P-O5'-C5'   | -5.82 | 111.58      | 120.90   |
| 39  | BF    | 86   | CYS  | CB-CA-C     | -5.82 | 98.75       | 110.40   |
| 43  | BJ    | 31   | GLU  | N-CA-CB     | 5.82  | 121.08      | 110.60   |
| 1   | AA    | 112  | G    | C2-N3-C4    | 5.82  | 114.81      | 111.90   |
| 1   | AA    | 613  | C    | O4'-C1'-N1  | 5.82  | 112.86      | 108.20   |
| 1   | AA    | 1456 | A    | C5-C6-N1    | -5.82 | 114.79      | 117.70   |
| 30  | B5    | 39   | VAL  | CG1-CB-CG2  | 5.82  | 120.22      | 110.90   |
| 35  | BB    | 145  | C    | C5-C6-N1    | 5.82  | 123.91      | 121.00   |
| 35  | BB    | 1085 | A    | C5-N7-C8    | 5.82  | 106.81      | 103.90   |
| 35  | BB    | 1380 | G    | C8-N9-C1'   | -5.82 | 119.43      | 127.00   |
| 35  | BB    | 1498 | C    | C4'-C3'-C2' | 5.82  | 108.42      | 102.60   |
| 35  | BB    | 1733 | G    | O4'-C1'-N9  | 5.82  | 112.86      | 108.20   |
| 35  | BB    | 2438 | U    | C5-C6-N1    | 5.82  | 125.61      | 122.70   |
| 1   | AA    | 129  | A    | C4-C5-C6    | 5.82  | 119.91      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 597  | G    | N7-C8-N9    | -5.82 | 110.19      | 113.10   |
| 1   | AA    | 600  | A    | N7-C8-N9    | -5.82 | 110.89      | 113.80   |
| 1   | AA    | 642  | A    | C2-N3-C4    | -5.82 | 107.69      | 110.60   |
| 1   | AA    | 800  | G    | O4'-C1'-N9  | 5.82  | 112.86      | 108.20   |
| 1   | AA    | 1508 | A    | C5-C6-N1    | -5.82 | 114.79      | 117.70   |
| 4   | AD    | 203  | TYR  | CB-CG-CD1   | -5.82 | 117.51      | 121.00   |
| 34  | BA    | 21   | G    | N9-C4-C5    | -5.82 | 103.07      | 105.40   |
| 35  | BB    | 3    | U    | C3'-C2'-C1' | 5.82  | 106.16      | 101.50   |
| 35  | BB    | 298  | G    | C5-C6-O6    | -5.82 | 125.11      | 128.60   |
| 35  | BB    | 390  | U    | N3-C4-O4    | 5.82  | 123.47      | 119.40   |
| 35  | BB    | 1689 | A    | N7-C8-N9    | -5.82 | 110.89      | 113.80   |
| 35  | BB    | 2050 | C    | C6-N1-C2    | 5.82  | 122.63      | 120.30   |
| 35  | BB    | 2608 | G    | C8-N9-C4    | -5.82 | 104.07      | 106.40   |
| 1   | AA    | 586  | C    | C6-N1-C2    | 5.82  | 122.63      | 120.30   |
| 1   | AA    | 1092 | A    | N9-C4-C5    | 5.82  | 108.13      | 105.80   |
| 1   | AA    | 1481 | U    | P-O3'-C3'   | -5.82 | 112.72      | 119.70   |
| 35  | BB    | 317  | G    | O4'-C1'-N9  | 5.82  | 112.86      | 108.20   |
| 35  | BB    | 1182 | G    | N1-C2-N3    | -5.82 | 120.41      | 123.90   |
| 35  | BB    | 1408 | G    | C4-C5-N7    | -5.82 | 108.47      | 110.80   |
| 35  | BB    | 1722 | A    | N1-C6-N6    | 5.82  | 122.09      | 118.60   |
| 35  | BB    | 2658 | C    | P-O3'-C3'   | -5.82 | 112.72      | 119.70   |
| 1   | AA    | 195  | A    | N1-C2-N3    | 5.82  | 132.21      | 129.30   |
| 1   | AA    | 545  | C    | C5'-C4'-C3' | -5.82 | 106.69      | 116.00   |
| 1   | AA    | 658  | C    | N1-C2-O2    | -5.82 | 115.41      | 118.90   |
| 1   | AA    | 716  | A    | N3-C4-C5    | -5.82 | 122.73      | 126.80   |
| 1   | AA    | 913  | A    | N1-C6-N6    | 5.82  | 122.09      | 118.60   |
| 1   | AA    | 1437 | A    | C2-N3-C4    | -5.82 | 107.69      | 110.60   |
| 1   | AA    | 1482 | G    | N9-C4-C5    | 5.82  | 107.73      | 105.40   |
| 1   | AA    | 1502 | A    | O4'-C1'-N9  | 5.82  | 112.85      | 108.20   |
| 35  | BB    | 5    | A    | C5-C6-N1    | -5.82 | 114.79      | 117.70   |
| 35  | BB    | 204  | A    | C4-C5-C6    | 5.82  | 119.91      | 117.00   |
| 35  | BB    | 464  | U    | N3-C4-O4    | 5.82  | 123.47      | 119.40   |
| 35  | BB    | 871  | U    | C1'-O4'-C4' | 5.82  | 114.55      | 109.90   |
| 35  | BB    | 1008 | A    | C5-C6-N1    | -5.82 | 114.79      | 117.70   |
| 35  | BB    | 1211 | C    | P-O5'-C5'   | -5.82 | 111.59      | 120.90   |
| 35  | BB    | 1377 | G    | N1-C2-N2    | -5.82 | 110.96      | 116.20   |
| 35  | BB    | 1669 | A    | O4'-C1'-N9  | 5.82  | 112.86      | 108.20   |
| 35  | BB    | 1804 | C    | C4-C5-C6    | -5.82 | 114.49      | 117.40   |
| 35  | BB    | 1995 | U    | C2-N1-C1'   | -5.82 | 110.72      | 117.70   |
| 35  | BB    | 2151 | U    | C5-C6-N1    | 5.82  | 125.61      | 122.70   |
| 35  | BB    | 2648 | G    | C8-N9-C4    | -5.82 | 104.07      | 106.40   |
| 35  | BB    | 2868 | A    | C5-N7-C8    | 5.82  | 106.81      | 103.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 177  | G    | C2-N3-C4    | 5.82  | 114.81      | 111.90   |
| 1   | AA    | 258  | G    | P-O3'-C3'   | 5.82  | 126.68      | 119.70   |
| 1   | AA    | 566  | G    | C4-C5-C6    | 5.82  | 122.29      | 118.80   |
| 1   | AA    | 982  | U    | C5-C4-O4    | -5.82 | 122.41      | 125.90   |
| 35  | BB    | 496  | G    | N1-C6-O6    | 5.82  | 123.39      | 119.90   |
| 35  | BB    | 638  | G    | C8-N9-C4    | -5.82 | 104.07      | 106.40   |
| 35  | BB    | 1295 | C    | C5-C4-N4    | -5.82 | 116.13      | 120.20   |
| 35  | BB    | 1377 | G    | C6-C5-N7    | -5.82 | 126.91      | 130.40   |
| 35  | BB    | 1589 | U    | P-O5'-C5'   | 5.82  | 130.20      | 120.90   |
| 35  | BB    | 1668 | A    | C8-N9-C4    | 5.82  | 108.13      | 105.80   |
| 35  | BB    | 2452 | C    | C6-N1-C1'   | -5.82 | 113.82      | 120.80   |
| 43  | BJ    | 37   | ARG  | NE-CZ-NH2   | 5.82  | 123.21      | 120.30   |
| 1   | AA    | 454  | G    | C5'-C4'-C3' | -5.81 | 106.70      | 116.00   |
| 1   | AA    | 482  | A    | N1-C6-N6    | 5.81  | 122.09      | 118.60   |
| 1   | AA    | 622  | A    | O4'-C1'-N9  | 5.81  | 112.85      | 108.20   |
| 35  | BB    | 263  | G    | C8-N9-C4    | -5.81 | 104.07      | 106.40   |
| 35  | BB    | 1358 | G    | C5-C6-N1    | 5.81  | 114.41      | 111.50   |
| 35  | BB    | 1520 | U    | C4-C5-C6    | -5.81 | 116.21      | 119.70   |
| 35  | BB    | 1871 | A    | N3-C4-C5    | -5.81 | 122.73      | 126.80   |
| 47  | BN    | 4    | ARG  | NE-CZ-NH2   | -5.81 | 117.39      | 120.30   |
| 1   | AA    | 206  | C    | N3-C2-O2    | 5.81  | 125.97      | 121.90   |
| 1   | AA    | 289  | G    | N9-C4-C5    | 5.81  | 107.72      | 105.40   |
| 1   | AA    | 971  | G    | C3'-C2'-C1' | -5.81 | 96.85       | 101.50   |
| 1   | AA    | 1039 | G    | N3-C2-N2    | 5.81  | 123.97      | 119.90   |
| 1   | AA    | 1138 | G    | C5-C6-N1    | -5.81 | 108.59      | 111.50   |
| 35  | BB    | 176  | A    | C4-C5-C6    | 5.81  | 119.91      | 117.00   |
| 35  | BB    | 241  | A    | C3'-C2'-C1' | -5.81 | 96.85       | 101.50   |
| 35  | BB    | 490  | C    | N3-C4-N4    | 5.81  | 122.07      | 118.00   |
| 35  | BB    | 1061 | U    | C5-C6-N1    | 5.81  | 125.61      | 122.70   |
| 35  | BB    | 1318 | U    | C5'-C4'-C3' | -5.81 | 106.70      | 116.00   |
| 35  | BB    | 1390 | U    | C4-C5-C6    | 5.81  | 123.19      | 119.70   |
| 35  | BB    | 1469 | A    | C6-C5-N7    | -5.81 | 128.23      | 132.30   |
| 35  | BB    | 1575 | C    | C5'-C4'-O4' | 5.81  | 116.08      | 109.10   |
| 35  | BB    | 1798 | U    | C4-C5-C6    | -5.81 | 116.21      | 119.70   |
| 35  | BB    | 2778 | A    | C4-C5-C6    | 5.81  | 119.91      | 117.00   |
| 1   | AA    | 106  | C    | P-O5'-C5'   | 5.81  | 130.20      | 120.90   |
| 35  | BB    | 1170 | C    | N3-C4-N4    | 5.81  | 122.07      | 118.00   |
| 35  | BB    | 1700 | A    | C5-C6-N6    | -5.81 | 119.05      | 123.70   |
| 35  | BB    | 1787 | A    | O4'-C1'-N9  | 5.81  | 112.85      | 108.20   |
| 35  | BB    | 1945 | G    | O4'-C1'-N9  | 5.81  | 112.85      | 108.20   |
| 1   | AA    | 207  | C    | N3-C4-N4    | 5.81  | 122.07      | 118.00   |
| 1   | AA    | 275  | G    | C5-C6-O6    | -5.81 | 125.11      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 369  | G    | O4'-C1'-N9  | 5.81  | 112.85      | 108.20   |
| 1   | AA    | 850  | U    | N3-C4-C5    | -5.81 | 111.11      | 114.60   |
| 1   | AA    | 904  | U    | N3-C4-O4    | 5.81  | 123.47      | 119.40   |
| 1   | AA    | 1276 | G    | N7-C8-N9    | 5.81  | 116.00      | 113.10   |
| 1   | AA    | 1534 | A    | C4-C5-N7    | -5.81 | 107.80      | 110.70   |
| 35  | BB    | 611  | C    | C2-N3-C4    | 5.81  | 122.81      | 119.90   |
| 35  | BB    | 659  | G    | N1-C2-N3    | -5.81 | 120.42      | 123.90   |
| 35  | BB    | 945  | A    | C6-C5-N7    | -5.81 | 128.23      | 132.30   |
| 35  | BB    | 1175 | A    | C6-C5-N7    | -5.81 | 128.23      | 132.30   |
| 35  | BB    | 1490 | A    | C5-N7-C8    | 5.81  | 106.81      | 103.90   |
| 1   | AA    | 286  | C    | P-O3'-C3'   | -5.81 | 112.73      | 119.70   |
| 1   | AA    | 711  | G    | C6-N1-C2    | 5.81  | 128.58      | 125.10   |
| 1   | AA    | 870  | U    | N3-C4-O4    | 5.81  | 123.47      | 119.40   |
| 34  | BA    | 104  | A    | C2-N3-C4    | -5.81 | 107.70      | 110.60   |
| 35  | BB    | 219  | A    | N9-C1'-C2'  | -5.81 | 105.61      | 112.00   |
| 35  | BB    | 379  | G    | O4'-C1'-N9  | 5.81  | 112.85      | 108.20   |
| 35  | BB    | 395  | U    | N3-C4-O4    | 5.81  | 123.47      | 119.40   |
| 35  | BB    | 769  | U    | P-O5'-C5'   | 5.81  | 130.19      | 120.90   |
| 35  | BB    | 1266 | G    | N3-C4-C5    | -5.81 | 125.70      | 128.60   |
| 35  | BB    | 1296 | G    | N7-C8-N9    | 5.81  | 116.00      | 113.10   |
| 35  | BB    | 1765 | U    | C2-N3-C4    | -5.81 | 123.52      | 127.00   |
| 35  | BB    | 1960 | A    | C5'-C4'-C3' | -5.81 | 106.71      | 116.00   |
| 35  | BB    | 2421 | G    | C6-N1-C2    | 5.81  | 128.58      | 125.10   |
| 35  | BB    | 2662 | A    | C5'-C4'-C3' | 5.81  | 125.29      | 116.00   |
| 35  | BB    | 2835 | A    | O4'-C1'-N9  | 5.81  | 112.85      | 108.20   |
| 1   | AA    | 180  | U    | N3-C4-O4    | 5.81  | 123.46      | 119.40   |
| 1   | AA    | 370  | C    | C6-N1-C2    | -5.81 | 117.98      | 120.30   |
| 1   | AA    | 837  | U    | N3-C4-C5    | -5.81 | 111.12      | 114.60   |
| 1   | AA    | 1454 | G    | O4'-C4'-C3' | -5.81 | 98.19       | 104.00   |
| 35  | BB    | 46   | G    | N1-C6-O6    | 5.81  | 123.38      | 119.90   |
| 35  | BB    | 1315 | C    | C5-C4-N4    | -5.81 | 116.14      | 120.20   |
| 35  | BB    | 1530 | G    | P-O3'-C3'   | 5.81  | 126.67      | 119.70   |
| 35  | BB    | 1897 | G    | C6-N1-C2    | -5.81 | 121.62      | 125.10   |
| 35  | BB    | 2064 | C    | P-O3'-C3'   | -5.81 | 112.73      | 119.70   |
| 35  | BB    | 2867 | G    | C6-C5-N7    | -5.81 | 126.92      | 130.40   |
| 45  | BL    | 113  | ALA  | N-CA-CB     | 5.81  | 118.23      | 110.10   |
| 1   | AA    | 365  | U    | C2-N1-C1'   | 5.80  | 124.67      | 117.70   |
| 1   | AA    | 459  | A    | O4'-C1'-N9  | 5.80  | 112.84      | 108.20   |
| 1   | AA    | 615  | G    | C5-C6-O6    | -5.80 | 125.12      | 128.60   |
| 7   | AG    | 78   | ARG  | NE-CZ-NH1   | 5.80  | 123.20      | 120.30   |
| 30  | B5    | 12   | ARG  | N-CA-CB     | 5.80  | 121.05      | 110.60   |
| 35  | BB    | 196  | A    | C4-N9-C1'   | 5.80  | 136.75      | 126.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 694  | U    | N3-C4-C5    | -5.80 | 111.12      | 114.60   |
| 35  | BB    | 932  | U    | N3-C4-O4    | 5.80  | 123.46      | 119.40   |
| 35  | BB    | 967  | U    | C6-N1-C2    | 5.80  | 124.48      | 121.00   |
| 35  | BB    | 1239 | G    | C2-N3-C4    | 5.80  | 114.80      | 111.90   |
| 35  | BB    | 1391 | U    | N3-C4-C5    | -5.80 | 111.12      | 114.60   |
| 35  | BB    | 1546 | G    | C4-C5-C6    | 5.80  | 122.28      | 118.80   |
| 35  | BB    | 1707 | G    | C5'-C4'-C3' | -5.80 | 106.71      | 116.00   |
| 35  | BB    | 1904 | G    | C4-C5-N7    | -5.80 | 108.48      | 110.80   |
| 35  | BB    | 2054 | A    | C5-C6-N6    | -5.80 | 119.06      | 123.70   |
| 35  | BB    | 2110 | G    | N3-C4-N9    | -5.80 | 122.52      | 126.00   |
| 35  | BB    | 2539 | C    | N3-C4-N4    | 5.80  | 122.06      | 118.00   |
| 35  | BB    | 2608 | G    | N9-C1'-C2'  | -5.80 | 105.62      | 112.00   |
| 35  | BB    | 2722 | G    | C6-N1-C2    | 5.80  | 128.58      | 125.10   |
| 1   | AA    | 1079 | G    | C4-C5-N7    | -5.80 | 108.48      | 110.80   |
| 34  | BA    | 22   | U    | C5-C6-N1    | 5.80  | 125.60      | 122.70   |
| 35  | BB    | 2009 | A    | C2-N3-C4    | 5.80  | 113.50      | 110.60   |
| 1   | AA    | 364  | A    | N1-C2-N3    | 5.80  | 132.20      | 129.30   |
| 1   | AA    | 496  | A    | C6-C5-N7    | -5.80 | 128.24      | 132.30   |
| 1   | AA    | 1306 | A    | C5-N7-C8    | 5.80  | 106.80      | 103.90   |
| 1   | AA    | 1362 | A    | C2-N3-C4    | -5.80 | 107.70      | 110.60   |
| 1   | AA    | 1490 | U    | N1-C2-O2    | -5.80 | 118.74      | 122.80   |
| 35  | BB    | 154  | U    | N3-C4-O4    | 5.80  | 123.46      | 119.40   |
| 35  | BB    | 608  | A    | C5-C6-N1    | -5.80 | 114.80      | 117.70   |
| 35  | BB    | 1095 | A    | C5'-C4'-O4' | 5.80  | 116.06      | 109.10   |
| 35  | BB    | 1403 | A    | C5-C6-N1    | -5.80 | 114.80      | 117.70   |
| 35  | BB    | 1754 | A    | OP1-P-OP2   | -5.80 | 110.90      | 119.60   |
| 35  | BB    | 2259 | U    | P-O3'-C3'   | -5.80 | 112.74      | 119.70   |
| 35  | BB    | 2617 | U    | P-O5'-C5'   | -5.80 | 111.62      | 120.90   |
| 35  | BB    | 2754 | U    | C4-C5-C6    | -5.80 | 116.22      | 119.70   |
| 50  | BQ    | 86   | SER  | N-CA-CB     | 5.80  | 119.20      | 110.50   |
| 1   | AA    | 342  | C    | C6-N1-C2    | -5.80 | 117.98      | 120.30   |
| 1   | AA    | 347  | G    | N1-C2-N3    | -5.80 | 120.42      | 123.90   |
| 1   | AA    | 605  | U    | C4'-C3'-C2' | -5.80 | 96.80       | 102.60   |
| 1   | AA    | 1258 | G    | O4'-C1'-N9  | 5.80  | 112.84      | 108.20   |
| 1   | AA    | 1292 | G    | N1-C2-N3    | -5.80 | 120.42      | 123.90   |
| 1   | AA    | 1507 | A    | N1-C2-N3    | 5.80  | 132.20      | 129.30   |
| 35  | BB    | 701  | G    | C5-C6-O6    | -5.80 | 125.12      | 128.60   |
| 35  | BB    | 716  | A    | C2-N3-C4    | -5.80 | 107.70      | 110.60   |
| 35  | BB    | 745  | G    | C6-C5-N7    | -5.80 | 126.92      | 130.40   |
| 35  | BB    | 814  | C    | N3-C4-C5    | -5.80 | 119.58      | 121.90   |
| 35  | BB    | 821  | A    | C1'-O4'-C4' | 5.80  | 114.54      | 109.90   |
| 35  | BB    | 2083 | G    | N3-C2-N2    | 5.80  | 123.96      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2358 | A    | P-O3'-C3'   | -5.80 | 112.74      | 119.70   |
| 35  | BB    | 2714 | G    | C4-C5-C6    | 5.80  | 122.28      | 118.80   |
| 1   | AA    | 789  | U    | C5'-C4'-C3' | -5.80 | 106.72      | 116.00   |
| 1   | AA    | 833  | G    | N1-C2-N3    | -5.80 | 120.42      | 123.90   |
| 34  | BA    | 83   | G    | N3-C2-N2    | 5.80  | 123.96      | 119.90   |
| 35  | BB    | 83   | A    | N3-C4-C5    | -5.80 | 122.74      | 126.80   |
| 35  | BB    | 1683 | U    | N3-C2-O2    | 5.80  | 126.26      | 122.20   |
| 35  | BB    | 1754 | A    | C5-N7-C8    | 5.80  | 106.80      | 103.90   |
| 35  | BB    | 2314 | A    | C5-C6-N1    | -5.80 | 114.80      | 117.70   |
| 1   | AA    | 435  | A    | C4-C5-C6    | 5.80  | 119.90      | 117.00   |
| 1   | AA    | 470  | C    | C5-C6-N1    | 5.80  | 123.90      | 121.00   |
| 1   | AA    | 718  | A    | C4-C5-N7    | -5.80 | 107.80      | 110.70   |
| 1   | AA    | 891  | U    | C6-N1-C2    | -5.80 | 117.52      | 121.00   |
| 1   | AA    | 981  | U    | P-O3'-C3'   | 5.80  | 126.66      | 119.70   |
| 1   | AA    | 985  | C    | C2-N3-C4    | 5.80  | 122.80      | 119.90   |
| 1   | AA    | 1029 | U    | N1-C2-O2    | -5.80 | 118.74      | 122.80   |
| 1   | AA    | 1262 | C    | N3-C4-N4    | 5.80  | 122.06      | 118.00   |
| 1   | AA    | 1392 | G    | C2-N3-C4    | 5.80  | 114.80      | 111.90   |
| 7   | AG    | 137  | ARG  | NE-CZ-NH2   | -5.80 | 117.40      | 120.30   |
| 15  | AO    | 67   | ASP  | CB-CG-OD1   | 5.80  | 123.52      | 118.30   |
| 34  | BA    | 57   | A    | C2-N3-C4    | -5.80 | 107.70      | 110.60   |
| 35  | BB    | 36   | G    | N3-C4-C5    | -5.80 | 125.70      | 128.60   |
| 35  | BB    | 929  | U    | P-O5'-C5'   | -5.80 | 111.63      | 120.90   |
| 35  | BB    | 1040 | A    | C5-N7-C8    | 5.80  | 106.80      | 103.90   |
| 35  | BB    | 1332 | G    | C5-C6-O6    | -5.80 | 125.12      | 128.60   |
| 35  | BB    | 2067 | G    | C6-C5-N7    | -5.80 | 126.92      | 130.40   |
| 35  | BB    | 2407 | A    | C4-N9-C1'   | 5.80  | 136.73      | 126.30   |
| 35  | BB    | 2786 | U    | O4'-C1'-N1  | 5.80  | 112.84      | 108.20   |
| 46  | BM    | 103  | TYR  | CB-CG-CD2   | 5.80  | 124.48      | 121.00   |
| 1   | AA    | 608  | A    | N3-C4-N9    | 5.79  | 132.04      | 127.40   |
| 1   | AA    | 615  | G    | N1-C6-O6    | 5.79  | 123.38      | 119.90   |
| 1   | AA    | 729  | A    | C6-N1-C2    | 5.79  | 122.08      | 118.60   |
| 35  | BB    | 777  | G    | O5'-C5'-C4' | -5.79 | 100.69      | 111.70   |
| 35  | BB    | 872  | U    | N3-C4-C5    | -5.79 | 111.12      | 114.60   |
| 35  | BB    | 1369 | G    | C1'-O4'-C4' | 5.79  | 114.54      | 109.90   |
| 35  | BB    | 1710 | G    | N9-C4-C5    | 5.79  | 107.72      | 105.40   |
| 35  | BB    | 2229 | U    | C5-C6-N1    | 5.79  | 125.60      | 122.70   |
| 53  | BT    | 73   | ARG  | CG-CD-NE    | -5.79 | 99.63       | 111.80   |
| 1   | AA    | 343  | U    | N3-C4-C5    | -5.79 | 111.12      | 114.60   |
| 34  | BA    | 50   | A    | C5-C6-N1    | -5.79 | 114.80      | 117.70   |
| 35  | BB    | 486  | C    | C4-C5-C6    | 5.79  | 120.30      | 117.40   |
| 35  | BB    | 1170 | C    | C5-C4-N4    | -5.79 | 116.14      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1582 | C    | C6-N1-C2    | -5.79 | 117.98      | 120.30   |
| 35  | BB    | 1906 | G    | C5-N7-C8    | -5.79 | 101.40      | 104.30   |
| 35  | BB    | 2580 | U    | C5-C4-O4    | -5.79 | 122.42      | 125.90   |
| 35  | BB    | 2811 | G    | C5-N7-C8    | -5.79 | 101.40      | 104.30   |
| 46  | BM    | 85   | GLY  | N-CA-C      | -5.79 | 98.62       | 113.10   |
| 52  | BS    | 76   | VAL  | N-CA-C      | -5.79 | 95.36       | 111.00   |
| 1   | AA    | 1177 | G    | N1-C2-N2    | -5.79 | 110.99      | 116.20   |
| 1   | AA    | 1461 | G    | C5-C6-N1    | -5.79 | 108.60      | 111.50   |
| 1   | AA    | 1475 | G    | N9-C1'-C2'  | -5.79 | 105.63      | 112.00   |
| 35  | BB    | 267  | C    | C6-N1-C2    | -5.79 | 117.98      | 120.30   |
| 35  | BB    | 381  | G    | C8-N9-C4    | 5.79  | 108.72      | 106.40   |
| 35  | BB    | 400  | G    | C2-N3-C4    | -5.79 | 109.00      | 111.90   |
| 35  | BB    | 437  | U    | C6-N1-C2    | -5.79 | 117.53      | 121.00   |
| 35  | BB    | 719  | C    | C2-N3-C4    | -5.79 | 117.00      | 119.90   |
| 35  | BB    | 746  | U    | P-O3'-C3'   | 5.79  | 126.65      | 119.70   |
| 35  | BB    | 1738 | G    | C5-C6-N1    | 5.79  | 114.40      | 111.50   |
| 35  | BB    | 1792 | G    | C6-C5-N7    | -5.79 | 126.92      | 130.40   |
| 35  | BB    | 2169 | A    | C5-N7-C8    | 5.79  | 106.80      | 103.90   |
| 35  | BB    | 2559 | C    | N1-C2-O2    | -5.79 | 115.42      | 118.90   |
| 50  | BQ    | 49   | ARG  | NE-CZ-NH1   | 5.79  | 123.20      | 120.30   |
| 1   | AA    | 284  | C    | C6-N1-C1'   | -5.79 | 113.85      | 120.80   |
| 1   | AA    | 946  | A    | C1'-O4'-C4' | -5.79 | 105.27      | 109.90   |
| 35  | BB    | 28   | A    | N1-C2-N3    | 5.79  | 132.19      | 129.30   |
| 35  | BB    | 1409 | U    | C4'-C3'-C2' | -5.79 | 96.81       | 102.60   |
| 35  | BB    | 2011 | U    | C4'-C3'-C2' | -5.79 | 96.81       | 102.60   |
| 35  | BB    | 2375 | G    | C6-C5-N7    | -5.79 | 126.93      | 130.40   |
| 54  | BU    | 66   | VAL  | CG1-CB-CG2  | 5.79  | 120.16      | 110.90   |
| 1   | AA    | 807  | A    | N7-C8-N9    | -5.79 | 110.91      | 113.80   |
| 1   | AA    | 809  | G    | C2-N3-C4    | 5.79  | 114.80      | 111.90   |
| 1   | AA    | 1041 | G    | C5-C6-N1    | -5.79 | 108.61      | 111.50   |
| 1   | AA    | 1368 | A    | P-O3'-C3'   | -5.79 | 112.75      | 119.70   |
| 35  | BB    | 1289 | C    | C2-N1-C1'   | 5.79  | 125.17      | 118.80   |
| 35  | BB    | 1490 | A    | N7-C8-N9    | -5.79 | 110.91      | 113.80   |
| 35  | BB    | 1681 | G    | C2-N3-C4    | 5.79  | 114.79      | 111.90   |
| 35  | BB    | 2294 | G    | C6-N1-C2    | 5.79  | 128.57      | 125.10   |
| 35  | BB    | 2379 | G    | C5-N7-C8    | -5.79 | 101.41      | 104.30   |
| 35  | BB    | 2518 | A    | C1'-O4'-C4' | 5.79  | 114.53      | 109.90   |
| 35  | BB    | 2682 | A    | C4-C5-C6    | 5.79  | 119.89      | 117.00   |
| 1   | AA    | 962  | C    | C2-N3-C4    | 5.79  | 122.79      | 119.90   |
| 22  | AV    | 16   | C    | O4'-C1'-N1  | 5.79  | 112.83      | 108.20   |
| 34  | BA    | 53   | A    | C6-C5-N7    | -5.79 | 128.25      | 132.30   |
| 34  | BA    | 58   | A    | C3'-C2'-C1' | 5.79  | 106.13      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 770  | G    | C5-N7-C8    | -5.79 | 101.41      | 104.30   |
| 35  | BB    | 1433 | A    | N1-C2-N3    | 5.79  | 132.19      | 129.30   |
| 35  | BB    | 1745 | A    | C4'-C3'-C2' | -5.79 | 96.81       | 102.60   |
| 35  | BB    | 1997 | C    | C6-N1-C2    | 5.79  | 122.61      | 120.30   |
| 35  | BB    | 2267 | A    | N1-C2-N3    | 5.79  | 132.19      | 129.30   |
| 35  | BB    | 2868 | A    | C2-N3-C4    | -5.79 | 107.71      | 110.60   |
| 1   | AA    | 557  | G    | N1-C6-O6    | 5.79  | 123.37      | 119.90   |
| 7   | AG    | 139  | ASP  | CB-CG-OD1   | 5.79  | 123.51      | 118.30   |
| 17  | AQ    | 77   | VAL  | CA-CB-CG2   | -5.79 | 102.22      | 110.90   |
| 34  | BA    | 86   | G    | C4-C5-N7    | 5.79  | 113.11      | 110.80   |
| 35  | BB    | 61   | C    | C6-N1-C2    | 5.79  | 122.61      | 120.30   |
| 35  | BB    | 384  | A    | N7-C8-N9    | -5.79 | 110.91      | 113.80   |
| 35  | BB    | 1143 | A    | C6-C5-N7    | -5.79 | 128.25      | 132.30   |
| 35  | BB    | 1423 | G    | C4'-C3'-C2' | 5.79  | 108.39      | 102.60   |
| 35  | BB    | 1556 | C    | C4-C5-C6    | 5.79  | 120.29      | 117.40   |
| 35  | BB    | 1903 | G    | N7-C8-N9    | -5.79 | 110.21      | 113.10   |
| 35  | BB    | 1909 | C    | C2-N1-C1'   | 5.79  | 125.17      | 118.80   |
| 35  | BB    | 2370 | G    | C6-N1-C2    | 5.79  | 128.57      | 125.10   |
| 35  | BB    | 2409 | G    | N3-C4-C5    | 5.79  | 131.49      | 128.60   |
| 35  | BB    | 2441 | U    | P-O3'-C3'   | -5.79 | 112.76      | 119.70   |
| 35  | BB    | 2770 | G    | N1-C6-O6    | 5.79  | 123.37      | 119.90   |
| 1   | AA    | 50   | A    | C1'-O4'-C4' | -5.78 | 105.27      | 109.90   |
| 1   | AA    | 1131 | G    | C1'-O4'-C4' | -5.78 | 105.27      | 109.90   |
| 1   | AA    | 1361 | G    | C5-C6-O6    | -5.78 | 125.13      | 128.60   |
| 35  | BB    | 949  | G    | N3-C2-N2    | 5.78  | 123.95      | 119.90   |
| 35  | BB    | 1542 | U    | N3-C4-C5    | 5.78  | 118.07      | 114.60   |
| 35  | BB    | 2070 | A    | C2-N3-C4    | -5.78 | 107.71      | 110.60   |
| 35  | BB    | 2170 | A    | C5-C6-N6    | -5.78 | 119.07      | 123.70   |
| 35  | BB    | 2176 | A    | N3-C4-C5    | -5.78 | 122.75      | 126.80   |
| 35  | BB    | 2511 | U    | C5'-C4'-O4' | -5.78 | 102.16      | 109.10   |
| 35  | BB    | 2871 | U    | C1'-O4'-C4' | 5.78  | 114.53      | 109.90   |
| 48  | BO    | 108  | ASP  | CB-CG-OD2   | -5.78 | 113.09      | 118.30   |
| 1   | AA    | 108  | G    | C8-N9-C4    | -5.78 | 104.09      | 106.40   |
| 1   | AA    | 464  | U    | N3-C4-C5    | -5.78 | 111.13      | 114.60   |
| 1   | AA    | 709  | U    | C4'-C3'-C2' | -5.78 | 96.82       | 102.60   |
| 22  | AV    | 70   | C    | N3-C2-O2    | -5.78 | 117.85      | 121.90   |
| 35  | BB    | 280  | U    | N1-C2-O2    | -5.78 | 118.75      | 122.80   |
| 35  | BB    | 546  | U    | N3-C4-O4    | 5.78  | 123.45      | 119.40   |
| 35  | BB    | 646  | U    | N3-C4-O4    | 5.78  | 123.45      | 119.40   |
| 35  | BB    | 977  | G    | C8-N9-C4    | -5.78 | 104.09      | 106.40   |
| 35  | BB    | 1067 | A    | C8-N9-C4    | -5.78 | 103.49      | 105.80   |
| 35  | BB    | 2347 | C    | OP1-P-OP2   | -5.78 | 110.93      | 119.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2824 | C    | C2-N1-C1'   | 5.78  | 125.16      | 118.80   |
| 1   | AA    | 176  | C    | C4-C5-C6    | 5.78  | 120.29      | 117.40   |
| 1   | AA    | 698  | G    | C6-N1-C2    | 5.78  | 128.57      | 125.10   |
| 1   | AA    | 1284 | C    | C5'-C4'-O4' | 5.78  | 116.04      | 109.10   |
| 1   | AA    | 1459 | G    | N7-C8-N9    | -5.78 | 110.21      | 113.10   |
| 10  | AJ    | 31   | ARG  | NE-CZ-NH2   | 5.78  | 123.19      | 120.30   |
| 19  | AS    | 21   | ALA  | CB-CA-C     | -5.78 | 101.43      | 110.10   |
| 22  | AV    | 27   | C    | N3-C4-N4    | 5.78  | 122.05      | 118.00   |
| 34  | BA    | 94   | A    | P-O3'-C3'   | -5.78 | 112.76      | 119.70   |
| 35  | BB    | 19   | A    | C5-N7-C8    | 5.78  | 106.79      | 103.90   |
| 35  | BB    | 602  | A    | P-O3'-C3'   | -5.78 | 112.76      | 119.70   |
| 35  | BB    | 948  | C    | O5'-P-OP2   | -5.78 | 100.50      | 105.70   |
| 35  | BB    | 949  | G    | C4-C5-N7    | 5.78  | 113.11      | 110.80   |
| 35  | BB    | 969  | G    | C4-C5-C6    | 5.78  | 122.27      | 118.80   |
| 35  | BB    | 1042 | G    | C5-C6-N1    | -5.78 | 108.61      | 111.50   |
| 35  | BB    | 1446 | C    | O4'-C1'-N1  | 5.78  | 112.82      | 108.20   |
| 35  | BB    | 1479 | G    | N1-C6-O6    | 5.78  | 123.37      | 119.90   |
| 35  | BB    | 1536 | C    | C5-C6-N1    | 5.78  | 123.89      | 121.00   |
| 35  | BB    | 1863 | G    | O4'-C1'-N9  | 5.78  | 112.83      | 108.20   |
| 35  | BB    | 1918 | A    | P-O3'-C3'   | 5.78  | 126.64      | 119.70   |
| 35  | BB    | 2203 | U    | N3-C4-C5    | -5.78 | 111.13      | 114.60   |
| 35  | BB    | 2421 | G    | N3-C2-N2    | 5.78  | 123.95      | 119.90   |
| 35  | BB    | 2447 | G    | C4-C5-N7    | 5.78  | 113.11      | 110.80   |
| 35  | BB    | 2582 | G    | C2-N3-C4    | -5.78 | 109.01      | 111.90   |
| 35  | BB    | 2614 | A    | C4-C5-C6    | 5.78  | 119.89      | 117.00   |
| 35  | BB    | 2883 | A    | OP1-P-OP2   | -5.78 | 110.93      | 119.60   |
| 1   | AA    | 760  | G    | OP1-P-OP2   | -5.78 | 110.93      | 119.60   |
| 3   | AC    | 105  | VAL  | O-C-N       | 5.78  | 131.95      | 122.70   |
| 35  | BB    | 441  | U    | N3-C4-O4    | 5.78  | 123.45      | 119.40   |
| 35  | BB    | 782  | A    | C4-C5-N7    | -5.78 | 107.81      | 110.70   |
| 35  | BB    | 926  | G    | O4'-C1'-N9  | 5.78  | 112.82      | 108.20   |
| 35  | BB    | 975  | A    | N9-C4-C5    | 5.78  | 108.11      | 105.80   |
| 35  | BB    | 1386 | C    | O4'-C1'-N1  | 5.78  | 112.82      | 108.20   |
| 35  | BB    | 2492 | U    | C4'-C3'-C2' | -5.78 | 96.82       | 102.60   |
| 56  | BY    | 78   | PHE  | CB-CG-CD1   | 5.78  | 124.84      | 120.80   |
| 1   | AA    | 801  | U    | C3'-C2'-C1' | -5.78 | 96.88       | 101.50   |
| 1   | AA    | 1098 | C    | O4'-C1'-N1  | 5.78  | 112.82      | 108.20   |
| 35  | BB    | 116  | C    | N1-C2-O2    | -5.78 | 115.43      | 118.90   |
| 35  | BB    | 498  | G    | C1'-O4'-C4' | 5.78  | 114.52      | 109.90   |
| 35  | BB    | 1006 | C    | C6-N1-C1'   | -5.78 | 113.87      | 120.80   |
| 35  | BB    | 2316 | G    | N1-C6-O6    | 5.78  | 123.37      | 119.90   |
| 35  | BB    | 2801 | G    | C4-C5-N7    | 5.78  | 113.11      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 47  | BN    | 14   | SER  | N-CA-CB     | 5.78  | 119.17      | 110.50   |
| 1   | AA    | 76   | G    | C5-C6-N1    | -5.78 | 108.61      | 111.50   |
| 1   | AA    | 281  | G    | C5'-C4'-O4' | 5.78  | 116.03      | 109.10   |
| 1   | AA    | 638  | U    | P-O3'-C3'   | -5.78 | 112.77      | 119.70   |
| 14  | AN    | 76   | PHE  | CB-CG-CD1   | -5.78 | 116.76      | 120.80   |
| 33  | B8    | 37   | GLN  | N-CA-C      | -5.78 | 95.41       | 111.00   |
| 35  | BB    | 110  | G    | C2-N3-C4    | -5.78 | 109.01      | 111.90   |
| 35  | BB    | 273  | G    | N1-C2-N3    | -5.78 | 120.44      | 123.90   |
| 35  | BB    | 456  | C    | O4'-C1'-N1  | 5.78  | 112.82      | 108.20   |
| 35  | BB    | 988  | A    | C5-C6-N1    | -5.78 | 114.81      | 117.70   |
| 35  | BB    | 1132 | U    | O4'-C1'-N1  | 5.78  | 112.82      | 108.20   |
| 35  | BB    | 1159 | U    | N1-C1'-C2'  | 5.78  | 121.51      | 114.00   |
| 35  | BB    | 1394 | U    | C1'-O4'-C4' | -5.78 | 105.28      | 109.90   |
| 35  | BB    | 1732 | C    | C4'-C3'-C2' | 5.78  | 108.38      | 102.60   |
| 35  | BB    | 1793 | C    | C6-N1-C2    | -5.78 | 117.99      | 120.30   |
| 35  | BB    | 1864 | U    | C2-N3-C4    | -5.78 | 123.53      | 127.00   |
| 35  | BB    | 1890 | A    | O4'-C1'-N9  | 5.78  | 112.82      | 108.20   |
| 35  | BB    | 1890 | A    | N7-C8-N9    | 5.78  | 116.69      | 113.80   |
| 35  | BB    | 2073 | C    | N3-C4-N4    | 5.78  | 122.04      | 118.00   |
| 35  | BB    | 2297 | A    | N7-C8-N9    | 5.78  | 116.69      | 113.80   |
| 35  | BB    | 2872 | A    | N3-C4-C5    | -5.78 | 122.76      | 126.80   |
| 1   | AA    | 475  | C    | N1-C2-O2    | -5.77 | 115.44      | 118.90   |
| 1   | AA    | 766  | A    | C4-C5-C6    | 5.77  | 119.89      | 117.00   |
| 35  | BB    | 412  | A    | C6-N1-C2    | 5.77  | 122.06      | 118.60   |
| 35  | BB    | 1026 | G    | N1-C6-O6    | 5.77  | 123.36      | 119.90   |
| 35  | BB    | 1308 | A    | C5-C6-N6    | -5.77 | 119.08      | 123.70   |
| 35  | BB    | 2062 | A    | O4'-C1'-N9  | 5.77  | 112.82      | 108.20   |
| 35  | BB    | 2075 | U    | N3-C4-O4    | -5.77 | 115.36      | 119.40   |
| 35  | BB    | 2671 | G    | C6-N1-C2    | -5.77 | 121.64      | 125.10   |
| 1   | AA    | 81   | A    | C4'-C3'-C2' | 5.77  | 108.37      | 102.60   |
| 1   | AA    | 162  | A    | C4-C5-N7    | -5.77 | 107.81      | 110.70   |
| 1   | AA    | 192  | A    | C3'-C2'-C1' | 5.77  | 106.12      | 101.50   |
| 1   | AA    | 250  | A    | C2-N3-C4    | 5.77  | 113.49      | 110.60   |
| 1   | AA    | 368  | U    | C6-N1-C2    | -5.77 | 117.54      | 121.00   |
| 1   | AA    | 755  | G    | C5'-C4'-C3' | -5.77 | 106.76      | 116.00   |
| 1   | AA    | 870  | U    | C5'-C4'-C3' | -5.77 | 106.76      | 116.00   |
| 1   | AA    | 1500 | A    | OP1-P-O3'   | 5.77  | 117.90      | 105.20   |
| 34  | BA    | 102  | G    | C4-C5-C6    | 5.77  | 122.26      | 118.80   |
| 35  | BB    | 416  | U    | N3-C4-C5    | 5.77  | 118.06      | 114.60   |
| 35  | BB    | 621  | A    | O4'-C1'-N9  | 5.77  | 112.82      | 108.20   |
| 35  | BB    | 1351 | C    | C6-N1-C2    | 5.77  | 122.61      | 120.30   |
| 35  | BB    | 1610 | A    | O5'-P-OP1   | -5.77 | 100.50      | 105.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1738 | G    | O4'-C1'-N9  | 5.77  | 112.82      | 108.20   |
| 35  | BB    | 2365 | G    | N7-C8-N9    | 5.77  | 115.99      | 113.10   |
| 35  | BB    | 2384 | U    | C3'-C2'-C1' | -5.77 | 96.88       | 101.50   |
| 37  | BD    | 82   | PHE  | CD1-CG-CD2  | -5.77 | 110.80      | 118.30   |
| 1   | AA    | 759  | A    | C6-C5-N7    | -5.77 | 128.26      | 132.30   |
| 4   | AD    | 132  | ALA  | N-CA-CB     | 5.77  | 118.18      | 110.10   |
| 35  | BB    | 392  | U    | N3-C2-O2    | -5.77 | 118.16      | 122.20   |
| 35  | BB    | 1299 | G    | O4'-C1'-N9  | 5.77  | 112.82      | 108.20   |
| 35  | BB    | 1886 | U    | N3-C4-C5    | -5.77 | 111.14      | 114.60   |
| 35  | BB    | 2183 | A    | N1-C2-N3    | 5.77  | 132.19      | 129.30   |
| 35  | BB    | 2333 | A    | C2-N3-C4    | -5.77 | 107.71      | 110.60   |
| 1   | AA    | 31   | G    | C4-N9-C1'   | 5.77  | 134.00      | 126.50   |
| 1   | AA    | 763  | G    | C8-N9-C1'   | 5.77  | 134.50      | 127.00   |
| 1   | AA    | 1466 | C    | C5-C4-N4    | -5.77 | 116.16      | 120.20   |
| 1   | AA    | 1493 | A    | P-O5'-C5'   | 5.77  | 130.13      | 120.90   |
| 1   | AA    | 1522 | U    | O4'-C1'-N1  | 5.77  | 112.81      | 108.20   |
| 1   | AA    | 1529 | G    | P-O3'-C3'   | 5.77  | 126.62      | 119.70   |
| 26  | B1    | 51   | ALA  | N-CA-CB     | 5.77  | 118.18      | 110.10   |
| 35  | BB    | 371  | A    | N7-C8-N9    | 5.77  | 116.68      | 113.80   |
| 35  | BB    | 1394 | U    | C2-N1-C1'   | -5.77 | 110.78      | 117.70   |
| 35  | BB    | 2480 | C    | C3'-C2'-C1' | 5.77  | 106.11      | 101.50   |
| 1   | AA    | 618  | C    | C5-C4-N4    | -5.77 | 116.16      | 120.20   |
| 1   | AA    | 657  | U    | C6-N1-C2    | 5.77  | 124.46      | 121.00   |
| 1   | AA    | 1118 | U    | C6-N1-C1'   | -5.77 | 113.13      | 121.20   |
| 1   | AA    | 1257 | A    | C1'-O4'-C4' | -5.77 | 105.29      | 109.90   |
| 1   | AA    | 1302 | C    | N1-C1'-C2'  | 5.77  | 121.50      | 114.00   |
| 34  | BA    | 63   | C    | N3-C4-N4    | 5.77  | 122.04      | 118.00   |
| 35  | BB    | 917  | A    | O4'-C1'-N9  | 5.77  | 112.81      | 108.20   |
| 35  | BB    | 972  | A    | C4-C5-N7    | -5.77 | 107.82      | 110.70   |
| 35  | BB    | 1046 | A    | C4-C5-C6    | 5.77  | 119.88      | 117.00   |
| 35  | BB    | 1129 | A    | N3-C4-C5    | -5.77 | 122.76      | 126.80   |
| 35  | BB    | 1454 | C    | O4'-C1'-N1  | 5.77  | 112.81      | 108.20   |
| 35  | BB    | 1762 | A    | C6-C5-N7    | -5.77 | 128.26      | 132.30   |
| 35  | BB    | 1983 | G    | P-O5'-C5'   | -5.77 | 111.67      | 120.90   |
| 35  | BB    | 2279 | G    | C3'-C2'-C1' | 5.77  | 106.11      | 101.50   |
| 35  | BB    | 2825 | G    | C3'-C2'-C1' | -5.77 | 96.89       | 101.50   |
| 1   | AA    | 1461 | G    | C1'-O4'-C4' | 5.77  | 114.51      | 109.90   |
| 35  | BB    | 255  | A    | C4-C5-C6    | 5.77  | 119.88      | 117.00   |
| 35  | BB    | 776  | G    | N3-C2-N2    | 5.77  | 123.94      | 119.90   |
| 35  | BB    | 874  | G    | C4'-C3'-C2' | -5.77 | 96.83       | 102.60   |
| 35  | BB    | 1842 | G    | C4-C5-C6    | 5.77  | 122.26      | 118.80   |
| 35  | BB    | 2199 | A    | C5-C6-N6    | -5.77 | 119.09      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2765 | A    | C4-C5-C6    | 5.77  | 119.88      | 117.00   |
| 1   | AA    | 33   | A    | C5-N7-C8    | 5.76  | 106.78      | 103.90   |
| 1   | AA    | 366  | A    | N1-C2-N3    | 5.76  | 132.18      | 129.30   |
| 1   | AA    | 423  | G    | C5-C6-N1    | -5.76 | 108.62      | 111.50   |
| 1   | AA    | 693  | G    | N3-C2-N2    | 5.76  | 123.94      | 119.90   |
| 1   | AA    | 1465 | A    | C6-C5-N7    | -5.76 | 128.26      | 132.30   |
| 3   | AC    | 155  | ARG  | NE-CZ-NH2   | -5.76 | 117.42      | 120.30   |
| 35  | BB    | 110  | G    | N1-C2-N3    | -5.76 | 120.44      | 123.90   |
| 35  | BB    | 324  | A    | O4'-C1'-N9  | 5.76  | 112.81      | 108.20   |
| 35  | BB    | 808  | G    | C5-N7-C8    | -5.76 | 101.42      | 104.30   |
| 35  | BB    | 935  | C    | N3-C4-C5    | -5.76 | 119.59      | 121.90   |
| 35  | BB    | 1300 | G    | C8-N9-C4    | 5.76  | 108.71      | 106.40   |
| 35  | BB    | 1573 | G    | C8-N9-C1'   | 5.76  | 134.50      | 127.00   |
| 35  | BB    | 2216 | G    | C5-C6-N1    | 5.76  | 114.38      | 111.50   |
| 35  | BB    | 2232 | C    | OP1-P-OP2   | -5.76 | 110.95      | 119.60   |
| 35  | BB    | 2418 | A    | N3-C4-C5    | -5.76 | 122.77      | 126.80   |
| 35  | BB    | 2439 | A    | P-O3'-C3'   | 5.76  | 126.62      | 119.70   |
| 35  | BB    | 2695 | U    | O4'-C1'-N1  | 5.76  | 112.81      | 108.20   |
| 1   | AA    | 739  | C    | C4'-C3'-C2' | -5.76 | 96.84       | 102.60   |
| 22  | AV    | 59   | A    | C4-C5-C6    | 5.76  | 119.88      | 117.00   |
| 35  | BB    | 1734 | G    | C4'-C3'-C2' | -5.76 | 96.84       | 102.60   |
| 1   | AA    | 25   | C    | C6-N1-C1'   | -5.76 | 113.89      | 120.80   |
| 1   | AA    | 202  | G    | C5-N7-C8    | 5.76  | 107.18      | 104.30   |
| 1   | AA    | 557  | G    | C5-C6-N1    | -5.76 | 108.62      | 111.50   |
| 1   | AA    | 803  | G    | C6-C5-N7    | -5.76 | 126.94      | 130.40   |
| 1   | AA    | 1374 | A    | C5'-C4'-C3' | -5.76 | 106.78      | 116.00   |
| 2   | AB    | 204  | ASP  | CB-CA-C     | -5.76 | 98.88       | 110.40   |
| 35  | BB    | 79   | C    | O4'-C1'-N1  | 5.76  | 112.81      | 108.20   |
| 35  | BB    | 328  | U    | P-O3'-C3'   | 5.76  | 126.61      | 119.70   |
| 35  | BB    | 1820 | U    | O4'-C1'-N1  | 5.76  | 112.81      | 108.20   |
| 35  | BB    | 1856 | U    | N3-C2-O2    | 5.76  | 126.23      | 122.20   |
| 35  | BB    | 2070 | A    | C4'-C3'-C2' | -5.76 | 96.84       | 102.60   |
| 35  | BB    | 2079 | U    | O5'-P-OP2   | -5.76 | 100.51      | 105.70   |
| 1   | AA    | 977  | A    | N1-C2-N3    | -5.76 | 126.42      | 129.30   |
| 1   | AA    | 1043 | G    | C5-C6-N1    | -5.76 | 108.62      | 111.50   |
| 35  | BB    | 77   | G    | O4'-C1'-N9  | 5.76  | 112.81      | 108.20   |
| 35  | BB    | 119  | A    | C8-N9-C4    | 5.76  | 108.10      | 105.80   |
| 35  | BB    | 633  | A    | N1-C2-N3    | 5.76  | 132.18      | 129.30   |
| 35  | BB    | 721  | A    | C8-N9-C4    | -5.76 | 103.50      | 105.80   |
| 35  | BB    | 1327 | A    | C5'-C4'-O4' | 5.76  | 116.01      | 109.10   |
| 35  | BB    | 1338 | G    | OP1-P-OP2   | -5.76 | 110.96      | 119.60   |
| 35  | BB    | 1696 | G    | N1-C6-O6    | 5.76  | 123.36      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1799 | G    | N3-C4-C5    | 5.76  | 131.48      | 128.60   |
| 35  | BB    | 2123 | G    | N1-C2-N3    | 5.76  | 127.36      | 123.90   |
| 35  | BB    | 2327 | A    | C6-N1-C2    | -5.76 | 115.14      | 118.60   |
| 1   | AA    | 691  | G    | N3-C4-N9    | 5.76  | 129.46      | 126.00   |
| 1   | AA    | 873  | A    | C5-C6-N1    | -5.76 | 114.82      | 117.70   |
| 1   | AA    | 1115 | U    | O4'-C1'-N1  | 5.76  | 112.81      | 108.20   |
| 16  | AP    | 60   | TRP  | N-CA-CB     | 5.76  | 120.96      | 110.60   |
| 35  | BB    | 552  | U    | C1'-O4'-C4' | -5.76 | 105.29      | 109.90   |
| 1   | AA    | 426  | U    | C5'-C4'-C3' | -5.76 | 106.79      | 116.00   |
| 1   | AA    | 1134 | G    | C6-N1-C2    | -5.76 | 121.65      | 125.10   |
| 1   | AA    | 1157 | A    | C5-C6-N6    | -5.76 | 119.09      | 123.70   |
| 1   | AA    | 1518 | A    | C4-C5-C6    | 5.76  | 119.88      | 117.00   |
| 1   | AA    | 1524 | C    | C5-C4-N4    | -5.76 | 116.17      | 120.20   |
| 3   | AC    | 88   | LYS  | CB-CG-CD    | 5.76  | 126.57      | 111.60   |
| 3   | AC    | 131  | ARG  | NH1-CZ-NH2  | 5.76  | 125.73      | 119.40   |
| 19  | AS    | 13   | HIS  | CA-CB-CG    | -5.76 | 103.81      | 113.60   |
| 35  | BB    | 313  | G    | P-O3'-C3'   | -5.76 | 112.79      | 119.70   |
| 35  | BB    | 319  | G    | OP1-P-OP2   | -5.76 | 110.97      | 119.60   |
| 35  | BB    | 889  | C    | O4'-C1'-N1  | 5.76  | 112.81      | 108.20   |
| 35  | BB    | 1649 | G    | C8-N9-C4    | -5.76 | 104.10      | 106.40   |
| 35  | BB    | 2054 | A    | N7-C8-N9    | -5.76 | 110.92      | 113.80   |
| 35  | BB    | 2414 | G    | C2-N3-C4    | -5.76 | 109.02      | 111.90   |
| 1   | AA    | 85   | U    | C6-N1-C2    | 5.75  | 124.45      | 121.00   |
| 1   | AA    | 1268 | G    | N3-C2-N2    | 5.75  | 123.93      | 119.90   |
| 35  | BB    | 788  | A    | C8-N9-C4    | 5.75  | 108.10      | 105.80   |
| 35  | BB    | 1715 | G    | C5-C6-O6    | -5.75 | 125.15      | 128.60   |
| 35  | BB    | 2736 | A    | O4'-C1'-N9  | 5.75  | 112.80      | 108.20   |
| 35  | BB    | 2782 | G    | C5'-C4'-O4' | 5.75  | 116.00      | 109.10   |
| 35  | BB    | 2896 | C    | C1'-O4'-C4' | -5.75 | 105.30      | 109.90   |
| 56  | BY    | 25   | PHE  | CB-CG-CD1   | 5.75  | 124.83      | 120.80   |
| 1   | AA    | 328  | C    | C2-N1-C1'   | 5.75  | 125.13      | 118.80   |
| 1   | AA    | 900  | A    | N9-C4-C5    | -5.75 | 103.50      | 105.80   |
| 1   | AA    | 1168 | U    | P-O3'-C3'   | 5.75  | 126.60      | 119.70   |
| 1   | AA    | 1340 | A    | C6-N1-C2    | -5.75 | 115.15      | 118.60   |
| 35  | BB    | 420  | C    | O4'-C1'-N1  | 5.75  | 112.80      | 108.20   |
| 35  | BB    | 531  | C    | C6-N1-C2    | -5.75 | 118.00      | 120.30   |
| 35  | BB    | 825  | A    | C5-C6-N6    | -5.75 | 119.10      | 123.70   |
| 35  | BB    | 1021 | A    | O4'-C1'-N9  | 5.75  | 112.80      | 108.20   |
| 35  | BB    | 1389 | G    | N3-C4-C5    | -5.75 | 125.72      | 128.60   |
| 35  | BB    | 1409 | U    | N1-C2-O2    | 5.75  | 126.83      | 122.80   |
| 35  | BB    | 1476 | U    | N1-C2-N3    | -5.75 | 111.45      | 114.90   |
| 35  | BB    | 1526 | C    | C5-C4-N4    | -5.75 | 116.17      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1697 | G    | C5'-C4'-O4' | 5.75  | 116.00      | 109.10   |
| 35  | BB    | 2198 | A    | C8-N9-C4    | -5.75 | 103.50      | 105.80   |
| 35  | BB    | 2839 | G    | C6-N1-C2    | 5.75  | 128.55      | 125.10   |
| 46  | BM    | 28   | PHE  | CB-CG-CD2   | 5.75  | 124.83      | 120.80   |
| 1   | AA    | 495  | A    | N1-C2-N3    | 5.75  | 132.18      | 129.30   |
| 34  | BA    | 88   | C    | C5-C6-N1    | -5.75 | 118.12      | 121.00   |
| 34  | BA    | 96   | G    | C5-N7-C8    | 5.75  | 107.17      | 104.30   |
| 35  | BB    | 1699 | G    | C4-C5-C6    | 5.75  | 122.25      | 118.80   |
| 35  | BB    | 2030 | A    | C5-N7-C8    | 5.75  | 106.78      | 103.90   |
| 35  | BB    | 2291 | U    | C5-C6-N1    | -5.75 | 119.83      | 122.70   |
| 1   | AA    | 198  | G    | C6-C5-N7    | -5.75 | 126.95      | 130.40   |
| 1   | AA    | 364  | A    | C6-C5-N7    | -5.75 | 128.28      | 132.30   |
| 1   | AA    | 1242 | G    | C2-N3-C4    | -5.75 | 109.03      | 111.90   |
| 6   | AF    | 63   | ASN  | N-CA-CB     | 5.75  | 120.95      | 110.60   |
| 26  | B1    | 11   | VAL  | CA-CB-CG1   | -5.75 | 102.27      | 110.90   |
| 35  | BB    | 290  | U    | N1-C2-N3    | 5.75  | 118.35      | 114.90   |
| 35  | BB    | 763  | G    | C5-C6-N1    | -5.75 | 108.62      | 111.50   |
| 35  | BB    | 829  | A    | C6-C5-N7    | -5.75 | 128.28      | 132.30   |
| 35  | BB    | 904  | G    | N7-C8-N9    | -5.75 | 110.22      | 113.10   |
| 35  | BB    | 2260 | C    | C4'-C3'-C2' | -5.75 | 96.85       | 102.60   |
| 35  | BB    | 2284 | A    | C4-C5-N7    | -5.75 | 107.83      | 110.70   |
| 35  | BB    | 2733 | A    | N1-C6-N6    | 5.75  | 122.05      | 118.60   |
| 1   | AA    | 288  | A    | C5-C6-N6    | -5.75 | 119.10      | 123.70   |
| 1   | AA    | 347  | G    | C5-C6-N1    | -5.75 | 108.63      | 111.50   |
| 1   | AA    | 676  | A    | C5-C6-N1    | -5.75 | 114.83      | 117.70   |
| 1   | AA    | 739  | C    | C6-N1-C2    | -5.75 | 118.00      | 120.30   |
| 1   | AA    | 1293 | C    | C2-N3-C4    | -5.75 | 117.03      | 119.90   |
| 22  | AV    | 7    | G    | N3-C4-C5    | -5.75 | 125.73      | 128.60   |
| 35  | BB    | 417  | C    | O4'-C1'-N1  | 5.75  | 112.80      | 108.20   |
| 35  | BB    | 1275 | A    | N1-C2-N3    | -5.75 | 126.43      | 129.30   |
| 35  | BB    | 1300 | G    | N7-C8-N9    | -5.75 | 110.23      | 113.10   |
| 35  | BB    | 1439 | A    | N1-C2-N3    | 5.75  | 132.17      | 129.30   |
| 35  | BB    | 1873 | G    | P-O3'-C3'   | -5.75 | 112.80      | 119.70   |
| 35  | BB    | 2013 | A    | C6-C5-N7    | -5.75 | 128.28      | 132.30   |
| 35  | BB    | 2267 | A    | O4'-C1'-N9  | 5.75  | 112.80      | 108.20   |
| 35  | BB    | 2662 | A    | N1-C2-N3    | 5.75  | 132.18      | 129.30   |
| 35  | BB    | 2665 | A    | N1-C2-N3    | 5.75  | 132.17      | 129.30   |
| 1   | AA    | 23   | C    | C6-N1-C2    | -5.75 | 118.00      | 120.30   |
| 1   | AA    | 108  | G    | N9-C1'-C2'  | -5.75 | 105.68      | 112.00   |
| 1   | AA    | 704  | A    | C4-C5-C6    | 5.75  | 119.87      | 117.00   |
| 5   | AE    | 47   | PHE  | O-C-N       | -5.75 | 113.43      | 123.20   |
| 35  | BB    | 1333 | G    | C5-C6-O6    | -5.75 | 125.15      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1397 | U    | C5-C6-N1    | 5.75  | 125.57      | 122.70   |
| 35  | BB    | 1865 | U    | C4-C5-C6    | 5.75  | 123.15      | 119.70   |
| 35  | BB    | 2029 | G    | N3-C2-N2    | 5.75  | 123.92      | 119.90   |
| 53  | BT    | 23   | ALA  | N-CA-CB     | 5.75  | 118.15      | 110.10   |
| 1   | AA    | 487  | A    | O4'-C1'-N9  | 5.75  | 112.80      | 108.20   |
| 1   | AA    | 604  | G    | O4'-C1'-N9  | 5.75  | 112.80      | 108.20   |
| 1   | AA    | 1226 | C    | N1-C2-O2    | 5.75  | 122.35      | 118.90   |
| 28  | B3    | 30   | ASP  | N-CA-CB     | 5.75  | 120.94      | 110.60   |
| 35  | BB    | 211  | C    | O4'-C1'-N1  | 5.75  | 112.80      | 108.20   |
| 35  | BB    | 518  | G    | C4-C5-N7    | 5.75  | 113.10      | 110.80   |
| 35  | BB    | 1332 | G    | C5'-C4'-O4' | 5.75  | 115.99      | 109.10   |
| 35  | BB    | 2615 | U    | O4'-C1'-N1  | 5.75  | 112.80      | 108.20   |
| 35  | BB    | 2725 | A    | N1-C6-N6    | 5.75  | 122.05      | 118.60   |
| 1   | AA    | 208  | U    | C1'-O4'-C4' | 5.74  | 114.49      | 109.90   |
| 1   | AA    | 295  | C    | O4'-C1'-C2' | 5.74  | 112.77      | 107.60   |
| 1   | AA    | 763  | G    | O4'-C1'-N9  | 5.74  | 112.80      | 108.20   |
| 1   | AA    | 1389 | C    | N3-C2-O2    | 5.74  | 125.92      | 121.90   |
| 16  | AP    | 70   | ARG  | CD-NE-CZ    | 5.74  | 131.64      | 123.60   |
| 35  | BB    | 232  | G    | C5'-C4'-O4' | 5.74  | 115.99      | 109.10   |
| 35  | BB    | 373  | U    | N3-C4-O4    | 5.74  | 123.42      | 119.40   |
| 35  | BB    | 506  | G    | P-O3'-C3'   | 5.74  | 126.59      | 119.70   |
| 35  | BB    | 511  | U    | C6-N1-C2    | -5.74 | 117.55      | 121.00   |
| 35  | BB    | 709  | U    | N3-C4-C5    | -5.74 | 111.15      | 114.60   |
| 35  | BB    | 966  | G    | N3-C2-N2    | 5.74  | 123.92      | 119.90   |
| 35  | BB    | 1406 | U    | C5-C4-O4    | -5.74 | 122.45      | 125.90   |
| 35  | BB    | 2408 | U    | P-O3'-C3'   | -5.74 | 112.81      | 119.70   |
| 35  | BB    | 2499 | C    | C6-N1-C2    | -5.74 | 118.00      | 120.30   |
| 39  | BF    | 174  | PHE  | CB-CG-CD1   | -5.74 | 116.78      | 120.80   |
| 1   | AA    | 183  | C    | C4'-C3'-C2' | 5.74  | 108.34      | 102.60   |
| 35  | BB    | 37   | C    | C5-C4-N4    | -5.74 | 116.18      | 120.20   |
| 35  | BB    | 91   | A    | N3-C4-C5    | -5.74 | 122.78      | 126.80   |
| 35  | BB    | 431  | U    | C5-C6-N1    | -5.74 | 119.83      | 122.70   |
| 35  | BB    | 804  | A    | N9-C4-C5    | -5.74 | 103.50      | 105.80   |
| 35  | BB    | 1695 | G    | C6-N1-C2    | -5.74 | 121.66      | 125.10   |
| 35  | BB    | 2191 | A    | N9-C1'-C2'  | -5.74 | 105.68      | 112.00   |
| 35  | BB    | 2324 | U    | C4-C5-C6    | 5.74  | 123.14      | 119.70   |
| 35  | BB    | 2577 | A    | O5'-P-OP2   | 5.74  | 117.59      | 110.70   |
| 35  | BB    | 2747 | G    | O4'-C1'-N9  | 5.74  | 112.79      | 108.20   |
| 1   | AA    | 181  | A    | C5-N7-C8    | 5.74  | 106.77      | 103.90   |
| 1   | AA    | 1017 | U    | C2-N3-C4    | -5.74 | 123.56      | 127.00   |
| 1   | AA    | 1259 | C    | N3-C4-C5    | -5.74 | 119.60      | 121.90   |
| 3   | AC    | 191  | THR  | CA-CB-CG2   | -5.74 | 104.36      | 112.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | AO    | 62   | ARG  | NE-CZ-NH1   | 5.74  | 123.17      | 120.30   |
| 26  | B1    | 49   | ASP  | CB-CG-OD2   | 5.74  | 123.47      | 118.30   |
| 35  | BB    | 74   | A    | C5'-C4'-O4' | 5.74  | 115.99      | 109.10   |
| 35  | BB    | 199  | A    | C6-C5-N7    | -5.74 | 128.28      | 132.30   |
| 35  | BB    | 750  | A    | C5-C6-N1    | -5.74 | 114.83      | 117.70   |
| 35  | BB    | 1165 | A    | C5'-C4'-C3' | -5.74 | 106.81      | 116.00   |
| 35  | BB    | 1950 | G    | C5-C6-O6    | -5.74 | 125.16      | 128.60   |
| 35  | BB    | 2046 | G    | C4-C5-C6    | 5.74  | 122.24      | 118.80   |
| 38  | BE    | 39   | ALA  | CB-CA-C     | -5.74 | 101.49      | 110.10   |
| 51  | BR    | 55   | ASP  | CB-CG-OD2   | -5.74 | 113.13      | 118.30   |
| 1   | AA    | 858  | G    | P-O5'-C5'   | 5.74  | 130.08      | 120.90   |
| 1   | AA    | 1009 | U    | N3-C4-C5    | -5.74 | 111.16      | 114.60   |
| 1   | AA    | 1364 | U    | C5-C6-N1    | 5.74  | 125.57      | 122.70   |
| 35  | BB    | 335  | C    | C1'-O4'-C4' | -5.74 | 105.31      | 109.90   |
| 35  | BB    | 341  | C    | C1'-O4'-C4' | -5.74 | 105.31      | 109.90   |
| 35  | BB    | 723  | C    | C3'-C2'-C1' | 5.74  | 106.09      | 101.50   |
| 35  | BB    | 768  | G    | C5-C6-O6    | -5.74 | 125.16      | 128.60   |
| 35  | BB    | 1477 | A    | C6-C5-N7    | -5.74 | 128.28      | 132.30   |
| 35  | BB    | 1610 | A    | C5-N7-C8    | -5.74 | 101.03      | 103.90   |
| 35  | BB    | 1677 | A    | C8-N9-C4    | -5.74 | 103.50      | 105.80   |
| 35  | BB    | 2181 | U    | N1-C2-N3    | 5.74  | 118.34      | 114.90   |
| 35  | BB    | 2634 | A    | P-O3'-C3'   | -5.74 | 112.81      | 119.70   |
| 2   | AB    | 31   | PHE  | CB-CG-CD1   | 5.74  | 124.82      | 120.80   |
| 35  | BB    | 43   | G    | O4'-C1'-N9  | 5.74  | 112.79      | 108.20   |
| 35  | BB    | 49   | A    | C2-N3-C4    | -5.74 | 107.73      | 110.60   |
| 35  | BB    | 330  | A    | O4'-C1'-N9  | 5.74  | 112.79      | 108.20   |
| 35  | BB    | 1911 | U    | C4-C5-C6    | -5.74 | 116.26      | 119.70   |
| 35  | BB    | 2031 | A    | O4'-C1'-N9  | 5.74  | 112.79      | 108.20   |
| 46  | BM    | 52   | ALA  | CB-CA-C     | -5.74 | 101.49      | 110.10   |
| 1   | AA    | 153  | C    | N3-C4-N4    | 5.74  | 122.02      | 118.00   |
| 1   | AA    | 249  | U    | C6-N1-C2    | 5.74  | 124.44      | 121.00   |
| 1   | AA    | 1433 | A    | C4-C5-N7    | -5.74 | 107.83      | 110.70   |
| 35  | BB    | 134  | G    | C5-N7-C8    | -5.74 | 101.43      | 104.30   |
| 35  | BB    | 246  | C    | C2-N3-C4    | 5.74  | 122.77      | 119.90   |
| 35  | BB    | 564  | C    | C6-N1-C2    | -5.74 | 118.01      | 120.30   |
| 35  | BB    | 771  | G    | C6-C5-N7    | -5.74 | 126.96      | 130.40   |
| 35  | BB    | 1146 | C    | N3-C4-C5    | -5.74 | 119.61      | 121.90   |
| 35  | BB    | 1226 | A    | C6-C5-N7    | -5.74 | 128.28      | 132.30   |
| 35  | BB    | 1727 | C    | C2-N3-C4    | 5.74  | 122.77      | 119.90   |
| 35  | BB    | 1816 | C    | C4-C5-C6    | 5.74  | 120.27      | 117.40   |
| 35  | BB    | 2268 | A    | C6-N1-C2    | 5.74  | 122.04      | 118.60   |
| 35  | BB    | 2532 | G    | P-O3'-C3'   | -5.74 | 112.82      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 87   | C    | C4'-C3'-C2' | 5.73  | 108.33      | 102.60   |
| 1   | AA    | 566  | G    | N1-C6-O6    | 5.73  | 123.34      | 119.90   |
| 32  | B7    | 6    | VAL  | N-CA-C      | -5.73 | 95.52       | 111.00   |
| 35  | BB    | 277  | G    | N1-C2-N3    | -5.73 | 120.46      | 123.90   |
| 35  | BB    | 352  | A    | N3-C4-C5    | -5.73 | 122.79      | 126.80   |
| 35  | BB    | 466  | A    | N7-C8-N9    | -5.73 | 110.93      | 113.80   |
| 35  | BB    | 494  | G    | C5-C6-N1    | 5.73  | 114.37      | 111.50   |
| 35  | BB    | 774  | G    | C4-N9-C1'   | 5.73  | 133.95      | 126.50   |
| 35  | BB    | 1645 | G    | C2-N3-C4    | 5.73  | 114.77      | 111.90   |
| 39  | BF    | 4    | HIS  | CA-CB-CG    | 5.73  | 123.35      | 113.60   |
| 49  | BP    | 52   | ARG  | NE-CZ-NH1   | -5.73 | 117.43      | 120.30   |
| 1   | AA    | 225  | C    | C4'-C3'-C2' | -5.73 | 96.87       | 102.60   |
| 1   | AA    | 1000 | A    | N3-C4-C5    | 5.73  | 130.81      | 126.80   |
| 35  | BB    | 1474 | U    | C3'-C2'-C1' | 5.73  | 106.09      | 101.50   |
| 35  | BB    | 1504 | A    | N9-C4-C5    | -5.73 | 103.51      | 105.80   |
| 1   | AA    | 208  | U    | N3-C4-O4    | 5.73  | 123.41      | 119.40   |
| 1   | AA    | 406  | G    | C5-C6-O6    | -5.73 | 125.16      | 128.60   |
| 1   | AA    | 1022 | A    | N3-C4-C5    | -5.73 | 122.79      | 126.80   |
| 1   | AA    | 1136 | C    | C2-N1-C1'   | 5.73  | 125.10      | 118.80   |
| 1   | AA    | 1498 | U    | O3'-P-O5'   | -5.73 | 93.11       | 104.00   |
| 17  | AQ    | 46   | HIS  | N-CA-CB     | 5.73  | 120.91      | 110.60   |
| 35  | BB    | 777  | G    | N3-C4-N9    | 5.73  | 129.44      | 126.00   |
| 35  | BB    | 1441 | G    | C4-N9-C1'   | -5.73 | 119.05      | 126.50   |
| 35  | BB    | 1723 | G    | N3-C2-N2    | 5.73  | 123.91      | 119.90   |
| 35  | BB    | 1833 | C    | N1-C2-O2    | 5.73  | 122.34      | 118.90   |
| 35  | BB    | 2050 | C    | O4'-C1'-N1  | 5.73  | 112.78      | 108.20   |
| 35  | BB    | 2110 | G    | N3-C2-N2    | 5.73  | 123.91      | 119.90   |
| 35  | BB    | 2472 | G    | N9-C4-C5    | -5.73 | 103.11      | 105.40   |
| 35  | BB    | 2704 | C    | C3'-C2'-C1' | 5.73  | 106.08      | 101.50   |
| 35  | BB    | 2719 | G    | C4-C5-C6    | 5.73  | 122.24      | 118.80   |
| 47  | BN    | 63   | ARG  | NE-CZ-NH1   | -5.73 | 117.44      | 120.30   |
| 1   | AA    | 166  | U    | O5'-P-OP1   | -5.73 | 100.54      | 105.70   |
| 1   | AA    | 370  | C    | C4'-C3'-C2' | -5.73 | 96.87       | 102.60   |
| 1   | AA    | 489  | C    | N1-C2-N3    | -5.73 | 115.19      | 119.20   |
| 35  | BB    | 1579 | A    | N9-C1'-C2'  | -5.73 | 105.70      | 112.00   |
| 35  | BB    | 2326 | C    | N3-C4-N4    | 5.73  | 122.01      | 118.00   |
| 35  | BB    | 2876 | G    | P-O5'-C5'   | -5.73 | 111.73      | 120.90   |
| 1   | AA    | 68   | G    | N1-C2-N2    | -5.73 | 111.05      | 116.20   |
| 1   | AA    | 81   | A    | N3-C4-C5    | -5.73 | 122.79      | 126.80   |
| 1   | AA    | 232  | G    | N7-C8-N9    | 5.73  | 115.96      | 113.10   |
| 1   | AA    | 988  | G    | P-O3'-C3'   | -5.73 | 112.83      | 119.70   |
| 1   | AA    | 1188 | A    | C4-C5-N7    | 5.73  | 113.56      | 110.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | AX    | 18   | C    | O4'-C1'-N1  | 5.73  | 112.78      | 108.20   |
| 35  | BB    | 280  | U    | N3-C4-O4    | 5.73  | 123.41      | 119.40   |
| 35  | BB    | 800  | A    | O4'-C1'-N9  | 5.73  | 112.78      | 108.20   |
| 35  | BB    | 1131 | G    | P-O3'-C3'   | 5.73  | 126.57      | 119.70   |
| 35  | BB    | 1136 | G    | O4'-C1'-N9  | 5.73  | 112.78      | 108.20   |
| 35  | BB    | 1633 | G    | C6-N1-C2    | 5.73  | 128.54      | 125.10   |
| 35  | BB    | 2259 | U    | C5-C4-O4    | -5.73 | 122.46      | 125.90   |
| 35  | BB    | 2283 | C    | O4'-C4'-C3' | -5.73 | 98.27       | 104.00   |
| 35  | BB    | 2704 | C    | C5-C6-N1    | -5.73 | 118.14      | 121.00   |
| 35  | BB    | 2845 | U    | O4'-C1'-N1  | 5.73  | 112.78      | 108.20   |
| 1   | AA    | 531  | U    | C2-N3-C4    | 5.73  | 130.44      | 127.00   |
| 1   | AA    | 1386 | G    | C5-N7-C8    | 5.73  | 107.16      | 104.30   |
| 35  | BB    | 234  | U    | C4'-C3'-C2' | -5.73 | 96.87       | 102.60   |
| 35  | BB    | 754  | U    | O4'-C1'-N1  | 5.73  | 112.78      | 108.20   |
| 35  | BB    | 2569 | G    | P-O3'-C3'   | -5.73 | 112.83      | 119.70   |
| 1   | AA    | 1376 | U    | N3-C4-O4    | 5.72  | 123.41      | 119.40   |
| 1   | AA    | 1395 | C    | O4'-C1'-N1  | 5.72  | 112.78      | 108.20   |
| 34  | BA    | 85   | G    | C4-C5-N7    | 5.72  | 113.09      | 110.80   |
| 35  | BB    | 71   | A    | C5-C6-N1    | -5.72 | 114.84      | 117.70   |
| 35  | BB    | 121  | G    | C6-C5-N7    | -5.72 | 126.97      | 130.40   |
| 35  | BB    | 176  | A    | C1'-O4'-C4' | 5.72  | 114.48      | 109.90   |
| 35  | BB    | 711  | G    | C6-N1-C2    | 5.72  | 128.53      | 125.10   |
| 35  | BB    | 1068 | G    | C5-C6-N1    | -5.72 | 108.64      | 111.50   |
| 35  | BB    | 1706 | C    | C2-N1-C1'   | 5.72  | 125.10      | 118.80   |
| 35  | BB    | 1808 | A    | C4-C5-C6    | 5.72  | 119.86      | 117.00   |
| 35  | BB    | 1827 | U    | C5-C4-O4    | -5.72 | 122.47      | 125.90   |
| 35  | BB    | 1905 | C    | O4'-C1'-N1  | 5.72  | 112.78      | 108.20   |
| 35  | BB    | 1915 | U    | N3-C4-C5    | 5.72  | 118.03      | 114.60   |
| 1   | AA    | 30   | U    | N1-C2-N3    | -5.72 | 111.47      | 114.90   |
| 1   | AA    | 180  | U    | C4-C5-C6    | 5.72  | 123.13      | 119.70   |
| 1   | AA    | 342  | C    | N3-C4-C5    | -5.72 | 119.61      | 121.90   |
| 1   | AA    | 710  | G    | C5-N7-C8    | 5.72  | 107.16      | 104.30   |
| 1   | AA    | 1468 | A    | C5'-C4'-O4' | -5.72 | 102.23      | 109.10   |
| 12  | AL    | 74   | GLN  | N-CA-C      | -5.72 | 95.55       | 111.00   |
| 34  | BA    | 45   | A    | C5-C6-N1    | -5.72 | 114.84      | 117.70   |
| 34  | BA    | 105  | G    | OP1-P-OP2   | -5.72 | 111.02      | 119.60   |
| 35  | BB    | 90   | U    | N1-C1'-C2'  | -5.72 | 105.70      | 112.00   |
| 35  | BB    | 1039 | A    | N9-C4-C5    | 5.72  | 108.09      | 105.80   |
| 35  | BB    | 1266 | G    | C6-N1-C2    | -5.72 | 121.67      | 125.10   |
| 35  | BB    | 1393 | A    | C6-N1-C2    | 5.72  | 122.03      | 118.60   |
| 35  | BB    | 1498 | C    | C1'-O4'-C4' | 5.72  | 114.48      | 109.90   |
| 35  | BB    | 1601 | G    | N3-C4-N9    | 5.72  | 129.43      | 126.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1862 | G    | C4-N9-C1'   | -5.72 | 119.06      | 126.50   |
| 35  | BB    | 1947 | C    | C5-C4-N4    | -5.72 | 116.19      | 120.20   |
| 35  | BB    | 2037 | A    | P-O3'-C3'   | -5.72 | 112.83      | 119.70   |
| 35  | BB    | 2330 | G    | C5-C6-O6    | -5.72 | 125.17      | 128.60   |
| 41  | BH    | 68   | ARG  | NE-CZ-NH1   | 5.72  | 123.16      | 120.30   |
| 1   | AA    | 385  | C    | C5-C6-N1    | 5.72  | 123.86      | 121.00   |
| 35  | BB    | 56   | A    | N1-C2-N3    | 5.72  | 132.16      | 129.30   |
| 35  | BB    | 1334 | G    | N7-C8-N9    | 5.72  | 115.96      | 113.10   |
| 35  | BB    | 2558 | C    | C4-C5-C6    | -5.72 | 114.54      | 117.40   |
| 1   | AA    | 253  | A    | N3-C4-C5    | -5.72 | 122.80      | 126.80   |
| 1   | AA    | 430  | A    | C4-C5-C6    | 5.72  | 119.86      | 117.00   |
| 1   | AA    | 484  | G    | N1-C2-N2    | -5.72 | 111.05      | 116.20   |
| 1   | AA    | 755  | G    | N9-C4-C5    | 5.72  | 107.69      | 105.40   |
| 1   | AA    | 776  | G    | C5-C6-O6    | -5.72 | 125.17      | 128.60   |
| 22  | AV    | 32   | A    | C5-N7-C8    | 5.72  | 106.76      | 103.90   |
| 35  | BB    | 911  | A    | C3'-C2'-C1' | 5.72  | 106.08      | 101.50   |
| 35  | BB    | 1010 | A    | C8-N9-C4    | -5.72 | 103.51      | 105.80   |
| 35  | BB    | 1301 | A    | C5-C6-N6    | -5.72 | 119.12      | 123.70   |
| 35  | BB    | 1776 | G    | O4'-C1'-N9  | 5.72  | 112.78      | 108.20   |
| 35  | BB    | 2395 | C    | C1'-O4'-C4' | 5.72  | 114.48      | 109.90   |
| 40  | BG    | 167  | VAL  | CA-CB-CG1   | -5.72 | 102.32      | 110.90   |
| 1   | AA    | 64   | G    | O4'-C1'-N9  | 5.72  | 112.77      | 108.20   |
| 1   | AA    | 801  | U    | N1-C2-N3    | -5.72 | 111.47      | 114.90   |
| 1   | AA    | 803  | G    | P-O3'-C3'   | -5.72 | 112.84      | 119.70   |
| 1   | AA    | 840  | C    | N1-C2-O2    | -5.72 | 115.47      | 118.90   |
| 1   | AA    | 907  | A    | N9-C4-C5    | 5.72  | 108.09      | 105.80   |
| 1   | AA    | 1289 | A    | N9-C4-C5    | 5.72  | 108.09      | 105.80   |
| 22  | AV    | 42   | G    | O4'-C1'-N9  | 5.72  | 112.77      | 108.20   |
| 35  | BB    | 1005 | C    | C3'-C2'-C1' | -5.72 | 96.93       | 101.50   |
| 35  | BB    | 1280 | G    | N1-C6-O6    | 5.72  | 123.33      | 119.90   |
| 35  | BB    | 1543 | G    | O4'-C1'-N9  | 5.72  | 112.77      | 108.20   |
| 1   | AA    | 167  | A    | C4'-C3'-C2' | -5.72 | 96.88       | 102.60   |
| 1   | AA    | 306  | A    | N3-C4-C5    | -5.72 | 122.80      | 126.80   |
| 1   | AA    | 1033 | G    | C8-N9-C4    | -5.72 | 104.11      | 106.40   |
| 1   | AA    | 1062 | U    | N3-C4-C5    | -5.72 | 111.17      | 114.60   |
| 1   | AA    | 1323 | G    | C5-C6-O6    | -5.72 | 125.17      | 128.60   |
| 6   | AF    | 59   | TYR  | O-C-N       | 5.72  | 131.84      | 122.70   |
| 35  | BB    | 18   | U    | N3-C4-O4    | 5.72  | 123.40      | 119.40   |
| 35  | BB    | 204  | A    | C2-N3-C4    | 5.72  | 113.46      | 110.60   |
| 35  | BB    | 862  | G    | N3-C2-N2    | 5.72  | 123.90      | 119.90   |
| 35  | BB    | 1166 | G    | O4'-C1'-N9  | 5.72  | 112.77      | 108.20   |
| 35  | BB    | 1521 | G    | C4-C5-N7    | 5.72  | 113.09      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1585 | C    | N1-C2-N3    | -5.72 | 115.20      | 119.20   |
| 35  | BB    | 2199 | A    | C4-C5-C6    | 5.72  | 119.86      | 117.00   |
| 35  | BB    | 2217 | G    | N7-C8-N9    | -5.72 | 110.24      | 113.10   |
| 1   | AA    | 215  | C    | C6-N1-C2    | -5.71 | 118.01      | 120.30   |
| 1   | AA    | 256  | U    | OP1-P-OP2   | -5.71 | 111.03      | 119.60   |
| 35  | BB    | 416  | U    | C4-C5-C6    | -5.71 | 116.27      | 119.70   |
| 35  | BB    | 730  | A    | C8-N9-C4    | -5.71 | 103.51      | 105.80   |
| 35  | BB    | 865  | C    | C5-C4-N4    | -5.71 | 116.20      | 120.20   |
| 35  | BB    | 1009 | A    | C4-C5-C6    | 5.71  | 119.86      | 117.00   |
| 35  | BB    | 2181 | U    | C6-N1-C2    | -5.71 | 117.57      | 121.00   |
| 35  | BB    | 2321 | U    | C2-N1-C1'   | 5.71  | 124.56      | 117.70   |
| 35  | BB    | 2462 | C    | N3-C4-C5    | -5.71 | 119.61      | 121.90   |
| 35  | BB    | 2631 | G    | C5-C6-N1    | 5.71  | 114.36      | 111.50   |
| 34  | BA    | 71   | C    | C2-N1-C1'   | 5.71  | 125.08      | 118.80   |
| 35  | BB    | 1341 | G    | N3-C4-C5    | -5.71 | 125.74      | 128.60   |
| 35  | BB    | 1431 | A    | N3-C4-N9    | 5.71  | 131.97      | 127.40   |
| 35  | BB    | 1862 | G    | O4'-C1'-N9  | 5.71  | 112.77      | 108.20   |
| 1   | AA    | 55   | A    | C5-C6-N6    | -5.71 | 119.13      | 123.70   |
| 1   | AA    | 172  | A    | O4'-C1'-N9  | 5.71  | 112.77      | 108.20   |
| 1   | AA    | 365  | U    | C4'-C3'-C2' | 5.71  | 108.31      | 102.60   |
| 1   | AA    | 1292 | G    | C6-C5-N7    | -5.71 | 126.97      | 130.40   |
| 35  | BB    | 56   | A    | C6-C5-N7    | -5.71 | 128.30      | 132.30   |
| 35  | BB    | 123  | G    | N3-C2-N2    | 5.71  | 123.90      | 119.90   |
| 35  | BB    | 138  | U    | C5-C4-O4    | -5.71 | 122.47      | 125.90   |
| 35  | BB    | 685  | A    | C2-N3-C4    | -5.71 | 107.75      | 110.60   |
| 35  | BB    | 2181 | U    | C5-C4-O4    | -5.71 | 122.47      | 125.90   |
| 35  | BB    | 2287 | A    | C3'-C2'-C1' | -5.71 | 96.93       | 101.50   |
| 50  | BQ    | 12   | ARG  | NE-CZ-NH2   | 5.71  | 123.16      | 120.30   |
| 1   | AA    | 446  | G    | N7-C8-N9    | 5.71  | 115.95      | 113.10   |
| 1   | AA    | 1356 | G    | N1-C6-O6    | 5.71  | 123.33      | 119.90   |
| 35  | BB    | 536  | G    | N7-C8-N9    | -5.71 | 110.25      | 113.10   |
| 35  | BB    | 1559 | U    | N3-C4-C5    | -5.71 | 111.17      | 114.60   |
| 35  | BB    | 2206 | C    | C5-C6-N1    | 5.71  | 123.86      | 121.00   |
| 35  | BB    | 2622 | U    | C4-C5-C6    | -5.71 | 116.27      | 119.70   |
| 35  | BB    | 2899 | A    | C8-N9-C4    | -5.71 | 103.52      | 105.80   |
| 36  | BC    | 169  | ALA  | CB-CA-C     | 5.71  | 118.66      | 110.10   |
| 1   | AA    | 1088 | G    | N3-C2-N2    | 5.71  | 123.90      | 119.90   |
| 1   | AA    | 1329 | A    | O4'-C4'-C3' | -5.71 | 98.29       | 104.00   |
| 10  | AJ    | 66   | GLU  | N-CA-CB     | 5.71  | 120.88      | 110.60   |
| 34  | BA    | 89   | U    | N1-C1'-C2'  | -5.71 | 105.72      | 112.00   |
| 35  | BB    | 962  | G    | C4'-C3'-C2' | -5.71 | 96.89       | 102.60   |
| 35  | BB    | 1812 | U    | O4'-C4'-C3' | -5.71 | 98.29       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2072 | C    | C5-C4-N4    | -5.71 | 116.20      | 120.20   |
| 35  | BB    | 2439 | A    | O4'-C1'-N9  | 5.71  | 112.77      | 108.20   |
| 1   | AA    | 544  | G    | C4-C5-N7    | 5.71  | 113.08      | 110.80   |
| 1   | AA    | 713  | G    | N1-C2-N3    | -5.71 | 120.48      | 123.90   |
| 1   | AA    | 1315 | U    | C2-N3-C4    | -5.71 | 123.58      | 127.00   |
| 4   | AD    | 154  | VAL  | CA-CB-CG2   | -5.71 | 102.34      | 110.90   |
| 14  | AN    | 35   | ALA  | CB-CA-C     | -5.71 | 101.54      | 110.10   |
| 35  | BB    | 143  | C    | N1-C2-O2    | 5.71  | 122.32      | 118.90   |
| 35  | BB    | 327  | G    | N3-C2-N2    | 5.71  | 123.89      | 119.90   |
| 35  | BB    | 1444 | G    | C6-C5-N7    | -5.71 | 126.98      | 130.40   |
| 35  | BB    | 1984 | G    | N3-C2-N2    | 5.71  | 123.89      | 119.90   |
| 35  | BB    | 2168 | G    | C6-N1-C2    | 5.71  | 128.52      | 125.10   |
| 35  | BB    | 2307 | G    | C3'-C2'-C1' | -5.71 | 96.94       | 101.50   |
| 35  | BB    | 2467 | C    | N1-C2-N3    | -5.71 | 115.20      | 119.20   |
| 35  | BB    | 2511 | U    | O4'-C1'-N1  | 5.71  | 112.77      | 108.20   |
| 38  | BE    | 59   | PRO  | O-C-N       | 5.71  | 131.83      | 122.70   |
| 1   | AA    | 856  | C    | O4'-C1'-N1  | 5.71  | 112.76      | 108.20   |
| 1   | AA    | 1319 | A    | C5'-C4'-O4' | 5.71  | 115.95      | 109.10   |
| 3   | AC    | 14   | VAL  | N-CA-C      | -5.71 | 95.60       | 111.00   |
| 34  | BA    | 76   | G    | N3-C4-C5    | -5.71 | 125.75      | 128.60   |
| 35  | BB    | 431  | U    | C4'-C3'-C2' | -5.71 | 96.89       | 102.60   |
| 35  | BB    | 616  | A    | C8-N9-C4    | -5.71 | 103.52      | 105.80   |
| 35  | BB    | 783  | A    | N9-C1'-C2'  | -5.71 | 105.72      | 112.00   |
| 35  | BB    | 808  | G    | N7-C8-N9    | 5.71  | 115.95      | 113.10   |
| 35  | BB    | 2015 | A    | C2-N3-C4    | -5.71 | 107.75      | 110.60   |
| 35  | BB    | 2265 | U    | C5-C4-O4    | -5.71 | 122.48      | 125.90   |
| 1   | AA    | 36   | C    | C2-N3-C4    | 5.70  | 122.75      | 119.90   |
| 1   | AA    | 214  | C    | C3'-C2'-C1' | 5.70  | 106.06      | 101.50   |
| 1   | AA    | 278  | G    | C2-N3-C4    | 5.70  | 114.75      | 111.90   |
| 1   | AA    | 870  | U    | C5-C6-N1    | -5.70 | 119.85      | 122.70   |
| 22  | AV    | 7    | G    | P-O5'-C5'   | 5.70  | 130.02      | 120.90   |
| 22  | AV    | 26   | A    | O4'-C1'-N9  | 5.70  | 112.76      | 108.20   |
| 35  | BB    | 620  | G    | C6-C5-N7    | -5.70 | 126.98      | 130.40   |
| 35  | BB    | 969  | G    | C8-N9-C1'   | 5.70  | 134.41      | 127.00   |
| 36  | BC    | 202  | ARG  | NH1-CZ-NH2  | -5.70 | 113.12      | 119.40   |
| 1   | AA    | 1083 | U    | C1'-O4'-C4' | 5.70  | 114.46      | 109.90   |
| 12  | AL    | 112  | ALA  | N-CA-CB     | 5.70  | 118.08      | 110.10   |
| 35  | BB    | 21   | A    | N1-C6-N6    | 5.70  | 122.02      | 118.60   |
| 35  | BB    | 1287 | A    | C8-N9-C4    | -5.70 | 103.52      | 105.80   |
| 35  | BB    | 2302 | U    | N3-C4-C5    | -5.70 | 111.18      | 114.60   |
| 35  | BB    | 2777 | G    | N9-C4-C5    | -5.70 | 103.12      | 105.40   |
| 1   | AA    | 170  | U    | C5-C6-N1    | 5.70  | 125.55      | 122.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 191  | G    | OP1-P-OP2   | -5.70 | 111.05      | 119.60   |
| 1   | AA    | 484  | G    | C6-C5-N7    | -5.70 | 126.98      | 130.40   |
| 18  | AR    | 50   | TYR  | CZ-CE2-CD2  | -5.70 | 114.67      | 119.80   |
| 35  | BB    | 363  | G    | C4-N9-C1'   | 5.70  | 133.91      | 126.50   |
| 35  | BB    | 458  | G    | C5-C6-O6    | -5.70 | 125.18      | 128.60   |
| 35  | BB    | 935  | C    | N3-C4-N4    | 5.70  | 121.99      | 118.00   |
| 35  | BB    | 1025 | G    | C5'-C4'-C3' | -5.70 | 106.88      | 116.00   |
| 35  | BB    | 1156 | A    | C5-C6-N1    | -5.70 | 114.85      | 117.70   |
| 35  | BB    | 1264 | A    | C5-C6-N1    | -5.70 | 114.85      | 117.70   |
| 35  | BB    | 1506 | U    | N3-C4-O4    | 5.70  | 123.39      | 119.40   |
| 35  | BB    | 1632 | A    | C5-C6-N1    | -5.70 | 114.85      | 117.70   |
| 35  | BB    | 1939 | U    | C5-C6-N1    | -5.70 | 119.85      | 122.70   |
| 35  | BB    | 2022 | U    | N3-C4-O4    | 5.70  | 123.39      | 119.40   |
| 35  | BB    | 2319 | G    | N1-C2-N3    | -5.70 | 120.48      | 123.90   |
| 35  | BB    | 2624 | G    | C4'-C3'-C2' | -5.70 | 96.90       | 102.60   |
| 35  | BB    | 2820 | A    | N3-C4-N9    | 5.70  | 131.96      | 127.40   |
| 1   | AA    | 28   | A    | C5-N7-C8    | 5.70  | 106.75      | 103.90   |
| 1   | AA    | 128  | G    | C4-C5-C6    | 5.70  | 122.22      | 118.80   |
| 1   | AA    | 271  | C    | N3-C2-O2    | 5.70  | 125.89      | 121.90   |
| 1   | AA    | 559  | A    | C5-C6-N1    | -5.70 | 114.85      | 117.70   |
| 1   | AA    | 1443 | C    | N3-C4-N4    | 5.70  | 121.99      | 118.00   |
| 22  | AV    | 16   | C    | N3-C4-C5    | -5.70 | 119.62      | 121.90   |
| 28  | B3    | 51   | ARG  | NH1-CZ-NH2  | -5.70 | 113.13      | 119.40   |
| 35  | BB    | 236  | C    | N3-C4-C5    | -5.70 | 119.62      | 121.90   |
| 35  | BB    | 286  | U    | OP2-P-O3'   | 5.70  | 117.74      | 105.20   |
| 35  | BB    | 401  | A    | O4'-C4'-C3' | -5.70 | 98.30       | 104.00   |
| 35  | BB    | 933  | A    | O3'-P-O5'   | -5.70 | 93.17       | 104.00   |
| 35  | BB    | 1277 | G    | N3-C4-N9    | -5.70 | 122.58      | 126.00   |
| 35  | BB    | 1962 | C    | P-O3'-C3'   | -5.70 | 112.86      | 119.70   |
| 35  | BB    | 2466 | C    | O5'-P-OP2   | -5.70 | 100.57      | 105.70   |
| 35  | BB    | 2880 | C    | P-O5'-C5'   | 5.70  | 130.02      | 120.90   |
| 1   | AA    | 166  | U    | P-O3'-C3'   | -5.70 | 112.86      | 119.70   |
| 1   | AA    | 167  | A    | N3-C4-C5    | -5.70 | 122.81      | 126.80   |
| 1   | AA    | 699  | C    | C5-C4-N4    | -5.70 | 116.21      | 120.20   |
| 1   | AA    | 825  | A    | O4'-C1'-N9  | 5.70  | 112.76      | 108.20   |
| 12  | AL    | 93   | ARG  | NH1-CZ-NH2  | 5.70  | 125.67      | 119.40   |
| 19  | AS    | 43   | MET  | CG-SD-CE    | -5.70 | 91.08       | 100.20   |
| 35  | BB    | 421  | C    | C4-C5-C6    | -5.70 | 114.55      | 117.40   |
| 35  | BB    | 642  | U    | O4'-C1'-N1  | 5.70  | 112.76      | 108.20   |
| 35  | BB    | 768  | G    | O4'-C1'-N9  | 5.70  | 112.76      | 108.20   |
| 35  | BB    | 1359 | A    | C4'-C3'-C2' | -5.70 | 96.90       | 102.60   |
| 45  | BL    | 95   | LEU  | CB-CG-CD2   | 5.70  | 120.68      | 111.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 196  | A    | C4-C5-C6    | 5.70  | 119.85      | 117.00   |
| 1   | AA    | 198  | G    | C1'-O4'-C4' | 5.70  | 114.46      | 109.90   |
| 1   | AA    | 266  | G    | O4'-C1'-N9  | 5.70  | 112.76      | 108.20   |
| 1   | AA    | 400  | C    | N1-C2-O2    | 5.70  | 122.32      | 118.90   |
| 1   | AA    | 682  | G    | C5-N7-C8    | 5.70  | 107.15      | 104.30   |
| 1   | AA    | 959  | A    | O4'-C1'-N9  | 5.70  | 112.76      | 108.20   |
| 1   | AA    | 1174 | G    | P-O5'-C5'   | -5.70 | 111.79      | 120.90   |
| 1   | AA    | 1332 | A    | C5-N7-C8    | 5.70  | 106.75      | 103.90   |
| 1   | AA    | 1410 | A    | O4'-C1'-C2' | 5.70  | 112.73      | 107.60   |
| 3   | AC    | 21   | TRP  | CZ3-CH2-CZ2 | 5.70  | 128.44      | 121.60   |
| 35  | BB    | 1012 | U    | C2-N1-C1'   | 5.70  | 124.53      | 117.70   |
| 35  | BB    | 1794 | A    | C4-C5-N7    | -5.70 | 107.85      | 110.70   |
| 35  | BB    | 1932 | A    | C4-C5-C6    | 5.70  | 119.85      | 117.00   |
| 35  | BB    | 2194 | U    | O4'-C1'-N1  | 5.70  | 112.76      | 108.20   |
| 35  | BB    | 2501 | C    | C4-C5-C6    | 5.70  | 120.25      | 117.40   |
| 1   | AA    | 106  | C    | C5-C4-N4    | -5.69 | 116.21      | 120.20   |
| 1   | AA    | 791  | G    | N9-C1'-C2'  | 5.69  | 121.40      | 114.00   |
| 1   | AA    | 1319 | A    | P-O3'-C3'   | 5.69  | 126.53      | 119.70   |
| 35  | BB    | 1073 | A    | N7-C8-N9    | -5.69 | 110.95      | 113.80   |
| 35  | BB    | 1121 | C    | C2-N3-C4    | 5.69  | 122.75      | 119.90   |
| 35  | BB    | 1527 | G    | C6-C5-N7    | -5.69 | 126.98      | 130.40   |
| 35  | BB    | 1654 | A    | O5'-P-OP2   | -5.69 | 100.58      | 105.70   |
| 35  | BB    | 2158 | A    | C6-C5-N7    | -5.69 | 128.31      | 132.30   |
| 38  | BE    | 44   | ARG  | NE-CZ-NH1   | -5.69 | 117.45      | 120.30   |
| 1   | AA    | 934  | C    | C1'-O4'-C4' | 5.69  | 114.45      | 109.90   |
| 1   | AA    | 1045 | C    | O4'-C1'-N1  | 5.69  | 112.75      | 108.20   |
| 35  | BB    | 904  | G    | C4-C5-C6    | 5.69  | 122.22      | 118.80   |
| 35  | BB    | 939  | G    | C6-C5-N7    | -5.69 | 126.98      | 130.40   |
| 35  | BB    | 1299 | G    | P-O3'-C3'   | 5.69  | 126.53      | 119.70   |
| 35  | BB    | 1887 | C    | O4'-C1'-N1  | 5.69  | 112.75      | 108.20   |
| 35  | BB    | 2244 | U    | C2-N1-C1'   | 5.69  | 124.53      | 117.70   |
| 35  | BB    | 2246 | G    | N1-C2-N3    | -5.69 | 120.48      | 123.90   |
| 35  | BB    | 2632 | A    | N7-C8-N9    | -5.69 | 110.95      | 113.80   |
| 1   | AA    | 886  | G    | C2-N3-C4    | -5.69 | 109.05      | 111.90   |
| 34  | BA    | 105  | G    | C8-N9-C4    | 5.69  | 108.68      | 106.40   |
| 34  | BA    | 113  | C    | C6-N1-C2    | -5.69 | 118.02      | 120.30   |
| 35  | BB    | 58   | G    | N3-C4-N9    | 5.69  | 129.41      | 126.00   |
| 35  | BB    | 597  | G    | N1-C6-O6    | 5.69  | 123.31      | 119.90   |
| 35  | BB    | 743  | A    | O4'-C1'-N9  | 5.69  | 112.75      | 108.20   |
| 35  | BB    | 1007 | C    | C5-C6-N1    | 5.69  | 123.85      | 121.00   |
| 35  | BB    | 1149 | G    | OP1-P-OP2   | -5.69 | 111.06      | 119.60   |
| 35  | BB    | 1299 | G    | OP1-P-OP2   | -5.69 | 111.06      | 119.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1552 | A    | N3-C4-N9    | 5.69  | 131.95      | 127.40   |
| 35  | BB    | 2184 | A    | C5-N7-C8    | 5.69  | 106.75      | 103.90   |
| 35  | BB    | 2350 | C    | C4-C5-C6    | 5.69  | 120.25      | 117.40   |
| 35  | BB    | 2522 | U    | C3'-C2'-C1' | 5.69  | 106.05      | 101.50   |
| 35  | BB    | 2555 | U    | N3-C2-O2    | 5.69  | 126.18      | 122.20   |
| 35  | BB    | 2614 | A    | O4'-C1'-N9  | 5.69  | 112.75      | 108.20   |
| 35  | BB    | 2688 | G    | N3-C2-N2    | 5.69  | 123.88      | 119.90   |
| 35  | BB    | 2810 | A    | N3-C4-C5    | -5.69 | 122.82      | 126.80   |
| 35  | BB    | 2883 | A    | N1-C2-N3    | 5.69  | 132.15      | 129.30   |
| 1   | AA    | 277  | C    | C1'-O4'-C4' | -5.69 | 105.35      | 109.90   |
| 1   | AA    | 1114 | C    | N3-C4-N4    | 5.69  | 121.98      | 118.00   |
| 1   | AA    | 1514 | G    | O4'-C1'-N9  | 5.69  | 112.75      | 108.20   |
| 35  | BB    | 409  | G    | C6-N1-C2    | -5.69 | 121.69      | 125.10   |
| 35  | BB    | 814  | C    | N3-C4-N4    | 5.69  | 121.98      | 118.00   |
| 35  | BB    | 989  | G    | O4'-C1'-C2' | -5.69 | 100.11      | 105.80   |
| 35  | BB    | 1732 | C    | C3'-C2'-C1' | -5.69 | 96.95       | 101.50   |
| 35  | BB    | 2116 | G    | C5-C6-O6    | -5.69 | 125.19      | 128.60   |
| 35  | BB    | 2849 | U    | C2-N3-C4    | 5.69  | 130.41      | 127.00   |
| 1   | AA    | 211  | G    | C4-N9-C1'   | 5.69  | 133.89      | 126.50   |
| 1   | AA    | 510  | A    | N9-C4-C5    | 5.69  | 108.08      | 105.80   |
| 1   | AA    | 586  | C    | N3-C2-O2    | 5.69  | 125.88      | 121.90   |
| 1   | AA    | 1015 | G    | C4-N9-C1'   | 5.69  | 133.89      | 126.50   |
| 1   | AA    | 1032 | G    | C4'-C3'-C2' | -5.69 | 96.91       | 102.60   |
| 19  | AS    | 25   | GLY  | N-CA-C      | -5.69 | 98.88       | 113.10   |
| 22  | AV    | 25   | C    | N3-C4-C5    | -5.69 | 119.62      | 121.90   |
| 35  | BB    | 611  | C    | O4'-C1'-N1  | 5.69  | 112.75      | 108.20   |
| 35  | BB    | 751  | A    | O4'-C1'-N9  | 5.69  | 112.75      | 108.20   |
| 35  | BB    | 1053 | C    | C1'-O4'-C4' | -5.69 | 105.35      | 109.90   |
| 35  | BB    | 1063 | G    | N1-C6-O6    | 5.69  | 123.31      | 119.90   |
| 35  | BB    | 1257 | C    | C2-N3-C4    | 5.69  | 122.74      | 119.90   |
| 35  | BB    | 1571 | A    | N9-C4-C5    | -5.69 | 103.53      | 105.80   |
| 35  | BB    | 1606 | C    | N3-C4-N4    | 5.69  | 121.98      | 118.00   |
| 35  | BB    | 1613 | G    | N3-C4-N9    | -5.69 | 122.59      | 126.00   |
| 35  | BB    | 1704 | C    | C5-C4-N4    | -5.69 | 116.22      | 120.20   |
| 35  | BB    | 1895 | C    | C5'-C4'-C3' | -5.69 | 106.90      | 116.00   |
| 35  | BB    | 2044 | C    | P-O3'-C3'   | -5.69 | 112.88      | 119.70   |
| 35  | BB    | 2149 | U    | O4'-C4'-C3' | -5.69 | 98.31       | 104.00   |
| 35  | BB    | 2410 | G    | N3-C4-N9    | 5.69  | 129.41      | 126.00   |
| 35  | BB    | 2619 | C    | C5'-C4'-C3' | -5.69 | 106.90      | 116.00   |
| 35  | BB    | 2647 | U    | N3-C4-C5    | -5.69 | 111.19      | 114.60   |
| 35  | BB    | 2654 | A    | N1-C2-N3    | 5.69  | 132.14      | 129.30   |
| 50  | BQ    | 31   | TYR  | CB-CG-CD1   | -5.69 | 117.59      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 21   | G    | N1-C2-N2    | -5.69 | 111.08      | 116.20   |
| 35  | BB    | 216  | A    | P-O3'-C3'   | 5.69  | 126.52      | 119.70   |
| 35  | BB    | 440  | C    | C2-N3-C4    | 5.69  | 122.74      | 119.90   |
| 35  | BB    | 581  | C    | N3-C2-O2    | -5.69 | 117.92      | 121.90   |
| 35  | BB    | 1653 | G    | C5-C6-O6    | -5.69 | 125.19      | 128.60   |
| 35  | BB    | 2834 | G    | N1-C6-O6    | 5.69  | 123.31      | 119.90   |
| 1   | AA    | 386  | C    | N1-C2-N3    | 5.68  | 123.18      | 119.20   |
| 1   | AA    | 446  | G    | N3-C4-N9    | 5.68  | 129.41      | 126.00   |
| 1   | AA    | 459  | A    | C6-C5-N7    | -5.68 | 128.32      | 132.30   |
| 1   | AA    | 728  | A    | C5'-C4'-O4' | 5.68  | 115.92      | 109.10   |
| 1   | AA    | 937  | A    | C4-C5-C6    | 5.68  | 119.84      | 117.00   |
| 1   | AA    | 1215 | G    | O5'-P-OP2   | -5.68 | 100.58      | 105.70   |
| 1   | AA    | 1430 | A    | C4-C5-C6    | 5.68  | 119.84      | 117.00   |
| 22  | AV    | 45   | G    | O4'-C1'-N9  | 5.68  | 112.75      | 108.20   |
| 34  | BA    | 101  | A    | N1-C2-N3    | 5.68  | 132.14      | 129.30   |
| 35  | BB    | 785  | G    | C4-C5-C6    | 5.68  | 122.21      | 118.80   |
| 35  | BB    | 902  | C    | C5-C4-N4    | -5.68 | 116.22      | 120.20   |
| 35  | BB    | 1133 | A    | N1-C2-N3    | -5.68 | 126.46      | 129.30   |
| 35  | BB    | 1210 | G    | C4-C5-C6    | 5.68  | 122.21      | 118.80   |
| 35  | BB    | 1529 | G    | C5-C6-O6    | -5.68 | 125.19      | 128.60   |
| 35  | BB    | 1672 | A    | C2-N3-C4    | -5.68 | 107.76      | 110.60   |
| 35  | BB    | 1702 | G    | N3-C2-N2    | 5.68  | 123.88      | 119.90   |
| 35  | BB    | 2038 | G    | O4'-C1'-N9  | 5.68  | 112.75      | 108.20   |
| 35  | BB    | 2134 | A    | C5-C6-N1    | -5.68 | 114.86      | 117.70   |
| 35  | BB    | 2328 | A    | C6-N1-C2    | -5.68 | 115.19      | 118.60   |
| 35  | BB    | 2346 | A    | N7-C8-N9    | 5.68  | 116.64      | 113.80   |
| 35  | BB    | 2446 | G    | N9-C4-C5    | -5.68 | 103.13      | 105.40   |
| 35  | BB    | 2530 | A    | O4'-C1'-N9  | 5.68  | 112.75      | 108.20   |
| 1   | AA    | 303  | A    | C4-C5-C6    | 5.68  | 119.84      | 117.00   |
| 1   | AA    | 344  | A    | C3'-C2'-C1' | 5.68  | 106.05      | 101.50   |
| 1   | AA    | 654  | G    | O5'-P-OP1   | 5.68  | 117.52      | 110.70   |
| 1   | AA    | 1225 | A    | O4'-C1'-C2' | -5.68 | 100.12      | 105.80   |
| 2   | AB    | 133  | ALA  | CB-CA-C     | -5.68 | 101.58      | 110.10   |
| 3   | AC    | 19   | SER  | N-CA-CB     | 5.68  | 119.03      | 110.50   |
| 35  | BB    | 975  | A    | C5-N7-C8    | 5.68  | 106.74      | 103.90   |
| 35  | BB    | 1361 | G    | C5-N7-C8    | -5.68 | 101.46      | 104.30   |
| 35  | BB    | 1839 | G    | C4-C5-C6    | 5.68  | 122.21      | 118.80   |
| 35  | BB    | 2250 | G    | C4-C5-C6    | 5.68  | 122.21      | 118.80   |
| 35  | BB    | 2524 | G    | C5-C6-O6    | -5.68 | 125.19      | 128.60   |
| 35  | BB    | 2613 | U    | P-O3'-C3'   | 5.68  | 126.52      | 119.70   |
| 35  | BB    | 2680 | U    | C6-N1-C2    | -5.68 | 117.59      | 121.00   |
| 35  | BB    | 2708 | G    | C4'-C3'-C2' | -5.68 | 96.92       | 102.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2823 | A    | C3'-C2'-C1' | 5.68  | 106.05      | 101.50   |
| 35  | BB    | 2887 | A    | C5-C6-N6    | -5.68 | 119.15      | 123.70   |
| 1   | AA    | 62   | U    | C2-N3-C4    | 5.68  | 130.41      | 127.00   |
| 1   | AA    | 973  | G    | N1-C2-N3    | -5.68 | 120.49      | 123.90   |
| 3   | AC    | 30   | ASP  | CB-CG-OD1   | 5.68  | 123.41      | 118.30   |
| 35  | BB    | 1165 | A    | C4-C5-C6    | 5.68  | 119.84      | 117.00   |
| 35  | BB    | 1247 | A    | N7-C8-N9    | 5.68  | 116.64      | 113.80   |
| 35  | BB    | 1389 | G    | N1-C2-N2    | -5.68 | 111.09      | 116.20   |
| 1   | AA    | 211  | G    | N3-C2-N2    | 5.68  | 123.88      | 119.90   |
| 1   | AA    | 265  | G    | C5-C6-O6    | -5.68 | 125.19      | 128.60   |
| 1   | AA    | 348  | G    | P-O5'-C5'   | 5.68  | 129.99      | 120.90   |
| 1   | AA    | 927  | G    | C5-C6-O6    | -5.68 | 125.19      | 128.60   |
| 1   | AA    | 1060 | U    | C4'-C3'-C2' | -5.68 | 96.92       | 102.60   |
| 34  | BA    | 72   | G    | N7-C8-N9    | 5.68  | 115.94      | 113.10   |
| 35  | BB    | 382  | A    | C5-C6-N6    | -5.68 | 119.16      | 123.70   |
| 35  | BB    | 1044 | C    | N3-C2-O2    | 5.68  | 125.88      | 121.90   |
| 35  | BB    | 1324 | G    | N9-C4-C5    | -5.68 | 103.13      | 105.40   |
| 35  | BB    | 1470 | A    | C2-N3-C4    | -5.68 | 107.76      | 110.60   |
| 35  | BB    | 1487 | U    | C6-N1-C2    | -5.68 | 117.59      | 121.00   |
| 35  | BB    | 2149 | U    | C4-C5-C6    | -5.68 | 116.29      | 119.70   |
| 35  | BB    | 2415 | G    | N1-C2-N2    | -5.68 | 111.09      | 116.20   |
| 35  | BB    | 2532 | G    | N3-C4-C5    | 5.68  | 131.44      | 128.60   |
| 35  | BB    | 2692 | G    | C8-N9-C4    | -5.68 | 104.13      | 106.40   |
| 35  | BB    | 2801 | G    | N1-C6-O6    | 5.68  | 123.31      | 119.90   |
| 49  | BP    | 14   | GLN  | N-CA-CB     | 5.68  | 120.82      | 110.60   |
| 34  | BA    | 62   | C    | N3-C4-C5    | -5.68 | 119.63      | 121.90   |
| 35  | BB    | 224  | U    | C6-N1-C2    | 5.68  | 124.41      | 121.00   |
| 35  | BB    | 363  | G    | N1-C2-N3    | 5.68  | 127.31      | 123.90   |
| 35  | BB    | 596  | U    | C5-C6-N1    | 5.68  | 125.54      | 122.70   |
| 35  | BB    | 796  | C    | N3-C4-N4    | 5.68  | 121.97      | 118.00   |
| 35  | BB    | 1627 | G    | N9-C1'-C2'  | -5.68 | 105.75      | 112.00   |
| 35  | BB    | 2118 | U    | O4'-C4'-C3' | 5.68  | 110.64      | 106.10   |
| 35  | BB    | 2230 | G    | N1-C2-N3    | -5.68 | 120.49      | 123.90   |
| 1   | AA    | 401  | C    | C5-C4-N4    | -5.68 | 116.23      | 120.20   |
| 1   | AA    | 540  | G    | P-O3'-C3'   | -5.68 | 112.89      | 119.70   |
| 1   | AA    | 857  | C    | C5-C6-N1    | -5.68 | 118.16      | 121.00   |
| 1   | AA    | 947  | G    | C4-C5-C6    | 5.68  | 122.21      | 118.80   |
| 1   | AA    | 1090 | U    | C2-N3-C4    | 5.68  | 130.41      | 127.00   |
| 1   | AA    | 1519 | A    | C5-C6-N6    | -5.68 | 119.16      | 123.70   |
| 13  | AM    | 109  | LYS  | CB-CA-C     | -5.68 | 99.05       | 110.40   |
| 35  | BB    | 43   | G    | N3-C4-N9    | 5.68  | 129.41      | 126.00   |
| 35  | BB    | 404  | A    | N3-C4-N9    | 5.68  | 131.94      | 127.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 720  | U    | O4'-C1'-N1  | 5.68  | 112.74      | 108.20   |
| 35  | BB    | 757  | G    | C5-C6-N1    | 5.68  | 114.34      | 111.50   |
| 35  | BB    | 1199 | U    | N1-C2-N3    | -5.68 | 111.49      | 114.90   |
| 35  | BB    | 1336 | A    | C8-N9-C4    | -5.68 | 103.53      | 105.80   |
| 35  | BB    | 1360 | G    | C4-C5-C6    | -5.68 | 115.39      | 118.80   |
| 35  | BB    | 1595 | C    | C3'-C2'-C1' | -5.68 | 96.96       | 101.50   |
| 35  | BB    | 1988 | G    | C5-N7-C8    | 5.68  | 107.14      | 104.30   |
| 35  | BB    | 2286 | G    | C6-N1-C2    | 5.68  | 128.51      | 125.10   |
| 1   | AA    | 366  | A    | N7-C8-N9    | -5.67 | 110.96      | 113.80   |
| 1   | AA    | 485  | U    | P-O5'-C5'   | 5.67  | 129.98      | 120.90   |
| 1   | AA    | 558  | G    | C6-N1-C2    | 5.67  | 128.50      | 125.10   |
| 1   | AA    | 1286 | U    | C5-C6-N1    | -5.67 | 119.86      | 122.70   |
| 1   | AA    | 1450 | U    | C2-N3-C4    | -5.67 | 123.59      | 127.00   |
| 1   | AA    | 1468 | A    | N3-C4-C5    | -5.67 | 122.83      | 126.80   |
| 2   | AB    | 122  | ASP  | CB-CG-OD1   | 5.67  | 123.41      | 118.30   |
| 22  | AV    | 12   | G    | O4'-C1'-N9  | 5.67  | 112.74      | 108.20   |
| 34  | BA    | 84   | G    | N1-C6-O6    | 5.67  | 123.31      | 119.90   |
| 34  | BA    | 112  | G    | N7-C8-N9    | 5.67  | 115.94      | 113.10   |
| 35  | BB    | 1111 | A    | P-O3'-C3'   | 5.67  | 126.51      | 119.70   |
| 35  | BB    | 1395 | A    | O4'-C1'-N9  | 5.67  | 112.74      | 108.20   |
| 35  | BB    | 2077 | A    | C2-N3-C4    | 5.67  | 113.44      | 110.60   |
| 1   | AA    | 1433 | A    | C5-N7-C8    | 5.67  | 106.74      | 103.90   |
| 35  | BB    | 663  | G    | C5-C6-O6    | -5.67 | 125.20      | 128.60   |
| 35  | BB    | 1171 | G    | C4-C5-N7    | 5.67  | 113.07      | 110.80   |
| 35  | BB    | 1706 | C    | C5'-C4'-C3' | -5.67 | 106.92      | 116.00   |
| 1   | AA    | 499  | A    | C1'-O4'-C4' | 5.67  | 114.44      | 109.90   |
| 1   | AA    | 763  | G    | C5-C6-O6    | -5.67 | 125.20      | 128.60   |
| 35  | BB    | 811  | U    | O4'-C1'-N1  | 5.67  | 112.74      | 108.20   |
| 35  | BB    | 956  | G    | N1-C2-N2    | -5.67 | 111.09      | 116.20   |
| 35  | BB    | 1405 | U    | N1-C2-N3    | -5.67 | 111.50      | 114.90   |
| 35  | BB    | 1975 | G    | N9-C4-C5    | -5.67 | 103.13      | 105.40   |
| 35  | BB    | 1988 | G    | C6-N1-C2    | -5.67 | 121.70      | 125.10   |
| 35  | BB    | 2003 | A    | N9-C4-C5    | 5.67  | 108.07      | 105.80   |
| 35  | BB    | 2239 | G    | C2-N3-C4    | 5.67  | 114.74      | 111.90   |
| 2   | AB    | 21   | TYR  | N-CA-CB     | 5.67  | 120.81      | 110.60   |
| 34  | BA    | 55   | U    | C4-C5-C6    | 5.67  | 123.10      | 119.70   |
| 35  | BB    | 330  | A    | C6-C5-N7    | -5.67 | 128.33      | 132.30   |
| 35  | BB    | 632  | A    | N9-C4-C5    | 5.67  | 108.07      | 105.80   |
| 35  | BB    | 691  | C    | N3-C4-C5    | -5.67 | 119.63      | 121.90   |
| 35  | BB    | 2059 | A    | C5-N7-C8    | 5.67  | 106.73      | 103.90   |
| 35  | BB    | 2765 | A    | O4'-C1'-N9  | 5.67  | 112.74      | 108.20   |
| 35  | BB    | 2897 | U    | C5-C4-O4    | -5.67 | 122.50      | 125.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 233  | C    | C6-N1-C2    | -5.67 | 118.03      | 120.30   |
| 1   | AA    | 448  | A    | C5-C6-N1    | -5.67 | 114.87      | 117.70   |
| 1   | AA    | 619  | U    | C4-C5-C6    | 5.67  | 123.10      | 119.70   |
| 1   | AA    | 807  | A    | C6-N1-C2    | 5.67  | 122.00      | 118.60   |
| 1   | AA    | 1044 | A    | C6-C5-N7    | -5.67 | 128.33      | 132.30   |
| 1   | AA    | 1123 | U    | N3-C4-O4    | 5.67  | 123.37      | 119.40   |
| 1   | AA    | 1318 | A    | N3-C4-C5    | -5.67 | 122.83      | 126.80   |
| 1   | AA    | 1340 | A    | C5-N7-C8    | 5.67  | 106.73      | 103.90   |
| 1   | AA    | 1395 | C    | P-O3'-C3'   | 5.67  | 126.50      | 119.70   |
| 2   | AB    | 124  | THR  | OG1-CB-CG2  | -5.67 | 96.96       | 110.00   |
| 31  | B6    | 19   | ARG  | NH1-CZ-NH2  | -5.67 | 113.16      | 119.40   |
| 35  | BB    | 71   | A    | C4'-C3'-C2' | 5.67  | 108.27      | 102.60   |
| 35  | BB    | 930  | G    | P-O3'-C3'   | 5.67  | 126.50      | 119.70   |
| 35  | BB    | 937  | C    | C5-C4-N4    | -5.67 | 116.23      | 120.20   |
| 35  | BB    | 958  | U    | C4-C5-C6    | 5.67  | 123.10      | 119.70   |
| 35  | BB    | 1159 | U    | N3-C4-C5    | -5.67 | 111.20      | 114.60   |
| 35  | BB    | 1290 | C    | C2-N3-C4    | 5.67  | 122.73      | 119.90   |
| 35  | BB    | 2102 | G    | N3-C2-N2    | 5.67  | 123.87      | 119.90   |
| 1   | AA    | 440  | C    | C4-C5-C6    | 5.67  | 120.23      | 117.40   |
| 1   | AA    | 713  | G    | C5-N7-C8    | -5.67 | 101.47      | 104.30   |
| 1   | AA    | 1030 | U    | O4'-C1'-N1  | 5.67  | 112.73      | 108.20   |
| 1   | AA    | 1164 | G    | C5-C6-O6    | -5.67 | 125.20      | 128.60   |
| 28  | B3    | 10   | SER  | N-CA-CB     | 5.67  | 119.00      | 110.50   |
| 34  | BA    | 84   | G    | C5-N7-C8    | -5.67 | 101.47      | 104.30   |
| 35  | BB    | 223  | A    | N7-C8-N9    | 5.67  | 116.63      | 113.80   |
| 35  | BB    | 444  | C    | C4'-C3'-C2' | -5.67 | 96.93       | 102.60   |
| 35  | BB    | 1037 | G    | C2-N3-C4    | -5.67 | 109.07      | 111.90   |
| 35  | BB    | 1374 | G    | C5-C6-N1    | -5.67 | 108.67      | 111.50   |
| 35  | BB    | 1710 | G    | C5'-C4'-O4' | 5.67  | 115.90      | 109.10   |
| 35  | BB    | 2051 | A    | O4'-C1'-N9  | 5.67  | 112.73      | 108.20   |
| 35  | BB    | 2856 | A    | N3-C4-N9    | 5.67  | 131.93      | 127.40   |
| 35  | BB    | 15   | G    | C4-C5-N7    | 5.67  | 113.07      | 110.80   |
| 35  | BB    | 923  | G    | C8-N9-C4    | 5.67  | 108.67      | 106.40   |
| 35  | BB    | 1090 | A    | C5-C6-N6    | -5.67 | 119.17      | 123.70   |
| 35  | BB    | 1306 | C    | P-O3'-C3'   | -5.67 | 112.90      | 119.70   |
| 35  | BB    | 1386 | C    | C2-N3-C4    | 5.67  | 122.73      | 119.90   |
| 35  | BB    | 2703 | C    | N3-C4-N4    | 5.67  | 121.97      | 118.00   |
| 1   | AA    | 27   | G    | N1-C2-N3    | -5.66 | 120.50      | 123.90   |
| 1   | AA    | 198  | G    | C2-N3-C4    | 5.66  | 114.73      | 111.90   |
| 1   | AA    | 229  | U    | O4'-C1'-N1  | 5.66  | 112.73      | 108.20   |
| 1   | AA    | 319  | G    | C2-N3-C4    | -5.66 | 109.07      | 111.90   |
| 1   | AA    | 368  | U    | N1-C2-N3    | 5.66  | 118.30      | 114.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 756  | C    | N1-C2-O2    | -5.66 | 115.50      | 118.90   |
| 1   | AA    | 1080 | A    | C5-C6-N1    | -5.66 | 114.87      | 117.70   |
| 34  | BA    | 32   | U    | C4-C5-C6    | -5.66 | 116.30      | 119.70   |
| 34  | BA    | 79   | G    | N7-C8-N9    | 5.66  | 115.93      | 113.10   |
| 35  | BB    | 36   | G    | N9-C4-C5    | 5.66  | 107.67      | 105.40   |
| 35  | BB    | 430  | A    | C1'-O4'-C4' | 5.66  | 114.43      | 109.90   |
| 35  | BB    | 1227 | G    | C6-C5-N7    | -5.66 | 127.00      | 130.40   |
| 35  | BB    | 1279 | G    | C4-C5-C6    | 5.66  | 122.20      | 118.80   |
| 35  | BB    | 1681 | G    | P-O3'-C3'   | -5.66 | 112.90      | 119.70   |
| 35  | BB    | 1988 | G    | N9-C4-C5    | -5.66 | 103.13      | 105.40   |
| 35  | BB    | 2053 | G    | C5-N7-C8    | 5.66  | 107.13      | 104.30   |
| 35  | BB    | 2389 | G    | C6-N1-C2    | -5.66 | 121.70      | 125.10   |
| 35  | BB    | 2425 | A    | N7-C8-N9    | 5.66  | 116.63      | 113.80   |
| 35  | BB    | 2464 | G    | C5-C6-N1    | -5.66 | 108.67      | 111.50   |
| 1   | AA    | 134  | G    | N9-C4-C5    | -5.66 | 103.14      | 105.40   |
| 1   | AA    | 743  | A    | C6-N1-C2    | -5.66 | 115.20      | 118.60   |
| 1   | AA    | 1020 | G    | N9-C4-C5    | 5.66  | 107.67      | 105.40   |
| 1   | AA    | 1245 | C    | C1'-O4'-C4' | -5.66 | 105.37      | 109.90   |
| 1   | AA    | 1358 | U    | P-O3'-C3'   | -5.66 | 112.91      | 119.70   |
| 35  | BB    | 1475 | G    | C6-C5-N7    | -5.66 | 127.00      | 130.40   |
| 35  | BB    | 2270 | A    | C6-N1-C2    | -5.66 | 115.20      | 118.60   |
| 39  | BF    | 174  | PHE  | N-CA-C      | -5.66 | 95.71       | 111.00   |
| 1   | AA    | 156  | C    | N1-C2-N3    | 5.66  | 123.16      | 119.20   |
| 8   | AH    | 98   | LEU  | CB-CG-CD2   | 5.66  | 120.62      | 111.00   |
| 8   | AH    | 121  | GLY  | N-CA-C      | -5.66 | 98.95       | 113.10   |
| 22  | AV    | 57   | A    | C5-C6-N6    | -5.66 | 119.17      | 123.70   |
| 35  | BB    | 172  | A    | C5'-C4'-O4' | 5.66  | 115.89      | 109.10   |
| 35  | BB    | 205  | G    | N1-C6-O6    | 5.66  | 123.30      | 119.90   |
| 35  | BB    | 385  | C    | N3-C2-O2    | 5.66  | 125.86      | 121.90   |
| 35  | BB    | 849  | A    | C5-C6-N6    | -5.66 | 119.17      | 123.70   |
| 35  | BB    | 931  | U    | P-O3'-C3'   | 5.66  | 126.49      | 119.70   |
| 35  | BB    | 960  | A    | C5-C6-N6    | -5.66 | 119.17      | 123.70   |
| 35  | BB    | 1112 | G    | N1-C2-N3    | -5.66 | 120.50      | 123.90   |
| 35  | BB    | 1275 | A    | C4-C5-N7    | -5.66 | 107.87      | 110.70   |
| 35  | BB    | 2059 | A    | C8-N9-C4    | 5.66  | 108.06      | 105.80   |
| 35  | BB    | 2142 | A    | C2-N3-C4    | -5.66 | 107.77      | 110.60   |
| 35  | BB    | 2543 | G    | N7-C8-N9    | 5.66  | 115.93      | 113.10   |
| 1   | AA    | 208  | U    | C5-C6-N1    | 5.66  | 125.53      | 122.70   |
| 1   | AA    | 1061 | G    | N1-C2-N3    | -5.66 | 120.50      | 123.90   |
| 1   | AA    | 1320 | C    | C6-N1-C2    | -5.66 | 118.04      | 120.30   |
| 1   | AA    | 1360 | A    | O5'-C5'-C4' | -5.66 | 100.95      | 111.70   |
| 22  | AV    | 2    | G    | N7-C8-N9    | 5.66  | 115.93      | 113.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 300  | A    | C8-N9-C4    | -5.66 | 103.54      | 105.80   |
| 35  | BB    | 535  | G    | O4'-C1'-N9  | 5.66  | 112.73      | 108.20   |
| 35  | BB    | 753  | A    | C5-C6-N1    | -5.66 | 114.87      | 117.70   |
| 35  | BB    | 2008 | C    | N3-C4-N4    | 5.66  | 121.96      | 118.00   |
| 35  | BB    | 2679 | A    | C6-C5-N7    | -5.66 | 128.34      | 132.30   |
| 1   | AA    | 362  | G    | C1'-O4'-C4' | -5.66 | 105.37      | 109.90   |
| 30  | B5    | 164  | ARG  | NE-CZ-NH2   | -5.66 | 117.47      | 120.30   |
| 34  | BA    | 52   | A    | C4'-C3'-C2' | -5.66 | 96.94       | 102.60   |
| 35  | BB    | 322  | A    | C4-C5-N7    | -5.66 | 107.87      | 110.70   |
| 35  | BB    | 1032 | A    | N7-C8-N9    | -5.66 | 110.97      | 113.80   |
| 35  | BB    | 1794 | A    | N9-C1'-C2'  | -5.66 | 105.78      | 112.00   |
| 35  | BB    | 1823 | G    | P-O3'-C3'   | -5.66 | 112.91      | 119.70   |
| 35  | BB    | 1937 | A    | N1-C2-N3    | -5.66 | 126.47      | 129.30   |
| 35  | BB    | 2272 | U    | C5-C4-O4    | -5.66 | 122.51      | 125.90   |
| 1   | AA    | 388  | G    | C5'-C4'-O4' | 5.66  | 115.89      | 109.10   |
| 1   | AA    | 407  | U    | C5-C4-O4    | -5.66 | 122.51      | 125.90   |
| 1   | AA    | 607  | A    | C5-C6-N6    | -5.66 | 119.18      | 123.70   |
| 1   | AA    | 873  | A    | O4'-C1'-N9  | 5.66  | 112.72      | 108.20   |
| 1   | AA    | 874  | G    | N1-C2-N2    | 5.66  | 121.29      | 116.20   |
| 1   | AA    | 1175 | G    | N3-C2-N2    | 5.66  | 123.86      | 119.90   |
| 22  | AV    | 14   | A    | C5-C6-N6    | -5.66 | 119.18      | 123.70   |
| 35  | BB    | 120  | U    | C4-C5-C6    | 5.66  | 123.09      | 119.70   |
| 35  | BB    | 696  | G    | C5-C6-O6    | 5.66  | 131.99      | 128.60   |
| 35  | BB    | 1002 | G    | N9-C4-C5    | -5.66 | 103.14      | 105.40   |
| 35  | BB    | 1991 | U    | C5-C4-O4    | 5.66  | 129.29      | 125.90   |
| 35  | BB    | 2392 | A    | N9-C1'-C2'  | -5.66 | 105.78      | 112.00   |
| 35  | BB    | 2654 | A    | N7-C8-N9    | 5.66  | 116.63      | 113.80   |
| 1   | AA    | 1065 | U    | C2-N3-C4    | -5.65 | 123.61      | 127.00   |
| 1   | AA    | 1135 | U    | O4'-C1'-N1  | 5.65  | 112.72      | 108.20   |
| 1   | AA    | 1238 | A    | C5'-C4'-C3' | 5.65  | 125.05      | 116.00   |
| 6   | AF    | 61   | LEU  | CB-CA-C     | 5.65  | 120.94      | 110.20   |
| 19  | AS    | 54   | ARG  | NE-CZ-NH2   | -5.65 | 117.47      | 120.30   |
| 22  | AV    | 61   | C    | N3-C4-N4    | 5.65  | 121.96      | 118.00   |
| 35  | BB    | 302  | C    | C4-C5-C6    | 5.65  | 120.23      | 117.40   |
| 35  | BB    | 407  | G    | C3'-C2'-C1' | 5.65  | 106.02      | 101.50   |
| 35  | BB    | 498  | G    | N1-C2-N3    | -5.65 | 120.51      | 123.90   |
| 35  | BB    | 2453 | A    | C4-C5-C6    | 5.65  | 119.83      | 117.00   |
| 35  | BB    | 2745 | C    | N1-C2-N3    | -5.65 | 115.24      | 119.20   |
| 1   | AA    | 515  | G    | C4'-C3'-C2' | -5.65 | 96.95       | 102.60   |
| 1   | AA    | 1207 | G    | C6-C5-N7    | -5.65 | 127.01      | 130.40   |
| 1   | AA    | 1392 | G    | C5-C6-N1    | -5.65 | 108.67      | 111.50   |
| 35  | BB    | 11   | C    | N1-C2-O2    | 5.65  | 122.29      | 118.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1702 | G    | C4-C5-N7    | -5.65 | 108.54      | 110.80   |
| 35  | BB    | 2636 | C    | N3-C4-C5    | -5.65 | 119.64      | 121.90   |
| 35  | BB    | 2782 | G    | C4-N9-C1'   | 5.65  | 133.85      | 126.50   |
| 1   | AA    | 371  | A    | O4'-C1'-N9  | 5.65  | 112.72      | 108.20   |
| 1   | AA    | 456  | A    | N7-C8-N9    | 5.65  | 116.62      | 113.80   |
| 1   | AA    | 460  | A    | C8-N9-C4    | 5.65  | 108.06      | 105.80   |
| 1   | AA    | 556  | C    | C2-N3-C4    | 5.65  | 122.72      | 119.90   |
| 1   | AA    | 732  | C    | C5-C6-N1    | 5.65  | 123.83      | 121.00   |
| 1   | AA    | 968  | A    | C4-N9-C1'   | 5.65  | 136.47      | 126.30   |
| 1   | AA    | 1046 | A    | C5-C6-N1    | -5.65 | 114.88      | 117.70   |
| 1   | AA    | 1151 | A    | C6-C5-N7    | -5.65 | 128.34      | 132.30   |
| 15  | AO    | 71   | ARG  | NE-CZ-NH2   | -5.65 | 117.47      | 120.30   |
| 34  | BA    | 54   | G    | C6-C5-N7    | -5.65 | 127.01      | 130.40   |
| 35  | BB    | 637  | A    | N3-C4-C5    | -5.65 | 122.84      | 126.80   |
| 35  | BB    | 1600 | C    | C6-N1-C2    | 5.65  | 122.56      | 120.30   |
| 35  | BB    | 1666 | G    | C4-N9-C1'   | -5.65 | 119.16      | 126.50   |
| 35  | BB    | 2090 | A    | C5-C6-N1    | -5.65 | 114.88      | 117.70   |
| 1   | AA    | 144  | G    | C1'-O4'-C4' | -5.65 | 105.38      | 109.90   |
| 1   | AA    | 646  | G    | N3-C2-N2    | 5.65  | 123.85      | 119.90   |
| 1   | AA    | 977  | A    | C5'-C4'-C3' | -5.65 | 106.96      | 116.00   |
| 1   | AA    | 1252 | A    | C8-N9-C4    | -5.65 | 103.54      | 105.80   |
| 35  | BB    | 184  | C    | N1-C2-N3    | -5.65 | 115.25      | 119.20   |
| 35  | BB    | 282  | A    | N3-C4-N9    | -5.65 | 122.88      | 127.40   |
| 35  | BB    | 882  | G    | C5-C6-O6    | -5.65 | 125.21      | 128.60   |
| 35  | BB    | 1266 | G    | C2-N3-C4    | 5.65  | 114.72      | 111.90   |
| 35  | BB    | 1347 | A    | C6-C5-N7    | -5.65 | 128.35      | 132.30   |
| 35  | BB    | 2109 | U    | C4'-C3'-C2' | -5.65 | 96.95       | 102.60   |
| 1   | AA    | 32   | A    | C4-C5-N7    | -5.65 | 107.88      | 110.70   |
| 1   | AA    | 1189 | U    | P-O5'-C5'   | 5.65  | 129.94      | 120.90   |
| 31  | B6    | 28   | ARG  | NE-CZ-NH1   | -5.65 | 117.48      | 120.30   |
| 35  | BB    | 1789 | A    | C5-C6-N1    | -5.65 | 114.88      | 117.70   |
| 35  | BB    | 2352 | A    | O4'-C1'-N9  | 5.65  | 112.72      | 108.20   |
| 35  | BB    | 2400 | G    | C6-C5-N7    | -5.65 | 127.01      | 130.40   |
| 1   | AA    | 30   | U    | C1'-O4'-C4' | -5.65 | 105.38      | 109.90   |
| 1   | AA    | 205  | A    | N9-C1'-C2'  | -5.65 | 105.79      | 112.00   |
| 1   | AA    | 363  | A    | C6-C5-N7    | -5.65 | 128.35      | 132.30   |
| 1   | AA    | 550  | G    | O4'-C1'-N9  | 5.65  | 112.72      | 108.20   |
| 1   | AA    | 1175 | G    | C4-N9-C1'   | -5.65 | 119.16      | 126.50   |
| 7   | AG    | 100  | MET  | CG-SD-CE    | -5.65 | 91.17       | 100.20   |
| 35  | BB    | 186  | G    | C8-N9-C4    | -5.65 | 104.14      | 106.40   |
| 35  | BB    | 569  | U    | C5'-C4'-O4' | -5.65 | 102.33      | 109.10   |
| 35  | BB    | 2104 | C    | C5-C6-N1    | 5.65  | 123.82      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2221 | G    | C4-C5-N7    | 5.65  | 113.06      | 110.80   |
| 1   | AA    | 225  | C    | OP1-P-OP2   | -5.64 | 111.13      | 119.60   |
| 1   | AA    | 324  | G    | N9-C4-C5    | -5.64 | 103.14      | 105.40   |
| 1   | AA    | 429  | U    | O5'-P-OP1   | 5.64  | 117.47      | 110.70   |
| 1   | AA    | 778  | G    | C5-C6-O6    | -5.64 | 125.21      | 128.60   |
| 1   | AA    | 941  | G    | O5'-P-OP1   | 5.64  | 117.47      | 110.70   |
| 1   | AA    | 1468 | A    | C5-C6-N6    | -5.64 | 119.19      | 123.70   |
| 34  | BA    | 48   | U    | C3'-C2'-C1' | 5.64  | 106.02      | 101.50   |
| 35  | BB    | 24   | G    | C5-C6-O6    | -5.64 | 125.21      | 128.60   |
| 35  | BB    | 129  | C    | O3'-P-O5'   | -5.64 | 93.28       | 104.00   |
| 35  | BB    | 667  | U    | N1-C2-O2    | -5.64 | 118.85      | 122.80   |
| 35  | BB    | 882  | G    | C8-N9-C4    | 5.64  | 108.66      | 106.40   |
| 35  | BB    | 1613 | G    | N3-C4-C5    | 5.64  | 131.42      | 128.60   |
| 35  | BB    | 2481 | G    | C6-C5-N7    | -5.64 | 127.01      | 130.40   |
| 35  | BB    | 2755 | C    | P-O5'-C5'   | -5.64 | 111.87      | 120.90   |
| 35  | BB    | 2835 | A    | C4'-C3'-C2' | -5.64 | 96.95       | 102.60   |
| 1   | AA    | 10   | A    | C4-N9-C1'   | -5.64 | 116.14      | 126.30   |
| 1   | AA    | 683  | G    | P-O5'-C5'   | -5.64 | 111.87      | 120.90   |
| 1   | AA    | 1222 | G    | C4-C5-C6    | 5.64  | 122.19      | 118.80   |
| 1   | AA    | 1232 | U    | N1-C1'-C2'  | -5.64 | 105.79      | 112.00   |
| 1   | AA    | 1316 | G    | C4-C5-N7    | -5.64 | 108.54      | 110.80   |
| 7   | AG    | 79   | VAL  | N-CA-C      | -5.64 | 95.76       | 111.00   |
| 35  | BB    | 1094 | U    | C2-N3-C4    | -5.64 | 123.61      | 127.00   |
| 35  | BB    | 1144 | A    | C4-C5-N7    | -5.64 | 107.88      | 110.70   |
| 35  | BB    | 1309 | G    | O4'-C1'-N9  | 5.64  | 112.72      | 108.20   |
| 35  | BB    | 2063 | C    | C5-C4-N4    | -5.64 | 116.25      | 120.20   |
| 35  | BB    | 2784 | U    | O4'-C1'-N1  | 5.64  | 112.71      | 108.20   |
| 36  | BC    | 212  | TRP  | CA-CB-CG    | 5.64  | 124.42      | 113.70   |
| 35  | BB    | 86   | G    | N9-C4-C5    | 5.64  | 107.66      | 105.40   |
| 35  | BB    | 665  | U    | N3-C4-O4    | 5.64  | 123.35      | 119.40   |
| 35  | BB    | 705  | A    | C5-C6-N1    | -5.64 | 114.88      | 117.70   |
| 35  | BB    | 2592 | G    | P-O3'-C3'   | -5.64 | 112.93      | 119.70   |
| 1   | AA    | 147  | G    | C4'-C3'-C2' | -5.64 | 96.96       | 102.60   |
| 1   | AA    | 258  | G    | N1-C2-N3    | -5.64 | 120.52      | 123.90   |
| 1   | AA    | 566  | G    | C4-C5-N7    | -5.64 | 108.54      | 110.80   |
| 1   | AA    | 1423 | G    | C6-C5-N7    | -5.64 | 127.02      | 130.40   |
| 3   | AC    | 38   | VAL  | CA-CB-CG1   | 5.64  | 119.36      | 110.90   |
| 35  | BB    | 1155 | A    | C5-N7-C8    | 5.64  | 106.72      | 103.90   |
| 35  | BB    | 1301 | A    | N7-C8-N9    | -5.64 | 110.98      | 113.80   |
| 35  | BB    | 1380 | G    | C4'-C3'-C2' | -5.64 | 96.96       | 102.60   |
| 35  | BB    | 1429 | G    | C8-N9-C4    | -5.64 | 104.14      | 106.40   |
| 35  | BB    | 2337 | G    | N3-C4-C5    | -5.64 | 125.78      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2443 | C    | N3-C4-N4    | 5.64  | 121.95      | 118.00   |
| 1   | AA    | 320  | A    | C8-N9-C4    | 5.64  | 108.06      | 105.80   |
| 6   | AF    | 8    | PHE  | N-CA-CB     | 5.64  | 120.75      | 110.60   |
| 35  | BB    | 219  | A    | N1-C6-N6    | 5.64  | 121.98      | 118.60   |
| 35  | BB    | 1191 | G    | N3-C4-C5    | -5.64 | 125.78      | 128.60   |
| 35  | BB    | 2775 | G    | N3-C4-N9    | 5.64  | 129.38      | 126.00   |
| 1   | AA    | 572  | A    | C4-C5-C6    | 5.64  | 119.82      | 117.00   |
| 1   | AA    | 927  | G    | N9-C4-C5    | -5.64 | 103.15      | 105.40   |
| 1   | AA    | 1241 | G    | P-O3'-C3'   | -5.64 | 112.94      | 119.70   |
| 1   | AA    | 1436 | U    | N3-C4-C5    | -5.64 | 111.22      | 114.60   |
| 34  | BA    | 79   | G    | O4'-C1'-N9  | 5.64  | 112.71      | 108.20   |
| 35  | BB    | 388  | G    | N3-C4-N9    | -5.64 | 122.62      | 126.00   |
| 35  | BB    | 603  | A    | C3'-C2'-C1' | -5.64 | 96.99       | 101.50   |
| 35  | BB    | 909  | A    | N3-C4-N9    | 5.64  | 131.91      | 127.40   |
| 35  | BB    | 954  | G    | C5-N7-C8    | 5.64  | 107.12      | 104.30   |
| 35  | BB    | 1070 | A    | C5-C6-N1    | -5.64 | 114.88      | 117.70   |
| 35  | BB    | 1396 | U    | OP1-P-OP2   | -5.64 | 111.14      | 119.60   |
| 35  | BB    | 1935 | G    | C2-N3-C4    | 5.64  | 114.72      | 111.90   |
| 35  | BB    | 2465 | C    | C2-N3-C4    | 5.64  | 122.72      | 119.90   |
| 35  | BB    | 2872 | A    | C6-N1-C2    | 5.64  | 121.98      | 118.60   |
| 1   | AA    | 913  | A    | C4-C5-C6    | 5.63  | 119.82      | 117.00   |
| 3   | AC    | 126  | ARG  | NE-CZ-NH1   | 5.63  | 123.12      | 120.30   |
| 14  | AN    | 42   | ASN  | CA-CB-CG    | -5.63 | 101.00      | 113.40   |
| 35  | BB    | 12   | U    | N3-C4-O4    | 5.63  | 123.34      | 119.40   |
| 35  | BB    | 784  | G    | C6-N1-C2    | 5.63  | 128.48      | 125.10   |
| 35  | BB    | 1809 | A    | O4'-C1'-N9  | 5.63  | 112.71      | 108.20   |
| 35  | BB    | 1881 | C    | C2-N3-C4    | 5.63  | 122.72      | 119.90   |
| 35  | BB    | 2163 | A    | N3-C4-C5    | -5.63 | 122.86      | 126.80   |
| 35  | BB    | 2228 | G    | C5'-C4'-O4' | 5.63  | 115.86      | 109.10   |
| 45  | BL    | 5    | THR  | CA-CB-CG2   | -5.63 | 104.51      | 112.40   |
| 1   | AA    | 701  | U    | N3-C4-C5    | -5.63 | 111.22      | 114.60   |
| 35  | BB    | 343  | C    | N3-C4-N4    | 5.63  | 121.94      | 118.00   |
| 35  | BB    | 774  | G    | C5-N7-C8    | -5.63 | 101.48      | 104.30   |
| 35  | BB    | 1630 | A    | N3-C4-C5    | -5.63 | 122.86      | 126.80   |
| 35  | BB    | 1760 | C    | P-O3'-C3'   | 5.63  | 126.46      | 119.70   |
| 35  | BB    | 2799 | A    | O4'-C4'-C3' | -5.63 | 98.37       | 104.00   |
| 1   | AA    | 112  | G    | C5-C6-N1    | -5.63 | 108.68      | 111.50   |
| 1   | AA    | 207  | C    | C4-C5-C6    | 5.63  | 120.22      | 117.40   |
| 1   | AA    | 679  | C    | C2-N3-C4    | 5.63  | 122.72      | 119.90   |
| 1   | AA    | 1475 | G    | C5-C6-N1    | -5.63 | 108.68      | 111.50   |
| 7   | AG    | 115  | MET  | CG-SD-CE    | -5.63 | 91.19       | 100.20   |
| 35  | BB    | 141  | G    | C5-C6-N1    | -5.63 | 108.69      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 725  | G    | C4-C5-N7    | 5.63  | 113.05      | 110.80   |
| 35  | BB    | 1061 | U    | C2-N3-C4    | -5.63 | 123.62      | 127.00   |
| 35  | BB    | 1330 | C    | N3-C4-C5    | -5.63 | 119.65      | 121.90   |
| 35  | BB    | 2024 | G    | N1-C2-N2    | 5.63  | 121.27      | 116.20   |
| 35  | BB    | 2053 | G    | N1-C2-N3    | -5.63 | 120.52      | 123.90   |
| 35  | BB    | 2637 | U    | N3-C4-O4    | 5.63  | 123.34      | 119.40   |
| 1   | AA    | 667  | G    | N1-C2-N3    | -5.63 | 120.52      | 123.90   |
| 1   | AA    | 1137 | C    | C6-N1-C1'   | -5.63 | 114.04      | 120.80   |
| 1   | AA    | 1448 | C    | N3-C4-N4    | 5.63  | 121.94      | 118.00   |
| 34  | BA    | 26   | C    | O4'-C1'-N1  | 5.63  | 112.70      | 108.20   |
| 35  | BB    | 595  | C    | C4-C5-C6    | 5.63  | 120.22      | 117.40   |
| 35  | BB    | 1136 | G    | C5-C6-N1    | 5.63  | 114.31      | 111.50   |
| 35  | BB    | 1585 | C    | P-O3'-C3'   | 5.63  | 126.46      | 119.70   |
| 36  | BC    | 202  | ARG  | CA-CB-CG    | 5.63  | 125.78      | 113.40   |
| 1   | AA    | 354  | G    | N1-C6-O6    | 5.63  | 123.28      | 119.90   |
| 1   | AA    | 378  | G    | C3'-C2'-C1' | -5.63 | 97.00       | 101.50   |
| 1   | AA    | 1328 | C    | C5-C6-N1    | 5.63  | 123.81      | 121.00   |
| 1   | AA    | 1511 | G    | N1-C2-N3    | -5.63 | 120.52      | 123.90   |
| 16  | AP    | 65   | ALA  | CB-CA-C     | -5.63 | 101.66      | 110.10   |
| 35  | BB    | 703  | U    | C4'-C3'-C2' | -5.63 | 96.97       | 102.60   |
| 35  | BB    | 1156 | A    | N7-C8-N9    | -5.63 | 110.99      | 113.80   |
| 35  | BB    | 1544 | A    | N3-C4-N9    | 5.63  | 131.90      | 127.40   |
| 35  | BB    | 1850 | G    | N3-C4-C5    | -5.63 | 125.79      | 128.60   |
| 35  | BB    | 1888 | G    | C5-C6-N1    | -5.63 | 108.69      | 111.50   |
| 35  | BB    | 2183 | A    | C4-C5-N7    | 5.63  | 113.51      | 110.70   |
| 35  | BB    | 2240 | U    | C2-N3-C4    | 5.63  | 130.38      | 127.00   |
| 1   | AA    | 34   | C    | N1-C2-N3    | -5.63 | 115.26      | 119.20   |
| 1   | AA    | 176  | C    | C3'-C2'-C1' | 5.63  | 106.00      | 101.50   |
| 1   | AA    | 380  | G    | C2-N3-C4    | 5.63  | 114.71      | 111.90   |
| 1   | AA    | 1005 | A    | C4-C5-N7    | -5.63 | 107.89      | 110.70   |
| 1   | AA    | 1480 | A    | N9-C1'-C2'  | -5.63 | 105.81      | 112.00   |
| 35  | BB    | 401  | A    | C4-C5-N7    | -5.63 | 107.89      | 110.70   |
| 35  | BB    | 582  | A    | C5'-C4'-C3' | -5.63 | 107.00      | 116.00   |
| 35  | BB    | 2089 | C    | C2-N1-C1'   | -5.63 | 112.61      | 118.80   |
| 35  | BB    | 2173 | A    | N1-C2-N3    | 5.63  | 132.11      | 129.30   |
| 35  | BB    | 2238 | G    | N1-C2-N3    | -5.63 | 120.52      | 123.90   |
| 35  | BB    | 2450 | A    | C6-N1-C2    | 5.63  | 121.98      | 118.60   |
| 35  | BB    | 2877 | G    | C4-C5-N7    | -5.63 | 108.55      | 110.80   |
| 1   | AA    | 71   | A    | O4'-C1'-N9  | 5.62  | 112.70      | 108.20   |
| 1   | AA    | 896  | C    | C4'-C3'-C2' | -5.62 | 96.97       | 102.60   |
| 1   | AA    | 901  | A    | O4'-C1'-N9  | 5.62  | 112.70      | 108.20   |
| 35  | BB    | 1043 | C    | O4'-C4'-C3' | -5.62 | 98.38       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1644 | C    | C2-N1-C1'   | 5.62  | 124.99      | 118.80   |
| 35  | BB    | 2033 | A    | C4-C5-N7    | -5.62 | 107.89      | 110.70   |
| 35  | BB    | 2199 | A    | N9-C4-C5    | 5.62  | 108.05      | 105.80   |
| 1   | AA    | 367  | U    | C5-C4-O4    | -5.62 | 122.53      | 125.90   |
| 1   | AA    | 1057 | G    | N1-C2-N2    | -5.62 | 111.14      | 116.20   |
| 1   | AA    | 1064 | G    | O4'-C1'-C2' | 5.62  | 112.66      | 107.60   |
| 5   | AE    | 127  | TYR  | CZ-CE2-CD2  | -5.62 | 114.74      | 119.80   |
| 34  | BA    | 9    | G    | C5'-C4'-C3' | -5.62 | 107.00      | 116.00   |
| 34  | BA    | 13   | G    | N1-C2-N3    | -5.62 | 120.53      | 123.90   |
| 35  | BB    | 19   | A    | C5-C6-N6    | -5.62 | 119.20      | 123.70   |
| 35  | BB    | 30   | G    | C5-C6-N1    | 5.62  | 114.31      | 111.50   |
| 35  | BB    | 247  | G    | C5-C6-O6    | -5.62 | 125.23      | 128.60   |
| 35  | BB    | 637  | A    | C5-C6-N1    | -5.62 | 114.89      | 117.70   |
| 35  | BB    | 904  | G    | C5-N7-C8    | 5.62  | 107.11      | 104.30   |
| 35  | BB    | 1098 | A    | O5'-P-OP2   | -5.62 | 100.64      | 105.70   |
| 35  | BB    | 1163 | G    | C4-N9-C1'   | -5.62 | 119.19      | 126.50   |
| 35  | BB    | 1479 | G    | O5'-P-OP2   | -5.62 | 100.64      | 105.70   |
| 35  | BB    | 1790 | C    | O4'-C1'-N1  | 5.62  | 112.70      | 108.20   |
| 35  | BB    | 2670 | A    | O4'-C1'-N9  | 5.62  | 112.70      | 108.20   |
| 35  | BB    | 2700 | A    | C6-N1-C2    | 5.62  | 121.97      | 118.60   |
| 46  | BM    | 10   | ARG  | NE-CZ-NH1   | 5.62  | 123.11      | 120.30   |
| 1   | AA    | 778  | G    | N1-C6-O6    | 5.62  | 123.27      | 119.90   |
| 1   | AA    | 786  | G    | C1'-O4'-C4' | 5.62  | 114.40      | 109.90   |
| 1   | AA    | 876  | C    | N3-C4-N4    | 5.62  | 121.93      | 118.00   |
| 1   | AA    | 1019 | A    | N3-C4-C5    | -5.62 | 122.86      | 126.80   |
| 35  | BB    | 323  | C    | N3-C4-N4    | 5.62  | 121.94      | 118.00   |
| 35  | BB    | 665  | U    | C3'-C2'-C1' | 5.62  | 106.00      | 101.50   |
| 35  | BB    | 919  | U    | C1'-O4'-C4' | 5.62  | 114.40      | 109.90   |
| 35  | BB    | 1072 | C    | N3-C4-C5    | -5.62 | 119.65      | 121.90   |
| 35  | BB    | 1135 | C    | C2-N1-C1'   | 5.62  | 124.98      | 118.80   |
| 35  | BB    | 1289 | C    | C5-C6-N1    | 5.62  | 123.81      | 121.00   |
| 35  | BB    | 2037 | A    | C6-C5-N7    | -5.62 | 128.37      | 132.30   |
| 35  | BB    | 2157 | G    | C5-N7-C8    | 5.62  | 107.11      | 104.30   |
| 35  | BB    | 2277 | G    | C5'-C4'-C3' | -5.62 | 107.00      | 116.00   |
| 35  | BB    | 2314 | A    | N7-C8-N9    | 5.62  | 116.61      | 113.80   |
| 35  | BB    | 2326 | C    | C4-C5-C6    | -5.62 | 114.59      | 117.40   |
| 35  | BB    | 2451 | A    | C3'-C2'-C1' | 5.62  | 106.00      | 101.50   |
| 35  | BB    | 2807 | U    | C3'-C2'-C1' | -5.62 | 97.00       | 101.50   |
| 1   | AA    | 91   | U    | P-O3'-C3'   | -5.62 | 112.96      | 119.70   |
| 1   | AA    | 400  | C    | N3-C4-C5    | -5.62 | 119.65      | 121.90   |
| 1   | AA    | 1205 | U    | N3-C4-O4    | 5.62  | 123.33      | 119.40   |
| 1   | AA    | 1215 | G    | C4-C5-C6    | 5.62  | 122.17      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1392 | G    | N9-C4-C5    | 5.62  | 107.65      | 105.40   |
| 1   | AA    | 1441 | A    | C4-C5-N7    | -5.62 | 107.89      | 110.70   |
| 35  | BB    | 126  | A    | C5-C6-N1    | -5.62 | 114.89      | 117.70   |
| 35  | BB    | 931  | U    | C5'-C4'-O4' | -5.62 | 102.36      | 109.10   |
| 35  | BB    | 1003 | G    | O4'-C1'-N9  | 5.62  | 112.70      | 108.20   |
| 35  | BB    | 1608 | A    | N3-C4-N9    | 5.62  | 131.90      | 127.40   |
| 35  | BB    | 1761 | C    | C5'-C4'-O4' | 5.62  | 115.84      | 109.10   |
| 35  | BB    | 1943 | U    | C3'-C2'-C1' | -5.62 | 97.00       | 101.50   |
| 35  | BB    | 2671 | G    | N1-C6-O6    | 5.62  | 123.27      | 119.90   |
| 35  | BB    | 2776 | A    | N1-C2-N3    | -5.62 | 126.49      | 129.30   |
| 1   | AA    | 39   | G    | O4'-C1'-N9  | 5.62  | 112.69      | 108.20   |
| 1   | AA    | 736  | C    | O4'-C1'-N1  | 5.62  | 112.69      | 108.20   |
| 1   | AA    | 782  | A    | N1-C2-N3    | -5.62 | 126.49      | 129.30   |
| 17  | AQ    | 11   | VAL  | CA-CB-CG1   | 5.62  | 119.33      | 110.90   |
| 34  | BA    | 50   | A    | C4-C5-C6    | 5.62  | 119.81      | 117.00   |
| 35  | BB    | 456  | C    | C5'-C4'-C3' | -5.62 | 107.01      | 116.00   |
| 35  | BB    | 1146 | C    | C5-C4-N4    | -5.62 | 116.27      | 120.20   |
| 35  | BB    | 1231 | U    | N3-C4-C5    | -5.62 | 111.23      | 114.60   |
| 35  | BB    | 1514 | G    | OP1-P-OP2   | -5.62 | 111.17      | 119.60   |
| 35  | BB    | 1846 | G    | C5'-C4'-C3' | -5.62 | 107.01      | 116.00   |
| 35  | BB    | 1946 | U    | N1-C2-N3    | -5.62 | 111.53      | 114.90   |
| 35  | BB    | 2114 | A    | O4'-C1'-N9  | 5.62  | 112.69      | 108.20   |
| 35  | BB    | 2864 | G    | C4'-C3'-C2' | -5.62 | 96.98       | 102.60   |
| 54  | BU    | 50   | ALA  | N-CA-CB     | 5.62  | 117.97      | 110.10   |
| 1   | AA    | 401  | C    | P-O5'-C5'   | -5.62 | 111.91      | 120.90   |
| 1   | AA    | 813  | U    | C5-C4-O4    | 5.62  | 129.27      | 125.90   |
| 1   | AA    | 918  | A    | C3'-C2'-C1' | -5.62 | 97.01       | 101.50   |
| 35  | BB    | 402  | A    | N1-C2-N3    | 5.62  | 132.11      | 129.30   |
| 35  | BB    | 560  | C    | C1'-O4'-C4' | 5.62  | 114.39      | 109.90   |
| 35  | BB    | 1082 | U    | C5'-C4'-C3' | -5.62 | 107.01      | 116.00   |
| 35  | BB    | 1462 | C    | N3-C2-O2    | -5.62 | 117.97      | 121.90   |
| 35  | BB    | 2042 | A    | C6-C5-N7    | -5.62 | 128.37      | 132.30   |
| 1   | AA    | 167  | A    | N3-C4-N9    | 5.62  | 131.89      | 127.40   |
| 1   | AA    | 1071 | C    | C2-N3-C4    | 5.62  | 122.71      | 119.90   |
| 1   | AA    | 1146 | A    | C4-C5-C6    | 5.62  | 119.81      | 117.00   |
| 1   | AA    | 1228 | C    | O4'-C1'-N1  | 5.62  | 112.69      | 108.20   |
| 1   | AA    | 1426 | G    | N1-C2-N2    | -5.62 | 111.15      | 116.20   |
| 26  | B1    | 24   | GLU  | N-CA-CB     | 5.62  | 120.71      | 110.60   |
| 35  | BB    | 334  | C    | C5-C4-N4    | -5.62 | 116.27      | 120.20   |
| 35  | BB    | 561  | G    | C8-N9-C4    | -5.62 | 104.15      | 106.40   |
| 35  | BB    | 712  | G    | N7-C8-N9    | -5.62 | 110.29      | 113.10   |
| 35  | BB    | 1431 | A    | N9-C4-C5    | -5.62 | 103.55      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1977 | A    | C2-N3-C4    | 5.62  | 113.41      | 110.60   |
| 35  | BB    | 2235 | G    | N1-C2-N2    | -5.62 | 111.15      | 116.20   |
| 35  | BB    | 2319 | G    | C6-N1-C2    | 5.62  | 128.47      | 125.10   |
| 35  | BB    | 2390 | U    | C6-N1-C2    | 5.62  | 124.37      | 121.00   |
| 35  | BB    | 2677 | G    | C5-N7-C8    | 5.62  | 107.11      | 104.30   |
| 35  | BB    | 2686 | G    | C3'-C2'-C1' | -5.62 | 97.01       | 101.50   |
| 35  | BB    | 2731 | G    | O4'-C1'-N9  | 5.62  | 112.69      | 108.20   |
| 1   | AA    | 146  | G    | C8-N9-C4    | -5.61 | 104.16      | 106.40   |
| 1   | AA    | 444  | G    | C5-C6-N1    | -5.61 | 108.69      | 111.50   |
| 1   | AA    | 511  | C    | P-O3'-C3'   | 5.61  | 126.44      | 119.70   |
| 1   | AA    | 787  | A    | N1-C6-N6    | 5.61  | 121.97      | 118.60   |
| 1   | AA    | 940  | C    | C5-C4-N4    | -5.61 | 116.27      | 120.20   |
| 1   | AA    | 1145 | A    | N9-C1'-C2'  | -5.61 | 105.82      | 112.00   |
| 1   | AA    | 1236 | A    | C8-N9-C4    | 5.61  | 108.05      | 105.80   |
| 1   | AA    | 1426 | G    | C6-C5-N7    | -5.61 | 127.03      | 130.40   |
| 1   | AA    | 1453 | G    | C4-C5-N7    | -5.61 | 108.56      | 110.80   |
| 7   | AG    | 112  | ASP  | CB-CG-OD1   | -5.61 | 113.25      | 118.30   |
| 35  | BB    | 70   | G    | O4'-C1'-N9  | 5.61  | 112.69      | 108.20   |
| 35  | BB    | 439  | A    | C5-C6-N6    | -5.61 | 119.21      | 123.70   |
| 35  | BB    | 767  | U    | C6-N1-C2    | -5.61 | 117.63      | 121.00   |
| 35  | BB    | 2259 | U    | C5-C6-N1    | 5.61  | 125.51      | 122.70   |
| 35  | BB    | 2507 | C    | C4-C5-C6    | 5.61  | 120.21      | 117.40   |
| 35  | BB    | 2894 | G    | C5-N7-C8    | 5.61  | 107.11      | 104.30   |
| 1   | AA    | 887  | G    | N9-C4-C5    | 5.61  | 107.64      | 105.40   |
| 34  | BA    | 39   | A    | N3-C4-C5    | -5.61 | 122.87      | 126.80   |
| 35  | BB    | 1669 | A    | N3-C4-C5    | -5.61 | 122.87      | 126.80   |
| 35  | BB    | 2240 | U    | N3-C2-O2    | 5.61  | 126.13      | 122.20   |
| 35  | BB    | 2429 | G    | C5-N7-C8    | 5.61  | 107.11      | 104.30   |
| 35  | BB    | 2650 | U    | C6-N1-C2    | -5.61 | 117.63      | 121.00   |
| 35  | BB    | 2754 | U    | N1-C2-N3    | 5.61  | 118.27      | 114.90   |
| 1   | AA    | 46   | G    | C4-C5-N7    | 5.61  | 113.04      | 110.80   |
| 1   | AA    | 57   | G    | C6-C5-N7    | -5.61 | 127.03      | 130.40   |
| 1   | AA    | 331  | G    | N9-C4-C5    | 5.61  | 107.64      | 105.40   |
| 1   | AA    | 1054 | C    | N3-C2-O2    | -5.61 | 117.97      | 121.90   |
| 1   | AA    | 1212 | U    | O4'-C1'-C2' | 5.61  | 112.65      | 107.60   |
| 31  | B6    | 35   | ARG  | NE-CZ-NH1   | 5.61  | 123.11      | 120.30   |
| 35  | BB    | 749  | A    | N3-C4-C5    | -5.61 | 122.87      | 126.80   |
| 35  | BB    | 804  | A    | P-O3'-C3'   | 5.61  | 126.43      | 119.70   |
| 35  | BB    | 935  | C    | N1-C2-N3    | 5.61  | 123.13      | 119.20   |
| 35  | BB    | 1258 | U    | C5-C6-N1    | 5.61  | 125.50      | 122.70   |
| 35  | BB    | 1486 | U    | C4-C5-C6    | -5.61 | 116.33      | 119.70   |
| 35  | BB    | 1628 | G    | C5-N7-C8    | -5.61 | 101.50      | 104.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1848 | A    | C6-C5-N7    | -5.61 | 128.37      | 132.30   |
| 35  | BB    | 2149 | U    | N1-C2-O2    | -5.61 | 118.87      | 122.80   |
| 35  | BB    | 2221 | G    | N7-C8-N9    | 5.61  | 115.91      | 113.10   |
| 1   | AA    | 773  | G    | P-O3'-C3'   | -5.61 | 112.97      | 119.70   |
| 1   | AA    | 1238 | A    | N7-C8-N9    | -5.61 | 111.00      | 113.80   |
| 35  | BB    | 1425 | G    | C4-C5-N7    | 5.61  | 113.04      | 110.80   |
| 35  | BB    | 1500 | G    | N1-C2-N3    | -5.61 | 120.53      | 123.90   |
| 35  | BB    | 2273 | A    | N7-C8-N9    | -5.61 | 111.00      | 113.80   |
| 1   | AA    | 315  | A    | N3-C4-N9    | -5.61 | 122.91      | 127.40   |
| 1   | AA    | 490  | C    | C2-N3-C4    | 5.61  | 122.70      | 119.90   |
| 1   | AA    | 814  | A    | N7-C8-N9    | 5.61  | 116.60      | 113.80   |
| 1   | AA    | 1040 | U    | N3-C4-C5    | -5.61 | 111.23      | 114.60   |
| 1   | AA    | 1442 | G    | C5-C6-O6    | -5.61 | 125.24      | 128.60   |
| 34  | BA    | 26   | C    | O4'-C1'-C2' | 5.61  | 112.65      | 107.60   |
| 35  | BB    | 329  | G    | C5'-C4'-O4' | 5.61  | 115.83      | 109.10   |
| 35  | BB    | 774  | G    | N1-C6-O6    | 5.61  | 123.27      | 119.90   |
| 35  | BB    | 863  | A    | O4'-C1'-N9  | 5.61  | 112.69      | 108.20   |
| 35  | BB    | 1425 | G    | C4-C5-C6    | 5.61  | 122.17      | 118.80   |
| 35  | BB    | 1469 | A    | C2-N3-C4    | -5.61 | 107.80      | 110.60   |
| 35  | BB    | 1697 | G    | N1-C2-N3    | -5.61 | 120.54      | 123.90   |
| 35  | BB    | 2295 | C    | C6-N1-C2    | -5.61 | 118.06      | 120.30   |
| 35  | BB    | 2340 | A    | N9-C1'-C2'  | -5.61 | 105.83      | 112.00   |
| 35  | BB    | 2618 | G    | C4-C5-C6    | 5.61  | 122.16      | 118.80   |
| 35  | BB    | 2665 | A    | P-O3'-C3'   | -5.61 | 112.97      | 119.70   |
| 35  | BB    | 2863 | C    | C2-N3-C4    | 5.61  | 122.70      | 119.90   |
| 1   | AA    | 525  | C    | N3-C4-N4    | 5.61  | 121.92      | 118.00   |
| 1   | AA    | 1043 | G    | C8-N9-C4    | -5.61 | 104.16      | 106.40   |
| 35  | BB    | 1735 | A    | C6-C5-N7    | -5.61 | 128.38      | 132.30   |
| 35  | BB    | 1884 | G    | N3-C4-N9    | -5.61 | 122.64      | 126.00   |
| 35  | BB    | 2009 | A    | N3-C4-N9    | 5.61  | 131.88      | 127.40   |
| 35  | BB    | 2092 | U    | O3'-P-O5'   | -5.61 | 93.35       | 104.00   |
| 35  | BB    | 2111 | U    | N3-C4-C5    | -5.61 | 111.24      | 114.60   |
| 45  | BL    | 48   | ARG  | NE-CZ-NH1   | 5.61  | 123.10      | 120.30   |
| 46  | BM    | 129  | THR  | CA-CB-OG1   | 5.61  | 120.77      | 109.00   |
| 1   | AA    | 122  | G    | C4-C5-C6    | 5.60  | 122.16      | 118.80   |
| 1   | AA    | 981  | U    | C3'-C2'-C1' | -5.60 | 97.02       | 101.50   |
| 1   | AA    | 1269 | A    | C6-C5-N7    | -5.60 | 128.38      | 132.30   |
| 35  | BB    | 325  | G    | N3-C4-C5    | 5.60  | 131.40      | 128.60   |
| 35  | BB    | 500  | G    | O4'-C4'-C3' | -5.60 | 98.40       | 104.00   |
| 35  | BB    | 535  | G    | C5-N7-C8    | 5.60  | 107.10      | 104.30   |
| 1   | AA    | 477  | C    | C5-C4-N4    | -5.60 | 116.28      | 120.20   |
| 1   | AA    | 743  | A    | C8-N9-C4    | 5.60  | 108.04      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 787  | A    | C3'-C2'-C1' | 5.60  | 105.98      | 101.50   |
| 1   | AA    | 833  | G    | C2-N3-C4    | 5.60  | 114.70      | 111.90   |
| 1   | AA    | 872  | A    | C5-C6-N6    | -5.60 | 119.22      | 123.70   |
| 1   | AA    | 1410 | A    | C5-C6-N1    | -5.60 | 114.90      | 117.70   |
| 1   | AA    | 1534 | A    | C6-C5-N7    | -5.60 | 128.38      | 132.30   |
| 35  | BB    | 156  | A    | O4'-C4'-C3' | -5.60 | 98.40       | 104.00   |
| 35  | BB    | 518  | G    | N9-C4-C5    | -5.60 | 103.16      | 105.40   |
| 35  | BB    | 907  | G    | O4'-C1'-N9  | 5.60  | 112.68      | 108.20   |
| 35  | BB    | 1382 | G    | C8-N9-C1'   | -5.60 | 119.72      | 127.00   |
| 35  | BB    | 1433 | A    | O4'-C1'-N9  | 5.60  | 112.68      | 108.20   |
| 35  | BB    | 1491 | G    | C4-C5-N7    | 5.60  | 113.04      | 110.80   |
| 35  | BB    | 1606 | C    | C2-N1-C1'   | 5.60  | 124.96      | 118.80   |
| 35  | BB    | 1776 | G    | O4'-C1'-C2' | -5.60 | 100.20      | 105.80   |
| 35  | BB    | 2422 | C    | C2-N3-C4    | -5.60 | 117.10      | 119.90   |
| 35  | BB    | 2820 | A    | C5-N7-C8    | 5.60  | 106.70      | 103.90   |
| 1   | AA    | 33   | A    | C5-C6-N1    | 5.60  | 120.50      | 117.70   |
| 1   | AA    | 227  | G    | C8-N9-C4    | -5.60 | 104.16      | 106.40   |
| 1   | AA    | 909  | A    | C1'-O4'-C4' | 5.60  | 114.38      | 109.90   |
| 6   | AF    | 86   | ARG  | NE-CZ-NH1   | 5.60  | 123.10      | 120.30   |
| 22  | AV    | 22   | G    | O4'-C1'-N9  | 5.60  | 112.68      | 108.20   |
| 35  | BB    | 1061 | U    | OP1-P-OP2   | -5.60 | 111.20      | 119.60   |
| 35  | BB    | 2206 | C    | C4'-C3'-C2' | -5.60 | 97.00       | 102.60   |
| 35  | BB    | 2575 | C    | P-O3'-C3'   | 5.60  | 126.42      | 119.70   |
| 45  | BL    | 47   | ARG  | CD-NE-CZ    | -5.60 | 115.76      | 123.60   |
| 1   | AA    | 282  | A    | C6-C5-N7    | -5.60 | 128.38      | 132.30   |
| 1   | AA    | 427  | U    | N3-C2-O2    | 5.60  | 126.12      | 122.20   |
| 1   | AA    | 1143 | G    | C8-N9-C4    | -5.60 | 104.16      | 106.40   |
| 1   | AA    | 1398 | A    | C6-N1-C2    | -5.60 | 115.24      | 118.60   |
| 1   | AA    | 1518 | A    | C8-N9-C4    | -5.60 | 103.56      | 105.80   |
| 12  | AL    | 55   | ARG  | NE-CZ-NH2   | -5.60 | 117.50      | 120.30   |
| 35  | BB    | 321  | U    | C2-N3-C4    | 5.60  | 130.36      | 127.00   |
| 35  | BB    | 506  | G    | C5-C6-O6    | -5.60 | 125.24      | 128.60   |
| 35  | BB    | 957  | C    | N3-C4-C5    | -5.60 | 119.66      | 121.90   |
| 35  | BB    | 997  | G    | C8-N9-C1'   | 5.60  | 134.28      | 127.00   |
| 35  | BB    | 1442 | U    | C5-C6-N1    | 5.60  | 125.50      | 122.70   |
| 35  | BB    | 1482 | G    | N1-C2-N3    | -5.60 | 120.54      | 123.90   |
| 35  | BB    | 1546 | G    | C6-C5-N7    | -5.60 | 127.04      | 130.40   |
| 35  | BB    | 1738 | G    | N3-C4-N9    | 5.60  | 129.36      | 126.00   |
| 35  | BB    | 2169 | A    | C2-N3-C4    | 5.60  | 113.40      | 110.60   |
| 35  | BB    | 2340 | A    | C5-C6-N1    | -5.60 | 114.90      | 117.70   |
| 35  | BB    | 2744 | G    | N7-C8-N9    | -5.60 | 110.30      | 113.10   |
| 35  | BB    | 2851 | A    | C5-C6-N1    | -5.60 | 114.90      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 498  | A    | C1'-O4'-C4' | 5.60  | 114.38      | 109.90   |
| 1   | AA    | 566  | G    | N3-C2-N2    | 5.60  | 123.82      | 119.90   |
| 1   | AA    | 859  | G    | C5-C6-O6    | -5.60 | 125.24      | 128.60   |
| 1   | AA    | 1034 | G    | P-O3'-C3'   | -5.60 | 112.98      | 119.70   |
| 7   | AG    | 104  | VAL  | CA-CB-CG1   | 5.60  | 119.30      | 110.90   |
| 35  | BB    | 37   | C    | P-O3'-C3'   | -5.60 | 112.98      | 119.70   |
| 35  | BB    | 716  | A    | C6-N1-C2    | 5.60  | 121.96      | 118.60   |
| 35  | BB    | 969  | G    | C8-N9-C4    | -5.60 | 104.16      | 106.40   |
| 35  | BB    | 983  | A    | C1'-O4'-C4' | 5.60  | 114.38      | 109.90   |
| 35  | BB    | 1549 | A    | C6-C5-N7    | -5.60 | 128.38      | 132.30   |
| 35  | BB    | 2280 | G    | C4-C5-N7    | 5.60  | 113.04      | 110.80   |
| 35  | BB    | 2524 | G    | C3'-C2'-C1' | 5.60  | 105.98      | 101.50   |
| 35  | BB    | 2869 | G    | O4'-C1'-N9  | 5.60  | 112.68      | 108.20   |
| 1   | AA    | 491  | G    | N1-C6-O6    | 5.60  | 123.26      | 119.90   |
| 1   | AA    | 1308 | U    | C4'-C3'-C2' | 5.60  | 108.20      | 102.60   |
| 35  | BB    | 282  | A    | N1-C6-N6    | 5.60  | 121.96      | 118.60   |
| 35  | BB    | 1589 | U    | C3'-C2'-C1' | -5.60 | 97.02       | 101.50   |
| 1   | AA    | 15   | G    | C5-N7-C8    | -5.59 | 101.50      | 104.30   |
| 1   | AA    | 98   | A    | N1-C2-N3    | 5.59  | 132.10      | 129.30   |
| 1   | AA    | 551  | U    | P-O5'-C5'   | 5.59  | 129.85      | 120.90   |
| 1   | AA    | 614  | C    | C5-C6-N1    | 5.59  | 123.80      | 121.00   |
| 1   | AA    | 1154 | G    | C5-N7-C8    | 5.59  | 107.10      | 104.30   |
| 1   | AA    | 1459 | G    | C5-C6-N1    | -5.59 | 108.70      | 111.50   |
| 1   | AA    | 1497 | G    | C5-N7-C8    | 5.59  | 107.10      | 104.30   |
| 1   | AA    | 1513 | A    | N9-C4-C5    | -5.59 | 103.56      | 105.80   |
| 3   | AC    | 7    | ASN  | O-C-N       | -5.59 | 113.69      | 123.20   |
| 35  | BB    | 1596 | A    | N1-C2-N3    | 5.59  | 132.10      | 129.30   |
| 35  | BB    | 1912 | A    | C3'-C2'-C1' | 5.59  | 105.97      | 101.50   |
| 35  | BB    | 1930 | G    | C5-C6-N1    | -5.59 | 108.70      | 111.50   |
| 35  | BB    | 1975 | G    | C5-C6-N1    | -5.59 | 108.70      | 111.50   |
| 35  | BB    | 2188 | U    | N1-C2-O2    | -5.59 | 118.88      | 122.80   |
| 35  | BB    | 2229 | U    | N1-C2-N3    | 5.59  | 118.26      | 114.90   |
| 35  | BB    | 2331 | G    | C2-N3-C4    | -5.59 | 109.10      | 111.90   |
| 35  | BB    | 2526 | G    | C5-C6-O6    | -5.59 | 125.24      | 128.60   |
| 35  | BB    | 2619 | C    | C5-C6-N1    | 5.59  | 123.80      | 121.00   |
| 35  | BB    | 2824 | C    | C5-C6-N1    | 5.59  | 123.80      | 121.00   |
| 1   | AA    | 120  | A    | C5-N7-C8    | 5.59  | 106.70      | 103.90   |
| 35  | BB    | 242  | G    | C2-N3-C4    | -5.59 | 109.10      | 111.90   |
| 35  | BB    | 601  | C    | C4'-C3'-C2' | -5.59 | 97.01       | 102.60   |
| 35  | BB    | 1126 | A    | P-O5'-C5'   | -5.59 | 111.95      | 120.90   |
| 35  | BB    | 1168 | G    | C6-N1-C2    | 5.59  | 128.46      | 125.10   |
| 35  | BB    | 1725 | U    | C4'-C3'-C2' | -5.59 | 97.01       | 102.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1871 | A    | C4-C5-N7    | -5.59 | 107.90      | 110.70   |
| 35  | BB    | 2375 | G    | N9-C1'-C2'  | -5.59 | 105.85      | 112.00   |
| 1   | AA    | 469  | C    | C2-N3-C4    | -5.59 | 117.10      | 119.90   |
| 1   | AA    | 533  | A    | N7-C8-N9    | 5.59  | 116.59      | 113.80   |
| 1   | AA    | 1162 | C    | C6-N1-C2    | -5.59 | 118.06      | 120.30   |
| 1   | AA    | 1222 | G    | C4'-C3'-C2' | -5.59 | 97.01       | 102.60   |
| 1   | AA    | 1231 | G    | N3-C2-N2    | 5.59  | 123.81      | 119.90   |
| 1   | AA    | 1334 | G    | C5-C6-N1    | -5.59 | 108.70      | 111.50   |
| 5   | AE    | 113  | VAL  | CA-CB-CG2   | 5.59  | 119.29      | 110.90   |
| 22  | AV    | 58   | A    | C5-C6-N1    | -5.59 | 114.90      | 117.70   |
| 34  | BA    | 84   | G    | C5-C6-N1    | 5.59  | 114.30      | 111.50   |
| 35  | BB    | 87   | U    | C2-N3-C4    | -5.59 | 123.64      | 127.00   |
| 35  | BB    | 166  | U    | O4'-C1'-N1  | 5.59  | 112.67      | 108.20   |
| 35  | BB    | 505  | A    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 35  | BB    | 665  | U    | C6-N1-C2    | -5.59 | 117.64      | 121.00   |
| 35  | BB    | 868  | U    | C4'-C3'-C2' | -5.59 | 97.01       | 102.60   |
| 35  | BB    | 934  | U    | C5-C4-O4    | -5.59 | 122.55      | 125.90   |
| 35  | BB    | 1098 | A    | N1-C6-N6    | 5.59  | 121.95      | 118.60   |
| 35  | BB    | 1126 | A    | C5-C6-N1    | -5.59 | 114.90      | 117.70   |
| 35  | BB    | 1817 | G    | N1-C2-N3    | -5.59 | 120.55      | 123.90   |
| 35  | BB    | 1914 | C    | N3-C4-C5    | -5.59 | 119.66      | 121.90   |
| 35  | BB    | 2355 | G    | N3-C2-N2    | -5.59 | 115.99      | 119.90   |
| 35  | BB    | 2579 | C    | O4'-C1'-N1  | 5.59  | 112.67      | 108.20   |
| 35  | BB    | 2598 | A    | C3'-C2'-C1' | 5.59  | 105.97      | 101.50   |
| 35  | BB    | 2688 | G    | N1-C2-N2    | -5.59 | 111.17      | 116.20   |
| 1   | AA    | 487  | A    | N9-C4-C5    | 5.59  | 108.03      | 105.80   |
| 1   | AA    | 666  | G    | C6-C5-N7    | -5.59 | 127.05      | 130.40   |
| 1   | AA    | 1511 | G    | C5-C6-N1    | -5.59 | 108.70      | 111.50   |
| 35  | BB    | 70   | G    | N1-C2-N3    | -5.59 | 120.55      | 123.90   |
| 35  | BB    | 528  | A    | C4-C5-C6    | 5.59  | 119.80      | 117.00   |
| 35  | BB    | 726  | G    | C5-C6-O6    | -5.59 | 125.25      | 128.60   |
| 35  | BB    | 1514 | G    | C3'-C2'-C1' | -5.59 | 97.03       | 101.50   |
| 35  | BB    | 1594 | U    | C5-C6-N1    | 5.59  | 125.50      | 122.70   |
| 35  | BB    | 2062 | A    | N9-C4-C5    | -5.59 | 103.56      | 105.80   |
| 35  | BB    | 2864 | G    | N3-C4-C5    | 5.59  | 131.40      | 128.60   |
| 35  | BB    | 2899 | A    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 1   | AA    | 750  | C    | C1'-O4'-C4' | 5.59  | 114.37      | 109.90   |
| 1   | AA    | 845  | A    | N3-C4-C5    | -5.59 | 122.89      | 126.80   |
| 22  | AV    | 76   | A    | OP1-P-OP2   | -5.59 | 111.22      | 119.60   |
| 34  | BA    | 84   | G    | N9-C4-C5    | -5.59 | 103.17      | 105.40   |
| 35  | BB    | 407  | G    | C4-C5-N7    | -5.59 | 108.56      | 110.80   |
| 35  | BB    | 1559 | U    | C2-N1-C1'   | 5.59  | 124.41      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2178 | C    | N1-C2-N3    | -5.59 | 115.29      | 119.20   |
| 35  | BB    | 2204 | G    | N3-C4-N9    | 5.59  | 129.35      | 126.00   |
| 1   | AA    | 213  | G    | N1-C2-N2    | 5.59  | 121.23      | 116.20   |
| 1   | AA    | 353  | A    | C8-N9-C4    | -5.59 | 103.56      | 105.80   |
| 1   | AA    | 484  | G    | N7-C8-N9    | -5.59 | 110.31      | 113.10   |
| 1   | AA    | 554  | A    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 1   | AA    | 826  | C    | C4-C5-C6    | 5.59  | 120.19      | 117.40   |
| 1   | AA    | 888  | G    | N3-C4-C5    | 5.59  | 131.39      | 128.60   |
| 1   | AA    | 942  | G    | C2-N3-C4    | -5.59 | 109.11      | 111.90   |
| 1   | AA    | 1014 | A    | C6-N1-C2    | 5.59  | 121.95      | 118.60   |
| 1   | AA    | 1068 | G    | C6-C5-N7    | -5.59 | 127.05      | 130.40   |
| 1   | AA    | 1118 | U    | C2-N1-C1'   | 5.59  | 124.40      | 117.70   |
| 13  | AM    | 100  | ARG  | NE-CZ-NH2   | -5.59 | 117.51      | 120.30   |
| 22  | AV    | 48   | C    | N3-C4-N4    | 5.59  | 121.91      | 118.00   |
| 35  | BB    | 197  | A    | C8-N9-C4    | -5.59 | 103.56      | 105.80   |
| 35  | BB    | 494  | G    | C4'-C3'-C2' | -5.59 | 97.01       | 102.60   |
| 35  | BB    | 1448 | G    | N9-C1'-C2'  | -5.59 | 105.85      | 112.00   |
| 35  | BB    | 1633 | G    | C4-N9-C1'   | 5.59  | 133.76      | 126.50   |
| 35  | BB    | 1729 | U    | C4'-C3'-C2' | -5.59 | 97.01       | 102.60   |
| 35  | BB    | 1883 | U    | O3'-P-O5'   | -5.59 | 93.39       | 104.00   |
| 35  | BB    | 2121 | G    | C5-N7-C8    | -5.59 | 101.51      | 104.30   |
| 35  | BB    | 2235 | G    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 35  | BB    | 2389 | G    | C5-N7-C8    | 5.59  | 107.09      | 104.30   |
| 53  | BT    | 6    | ARG  | NE-CZ-NH1   | 5.59  | 123.09      | 120.30   |
| 35  | BB    | 840  | C    | C5-C6-N1    | -5.58 | 118.21      | 121.00   |
| 35  | BB    | 1500 | G    | N3-C2-N2    | 5.58  | 123.81      | 119.90   |
| 1   | AA    | 52   | C    | C5'-C4'-O4' | 5.58  | 115.80      | 109.10   |
| 1   | AA    | 120  | A    | C5-C6-N1    | -5.58 | 114.91      | 117.70   |
| 1   | AA    | 129  | A    | C5-C6-N1    | -5.58 | 114.91      | 117.70   |
| 1   | AA    | 297  | G    | C8-N9-C1'   | 5.58  | 134.26      | 127.00   |
| 1   | AA    | 753  | A    | P-O3'-C3'   | -5.58 | 113.00      | 119.70   |
| 1   | AA    | 1036 | A    | P-O5'-C5'   | 5.58  | 129.84      | 120.90   |
| 1   | AA    | 1477 | U    | C5'-C4'-C3' | -5.58 | 107.07      | 116.00   |
| 7   | AG    | 43   | TYR  | CG-CD1-CE1  | 5.58  | 125.77      | 121.30   |
| 35  | BB    | 879  | G    | C4'-C3'-C2' | -5.58 | 97.02       | 102.60   |
| 35  | BB    | 1604 | C    | O5'-C5'-C4' | -5.58 | 101.09      | 111.70   |
| 35  | BB    | 1620 | G    | P-O3'-C3'   | -5.58 | 113.00      | 119.70   |
| 35  | BB    | 1905 | C    | P-O3'-C3'   | 5.58  | 126.40      | 119.70   |
| 35  | BB    | 2077 | A    | N3-C4-C5    | -5.58 | 122.89      | 126.80   |
| 35  | BB    | 2296 | U    | C5-C6-N1    | 5.58  | 125.49      | 122.70   |
| 35  | BB    | 2537 | U    | C4-C5-C6    | -5.58 | 116.35      | 119.70   |
| 35  | BB    | 2656 | U    | O4'-C1'-N1  | 5.58  | 112.67      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2726 | A    | C6-N1-C2    | 5.58  | 121.95      | 118.60   |
| 1   | AA    | 716  | A    | N1-C6-N6    | 5.58  | 121.95      | 118.60   |
| 1   | AA    | 831  | A    | C1'-O4'-C4' | -5.58 | 105.44      | 109.90   |
| 1   | AA    | 863  | U    | N1-C2-O2    | 5.58  | 126.71      | 122.80   |
| 1   | AA    | 996  | A    | N7-C8-N9    | -5.58 | 111.01      | 113.80   |
| 1   | AA    | 1114 | C    | C2-N1-C1'   | 5.58  | 124.94      | 118.80   |
| 1   | AA    | 1258 | G    | C6-N1-C2    | -5.58 | 121.75      | 125.10   |
| 19  | AS    | 35   | ARG  | CB-CA-C     | -5.58 | 99.24       | 110.40   |
| 35  | BB    | 328  | U    | C4-C5-C6    | -5.58 | 116.35      | 119.70   |
| 35  | BB    | 479  | A    | N9-C4-C5    | -5.58 | 103.57      | 105.80   |
| 35  | BB    | 914  | G    | C8-N9-C4    | -5.58 | 104.17      | 106.40   |
| 35  | BB    | 1283 | G    | N3-C2-N2    | 5.58  | 123.81      | 119.90   |
| 35  | BB    | 1413 | A    | C5-C6-N1    | -5.58 | 114.91      | 117.70   |
| 35  | BB    | 1448 | G    | O4'-C1'-N9  | 5.58  | 112.67      | 108.20   |
| 35  | BB    | 1630 | A    | O5'-C5'-C4' | -5.58 | 101.10      | 111.70   |
| 35  | BB    | 1669 | A    | C5-C6-N6    | -5.58 | 119.23      | 123.70   |
| 35  | BB    | 2634 | A    | C4-C5-N7    | -5.58 | 107.91      | 110.70   |
| 35  | BB    | 2741 | A    | N7-C8-N9    | -5.58 | 111.01      | 113.80   |
| 49  | BP    | 101  | GLU  | O-C-N       | -5.58 | 113.77      | 122.70   |
| 1   | AA    | 393  | A    | C5-C6-N1    | -5.58 | 114.91      | 117.70   |
| 1   | AA    | 415  | A    | N1-C2-N3    | -5.58 | 126.51      | 129.30   |
| 1   | AA    | 468  | A    | P-O3'-C3'   | 5.58  | 126.40      | 119.70   |
| 1   | AA    | 954  | G    | C4-C5-C6    | 5.58  | 122.15      | 118.80   |
| 1   | AA    | 1343 | G    | N9-C4-C5    | 5.58  | 107.63      | 105.40   |
| 35  | BB    | 381  | G    | C8-N9-C1'   | -5.58 | 119.75      | 127.00   |
| 35  | BB    | 2132 | U    | O3'-P-O5'   | 5.58  | 114.60      | 104.00   |
| 1   | AA    | 39   | G    | C4-C5-N7    | 5.58  | 113.03      | 110.80   |
| 1   | AA    | 298  | A    | N1-C6-N6    | 5.58  | 121.95      | 118.60   |
| 16  | AP    | 77   | GLU  | OE1-CD-OE2  | 5.58  | 130.00      | 123.30   |
| 35  | BB    | 200  | U    | C4-C5-C6    | 5.58  | 123.05      | 119.70   |
| 35  | BB    | 879  | G    | C4-C5-N7    | 5.58  | 113.03      | 110.80   |
| 35  | BB    | 1199 | U    | C4-C5-C6    | -5.58 | 116.35      | 119.70   |
| 35  | BB    | 1327 | A    | C2-N3-C4    | -5.58 | 107.81      | 110.60   |
| 35  | BB    | 1435 | G    | C8-N9-C4    | -5.58 | 104.17      | 106.40   |
| 35  | BB    | 1471 | G    | C4-C5-N7    | -5.58 | 108.57      | 110.80   |
| 35  | BB    | 1478 | G    | N9-C4-C5    | 5.58  | 107.63      | 105.40   |
| 35  | BB    | 2813 | A    | C1'-O4'-C4' | 5.58  | 114.36      | 109.90   |
| 35  | BB    | 2830 | C    | C4-C5-C6    | 5.58  | 120.19      | 117.40   |
| 35  | BB    | 503  | A    | C5-N7-C8    | 5.58  | 106.69      | 103.90   |
| 35  | BB    | 2056 | G    | C1'-O4'-C4' | 5.58  | 114.36      | 109.90   |
| 35  | BB    | 2105 | U    | N3-C2-O2    | 5.58  | 126.10      | 122.20   |
| 1   | AA    | 201  | G    | C5-C6-N1    | -5.58 | 108.71      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 587  | G    | N7-C8-N9    | -5.58 | 110.31      | 113.10   |
| 1   | AA    | 760  | G    | N1-C6-O6    | 5.58  | 123.25      | 119.90   |
| 1   | AA    | 1162 | C    | C5-C6-N1    | 5.58  | 123.79      | 121.00   |
| 22  | AV    | 43   | G    | O4'-C1'-N9  | 5.58  | 112.66      | 108.20   |
| 35  | BB    | 119  | A    | C2-N3-C4    | -5.58 | 107.81      | 110.60   |
| 35  | BB    | 584  | C    | C6-N1-C2    | -5.58 | 118.07      | 120.30   |
| 35  | BB    | 1336 | A    | O4'-C1'-N9  | 5.58  | 112.66      | 108.20   |
| 35  | BB    | 1927 | A    | C6-C5-N7    | -5.58 | 128.40      | 132.30   |
| 35  | BB    | 2106 | U    | N3-C2-O2    | 5.58  | 126.10      | 122.20   |
| 35  | BB    | 2354 | C    | N3-C2-O2    | 5.58  | 125.80      | 121.90   |
| 35  | BB    | 2443 | C    | N1-C2-N3    | -5.58 | 115.30      | 119.20   |
| 35  | BB    | 2714 | G    | N3-C2-N2    | 5.58  | 123.80      | 119.90   |
| 35  | BB    | 2751 | G    | C6-C5-N7    | -5.58 | 127.05      | 130.40   |
| 1   | AA    | 54   | C    | O5'-C5'-C4' | -5.57 | 101.11      | 111.70   |
| 1   | AA    | 63   | C    | C5'-C4'-O4' | 5.57  | 115.79      | 109.10   |
| 1   | AA    | 826  | C    | P-O3'-C3'   | 5.57  | 126.39      | 119.70   |
| 1   | AA    | 900  | A    | N3-C4-N9    | 5.57  | 131.86      | 127.40   |
| 1   | AA    | 908  | A    | C6-N1-C2    | 5.57  | 121.94      | 118.60   |
| 1   | AA    | 1068 | G    | C4-C5-C6    | 5.57  | 122.14      | 118.80   |
| 1   | AA    | 1505 | G    | N9-C4-C5    | -5.57 | 103.17      | 105.40   |
| 8   | AH    | 44   | PHE  | N-CA-CB     | 5.57  | 120.63      | 110.60   |
| 10  | AJ    | 68   | ARG  | NE-CZ-NH1   | 5.57  | 123.09      | 120.30   |
| 35  | BB    | 207  | A    | C4-C5-N7    | 5.57  | 113.49      | 110.70   |
| 35  | BB    | 674  | G    | O5'-C5'-C4' | -5.57 | 101.11      | 111.70   |
| 35  | BB    | 907  | G    | C2-N3-C4    | -5.57 | 109.11      | 111.90   |
| 35  | BB    | 995  | C    | O4'-C4'-C3' | -5.57 | 98.43       | 104.00   |
| 35  | BB    | 1020 | A    | C4-C5-C6    | 5.57  | 119.79      | 117.00   |
| 35  | BB    | 1468 | U    | O4'-C4'-C3' | -5.57 | 98.43       | 104.00   |
| 35  | BB    | 1776 | G    | N3-C4-C5    | -5.57 | 125.81      | 128.60   |
| 35  | BB    | 1901 | A    | N3-C4-C5    | -5.57 | 122.90      | 126.80   |
| 35  | BB    | 2068 | U    | N3-C4-O4    | 5.57  | 123.30      | 119.40   |
| 35  | BB    | 2068 | U    | C4-C5-C6    | 5.57  | 123.04      | 119.70   |
| 35  | BB    | 2714 | G    | C8-N9-C4    | 5.57  | 108.63      | 106.40   |
| 35  | BB    | 2903 | U    | O4'-C4'-C3' | -5.57 | 98.43       | 104.00   |
| 1   | AA    | 255  | G    | N9-C4-C5    | 5.57  | 107.63      | 105.40   |
| 1   | AA    | 837  | U    | N1-C2-O2    | -5.57 | 118.90      | 122.80   |
| 1   | AA    | 1199 | U    | N3-C4-O4    | -5.57 | 115.50      | 119.40   |
| 1   | AA    | 1494 | G    | C8-N9-C4    | -5.57 | 104.17      | 106.40   |
| 35  | BB    | 965  | C    | P-O3'-C3'   | -5.57 | 113.01      | 119.70   |
| 35  | BB    | 1877 | A    | N9-C4-C5    | -5.57 | 103.57      | 105.80   |
| 35  | BB    | 2640 | G    | C2-N3-C4    | -5.57 | 109.11      | 111.90   |
| 1   | AA    | 10   | A    | N7-C8-N9    | -5.57 | 111.02      | 113.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 378  | G    | C4-C5-N7    | 5.57  | 113.03      | 110.80   |
| 1   | AA    | 385  | C    | P-O5'-C5'   | 5.57  | 129.81      | 120.90   |
| 1   | AA    | 1050 | G    | N1-C2-N3    | -5.57 | 120.56      | 123.90   |
| 1   | AA    | 1433 | A    | N7-C8-N9    | -5.57 | 111.01      | 113.80   |
| 4   | AD    | 62   | ARG  | NE-CZ-NH1   | -5.57 | 117.52      | 120.30   |
| 5   | AE    | 13   | LYS  | N-CA-CB     | 5.57  | 120.63      | 110.60   |
| 35  | BB    | 882  | G    | C5'-C4'-O4' | 5.57  | 115.78      | 109.10   |
| 35  | BB    | 904  | G    | O4'-C1'-N9  | 5.57  | 112.66      | 108.20   |
| 35  | BB    | 1043 | C    | C5-C4-N4    | -5.57 | 116.30      | 120.20   |
| 35  | BB    | 1194 | A    | N3-C4-C5    | -5.57 | 122.90      | 126.80   |
| 35  | BB    | 1866 | A    | C5-C6-N6    | -5.57 | 119.24      | 123.70   |
| 35  | BB    | 1906 | G    | O4'-C1'-N9  | 5.57  | 112.66      | 108.20   |
| 35  | BB    | 1939 | U    | N1-C2-O2    | -5.57 | 118.90      | 122.80   |
| 35  | BB    | 2286 | G    | C1'-O4'-C4' | -5.57 | 105.44      | 109.90   |
| 35  | BB    | 2482 | A    | N3-C4-C5    | -5.57 | 122.90      | 126.80   |
| 35  | BB    | 2608 | G    | N7-C8-N9    | 5.57  | 115.89      | 113.10   |
| 35  | BB    | 2690 | U    | C4-C5-C6    | 5.57  | 123.04      | 119.70   |
| 38  | BE    | 184  | ASP  | CB-CG-OD2   | 5.57  | 123.31      | 118.30   |
| 44  | BK    | 120  | PRO  | N-CA-CB     | -5.57 | 96.47       | 102.60   |
| 35  | BB    | 409  | G    | C4-C5-C6    | 5.57  | 122.14      | 118.80   |
| 35  | BB    | 589  | U    | N1-C2-N3    | -5.57 | 111.56      | 114.90   |
| 35  | BB    | 604  | G    | C5-C6-O6    | -5.57 | 125.26      | 128.60   |
| 35  | BB    | 1307 | A    | OP1-P-O3'   | 5.57  | 117.45      | 105.20   |
| 35  | BB    | 1462 | C    | C2-N1-C1'   | 5.57  | 124.92      | 118.80   |
| 35  | BB    | 2212 | A    | C4-C5-C6    | 5.57  | 119.78      | 117.00   |
| 35  | BB    | 2543 | G    | N1-C2-N3    | -5.57 | 120.56      | 123.90   |
| 1   | AA    | 777  | A    | O4'-C1'-N9  | 5.57  | 112.65      | 108.20   |
| 1   | AA    | 964  | A    | C8-N9-C4    | -5.57 | 103.57      | 105.80   |
| 1   | AA    | 1047 | G    | C5-C6-O6    | -5.57 | 125.26      | 128.60   |
| 1   | AA    | 1214 | C    | O4'-C1'-N1  | 5.57  | 112.65      | 108.20   |
| 1   | AA    | 1390 | U    | C5-C6-N1    | 5.57  | 125.48      | 122.70   |
| 24  | AZ    | 24   | ALA  | CB-CA-C     | -5.57 | 101.75      | 110.10   |
| 34  | BA    | 74   | U    | C2-N3-C4    | 5.57  | 130.34      | 127.00   |
| 35  | BB    | 16   | C    | N3-C4-N4    | 5.57  | 121.90      | 118.00   |
| 35  | BB    | 893  | C    | C2-N3-C4    | 5.57  | 122.68      | 119.90   |
| 35  | BB    | 1430 | G    | N1-C6-O6    | 5.57  | 123.24      | 119.90   |
| 35  | BB    | 1801 | A    | C6-C5-N7    | -5.57 | 128.40      | 132.30   |
| 35  | BB    | 1892 | C    | N3-C4-N4    | 5.57  | 121.90      | 118.00   |
| 35  | BB    | 2139 | U    | P-O5'-C5'   | -5.57 | 111.99      | 120.90   |
| 35  | BB    | 2227 | A    | P-O3'-C3'   | -5.57 | 113.02      | 119.70   |
| 35  | BB    | 2279 | G    | O4'-C1'-C2' | -5.57 | 100.23      | 105.80   |
| 35  | BB    | 2326 | C    | N1-C2-N3    | -5.57 | 115.30      | 119.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2507 | C    | C2-N3-C4    | -5.57 | 117.12      | 119.90   |
| 35  | BB    | 2690 | U    | N3-C4-O4    | 5.57  | 123.30      | 119.40   |
| 35  | BB    | 2862 | G    | P-O5'-C5'   | -5.57 | 111.99      | 120.90   |
| 1   | AA    | 848  | C    | C6-N1-C1'   | -5.57 | 114.12      | 120.80   |
| 1   | AA    | 1081 | A    | C8-N9-C4    | -5.57 | 103.57      | 105.80   |
| 1   | AA    | 1367 | C    | N3-C4-C5    | -5.57 | 119.67      | 121.90   |
| 34  | BA    | 94   | A    | C5-N7-C8    | 5.57  | 106.68      | 103.90   |
| 35  | BB    | 626  | A    | C5'-C4'-O4' | 5.57  | 115.78      | 109.10   |
| 35  | BB    | 1009 | A    | N1-C2-N3    | -5.57 | 126.52      | 129.30   |
| 35  | BB    | 1570 | A    | OP1-P-OP2   | -5.57 | 111.25      | 119.60   |
| 35  | BB    | 1938 | A    | C8-N9-C4    | 5.57  | 108.03      | 105.80   |
| 35  | BB    | 2238 | G    | N1-C6-O6    | -5.57 | 116.56      | 119.90   |
| 1   | AA    | 11   | G    | O4'-C1'-N9  | 5.56  | 112.65      | 108.20   |
| 1   | AA    | 359  | G    | C4'-C3'-C2' | -5.56 | 97.04       | 102.60   |
| 1   | AA    | 391  | G    | C5-N7-C8    | 5.56  | 107.08      | 104.30   |
| 1   | AA    | 945  | G    | N1-C6-O6    | 5.56  | 123.24      | 119.90   |
| 1   | AA    | 1037 | C    | C5-C4-N4    | -5.56 | 116.31      | 120.20   |
| 35  | BB    | 522  | A    | N1-C2-N3    | 5.56  | 132.08      | 129.30   |
| 35  | BB    | 1875 | G    | N9-C4-C5    | -5.56 | 103.17      | 105.40   |
| 35  | BB    | 2078 | C    | C4'-C3'-C2' | -5.56 | 97.04       | 102.60   |
| 35  | BB    | 2243 | U    | N1-C2-N3    | 5.56  | 118.24      | 114.90   |
| 35  | BB    | 2561 | U    | C2-N3-C4    | -5.56 | 123.66      | 127.00   |
| 1   | AA    | 647  | C    | N3-C2-O2    | 5.56  | 125.79      | 121.90   |
| 1   | AA    | 747  | A    | C6-N1-C2    | -5.56 | 115.26      | 118.60   |
| 1   | AA    | 768  | A    | N3-C4-N9    | 5.56  | 131.85      | 127.40   |
| 1   | AA    | 785  | G    | C5'-C4'-O4' | 5.56  | 115.78      | 109.10   |
| 1   | AA    | 1096 | C    | C4-C5-C6    | -5.56 | 114.62      | 117.40   |
| 1   | AA    | 1204 | A    | C4-C5-N7    | -5.56 | 107.92      | 110.70   |
| 1   | AA    | 1286 | U    | C4-C5-C6    | 5.56  | 123.04      | 119.70   |
| 30  | B5    | 16   | ASP  | CB-CG-OD1   | -5.56 | 113.29      | 118.30   |
| 34  | BA    | 33   | G    | C8-N9-C4    | 5.56  | 108.62      | 106.40   |
| 35  | BB    | 271  | G    | N1-C2-N3    | -5.56 | 120.56      | 123.90   |
| 35  | BB    | 283  | G    | N1-C2-N2    | 5.56  | 121.20      | 116.20   |
| 35  | BB    | 406  | G    | C4-N9-C1'   | -5.56 | 119.27      | 126.50   |
| 35  | BB    | 624  | C    | N3-C2-O2    | -5.56 | 118.01      | 121.90   |
| 35  | BB    | 1626 | A    | C5-C6-N6    | -5.56 | 119.25      | 123.70   |
| 35  | BB    | 1694 | C    | C2-N1-C1'   | 5.56  | 124.92      | 118.80   |
| 35  | BB    | 1768 | C    | O5'-C5'-C4' | -5.56 | 101.13      | 111.70   |
| 35  | BB    | 1822 | C    | C5-C4-N4    | -5.56 | 116.31      | 120.20   |
| 35  | BB    | 1828 | G    | C4'-C3'-C2' | -5.56 | 97.04       | 102.60   |
| 35  | BB    | 2201 | G    | N9-C4-C5    | -5.56 | 103.17      | 105.40   |
| 1   | AA    | 207  | C    | C1'-O4'-C4' | 5.56  | 114.35      | 109.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1010 | U    | N3-C4-C5    | -5.56 | 111.26      | 114.60   |
| 1   | AA    | 1133 | G    | C6-N1-C2    | 5.56  | 128.44      | 125.10   |
| 22  | AV    | 62   | C    | N3-C4-N4    | 5.56  | 121.89      | 118.00   |
| 35  | BB    | 78   | U    | N1-C2-O2    | -5.56 | 118.91      | 122.80   |
| 35  | BB    | 846  | U    | C1'-O4'-C4' | -5.56 | 105.45      | 109.90   |
| 35  | BB    | 1008 | A    | N9-C4-C5    | 5.56  | 108.03      | 105.80   |
| 35  | BB    | 1037 | G    | N9-C1'-C2'  | -5.56 | 105.88      | 112.00   |
| 35  | BB    | 1330 | C    | N3-C4-N4    | 5.56  | 121.89      | 118.00   |
| 35  | BB    | 1455 | G    | N7-C8-N9    | 5.56  | 115.88      | 113.10   |
| 35  | BB    | 1681 | G    | O4'-C4'-C3' | -5.56 | 98.44       | 104.00   |
| 35  | BB    | 2271 | G    | O4'-C1'-N9  | 5.56  | 112.65      | 108.20   |
| 1   | AA    | 39   | G    | N9-C4-C5    | -5.56 | 103.18      | 105.40   |
| 1   | AA    | 55   | A    | C1'-O4'-C4' | 5.56  | 114.35      | 109.90   |
| 1   | AA    | 75   | G    | C8-N9-C4    | 5.56  | 108.62      | 106.40   |
| 1   | AA    | 517  | G    | C8-N9-C4    | -5.56 | 104.18      | 106.40   |
| 1   | AA    | 1123 | U    | C2-N3-C4    | -5.56 | 123.66      | 127.00   |
| 1   | AA    | 1174 | G    | C5-C6-O6    | -5.56 | 125.26      | 128.60   |
| 1   | AA    | 1453 | G    | N7-C8-N9    | -5.56 | 110.32      | 113.10   |
| 35  | BB    | 70   | G    | O5'-C5'-C4' | -5.56 | 101.14      | 111.70   |
| 35  | BB    | 691  | C    | O4'-C1'-N1  | 5.56  | 112.65      | 108.20   |
| 35  | BB    | 916  | G    | N7-C8-N9    | 5.56  | 115.88      | 113.10   |
| 35  | BB    | 1070 | A    | N9-C4-C5    | 5.56  | 108.02      | 105.80   |
| 35  | BB    | 1598 | A    | N9-C4-C5    | 5.56  | 108.02      | 105.80   |
| 35  | BB    | 1669 | A    | C5-N7-C8    | 5.56  | 106.68      | 103.90   |
| 35  | BB    | 2086 | U    | P-O5'-C5'   | -5.56 | 112.00      | 120.90   |
| 35  | BB    | 2587 | A    | P-O3'-C3'   | -5.56 | 113.03      | 119.70   |
| 35  | BB    | 2832 | U    | O4'-C1'-N1  | 5.56  | 112.65      | 108.20   |
| 1   | AA    | 138  | G    | C2-N3-C4    | -5.56 | 109.12      | 111.90   |
| 1   | AA    | 406  | G    | C2-N3-C4    | 5.56  | 114.68      | 111.90   |
| 1   | AA    | 555  | U    | C5-C4-O4    | -5.56 | 122.56      | 125.90   |
| 1   | AA    | 563  | A    | C6-C5-N7    | -5.56 | 128.41      | 132.30   |
| 1   | AA    | 931  | C    | N3-C4-C5    | 5.56  | 124.12      | 121.90   |
| 1   | AA    | 964  | A    | C5'-C4'-O4' | 5.56  | 115.77      | 109.10   |
| 35  | BB    | 85   | G    | N3-C2-N2    | 5.56  | 123.79      | 119.90   |
| 35  | BB    | 195  | A    | C4-C5-C6    | 5.56  | 119.78      | 117.00   |
| 35  | BB    | 597  | G    | OP1-P-OP2   | -5.56 | 111.26      | 119.60   |
| 35  | BB    | 733  | G    | C8-N9-C4    | -5.56 | 104.18      | 106.40   |
| 35  | BB    | 810  | U    | C3'-C2'-C1' | -5.56 | 97.05       | 101.50   |
| 35  | BB    | 934  | U    | N1-C2-N3    | -5.56 | 111.57      | 114.90   |
| 35  | BB    | 1060 | U    | N3-C4-O4    | 5.56  | 123.29      | 119.40   |
| 35  | BB    | 1529 | G    | N7-C8-N9    | 5.56  | 115.88      | 113.10   |
| 35  | BB    | 1814 | G    | N1-C2-N3    | -5.56 | 120.57      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1925 | C    | C2-N3-C4    | -5.56 | 117.12      | 119.90   |
| 35  | BB    | 1947 | C    | C6-N1-C2    | 5.56  | 122.52      | 120.30   |
| 35  | BB    | 2823 | A    | P-O3'-C3'   | -5.56 | 113.03      | 119.70   |
| 35  | BB    | 213  | A    | C4-C5-N7    | -5.56 | 107.92      | 110.70   |
| 35  | BB    | 453  | A    | N1-C2-N3    | 5.56  | 132.08      | 129.30   |
| 35  | BB    | 543  | G    | C5-C6-O6    | -5.56 | 125.27      | 128.60   |
| 35  | BB    | 684  | G    | O5'-P-OP2   | 5.56  | 117.37      | 110.70   |
| 35  | BB    | 1650 | A    | P-O5'-C5'   | 5.56  | 129.79      | 120.90   |
| 34  | BA    | 47   | C    | C1'-O4'-C4' | -5.55 | 105.46      | 109.90   |
| 35  | BB    | 8    | C    | O5'-P-OP2   | 5.55  | 117.37      | 110.70   |
| 35  | BB    | 23   | G    | N3-C4-C5    | -5.55 | 125.82      | 128.60   |
| 35  | BB    | 98   | G    | N7-C8-N9    | 5.55  | 115.88      | 113.10   |
| 35  | BB    | 242  | G    | C8-N9-C4    | 5.55  | 108.62      | 106.40   |
| 35  | BB    | 506  | G    | C5-N7-C8    | -5.55 | 101.52      | 104.30   |
| 35  | BB    | 520  | G    | C8-N9-C1'   | 5.55  | 134.22      | 127.00   |
| 35  | BB    | 1134 | A    | C2-N3-C4    | -5.55 | 107.82      | 110.60   |
| 35  | BB    | 1382 | G    | P-O3'-C3'   | -5.55 | 113.03      | 119.70   |
| 35  | BB    | 1641 | A    | C4-C5-N7    | -5.55 | 107.92      | 110.70   |
| 35  | BB    | 1819 | A    | P-O5'-C5'   | 5.55  | 129.79      | 120.90   |
| 35  | BB    | 2159 | G    | C3'-C2'-C1' | 5.55  | 105.94      | 101.50   |
| 35  | BB    | 2433 | A    | C4-C5-N7    | -5.55 | 107.92      | 110.70   |
| 35  | BB    | 2707 | U    | N3-C4-O4    | 5.55  | 123.29      | 119.40   |
| 35  | BB    | 2799 | A    | C4-N9-C1'   | 5.55  | 136.30      | 126.30   |
| 16  | AP    | 35   | ARG  | NE-CZ-NH2   | -5.55 | 117.52      | 120.30   |
| 35  | BB    | 686  | U    | O4'-C4'-C3' | 5.55  | 110.54      | 106.10   |
| 35  | BB    | 1235 | G    | C2-N3-C4    | -5.55 | 109.12      | 111.90   |
| 35  | BB    | 1466 | U    | C2-N3-C4    | -5.55 | 123.67      | 127.00   |
| 35  | BB    | 1540 | G    | C4-C5-C6    | 5.55  | 122.13      | 118.80   |
| 35  | BB    | 1942 | C    | O4'-C1'-N1  | 5.55  | 112.64      | 108.20   |
| 37  | BD    | 184  | ARG  | NE-CZ-NH2   | 5.55  | 123.08      | 120.30   |
| 1   | AA    | 79   | G    | N1-C2-N2    | -5.55 | 111.20      | 116.20   |
| 1   | AA    | 1020 | G    | N1-C2-N3    | -5.55 | 120.57      | 123.90   |
| 1   | AA    | 1050 | G    | N3-C2-N2    | 5.55  | 123.79      | 119.90   |
| 1   | AA    | 1189 | U    | N3-C4-C5    | -5.55 | 111.27      | 114.60   |
| 1   | AA    | 1235 | U    | N3-C4-C5    | -5.55 | 111.27      | 114.60   |
| 1   | AA    | 1266 | G    | N3-C4-N9    | -5.55 | 122.67      | 126.00   |
| 1   | AA    | 1305 | G    | N1-C2-N3    | -5.55 | 120.57      | 123.90   |
| 1   | AA    | 1518 | A    | N1-C6-N6    | 5.55  | 121.93      | 118.60   |
| 34  | BA    | 53   | A    | O5'-P-OP2   | 5.55  | 117.36      | 110.70   |
| 35  | BB    | 271  | G    | N3-C4-C5    | 5.55  | 131.38      | 128.60   |
| 35  | BB    | 829  | A    | C4-C5-C6    | 5.55  | 119.78      | 117.00   |
| 35  | BB    | 1828 | G    | C2-N3-C4    | 5.55  | 114.68      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1922 | G    | C4'-C3'-C2' | -5.55 | 97.05       | 102.60   |
| 35  | BB    | 2033 | A    | N7-C8-N9    | -5.55 | 111.02      | 113.80   |
| 35  | BB    | 2200 | C    | C2-N1-C1'   | 5.55  | 124.91      | 118.80   |
| 35  | BB    | 2693 | G    | O4'-C1'-N9  | 5.55  | 112.64      | 108.20   |
| 38  | BE    | 182  | ALA  | N-CA-CB     | 5.55  | 117.87      | 110.10   |
| 1   | AA    | 498  | A    | C8-N9-C4    | -5.55 | 103.58      | 105.80   |
| 1   | AA    | 903  | G    | O4'-C1'-N9  | 5.55  | 112.64      | 108.20   |
| 1   | AA    | 936  | C    | N1-C2-N3    | 5.55  | 123.08      | 119.20   |
| 1   | AA    | 1231 | G    | C6-C5-N7    | -5.55 | 127.07      | 130.40   |
| 1   | AA    | 1282 | C    | C5-C4-N4    | -5.55 | 116.31      | 120.20   |
| 1   | AA    | 1426 | G    | C2-N3-C4    | -5.55 | 109.12      | 111.90   |
| 35  | BB    | 813  | U    | N1-C2-N3    | -5.55 | 111.57      | 114.90   |
| 35  | BB    | 876  | C    | O4'-C4'-C3' | -5.55 | 98.45       | 104.00   |
| 35  | BB    | 1013 | C    | P-O3'-C3'   | -5.55 | 113.04      | 119.70   |
| 35  | BB    | 1290 | C    | C6-N1-C2    | -5.55 | 118.08      | 120.30   |
| 35  | BB    | 2355 | G    | C4-C5-N7    | 5.55  | 113.02      | 110.80   |
| 35  | BB    | 2569 | G    | N9-C4-C5    | 5.55  | 107.62      | 105.40   |
| 35  | BB    | 2672 | U    | N3-C4-O4    | -5.55 | 115.52      | 119.40   |
| 35  | BB    | 2886 | A    | N9-C1'-C2'  | -5.55 | 105.89      | 112.00   |
| 45  | BL    | 41   | ARG  | NE-CZ-NH1   | -5.55 | 117.53      | 120.30   |
| 1   | AA    | 762  | U    | C5'-C4'-O4' | 5.55  | 115.76      | 109.10   |
| 1   | AA    | 769  | G    | N7-C8-N9    | -5.55 | 110.33      | 113.10   |
| 1   | AA    | 922  | G    | C1'-O4'-C4' | -5.55 | 105.46      | 109.90   |
| 1   | AA    | 978  | A    | N3-C4-N9    | 5.55  | 131.84      | 127.40   |
| 1   | AA    | 1106 | G    | N1-C6-O6    | 5.55  | 123.23      | 119.90   |
| 22  | AV    | 25   | C    | N3-C4-N4    | 5.55  | 121.88      | 118.00   |
| 1   | AA    | 157  | U    | P-O5'-C5'   | 5.55  | 129.77      | 120.90   |
| 1   | AA    | 291  | U    | N3-C2-O2    | 5.55  | 126.08      | 122.20   |
| 1   | AA    | 1261 | A    | C4'-C3'-C2' | -5.55 | 97.05       | 102.60   |
| 1   | AA    | 1292 | G    | N7-C8-N9    | -5.55 | 110.33      | 113.10   |
| 8   | AH    | 110  | MET  | N-CA-CB     | -5.55 | 100.62      | 110.60   |
| 12  | AL    | 94   | TYR  | CA-CB-CG    | -5.55 | 102.86      | 113.40   |
| 35  | BB    | 264  | C    | C2-N3-C4    | 5.55  | 122.67      | 119.90   |
| 35  | BB    | 1205 | A    | C8-N9-C4    | 5.55  | 108.02      | 105.80   |
| 35  | BB    | 1297 | C    | C5-C6-N1    | 5.55  | 123.77      | 121.00   |
| 35  | BB    | 1306 | C    | N3-C4-C5    | -5.55 | 119.68      | 121.90   |
| 35  | BB    | 1482 | G    | N9-C4-C5    | 5.55  | 107.62      | 105.40   |
| 35  | BB    | 1579 | A    | C5-C6-N6    | -5.55 | 119.26      | 123.70   |
| 35  | BB    | 1603 | A    | C4'-C3'-C2' | -5.55 | 97.05       | 102.60   |
| 35  | BB    | 2055 | C    | N1-C2-N3    | 5.55  | 123.08      | 119.20   |
| 35  | BB    | 2135 | A    | N1-C6-N6    | 5.55  | 121.93      | 118.60   |
| 1   | AA    | 63   | C    | N3-C4-C5    | -5.54 | 119.68      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 123  | U    | N3-C4-O4    | 5.54  | 123.28      | 119.40   |
| 35  | BB    | 1061 | U    | N3-C4-O4    | 5.54  | 123.28      | 119.40   |
| 35  | BB    | 2074 | U    | N1-C2-N3    | -5.54 | 111.57      | 114.90   |
| 35  | BB    | 2770 | G    | C2-N3-C4    | -5.54 | 109.13      | 111.90   |
| 1   | AA    | 289  | G    | C4-C5-N7    | -5.54 | 108.58      | 110.80   |
| 1   | AA    | 847  | G    | N7-C8-N9    | 5.54  | 115.87      | 113.10   |
| 1   | AA    | 1163 | A    | C5-N7-C8    | -5.54 | 101.13      | 103.90   |
| 1   | AA    | 1274 | A    | N7-C8-N9    | 5.54  | 116.57      | 113.80   |
| 1   | AA    | 1399 | C    | N3-C2-O2    | 5.54  | 125.78      | 121.90   |
| 10  | AJ    | 77   | VAL  | CA-CB-CG1   | 5.54  | 119.21      | 110.90   |
| 35  | BB    | 139  | U    | C1'-O4'-C4' | -5.54 | 105.47      | 109.90   |
| 35  | BB    | 643  | A    | C3'-C2'-C1' | 5.54  | 105.93      | 101.50   |
| 35  | BB    | 672  | C    | N1-C2-O2    | 5.54  | 122.23      | 118.90   |
| 35  | BB    | 708  | G    | C5'-C4'-C3' | -5.54 | 107.13      | 116.00   |
| 35  | BB    | 992  | C    | C4'-C3'-C2' | -5.54 | 97.06       | 102.60   |
| 35  | BB    | 1280 | G    | C5'-C4'-O4' | 5.54  | 115.75      | 109.10   |
| 35  | BB    | 1452 | G    | C2-N3-C4    | 5.54  | 114.67      | 111.90   |
| 35  | BB    | 1797 | G    | N3-C4-C5    | -5.54 | 125.83      | 128.60   |
| 35  | BB    | 1904 | G    | O4'-C4'-C3' | -5.54 | 98.46       | 104.00   |
| 35  | BB    | 1906 | G    | OP1-P-OP2   | -5.54 | 111.28      | 119.60   |
| 35  | BB    | 2024 | G    | C5-C6-N1    | -5.54 | 108.73      | 111.50   |
| 35  | BB    | 2449 | U    | N3-C4-O4    | 5.54  | 123.28      | 119.40   |
| 35  | BB    | 2618 | G    | OP2-P-O3'   | 5.54  | 117.40      | 105.20   |
| 35  | BB    | 2828 | G    | P-O3'-C3'   | -5.54 | 113.05      | 119.70   |
| 35  | BB    | 2868 | A    | N1-C6-N6    | 5.54  | 121.93      | 118.60   |
| 54  | BU    | 94   | PHE  | CG-CD2-CE2  | 5.54  | 126.90      | 120.80   |
| 1   | AA    | 290  | C    | C5-C4-N4    | -5.54 | 116.32      | 120.20   |
| 1   | AA    | 293  | G    | C6-C5-N7    | -5.54 | 127.08      | 130.40   |
| 1   | AA    | 1231 | G    | C5-C6-O6    | -5.54 | 125.28      | 128.60   |
| 1   | AA    | 1380 | U    | O4'-C1'-N1  | 5.54  | 112.63      | 108.20   |
| 35  | BB    | 282  | A    | N7-C8-N9    | -5.54 | 111.03      | 113.80   |
| 35  | BB    | 909  | A    | C4-C5-N7    | 5.54  | 113.47      | 110.70   |
| 35  | BB    | 1163 | G    | N3-C4-N9    | 5.54  | 129.32      | 126.00   |
| 35  | BB    | 1262 | A    | C8-N9-C4    | -5.54 | 103.58      | 105.80   |
| 35  | BB    | 1714 | U    | N3-C4-C5    | -5.54 | 111.28      | 114.60   |
| 35  | BB    | 1993 | U    | C5'-C4'-O4' | -5.54 | 102.45      | 109.10   |
| 35  | BB    | 2282 | G    | C6-N1-C2    | -5.54 | 121.78      | 125.10   |
| 35  | BB    | 2487 | G    | C5-N7-C8    | 5.54  | 107.07      | 104.30   |
| 35  | BB    | 2551 | C    | C5-C4-N4    | -5.54 | 116.32      | 120.20   |
| 35  | BB    | 2692 | G    | C4-C5-C6    | 5.54  | 122.12      | 118.80   |
| 35  | BB    | 2788 | C    | C2-N1-C1'   | 5.54  | 124.90      | 118.80   |
| 38  | BE    | 161  | ALA  | N-CA-CB     | 5.54  | 117.86      | 110.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 187  | G    | N3-C4-C5    | -5.54 | 125.83      | 128.60   |
| 35  | BB    | 1888 | G    | C1'-O4'-C4' | -5.54 | 105.47      | 109.90   |
| 35  | BB    | 2061 | G    | N1-C2-N2    | -5.54 | 111.21      | 116.20   |
| 35  | BB    | 2307 | G    | C5-C6-O6    | -5.54 | 125.28      | 128.60   |
| 35  | BB    | 2569 | G    | C6-C5-N7    | -5.54 | 127.08      | 130.40   |
| 1   | AA    | 255  | G    | C5-N7-C8    | 5.54  | 107.07      | 104.30   |
| 1   | AA    | 525  | C    | O4'-C1'-N1  | 5.54  | 112.63      | 108.20   |
| 1   | AA    | 1302 | C    | C5'-C4'-O4' | -5.54 | 102.45      | 109.10   |
| 1   | AA    | 1356 | G    | C4-C5-N7    | 5.54  | 113.02      | 110.80   |
| 1   | AA    | 1363 | A    | C2-N3-C4    | -5.54 | 107.83      | 110.60   |
| 1   | AA    | 1393 | U    | C4'-C3'-C2' | -5.54 | 97.06       | 102.60   |
| 22  | AV    | 14   | A    | C5-C6-N1    | -5.54 | 114.93      | 117.70   |
| 34  | BA    | 77   | U    | N1-C2-O2    | -5.54 | 118.92      | 122.80   |
| 35  | BB    | 141  | G    | OP1-P-OP2   | -5.54 | 111.29      | 119.60   |
| 35  | BB    | 143  | C    | N3-C2-O2    | -5.54 | 118.02      | 121.90   |
| 35  | BB    | 956  | G    | N3-C4-N9    | -5.54 | 122.68      | 126.00   |
| 35  | BB    | 1124 | G    | C5-C6-O6    | -5.54 | 125.28      | 128.60   |
| 35  | BB    | 1472 | C    | O4'-C4'-C3' | -5.54 | 98.46       | 104.00   |
| 35  | BB    | 1685 | C    | N3-C2-O2    | -5.54 | 118.02      | 121.90   |
| 35  | BB    | 2198 | A    | C4-C5-N7    | -5.54 | 107.93      | 110.70   |
| 35  | BB    | 2218 | G    | C6-C5-N7    | -5.54 | 127.08      | 130.40   |
| 35  | BB    | 2259 | U    | C4-C5-C6    | -5.54 | 116.38      | 119.70   |
| 35  | BB    | 2732 | G    | N3-C4-C5    | -5.54 | 125.83      | 128.60   |
| 35  | BB    | 2830 | C    | P-O5'-C5'   | -5.54 | 112.04      | 120.90   |
| 1   | AA    | 335  | C    | P-O3'-C3'   | 5.54  | 126.34      | 119.70   |
| 1   | AA    | 1028 | C    | C4-C5-C6    | -5.54 | 114.63      | 117.40   |
| 35  | BB    | 182  | A    | C8-N9-C4    | -5.54 | 103.58      | 105.80   |
| 35  | BB    | 401  | A    | C4'-C3'-C2' | -5.54 | 97.06       | 102.60   |
| 35  | BB    | 506  | G    | C5-C6-N1    | -5.54 | 108.73      | 111.50   |
| 35  | BB    | 656  | G    | C8-N9-C4    | -5.54 | 104.19      | 106.40   |
| 35  | BB    | 951  | C    | N1-C2-O2    | -5.54 | 115.58      | 118.90   |
| 35  | BB    | 962  | G    | N3-C2-N2    | 5.54  | 123.78      | 119.90   |
| 35  | BB    | 1718 | G    | O4'-C4'-C3' | -5.54 | 98.46       | 104.00   |
| 35  | BB    | 2145 | C    | C2-N3-C4    | 5.54  | 122.67      | 119.90   |
| 35  | BB    | 2157 | G    | N7-C8-N9    | -5.54 | 110.33      | 113.10   |
| 35  | BB    | 2831 | G    | P-O3'-C3'   | 5.54  | 126.34      | 119.70   |
| 1   | AA    | 624  | C    | N1-C2-O2    | -5.54 | 115.58      | 118.90   |
| 1   | AA    | 953  | G    | O4'-C1'-N9  | 5.54  | 112.63      | 108.20   |
| 1   | AA    | 1115 | U    | C2-N3-C4    | 5.54  | 130.32      | 127.00   |
| 1   | AA    | 1185 | G    | C3'-C2'-C1' | 5.54  | 105.93      | 101.50   |
| 35  | BB    | 82   | U    | C5'-C4'-O4' | 5.54  | 115.74      | 109.10   |
| 35  | BB    | 244  | A    | C2-N3-C4    | -5.54 | 107.83      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1042 | G    | C4-C5-C6    | 5.54  | 122.12      | 118.80   |
| 35  | BB    | 1202 | G    | O4'-C1'-N9  | 5.54  | 112.63      | 108.20   |
| 35  | BB    | 1395 | A    | C5-C6-N6    | -5.54 | 119.27      | 123.70   |
| 35  | BB    | 1439 | A    | C6-C5-N7    | -5.54 | 128.43      | 132.30   |
| 35  | BB    | 1838 | C    | C2-N3-C4    | 5.54  | 122.67      | 119.90   |
| 35  | BB    | 1973 | G    | O4'-C1'-N9  | 5.54  | 112.63      | 108.20   |
| 35  | BB    | 2431 | U    | O4'-C1'-N1  | 5.54  | 112.63      | 108.20   |
| 35  | BB    | 2597 | G    | C6-N1-C2    | 5.54  | 128.42      | 125.10   |
| 35  | BB    | 2764 | A    | C5-C6-N6    | -5.54 | 119.27      | 123.70   |
| 36  | BC    | 263  | ASP  | CB-CG-OD2   | 5.54  | 123.28      | 118.30   |
| 1   | AA    | 241  | G    | C5-C6-N1    | -5.53 | 108.73      | 111.50   |
| 1   | AA    | 731  | G    | N9-C4-C5    | 5.53  | 107.61      | 105.40   |
| 1   | AA    | 874  | G    | C4-C5-C6    | 5.53  | 122.12      | 118.80   |
| 1   | AA    | 1210 | C    | C3'-C2'-C1' | -5.53 | 97.07       | 101.50   |
| 1   | AA    | 1311 | A    | N7-C8-N9    | 5.53  | 116.57      | 113.80   |
| 1   | AA    | 1425 | U    | O4'-C1'-N1  | 5.53  | 112.63      | 108.20   |
| 34  | BA    | 43   | C    | N3-C4-C5    | -5.53 | 119.69      | 121.90   |
| 35  | BB    | 141  | G    | C5-C6-O6    | -5.53 | 125.28      | 128.60   |
| 35  | BB    | 626  | A    | C6-C5-N7    | -5.53 | 128.43      | 132.30   |
| 35  | BB    | 853  | C    | C5-C4-N4    | -5.53 | 116.33      | 120.20   |
| 35  | BB    | 1102 | C    | C5-C4-N4    | -5.53 | 116.33      | 120.20   |
| 35  | BB    | 1664 | A    | C5-C6-N6    | -5.53 | 119.27      | 123.70   |
| 35  | BB    | 1848 | A    | C8-N9-C4    | 5.53  | 108.01      | 105.80   |
| 35  | BB    | 2103 | C    | C5'-C4'-O4' | 5.53  | 115.74      | 109.10   |
| 35  | BB    | 2890 | G    | C6-C5-N7    | -5.53 | 127.08      | 130.40   |
| 1   | AA    | 119  | A    | O4'-C1'-N9  | 5.53  | 112.62      | 108.20   |
| 1   | AA    | 210  | C    | C6-N1-C2    | 5.53  | 122.51      | 120.30   |
| 35  | BB    | 197  | A    | C5-N7-C8    | 5.53  | 106.67      | 103.90   |
| 35  | BB    | 503  | A    | P-O5'-C5'   | -5.53 | 112.05      | 120.90   |
| 35  | BB    | 805  | G    | N3-C2-N2    | 5.53  | 123.77      | 119.90   |
| 35  | BB    | 875  | G    | C8-N9-C4    | -5.53 | 104.19      | 106.40   |
| 35  | BB    | 2304 | G    | N3-C4-C5    | 5.53  | 131.37      | 128.60   |
| 35  | BB    | 2406 | A    | C2-N3-C4    | -5.53 | 107.83      | 110.60   |
| 35  | BB    | 2420 | C    | O4'-C1'-N1  | 5.53  | 112.63      | 108.20   |
| 35  | BB    | 2780 | G    | C2-N3-C4    | 5.53  | 114.67      | 111.90   |
| 1   | AA    | 45   | G    | C4-C5-C6    | 5.53  | 122.12      | 118.80   |
| 1   | AA    | 182  | A    | C6-C5-N7    | -5.53 | 128.43      | 132.30   |
| 1   | AA    | 308  | C    | C2-N3-C4    | 5.53  | 122.67      | 119.90   |
| 1   | AA    | 346  | G    | C5'-C4'-O4' | 5.53  | 115.74      | 109.10   |
| 1   | AA    | 572  | A    | C5'-C4'-O4' | -5.53 | 102.46      | 109.10   |
| 1   | AA    | 792  | A    | C6-C5-N7    | -5.53 | 128.43      | 132.30   |
| 1   | AA    | 1249 | C    | C4'-C3'-C2' | -5.53 | 97.07       | 102.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1493 | A    | C5-C6-N1    | -5.53 | 114.93      | 117.70   |
| 6   | AF    | 53   | LYS  | N-CA-CB     | 5.53  | 120.55      | 110.60   |
| 9   | AI    | 38   | PHE  | CB-CG-CD1   | 5.53  | 124.67      | 120.80   |
| 9   | AI    | 72   | SER  | N-CA-CB     | 5.53  | 118.80      | 110.50   |
| 24  | AZ    | 23   | ALA  | O-C-N       | -5.53 | 113.85      | 122.70   |
| 35  | BB    | 465  | G    | O4'-C1'-N9  | 5.53  | 112.62      | 108.20   |
| 35  | BB    | 893  | C    | C6-N1-C1'   | -5.53 | 114.16      | 120.80   |
| 35  | BB    | 1245 | G    | C6-N1-C2    | -5.53 | 121.78      | 125.10   |
| 35  | BB    | 1281 | G    | C5-N7-C8    | 5.53  | 107.06      | 104.30   |
| 35  | BB    | 1382 | G    | C5-C6-N1    | 5.53  | 114.27      | 111.50   |
| 35  | BB    | 2263 | C    | C4'-C3'-C2' | -5.53 | 97.07       | 102.60   |
| 1   | AA    | 80   | A    | C6-C5-N7    | -5.53 | 128.43      | 132.30   |
| 1   | AA    | 1019 | A    | C4-C5-N7    | -5.53 | 107.94      | 110.70   |
| 1   | AA    | 1283 | U    | C5-C6-N1    | 5.53  | 125.46      | 122.70   |
| 35  | BB    | 432  | A    | N9-C4-C5    | 5.53  | 108.01      | 105.80   |
| 35  | BB    | 2182 | U    | O3'-P-O5'   | -5.53 | 93.50       | 104.00   |
| 35  | BB    | 2595 | G    | C5-C6-N1    | -5.53 | 108.74      | 111.50   |
| 1   | AA    | 82   | G    | C8-N9-C4    | -5.53 | 104.19      | 106.40   |
| 1   | AA    | 98   | A    | C6-C5-N7    | -5.53 | 128.43      | 132.30   |
| 1   | AA    | 204  | G    | C5'-C4'-O4' | -5.53 | 102.47      | 109.10   |
| 1   | AA    | 768  | A    | C4'-C3'-C2' | -5.53 | 97.07       | 102.60   |
| 1   | AA    | 823  | C    | P-O5'-C5'   | -5.53 | 112.06      | 120.90   |
| 1   | AA    | 918  | A    | C8-N9-C4    | -5.53 | 103.59      | 105.80   |
| 1   | AA    | 1311 | A    | C5-C6-N6    | -5.53 | 119.28      | 123.70   |
| 1   | AA    | 1318 | A    | C4'-C3'-C2' | -5.53 | 97.07       | 102.60   |
| 22  | AV    | 23   | C    | N3-C4-N4    | 5.53  | 121.87      | 118.00   |
| 35  | BB    | 87   | U    | O5'-C5'-C4' | -5.53 | 101.20      | 111.70   |
| 35  | BB    | 473  | G    | N1-C2-N3    | 5.53  | 127.22      | 123.90   |
| 35  | BB    | 563  | A    | C4-C5-C6    | 5.53  | 119.76      | 117.00   |
| 35  | BB    | 830  | G    | N3-C4-N9    | -5.53 | 122.68      | 126.00   |
| 35  | BB    | 932  | U    | C5'-C4'-O4' | 5.53  | 115.73      | 109.10   |
| 35  | BB    | 1789 | A    | N9-C4-C5    | 5.53  | 108.01      | 105.80   |
| 35  | BB    | 2112 | G    | C8-N9-C4    | -5.53 | 104.19      | 106.40   |
| 56  | BY    | 14   | ASP  | CB-CG-OD1   | -5.53 | 113.33      | 118.30   |
| 1   | AA    | 7    | A    | C5-C6-N1    | -5.53 | 114.94      | 117.70   |
| 1   | AA    | 115  | G    | C5-C6-O6    | -5.53 | 125.28      | 128.60   |
| 1   | AA    | 278  | G    | C4-C5-C6    | 5.53  | 122.11      | 118.80   |
| 1   | AA    | 573  | A    | C6-N1-C2    | -5.53 | 115.28      | 118.60   |
| 1   | AA    | 1222 | G    | C4-N9-C1'   | 5.53  | 133.68      | 126.50   |
| 1   | AA    | 1281 | C    | N1-C2-N3    | 5.53  | 123.07      | 119.20   |
| 1   | AA    | 1512 | U    | O4'-C1'-N1  | 5.53  | 112.62      | 108.20   |
| 23  | AX    | 19   | A    | C5-C6-N6    | -5.53 | 119.28      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 68   | G    | O4'-C1'-N9  | 5.53  | 112.62      | 108.20   |
| 35  | BB    | 462  | C    | P-O3'-C3'   | -5.53 | 113.07      | 119.70   |
| 35  | BB    | 1541 | C    | C4'-C3'-C2' | -5.53 | 97.08       | 102.60   |
| 35  | BB    | 1821 | A    | P-O5'-C5'   | 5.53  | 129.74      | 120.90   |
| 35  | BB    | 2106 | U    | C3'-C2'-C1' | 5.53  | 105.92      | 101.50   |
| 35  | BB    | 2766 | A    | C8-N9-C4    | -5.53 | 103.59      | 105.80   |
| 35  | BB    | 2862 | G    | C4-C5-N7    | -5.53 | 108.59      | 110.80   |
| 1   | AA    | 1500 | A    | OP1-P-OP2   | -5.52 | 111.31      | 119.60   |
| 35  | BB    | 192  | C    | C5-C6-N1    | -5.52 | 118.24      | 121.00   |
| 35  | BB    | 1098 | A    | C5-C6-N1    | -5.52 | 114.94      | 117.70   |
| 35  | BB    | 1110 | G    | O4'-C1'-N9  | 5.52  | 112.62      | 108.20   |
| 35  | BB    | 1143 | A    | P-O3'-C3'   | 5.52  | 126.33      | 119.70   |
| 35  | BB    | 2337 | G    | C6-C5-N7    | -5.52 | 127.09      | 130.40   |
| 1   | AA    | 306  | A    | N1-C2-N3    | -5.52 | 126.54      | 129.30   |
| 1   | AA    | 355  | C    | C4-C5-C6    | 5.52  | 120.16      | 117.40   |
| 1   | AA    | 648  | A    | C4-C5-C6    | 5.52  | 119.76      | 117.00   |
| 1   | AA    | 950  | U    | N3-C4-O4    | -5.52 | 115.53      | 119.40   |
| 1   | AA    | 1100 | C    | C2-N3-C4    | 5.52  | 122.66      | 119.90   |
| 1   | AA    | 1130 | A    | C5-C6-N1    | -5.52 | 114.94      | 117.70   |
| 22  | AV    | 3    | G    | C4-C5-C6    | 5.52  | 122.11      | 118.80   |
| 26  | B1    | 55   | THR  | CA-CB-CG2   | -5.52 | 104.67      | 112.40   |
| 35  | BB    | 439  | A    | O4'-C1'-N9  | 5.52  | 112.62      | 108.20   |
| 35  | BB    | 745  | G    | C5-C6-N1    | -5.52 | 108.74      | 111.50   |
| 35  | BB    | 877  | A    | C4-C5-N7    | -5.52 | 107.94      | 110.70   |
| 35  | BB    | 1053 | C    | C2-N3-C4    | 5.52  | 122.66      | 119.90   |
| 35  | BB    | 1074 | G    | C5-C6-N1    | -5.52 | 108.74      | 111.50   |
| 35  | BB    | 1107 | G    | C3'-C2'-C1' | 5.52  | 105.92      | 101.50   |
| 35  | BB    | 1280 | G    | C3'-C2'-C1' | -5.52 | 97.08       | 101.50   |
| 35  | BB    | 1584 | U    | C2-N3-C4    | 5.52  | 130.31      | 127.00   |
| 35  | BB    | 1873 | G    | N3-C2-N2    | 5.52  | 123.77      | 119.90   |
| 35  | BB    | 2063 | C    | C6-N1-C1'   | -5.52 | 114.17      | 120.80   |
| 35  | BB    | 2495 | G    | O4'-C1'-N9  | 5.52  | 112.62      | 108.20   |
| 35  | BB    | 2715 | C    | P-O5'-C5'   | 5.52  | 129.74      | 120.90   |
| 35  | BB    | 2850 | A    | C3'-C2'-C1' | 5.52  | 105.92      | 101.50   |
| 35  | BB    | 2889 | C    | C5-C4-N4    | -5.52 | 116.33      | 120.20   |
| 1   | AA    | 945  | G    | C4-C5-C6    | 5.52  | 122.11      | 118.80   |
| 1   | AA    | 989  | U    | C6-N1-C2    | -5.52 | 117.69      | 121.00   |
| 1   | AA    | 1013 | G    | N9-C4-C5    | -5.52 | 103.19      | 105.40   |
| 1   | AA    | 1198 | G    | N9-C4-C5    | -5.52 | 103.19      | 105.40   |
| 35  | BB    | 637  | A    | C5'-C4'-O4' | 5.52  | 115.72      | 109.10   |
| 35  | BB    | 820  | A    | C5-N7-C8    | 5.52  | 106.66      | 103.90   |
| 35  | BB    | 1692 | U    | P-O3'-C3'   | 5.52  | 126.33      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1744 | A    | N9-C4-C5    | 5.52  | 108.01      | 105.80   |
| 35  | BB    | 2800 | A    | C5-C6-N6    | -5.52 | 119.28      | 123.70   |
| 1   | AA    | 167  | A    | C5'-C4'-O4' | 5.52  | 115.72      | 109.10   |
| 1   | AA    | 199  | A    | C5-N7-C8    | 5.52  | 106.66      | 103.90   |
| 1   | AA    | 521  | G    | N9-C4-C5    | 5.52  | 107.61      | 105.40   |
| 35  | BB    | 617  | G    | C5-C6-O6    | -5.52 | 125.29      | 128.60   |
| 35  | BB    | 865  | C    | O4'-C1'-N1  | 5.52  | 112.62      | 108.20   |
| 35  | BB    | 1070 | A    | N3-C4-C5    | -5.52 | 122.94      | 126.80   |
| 35  | BB    | 1890 | A    | C4'-C3'-C2' | -5.52 | 97.08       | 102.60   |
| 35  | BB    | 2033 | A    | C4'-C3'-C2' | -5.52 | 97.08       | 102.60   |
| 35  | BB    | 2619 | C    | O4'-C1'-N1  | 5.52  | 112.61      | 108.20   |
| 1   | AA    | 332  | G    | C8-N9-C1'   | 5.52  | 134.17      | 127.00   |
| 1   | AA    | 891  | U    | O4'-C1'-N1  | 5.52  | 112.61      | 108.20   |
| 1   | AA    | 981  | U    | C5-C4-O4    | -5.52 | 122.59      | 125.90   |
| 1   | AA    | 1078 | U    | C4'-C3'-C2' | -5.52 | 97.08       | 102.60   |
| 1   | AA    | 1108 | G    | N3-C2-N2    | 5.52  | 123.76      | 119.90   |
| 1   | AA    | 1108 | G    | N1-C2-N3    | -5.52 | 120.59      | 123.90   |
| 1   | AA    | 1230 | C    | O4'-C1'-N1  | 5.52  | 112.61      | 108.20   |
| 1   | AA    | 1355 | G    | C5'-C4'-O4' | 5.52  | 115.72      | 109.10   |
| 35  | BB    | 391  | A    | C6-C5-N7    | -5.52 | 128.44      | 132.30   |
| 35  | BB    | 522  | A    | N3-C4-C5    | -5.52 | 122.94      | 126.80   |
| 35  | BB    | 1112 | G    | N3-C2-N2    | 5.52  | 123.76      | 119.90   |
| 35  | BB    | 1230 | A    | C4-C5-N7    | -5.52 | 107.94      | 110.70   |
| 35  | BB    | 1285 | A    | N1-C2-N3    | -5.52 | 126.54      | 129.30   |
| 35  | BB    | 1496 | A    | P-O3'-C3'   | 5.52  | 126.32      | 119.70   |
| 35  | BB    | 1641 | A    | N3-C4-C5    | -5.52 | 122.94      | 126.80   |
| 35  | BB    | 2105 | U    | N1-C2-O2    | -5.52 | 118.94      | 122.80   |
| 35  | BB    | 2421 | G    | N9-C4-C5    | -5.52 | 103.19      | 105.40   |
| 35  | BB    | 2704 | C    | C5-C4-N4    | -5.52 | 116.34      | 120.20   |
| 38  | BE    | 199  | MET  | N-CA-CB     | -5.52 | 100.67      | 110.60   |
| 56  | BY    | 75   | ASN  | CB-CG-OD1   | -5.52 | 110.56      | 121.60   |
| 1   | AA    | 892  | A    | O4'-C1'-N9  | 5.52  | 112.61      | 108.20   |
| 1   | AA    | 927  | G    | C2-N3-C4    | -5.52 | 109.14      | 111.90   |
| 1   | AA    | 1122 | U    | P-O5'-C5'   | 5.52  | 129.73      | 120.90   |
| 35  | BB    | 397  | U    | C1'-O4'-C4' | -5.52 | 105.49      | 109.90   |
| 35  | BB    | 1207 | C    | P-O5'-C5'   | -5.52 | 112.07      | 120.90   |
| 35  | BB    | 2082 | A    | N3-C4-C5    | -5.52 | 122.94      | 126.80   |
| 35  | BB    | 2108 | A    | C5'-C4'-O4' | -5.52 | 102.48      | 109.10   |
| 1   | AA    | 7    | A    | C6-C5-N7    | -5.51 | 128.44      | 132.30   |
| 1   | AA    | 71   | A    | C8-N9-C1'   | 5.51  | 137.63      | 127.70   |
| 1   | AA    | 241  | G    | C6-N1-C2    | 5.51  | 128.41      | 125.10   |
| 1   | AA    | 697  | U    | N3-C4-O4    | -5.51 | 115.54      | 119.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1086 | U    | N3-C4-C5    | -5.51 | 111.29      | 114.60   |
| 34  | BA    | 12   | C    | N3-C4-N4    | 5.51  | 121.86      | 118.00   |
| 34  | BA    | 62   | C    | P-O5'-C5'   | 5.51  | 129.72      | 120.90   |
| 35  | BB    | 6    | A    | C4'-C3'-C2' | -5.51 | 97.08       | 102.60   |
| 35  | BB    | 414  | C    | C3'-C2'-C1' | 5.51  | 105.91      | 101.50   |
| 35  | BB    | 661  | A    | C3'-C2'-C1' | -5.51 | 97.09       | 101.50   |
| 35  | BB    | 890  | C    | C5-C4-N4    | -5.51 | 116.34      | 120.20   |
| 35  | BB    | 969  | G    | O4'-C4'-C3' | -5.51 | 98.49       | 104.00   |
| 35  | BB    | 1844 | C    | N3-C4-N4    | 5.51  | 121.86      | 118.00   |
| 35  | BB    | 1914 | C    | C6-N1-C2    | -5.51 | 118.09      | 120.30   |
| 35  | BB    | 2001 | C    | N3-C4-C5    | -5.51 | 119.69      | 121.90   |
| 35  | BB    | 2038 | G    | N9-C4-C5    | 5.51  | 107.61      | 105.40   |
| 35  | BB    | 2178 | C    | N3-C4-N4    | 5.51  | 121.86      | 118.00   |
| 35  | BB    | 2594 | C    | P-O5'-C5'   | 5.51  | 129.72      | 120.90   |
| 35  | BB    | 2771 | C    | C2-N1-C1'   | 5.51  | 124.87      | 118.80   |
| 35  | BB    | 2781 | A    | P-O3'-C3'   | 5.51  | 126.32      | 119.70   |
| 1   | AA    | 52   | C    | C5'-C4'-C3' | -5.51 | 107.18      | 116.00   |
| 1   | AA    | 506  | G    | C3'-C2'-C1' | -5.51 | 97.09       | 101.50   |
| 1   | AA    | 943  | U    | C1'-O4'-C4' | 5.51  | 114.31      | 109.90   |
| 25  | B0    | 71   | ARG  | N-CA-CB     | 5.51  | 120.52      | 110.60   |
| 35  | BB    | 308  | G    | O4'-C1'-N9  | 5.51  | 112.61      | 108.20   |
| 35  | BB    | 1210 | G    | O4'-C1'-N9  | 5.51  | 112.61      | 108.20   |
| 35  | BB    | 2061 | G    | N9-C4-C5    | 5.51  | 107.61      | 105.40   |
| 35  | BB    | 2883 | A    | P-O3'-C3'   | 5.51  | 126.32      | 119.70   |
| 1   | AA    | 11   | G    | N3-C4-N9    | 5.51  | 129.31      | 126.00   |
| 1   | AA    | 219  | U    | P-O3'-C3'   | -5.51 | 113.09      | 119.70   |
| 1   | AA    | 363  | A    | P-O3'-C3'   | 5.51  | 126.31      | 119.70   |
| 34  | BA    | 55   | U    | C4'-C3'-C2' | -5.51 | 97.09       | 102.60   |
| 35  | BB    | 247  | G    | P-O3'-C3'   | 5.51  | 126.31      | 119.70   |
| 35  | BB    | 313  | G    | C4-C5-N7    | -5.51 | 108.60      | 110.80   |
| 35  | BB    | 319  | G    | N1-C2-N3    | -5.51 | 120.59      | 123.90   |
| 35  | BB    | 539  | G    | C6-N1-C2    | 5.51  | 128.41      | 125.10   |
| 35  | BB    | 883  | G    | C5-N7-C8    | 5.51  | 107.06      | 104.30   |
| 35  | BB    | 1332 | G    | N3-C4-N9    | 5.51  | 129.31      | 126.00   |
| 35  | BB    | 1653 | G    | C3'-C2'-C1' | -5.51 | 97.09       | 101.50   |
| 35  | BB    | 2118 | U    | O4'-C1'-N1  | 5.51  | 112.61      | 108.20   |
| 35  | BB    | 2221 | G    | C5-N7-C8    | -5.51 | 101.55      | 104.30   |
| 35  | BB    | 2356 | U    | C5'-C4'-C3' | -5.51 | 107.18      | 116.00   |
| 35  | BB    | 2473 | U    | N3-C4-C5    | -5.51 | 111.29      | 114.60   |
| 35  | BB    | 2688 | G    | C5-C6-N1    | 5.51  | 114.26      | 111.50   |
| 35  | BB    | 2702 | G    | N3-C2-N2    | 5.51  | 123.76      | 119.90   |
| 1   | AA    | 415  | A    | C5-C6-N1    | -5.51 | 114.95      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 852  | G    | C2-N3-C4    | -5.51 | 109.14      | 111.90   |
| 1   | AA    | 1137 | C    | N3-C4-C5    | -5.51 | 119.70      | 121.90   |
| 1   | AA    | 1151 | A    | C2-N3-C4    | 5.51  | 113.36      | 110.60   |
| 1   | AA    | 1531 | A    | C6-C5-N7    | -5.51 | 128.44      | 132.30   |
| 7   | AG    | 32   | ASP  | CB-CG-OD2   | -5.51 | 113.34      | 118.30   |
| 8   | AH    | 58   | LEU  | N-CA-C      | -5.51 | 96.12       | 111.00   |
| 22  | AV    | 2    | G    | N9-C4-C5    | -5.51 | 103.20      | 105.40   |
| 35  | BB    | 281  | C    | C5'-C4'-O4' | 5.51  | 115.71      | 109.10   |
| 35  | BB    | 923  | G    | C2-N3-C4    | -5.51 | 109.14      | 111.90   |
| 35  | BB    | 1313 | U    | P-O3'-C3'   | 5.51  | 126.31      | 119.70   |
| 35  | BB    | 1372 | U    | N3-C4-O4    | 5.51  | 123.26      | 119.40   |
| 35  | BB    | 1479 | G    | C3'-C2'-C1' | 5.51  | 105.91      | 101.50   |
| 35  | BB    | 1745 | A    | C1'-O4'-C4' | -5.51 | 105.49      | 109.90   |
| 35  | BB    | 1805 | A    | C4-C5-C6    | 5.51  | 119.75      | 117.00   |
| 35  | BB    | 2622 | U    | N3-C4-O4    | -5.51 | 115.54      | 119.40   |
| 35  | BB    | 168  | G    | N1-C6-O6    | 5.51  | 123.20      | 119.90   |
| 35  | BB    | 709  | U    | N1-C2-N3    | 5.51  | 118.20      | 114.90   |
| 35  | BB    | 980  | A    | C5-C6-N6    | -5.51 | 119.29      | 123.70   |
| 35  | BB    | 1093 | G    | C4-C5-C6    | 5.51  | 122.11      | 118.80   |
| 35  | BB    | 1869 | G    | C3'-C2'-C1' | -5.51 | 97.09       | 101.50   |
| 35  | BB    | 2601 | C    | C4-C5-C6    | 5.51  | 120.15      | 117.40   |
| 35  | BB    | 2766 | A    | O4'-C1'-N9  | 5.51  | 112.61      | 108.20   |
| 35  | BB    | 2775 | G    | N3-C4-C5    | -5.51 | 125.85      | 128.60   |
| 1   | AA    | 99   | C    | C2-N1-C1'   | -5.51 | 112.74      | 118.80   |
| 1   | AA    | 200  | G    | C4'-C3'-C2' | -5.51 | 97.09       | 102.60   |
| 1   | AA    | 857  | C    | C5'-C4'-C3' | 5.51  | 124.81      | 116.00   |
| 1   | AA    | 1092 | A    | C2-N3-C4    | 5.51  | 113.35      | 110.60   |
| 1   | AA    | 1220 | G    | C5-N7-C8    | 5.51  | 107.05      | 104.30   |
| 1   | AA    | 1305 | G    | C5-C6-O6    | -5.51 | 125.30      | 128.60   |
| 35  | BB    | 993  | G    | N1-C2-N3    | -5.51 | 120.60      | 123.90   |
| 35  | BB    | 1361 | G    | N9-C4-C5    | 5.51  | 107.60      | 105.40   |
| 35  | BB    | 1454 | C    | C2-N1-C1'   | 5.51  | 124.86      | 118.80   |
| 35  | BB    | 2027 | G    | N9-C4-C5    | -5.51 | 103.20      | 105.40   |
| 35  | BB    | 2128 | G    | N3-C2-N2    | 5.51  | 123.75      | 119.90   |
| 35  | BB    | 2502 | G    | N3-C2-N2    | 5.51  | 123.75      | 119.90   |
| 35  | BB    | 2634 | A    | O4'-C1'-N9  | 5.51  | 112.61      | 108.20   |
| 49  | BP    | 93   | LYS  | CD-CE-NZ    | 5.51  | 124.36      | 111.70   |
| 35  | BB    | 542  | C    | OP1-P-OP2   | -5.50 | 111.34      | 119.60   |
| 35  | BB    | 730  | A    | P-O3'-C3'   | -5.50 | 113.09      | 119.70   |
| 35  | BB    | 1138 | G    | N3-C4-N9    | -5.50 | 122.70      | 126.00   |
| 35  | BB    | 1980 | G    | C4-C5-N7    | -5.50 | 108.60      | 110.80   |
| 35  | BB    | 2595 | G    | C2-N3-C4    | 5.50  | 114.65      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2848 | G    | OP2-P-O3'   | 5.50  | 117.31      | 105.20   |
| 35  | BB    | 2883 | A    | C4-C5-C6    | 5.50  | 119.75      | 117.00   |
| 44  | BK    | 56   | ASP  | CB-CG-OD2   | 5.50  | 123.25      | 118.30   |
| 1   | AA    | 90   | C    | N1-C1'-C2'  | -5.50 | 105.95      | 112.00   |
| 1   | AA    | 142  | G    | OP1-P-OP2   | -5.50 | 111.34      | 119.60   |
| 1   | AA    | 205  | A    | C8-N9-C4    | -5.50 | 103.60      | 105.80   |
| 1   | AA    | 211  | G    | C5-C6-N1    | -5.50 | 108.75      | 111.50   |
| 1   | AA    | 338  | A    | C4'-C3'-C2' | -5.50 | 97.10       | 102.60   |
| 1   | AA    | 622  | A    | N1-C6-N6    | 5.50  | 121.90      | 118.60   |
| 1   | AA    | 643  | C    | O4'-C1'-N1  | 5.50  | 112.60      | 108.20   |
| 1   | AA    | 750  | C    | N3-C4-C5    | -5.50 | 119.70      | 121.90   |
| 1   | AA    | 773  | G    | C5-C6-N1    | -5.50 | 108.75      | 111.50   |
| 1   | AA    | 811  | C    | O4'-C1'-N1  | 5.50  | 112.60      | 108.20   |
| 1   | AA    | 1277 | C    | OP2-P-O3'   | 5.50  | 117.31      | 105.20   |
| 15  | AO    | 14   | PHE  | CG-CD2-CE2  | -5.50 | 114.75      | 120.80   |
| 22  | AV    | 57   | A    | O4'-C1'-N9  | 5.50  | 112.60      | 108.20   |
| 35  | BB    | 255  | A    | C8-N9-C4    | -5.50 | 103.60      | 105.80   |
| 35  | BB    | 620  | G    | N3-C2-N2    | 5.50  | 123.75      | 119.90   |
| 35  | BB    | 886  | A    | C2-N3-C4    | 5.50  | 113.35      | 110.60   |
| 35  | BB    | 2353 | G    | N1-C2-N3    | -5.50 | 120.60      | 123.90   |
| 35  | BB    | 2433 | A    | C5-C6-N6    | -5.50 | 119.30      | 123.70   |
| 35  | BB    | 2588 | G    | C4-C5-N7    | -5.50 | 108.60      | 110.80   |
| 35  | BB    | 2609 | U    | C4-C5-C6    | -5.50 | 116.40      | 119.70   |
| 35  | BB    | 2693 | G    | N7-C8-N9    | -5.50 | 110.35      | 113.10   |
| 35  | BB    | 2871 | U    | N3-C4-C5    | -5.50 | 111.30      | 114.60   |
| 35  | BB    | 2885 | G    | N3-C4-N9    | -5.50 | 122.70      | 126.00   |
| 1   | AA    | 187  | G    | O4'-C1'-N9  | 5.50  | 112.60      | 108.20   |
| 1   | AA    | 678  | U    | C5-C6-N1    | 5.50  | 125.45      | 122.70   |
| 1   | AA    | 921  | U    | C5-C6-N1    | 5.50  | 125.45      | 122.70   |
| 1   | AA    | 1376 | U    | P-O5'-C5'   | -5.50 | 112.10      | 120.90   |
| 28  | B3    | 40   | HIS  | ND1-CG-CD2  | 5.50  | 116.50      | 108.80   |
| 35  | BB    | 367  | G    | N3-C2-N2    | 5.50  | 123.75      | 119.90   |
| 35  | BB    | 443  | A    | C4-C5-C6    | 5.50  | 119.75      | 117.00   |
| 35  | BB    | 608  | A    | C4'-C3'-C2' | -5.50 | 97.10       | 102.60   |
| 35  | BB    | 826  | U    | C1'-O4'-C4' | 5.50  | 114.30      | 109.90   |
| 35  | BB    | 941  | A    | N3-C4-N9    | 5.50  | 131.80      | 127.40   |
| 35  | BB    | 1050 | A    | O4'-C1'-N9  | 5.50  | 112.60      | 108.20   |
| 35  | BB    | 1125 | G    | O4'-C1'-N9  | 5.50  | 112.60      | 108.20   |
| 35  | BB    | 1597 | A    | C5-C6-N6    | -5.50 | 119.30      | 123.70   |
| 35  | BB    | 2199 | A    | C8-N9-C4    | -5.50 | 103.60      | 105.80   |
| 35  | BB    | 2314 | A    | C8-N9-C4    | -5.50 | 103.60      | 105.80   |
| 35  | BB    | 2352 | A    | N7-C8-N9    | 5.50  | 116.55      | 113.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2444 | G    | N1-C2-N3    | -5.50 | 120.60      | 123.90   |
| 35  | BB    | 2752 | C    | C4-C5-C6    | 5.50  | 120.15      | 117.40   |
| 1   | AA    | 881  | G    | C5-C6-N1    | -5.50 | 108.75      | 111.50   |
| 1   | AA    | 1496 | C    | P-O3'-C3'   | -5.50 | 113.10      | 119.70   |
| 35  | BB    | 1757 | A    | C8-N9-C4    | 5.50  | 108.00      | 105.80   |
| 35  | BB    | 2638 | G    | O4'-C1'-N9  | 5.50  | 112.60      | 108.20   |
| 1   | AA    | 178  | C    | C1'-O4'-C4' | -5.50 | 105.50      | 109.90   |
| 1   | AA    | 462  | G    | O4'-C1'-N9  | 5.50  | 112.60      | 108.20   |
| 1   | AA    | 611  | C    | C5-C4-N4    | 5.50  | 124.05      | 120.20   |
| 1   | AA    | 728  | A    | C2-N3-C4    | 5.50  | 113.35      | 110.60   |
| 1   | AA    | 846  | G    | C5-C6-N1    | 5.50  | 114.25      | 111.50   |
| 1   | AA    | 846  | G    | N3-C4-C5    | -5.50 | 125.85      | 128.60   |
| 1   | AA    | 968  | A    | N1-C2-N3    | 5.50  | 132.05      | 129.30   |
| 1   | AA    | 1497 | G    | C5-C6-N1    | -5.50 | 108.75      | 111.50   |
| 35  | BB    | 5    | A    | C6-C5-N7    | -5.50 | 128.45      | 132.30   |
| 35  | BB    | 326  | G    | N1-C2-N2    | -5.50 | 111.25      | 116.20   |
| 35  | BB    | 546  | U    | C2-N1-C1'   | 5.50  | 124.30      | 117.70   |
| 35  | BB    | 777  | G    | N3-C4-C5    | -5.50 | 125.85      | 128.60   |
| 35  | BB    | 995  | C    | N3-C2-O2    | -5.50 | 118.05      | 121.90   |
| 35  | BB    | 1156 | A    | O4'-C1'-C2' | 5.50  | 112.55      | 107.60   |
| 35  | BB    | 1332 | G    | N1-C2-N3    | -5.50 | 120.60      | 123.90   |
| 35  | BB    | 1798 | U    | C2-N3-C4    | -5.50 | 123.70      | 127.00   |
| 35  | BB    | 1895 | C    | P-O5'-C5'   | 5.50  | 129.70      | 120.90   |
| 35  | BB    | 1993 | U    | OP1-P-OP2   | -5.50 | 111.35      | 119.60   |
| 35  | BB    | 2229 | U    | N1-C1'-C2'  | -5.50 | 105.95      | 112.00   |
| 35  | BB    | 2288 | A    | C4-C5-N7    | -5.50 | 107.95      | 110.70   |
| 35  | BB    | 2829 | A    | OP1-P-OP2   | -5.50 | 111.35      | 119.60   |
| 41  | BH    | 15   | LEU  | N-CA-CB     | 5.50  | 121.40      | 110.40   |
| 53  | BT    | 30   | ILE  | CB-CA-C     | 5.50  | 122.60      | 111.60   |
| 55  | BW    | 28   | ALA  | N-CA-CB     | 5.50  | 117.80      | 110.10   |
| 1   | AA    | 98   | A    | C2-N3-C4    | -5.50 | 107.85      | 110.60   |
| 1   | AA    | 122  | G    | N9-C1'-C2'  | -5.50 | 105.95      | 112.00   |
| 1   | AA    | 151  | A    | N1-C2-N3    | -5.50 | 126.55      | 129.30   |
| 1   | AA    | 347  | G    | P-O3'-C3'   | -5.50 | 113.11      | 119.70   |
| 1   | AA    | 935  | A    | C4-C5-C6    | 5.50  | 119.75      | 117.00   |
| 1   | AA    | 1117 | A    | C5'-C4'-C3' | -5.50 | 107.21      | 116.00   |
| 1   | AA    | 1427 | C    | OP1-P-OP2   | -5.50 | 111.35      | 119.60   |
| 7   | AG    | 43   | TYR  | CB-CG-CD2   | -5.50 | 117.70      | 121.00   |
| 22  | AV    | 69   | G    | C6-N1-C2    | -5.50 | 121.80      | 125.10   |
| 35  | BB    | 221  | A    | C5-N7-C8    | 5.50  | 106.65      | 103.90   |
| 35  | BB    | 530  | G    | C1'-O4'-C4' | -5.50 | 105.50      | 109.90   |
| 35  | BB    | 612  | G    | C2-N3-C4    | 5.50  | 114.65      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 729  | G    | C5-C6-N1    | -5.50 | 108.75      | 111.50   |
| 35  | BB    | 1031 | G    | C8-N9-C4    | -5.50 | 104.20      | 106.40   |
| 35  | BB    | 1177 | G    | N9-C4-C5    | -5.50 | 103.20      | 105.40   |
| 35  | BB    | 1377 | G    | P-O5'-C5'   | 5.50  | 129.69      | 120.90   |
| 35  | BB    | 1560 | G    | C6-N1-C2    | -5.50 | 121.80      | 125.10   |
| 35  | BB    | 1660 | G    | C6-N1-C2    | 5.50  | 128.40      | 125.10   |
| 35  | BB    | 1774 | C    | C4-C5-C6    | -5.50 | 114.65      | 117.40   |
| 35  | BB    | 2171 | A    | C5-C6-N1    | -5.50 | 114.95      | 117.70   |
| 35  | BB    | 2304 | G    | N1-C2-N2    | 5.50  | 121.15      | 116.20   |
| 35  | BB    | 2387 | U    | N1-C2-N3    | 5.50  | 118.20      | 114.90   |
| 35  | BB    | 2849 | U    | N3-C4-O4    | 5.50  | 123.25      | 119.40   |
| 56  | BY    | 30   | VAL  | CA-CB-CG2   | -5.50 | 102.66      | 110.90   |
| 1   | AA    | 565  | U    | N1-C2-N3    | -5.50 | 111.60      | 114.90   |
| 1   | AA    | 1333 | A    | C4'-C3'-C2' | -5.50 | 97.11       | 102.60   |
| 34  | BA    | 23   | G    | C5-C6-O6    | -5.50 | 125.30      | 128.60   |
| 35  | BB    | 221  | A    | C5'-C4'-C3' | -5.50 | 107.21      | 116.00   |
| 35  | BB    | 1046 | A    | N3-C4-C5    | -5.50 | 122.95      | 126.80   |
| 35  | BB    | 1288 | G    | N3-C4-C5    | -5.50 | 125.85      | 128.60   |
| 35  | BB    | 2792 | A    | C1'-O4'-C4' | 5.50  | 114.30      | 109.90   |
| 1   | AA    | 562  | U    | O4'-C4'-C3' | -5.49 | 98.51       | 104.00   |
| 1   | AA    | 1025 | U    | O4'-C1'-N1  | 5.49  | 112.59      | 108.20   |
| 1   | AA    | 1050 | G    | N3-C4-C5    | 5.49  | 131.35      | 128.60   |
| 1   | AA    | 1488 | G    | C5-C6-O6    | -5.49 | 125.30      | 128.60   |
| 10  | AJ    | 68   | ARG  | CB-CA-C     | -5.49 | 99.41       | 110.40   |
| 11  | AK    | 115  | ILE  | N-CA-C      | -5.49 | 96.17       | 111.00   |
| 34  | BA    | 52   | A    | C3'-C2'-C1' | 5.49  | 105.89      | 101.50   |
| 35  | BB    | 119  | A    | C4'-C3'-C2' | -5.49 | 97.11       | 102.60   |
| 35  | BB    | 674  | G    | C5-C6-O6    | -5.49 | 125.30      | 128.60   |
| 35  | BB    | 698  | C    | C5-C6-N1    | 5.49  | 123.75      | 121.00   |
| 35  | BB    | 775  | G    | N1-C2-N2    | -5.49 | 111.26      | 116.20   |
| 35  | BB    | 1288 | G    | N3-C2-N2    | 5.49  | 123.75      | 119.90   |
| 35  | BB    | 2243 | U    | O4'-C1'-N1  | 5.49  | 112.59      | 108.20   |
| 35  | BB    | 2324 | U    | N1-C2-N3    | 5.49  | 118.20      | 114.90   |
| 35  | BB    | 2802 | G    | N1-C2-N3    | -5.49 | 120.60      | 123.90   |
| 35  | BB    | 2862 | G    | O4'-C1'-N9  | 5.49  | 112.59      | 108.20   |
| 1   | AA    | 699  | C    | C4-C5-C6    | 5.49  | 120.15      | 117.40   |
| 7   | AG    | 7    | GLY  | N-CA-C      | -5.49 | 99.37       | 113.10   |
| 22  | AV    | 33   | U    | O3'-P-O5'   | 5.49  | 114.43      | 104.00   |
| 35  | BB    | 6    | A    | C5-C6-N1    | -5.49 | 114.95      | 117.70   |
| 35  | BB    | 363  | G    | C8-N9-C1'   | -5.49 | 119.86      | 127.00   |
| 35  | BB    | 945  | A    | N1-C2-N3    | -5.49 | 126.55      | 129.30   |
| 35  | BB    | 1403 | A    | C5'-C4'-C3' | 5.49  | 124.79      | 116.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1426 | G    | C2-N3-C4    | 5.49  | 114.65      | 111.90   |
| 35  | BB    | 2054 | A    | N1-C2-N3    | -5.49 | 126.55      | 129.30   |
| 35  | BB    | 2763 | G    | N1-C2-N3    | 5.49  | 127.19      | 123.90   |
| 36  | BC    | 216  | ARG  | CD-NE-CZ    | 5.49  | 131.29      | 123.60   |
| 1   | AA    | 57   | G    | N1-C2-N2    | 5.49  | 121.14      | 116.20   |
| 1   | AA    | 131  | A    | O4'-C1'-N9  | 5.49  | 112.59      | 108.20   |
| 1   | AA    | 197  | A    | O4'-C1'-N9  | -5.49 | 103.81      | 108.20   |
| 1   | AA    | 939  | G    | N1-C6-O6    | 5.49  | 123.19      | 119.90   |
| 1   | AA    | 1003 | G    | C8-N9-C4    | -5.49 | 104.20      | 106.40   |
| 1   | AA    | 1373 | G    | N9-C1'-C2'  | -5.49 | 105.96      | 112.00   |
| 1   | AA    | 1395 | C    | C2-N1-C1'   | -5.49 | 112.76      | 118.80   |
| 1   | AA    | 1463 | U    | N3-C2-O2    | 5.49  | 126.04      | 122.20   |
| 22  | AV    | 50   | G    | O4'-C1'-N9  | 5.49  | 112.59      | 108.20   |
| 35  | BB    | 1215 | G    | C5-C6-N1    | 5.49  | 114.25      | 111.50   |
| 35  | BB    | 1609 | A    | C5-C6-N6    | -5.49 | 119.31      | 123.70   |
| 35  | BB    | 1972 | G    | O4'-C1'-N9  | 5.49  | 112.59      | 108.20   |
| 35  | BB    | 2091 | C    | C5-C4-N4    | -5.49 | 116.36      | 120.20   |
| 35  | BB    | 2116 | G    | OP2-P-O3'   | 5.49  | 117.28      | 105.20   |
| 1   | AA    | 175  | C    | C2-N1-C1'   | 5.49  | 124.84      | 118.80   |
| 1   | AA    | 468  | A    | C4-C5-C6    | -5.49 | 114.26      | 117.00   |
| 1   | AA    | 888  | G    | N3-C2-N2    | 5.49  | 123.74      | 119.90   |
| 1   | AA    | 1473 | G    | N1-C2-N2    | -5.49 | 111.26      | 116.20   |
| 1   | AA    | 1525 | G    | C5-C6-N1    | -5.49 | 108.76      | 111.50   |
| 3   | AC    | 126  | ARG  | NE-CZ-NH2   | -5.49 | 117.56      | 120.30   |
| 34  | BA    | 17   | C    | N3-C2-O2    | -5.49 | 118.06      | 121.90   |
| 35  | BB    | 220  | G    | N1-C2-N3    | -5.49 | 120.61      | 123.90   |
| 35  | BB    | 223  | A    | C2-N3-C4    | -5.49 | 107.86      | 110.60   |
| 35  | BB    | 298  | G    | C4-C5-N7    | 5.49  | 113.00      | 110.80   |
| 35  | BB    | 739  | A    | N9-C4-C5    | 5.49  | 108.00      | 105.80   |
| 35  | BB    | 752  | A    | C3'-C2'-C1' | -5.49 | 97.11       | 101.50   |
| 35  | BB    | 1110 | G    | C5-N7-C8    | -5.49 | 101.56      | 104.30   |
| 35  | BB    | 1152 | C    | N1-C2-O2    | 5.49  | 122.19      | 118.90   |
| 35  | BB    | 1212 | G    | C6-C5-N7    | -5.49 | 127.11      | 130.40   |
| 35  | BB    | 1295 | C    | N1-C2-O2    | -5.49 | 115.61      | 118.90   |
| 35  | BB    | 1497 | U    | C6-N1-C1'   | -5.49 | 113.52      | 121.20   |
| 35  | BB    | 1831 | G    | P-O5'-C5'   | -5.49 | 112.12      | 120.90   |
| 35  | BB    | 1987 | A    | N1-C2-N3    | 5.49  | 132.04      | 129.30   |
| 35  | BB    | 2120 | G    | N1-C2-N2    | -5.49 | 111.26      | 116.20   |
| 35  | BB    | 2229 | U    | OP1-P-OP2   | -5.49 | 111.37      | 119.60   |
| 35  | BB    | 2245 | U    | O4'-C1'-N1  | 5.49  | 112.59      | 108.20   |
| 35  | BB    | 2340 | A    | N3-C4-N9    | -5.49 | 123.01      | 127.40   |
| 35  | BB    | 2675 | A    | C6-N1-C2    | 5.49  | 121.89      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2696 | U    | N3-C4-C5    | -5.49 | 111.31      | 114.60   |
| 35  | BB    | 2787 | C    | N1-C2-O2    | 5.49  | 122.19      | 118.90   |
| 39  | BF    | 88   | VAL  | CG1-CB-CG2  | 5.49  | 119.68      | 110.90   |
| 30  | B5    | 78   | PHE  | CB-CG-CD2   | -5.49 | 116.96      | 120.80   |
| 35  | BB    | 403  | U    | P-O3'-C3'   | 5.49  | 126.28      | 119.70   |
| 35  | BB    | 420  | C    | C2-N1-C1'   | 5.49  | 124.83      | 118.80   |
| 35  | BB    | 1578 | U    | C5-C4-O4    | 5.49  | 129.19      | 125.90   |
| 35  | BB    | 1641 | A    | P-O5'-C5'   | -5.49 | 112.12      | 120.90   |
| 35  | BB    | 2294 | G    | C5-C6-N1    | -5.49 | 108.76      | 111.50   |
| 35  | BB    | 2563 | U    | C3'-C2'-C1' | 5.49  | 105.89      | 101.50   |
| 35  | BB    | 2857 | G    | C6-N1-C2    | 5.49  | 128.39      | 125.10   |
| 1   | AA    | 176  | C    | N1-C1'-C2'  | -5.49 | 105.97      | 112.00   |
| 1   | AA    | 241  | G    | O4'-C1'-N9  | 5.49  | 112.59      | 108.20   |
| 1   | AA    | 548  | G    | C6-C5-N7    | -5.49 | 127.11      | 130.40   |
| 1   | AA    | 852  | G    | N1-C6-O6    | 5.49  | 123.19      | 119.90   |
| 1   | AA    | 910  | C    | C5-C6-N1    | 5.49  | 123.74      | 121.00   |
| 1   | AA    | 936  | C    | C4-C5-C6    | -5.49 | 114.66      | 117.40   |
| 1   | AA    | 962  | C    | N1-C2-N3    | -5.49 | 115.36      | 119.20   |
| 1   | AA    | 1199 | U    | C5-C4-O4    | 5.49  | 129.19      | 125.90   |
| 12  | AL    | 65   | TYR  | CG-CD1-CE1  | -5.49 | 116.91      | 121.30   |
| 34  | BA    | 7    | G    | C8-N9-C4    | 5.49  | 108.59      | 106.40   |
| 35  | BB    | 693  | A    | N1-C6-N6    | 5.49  | 121.89      | 118.60   |
| 35  | BB    | 1085 | A    | C3'-C2'-C1' | 5.49  | 105.89      | 101.50   |
| 35  | BB    | 1628 | G    | C5-C6-O6    | -5.49 | 125.31      | 128.60   |
| 35  | BB    | 2283 | C    | C1'-O4'-C4' | 5.49  | 114.29      | 109.90   |
| 52  | BS    | 60   | HIS  | C-N-CA      | 5.49  | 135.41      | 121.70   |
| 1   | AA    | 113  | G    | C2-N3-C4    | -5.48 | 109.16      | 111.90   |
| 1   | AA    | 162  | A    | N1-C2-N3    | -5.48 | 126.56      | 129.30   |
| 1   | AA    | 629  | A    | N1-C2-N3    | 5.48  | 132.04      | 129.30   |
| 1   | AA    | 631  | C    | C4-C5-C6    | -5.48 | 114.66      | 117.40   |
| 1   | AA    | 633  | G    | C5-N7-C8    | -5.48 | 101.56      | 104.30   |
| 1   | AA    | 791  | G    | O4'-C1'-N9  | 5.48  | 112.59      | 108.20   |
| 1   | AA    | 1316 | G    | C5-C6-O6    | -5.48 | 125.31      | 128.60   |
| 22  | AV    | 28   | C    | N3-C4-N4    | 5.48  | 121.84      | 118.00   |
| 35  | BB    | 757  | G    | O4'-C1'-N9  | 5.48  | 112.59      | 108.20   |
| 35  | BB    | 1192 | G    | C6-C5-N7    | -5.48 | 127.11      | 130.40   |
| 35  | BB    | 1212 | G    | N7-C8-N9    | 5.48  | 115.84      | 113.10   |
| 35  | BB    | 1594 | U    | C2-N1-C1'   | 5.48  | 124.28      | 117.70   |
| 35  | BB    | 1632 | A    | N1-C2-N3    | -5.48 | 126.56      | 129.30   |
| 35  | BB    | 1871 | A    | O4'-C1'-N9  | 5.48  | 112.59      | 108.20   |
| 35  | BB    | 2316 | G    | C8-N9-C4    | 5.48  | 108.59      | 106.40   |
| 1   | AA    | 546  | A    | C5-N7-C8    | 5.48  | 106.64      | 103.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1088 | G    | N1-C6-O6    | 5.48  | 123.19      | 119.90   |
| 1   | AA    | 1514 | G    | N3-C2-N2    | 5.48  | 123.74      | 119.90   |
| 22  | AV    | 31   | C    | N3-C4-N4    | 5.48  | 121.84      | 118.00   |
| 33  | B8    | 20   | ASP  | CB-CG-OD2   | -5.48 | 113.37      | 118.30   |
| 35  | BB    | 126  | A    | C5-C6-N6    | -5.48 | 119.31      | 123.70   |
| 35  | BB    | 470  | A    | C8-N9-C4    | -5.48 | 103.61      | 105.80   |
| 35  | BB    | 508  | A    | C8-N9-C4    | -5.48 | 103.61      | 105.80   |
| 35  | BB    | 636  | G    | C6-N1-C2    | 5.48  | 128.39      | 125.10   |
| 35  | BB    | 689  | A    | C5-N7-C8    | 5.48  | 106.64      | 103.90   |
| 35  | BB    | 818  | G    | C8-N9-C4    | -5.48 | 104.21      | 106.40   |
| 35  | BB    | 938  | G    | N9-C4-C5    | -5.48 | 103.21      | 105.40   |
| 35  | BB    | 961  | C    | C1'-O4'-C4' | 5.48  | 114.29      | 109.90   |
| 35  | BB    | 1396 | U    | O4'-C1'-C2' | 5.48  | 112.53      | 107.60   |
| 35  | BB    | 2316 | G    | P-O5'-C5'   | 5.48  | 129.67      | 120.90   |
| 35  | BB    | 2329 | U    | C1'-O4'-C4' | -5.48 | 105.52      | 109.90   |
| 1   | AA    | 596  | A    | N7-C8-N9    | -5.48 | 111.06      | 113.80   |
| 1   | AA    | 633  | G    | N3-C4-C5    | -5.48 | 125.86      | 128.60   |
| 1   | AA    | 987  | G    | C5-N7-C8    | 5.48  | 107.04      | 104.30   |
| 22  | AV    | 23   | C    | N3-C4-C5    | -5.48 | 119.71      | 121.90   |
| 23  | AX    | 20   | G    | O4'-C1'-N9  | 5.48  | 112.58      | 108.20   |
| 35  | BB    | 551  | G    | N1-C2-N3    | -5.48 | 120.61      | 123.90   |
| 35  | BB    | 705  | A    | C5-C6-N6    | -5.48 | 119.32      | 123.70   |
| 35  | BB    | 849  | A    | N7-C8-N9    | -5.48 | 111.06      | 113.80   |
| 35  | BB    | 1154 | G    | N1-C2-N2    | -5.48 | 111.27      | 116.20   |
| 35  | BB    | 1329 | U    | C5-C6-N1    | 5.48  | 125.44      | 122.70   |
| 35  | BB    | 1543 | G    | C6-N1-C2    | 5.48  | 128.39      | 125.10   |
| 35  | BB    | 1900 | A    | C4-C5-C6    | 5.48  | 119.74      | 117.00   |
| 35  | BB    | 2319 | G    | P-O5'-C5'   | 5.48  | 129.67      | 120.90   |
| 35  | BB    | 2647 | U    | O4'-C1'-N1  | 5.48  | 112.58      | 108.20   |
| 35  | BB    | 2734 | A    | N7-C8-N9    | -5.48 | 111.06      | 113.80   |
| 37  | BD    | 82   | PHE  | CG-CD1-CE1  | 5.48  | 126.83      | 120.80   |
| 37  | BD    | 161  | MET  | CA-CB-CG    | 5.48  | 122.62      | 113.30   |
| 1   | AA    | 447  | G    | O4'-C1'-N9  | 5.48  | 112.58      | 108.20   |
| 1   | AA    | 634  | C    | N3-C4-N4    | 5.48  | 121.83      | 118.00   |
| 34  | BA    | 46   | A    | N1-C6-N6    | 5.48  | 121.89      | 118.60   |
| 35  | BB    | 108  | G    | C8-N9-C4    | -5.48 | 104.21      | 106.40   |
| 35  | BB    | 381  | G    | C5-C6-N1    | -5.48 | 108.76      | 111.50   |
| 35  | BB    | 880  | G    | C4'-C3'-C2' | -5.48 | 97.12       | 102.60   |
| 35  | BB    | 2139 | U    | N3-C4-O4    | 5.48  | 123.24      | 119.40   |
| 35  | BB    | 2162 | G    | O4'-C1'-N9  | 5.48  | 112.58      | 108.20   |
| 35  | BB    | 2363 | G    | N3-C4-C5    | 5.48  | 131.34      | 128.60   |
| 35  | BB    | 2844 | G    | C8-N9-C4    | -5.48 | 104.21      | 106.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2885 | G    | N3-C2-N2    | 5.48  | 123.73      | 119.90   |
| 1   | AA    | 24   | U    | O4'-C1'-N1  | 5.48  | 112.58      | 108.20   |
| 1   | AA    | 652  | U    | OP2-P-O3'   | 5.48  | 117.25      | 105.20   |
| 1   | AA    | 1065 | U    | C6-N1-C2    | -5.48 | 117.71      | 121.00   |
| 1   | AA    | 1101 | A    | O4'-C1'-N9  | 5.48  | 112.58      | 108.20   |
| 1   | AA    | 1136 | C    | C5'-C4'-O4' | 5.48  | 115.67      | 109.10   |
| 35  | BB    | 340  | A    | N3-C4-N9    | 5.48  | 131.78      | 127.40   |
| 35  | BB    | 372  | G    | O4'-C1'-N9  | 5.48  | 112.58      | 108.20   |
| 35  | BB    | 511  | U    | N1-C2-O2    | -5.48 | 118.97      | 122.80   |
| 35  | BB    | 891  | G    | C5-C6-O6    | -5.48 | 125.31      | 128.60   |
| 35  | BB    | 1303 | G    | C2-N3-C4    | 5.48  | 114.64      | 111.90   |
| 35  | BB    | 2127 | G    | N3-C4-N9    | -5.48 | 122.71      | 126.00   |
| 35  | BB    | 2129 | C    | C5'-C4'-C3' | -5.48 | 107.23      | 116.00   |
| 35  | BB    | 2281 | A    | C6-C5-N7    | -5.48 | 128.47      | 132.30   |
| 35  | BB    | 2611 | C    | N3-C4-C5    | -5.48 | 119.71      | 121.90   |
| 35  | BB    | 2623 | G    | C5-N7-C8    | -5.48 | 101.56      | 104.30   |
| 1   | AA    | 126  | G    | N3-C4-C5    | 5.48  | 131.34      | 128.60   |
| 1   | AA    | 269  | C    | C5-C6-N1    | -5.48 | 118.26      | 121.00   |
| 1   | AA    | 1273 | C    | C3'-C2'-C1' | 5.48  | 105.88      | 101.50   |
| 35  | BB    | 446  | G    | N7-C8-N9    | -5.48 | 110.36      | 113.10   |
| 35  | BB    | 668  | A    | C4'-C3'-C2' | -5.48 | 97.12       | 102.60   |
| 35  | BB    | 1244 | A    | C3'-C2'-C1' | -5.48 | 97.12       | 101.50   |
| 35  | BB    | 2035 | G    | N7-C8-N9    | -5.48 | 110.36      | 113.10   |
| 35  | BB    | 2058 | A    | C5-C6-N1    | -5.48 | 114.96      | 117.70   |
| 1   | AA    | 264  | C    | C1'-O4'-C4' | -5.47 | 105.52      | 109.90   |
| 1   | AA    | 668  | G    | C4'-C3'-C2' | -5.47 | 97.12       | 102.60   |
| 34  | BA    | 79   | G    | OP1-P-OP2   | -5.47 | 111.39      | 119.60   |
| 35  | BB    | 1    | G    | C6-C5-N7    | -5.47 | 127.11      | 130.40   |
| 35  | BB    | 45   | G    | OP1-P-O3'   | 5.47  | 117.24      | 105.20   |
| 35  | BB    | 97   | C    | C4-C5-C6    | 5.47  | 120.14      | 117.40   |
| 35  | BB    | 302  | C    | O5'-P-OP2   | 5.47  | 117.27      | 110.70   |
| 35  | BB    | 1829 | A    | C5-C6-N6    | -5.47 | 119.32      | 123.70   |
| 35  | BB    | 2203 | U    | C5'-C4'-C3' | -5.47 | 107.24      | 116.00   |
| 35  | BB    | 2677 | G    | C6-C5-N7    | -5.47 | 127.12      | 130.40   |
| 35  | BB    | 2872 | A    | C8-N9-C4    | -5.47 | 103.61      | 105.80   |
| 1   | AA    | 295  | C    | C3'-C2'-C1' | -5.47 | 97.12       | 101.50   |
| 1   | AA    | 804  | U    | C5-C4-O4    | -5.47 | 122.62      | 125.90   |
| 1   | AA    | 1185 | G    | C1'-O4'-C4' | 5.47  | 114.28      | 109.90   |
| 35  | BB    | 220  | G    | C6-N1-C2    | -5.47 | 121.82      | 125.10   |
| 35  | BB    | 247  | G    | C8-N9-C1'   | -5.47 | 119.89      | 127.00   |
| 35  | BB    | 673  | C    | O3'-P-O5'   | -5.47 | 93.60       | 104.00   |
| 35  | BB    | 1546 | G    | C5-C6-N1    | -5.47 | 108.76      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1552 | A    | OP1-P-OP2   | -5.47 | 111.39      | 119.60   |
| 35  | BB    | 2765 | A    | P-O3'-C3'   | 5.47  | 126.27      | 119.70   |
| 35  | BB    | 61   | C    | C5-C6-N1    | -5.47 | 118.27      | 121.00   |
| 35  | BB    | 460  | A    | C4-C5-C6    | 5.47  | 119.74      | 117.00   |
| 35  | BB    | 1603 | A    | C4-C5-C6    | 5.47  | 119.73      | 117.00   |
| 35  | BB    | 1993 | U    | C5-C6-N1    | 5.47  | 125.44      | 122.70   |
| 35  | BB    | 2289 | G    | N3-C4-C5    | 5.47  | 131.34      | 128.60   |
| 1   | AA    | 372  | C    | O4'-C1'-N1  | 5.47  | 112.58      | 108.20   |
| 1   | AA    | 856  | C    | P-O3'-C3'   | -5.47 | 113.14      | 119.70   |
| 1   | AA    | 1136 | C    | N1-C2-O2    | -5.47 | 115.62      | 118.90   |
| 1   | AA    | 1476 | A    | C1'-O4'-C4' | -5.47 | 105.52      | 109.90   |
| 34  | BA    | 10   | G    | N3-C2-N2    | 5.47  | 123.73      | 119.90   |
| 35  | BB    | 384  | A    | C5-C6-N6    | -5.47 | 119.33      | 123.70   |
| 35  | BB    | 491  | G    | C3'-C2'-C1' | -5.47 | 97.12       | 101.50   |
| 35  | BB    | 924  | G    | O4'-C4'-C3' | -5.47 | 98.53       | 104.00   |
| 35  | BB    | 975  | A    | N1-C2-N3    | 5.47  | 132.03      | 129.30   |
| 35  | BB    | 1512 | C    | C2-N1-C1'   | 5.47  | 124.82      | 118.80   |
| 35  | BB    | 1865 | U    | O3'-P-O5'   | -5.47 | 93.61       | 104.00   |
| 35  | BB    | 2502 | G    | P-O5'-C5'   | 5.47  | 129.65      | 120.90   |
| 35  | BB    | 2783 | U    | N1-C2-N3    | 5.47  | 118.18      | 114.90   |
| 1   | AA    | 1056 | U    | C5-C4-O4    | 5.47  | 129.18      | 125.90   |
| 35  | BB    | 38   | A    | C5-N7-C8    | 5.47  | 106.63      | 103.90   |
| 35  | BB    | 257  | C    | N3-C4-N4    | 5.47  | 121.83      | 118.00   |
| 35  | BB    | 2121 | G    | N3-C4-N9    | -5.47 | 122.72      | 126.00   |
| 35  | BB    | 2134 | A    | N1-C2-N3    | -5.47 | 126.57      | 129.30   |
| 35  | BB    | 2896 | C    | O4'-C1'-N1  | 5.47  | 112.57      | 108.20   |
| 1   | AA    | 78   | A    | C5-C6-N6    | -5.47 | 119.33      | 123.70   |
| 1   | AA    | 81   | A    | C2-N3-C4    | 5.47  | 113.33      | 110.60   |
| 1   | AA    | 199  | A    | O4'-C1'-N9  | 5.47  | 112.57      | 108.20   |
| 1   | AA    | 645  | G    | N9-C4-C5    | 5.47  | 107.59      | 105.40   |
| 1   | AA    | 910  | C    | N3-C4-N4    | 5.47  | 121.83      | 118.00   |
| 1   | AA    | 1076 | U    | N3-C4-C5    | -5.47 | 111.32      | 114.60   |
| 1   | AA    | 1295 | U    | O4'-C1'-C2' | -5.47 | 100.33      | 105.80   |
| 7   | AG    | 125  | ASP  | CB-CG-OD2   | 5.47  | 123.22      | 118.30   |
| 22  | AV    | 7    | G    | C1'-O4'-C4' | 5.47  | 114.27      | 109.90   |
| 35  | BB    | 1122 | G    | C4-C5-C6    | 5.47  | 122.08      | 118.80   |
| 35  | BB    | 1147 | A    | C6-C5-N7    | -5.47 | 128.47      | 132.30   |
| 35  | BB    | 2325 | G    | N1-C2-N2    | 5.47  | 121.12      | 116.20   |
| 35  | BB    | 2560 | A    | C2-N3-C4    | -5.47 | 107.87      | 110.60   |
| 35  | BB    | 2630 | G    | O4'-C1'-N9  | 5.47  | 112.57      | 108.20   |
| 1   | AA    | 120  | A    | C4'-C3'-C2' | -5.46 | 97.14       | 102.60   |
| 1   | AA    | 130  | A    | N7-C8-N9    | -5.46 | 111.07      | 113.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 671  | G    | N1-C2-N3    | -5.46 | 120.62      | 123.90   |
| 1   | AA    | 1463 | U    | N3-C4-O4    | 5.46  | 123.23      | 119.40   |
| 22  | AV    | 17   | C    | N3-C4-N4    | 5.46  | 121.83      | 118.00   |
| 22  | AV    | 28   | C    | N3-C4-C5    | -5.46 | 119.71      | 121.90   |
| 34  | BA    | 7    | G    | C5-C6-N1    | 5.46  | 114.23      | 111.50   |
| 35  | BB    | 614  | A    | O4'-C4'-C3' | 5.46  | 110.47      | 106.10   |
| 35  | BB    | 894  | U    | C4-C5-C6    | 5.46  | 122.98      | 119.70   |
| 35  | BB    | 1142 | A    | C5-C6-N6    | -5.46 | 119.33      | 123.70   |
| 35  | BB    | 1187 | G    | C5-C6-O6    | -5.46 | 125.32      | 128.60   |
| 35  | BB    | 1597 | A    | C6-C5-N7    | -5.46 | 128.47      | 132.30   |
| 35  | BB    | 1666 | G    | C5-C6-O6    | -5.46 | 125.32      | 128.60   |
| 35  | BB    | 1727 | C    | O4'-C1'-N1  | 5.46  | 112.57      | 108.20   |
| 35  | BB    | 1847 | A    | O4'-C1'-N9  | 5.46  | 112.57      | 108.20   |
| 1   | AA    | 793  | U    | N3-C4-O4    | 5.46  | 123.22      | 119.40   |
| 1   | AA    | 1426 | G    | C4'-C3'-C2' | -5.46 | 97.14       | 102.60   |
| 5   | AE    | 87   | VAL  | CA-CB-CG1   | 5.46  | 119.09      | 110.90   |
| 35  | BB    | 1432 | G    | N1-C2-N2    | -5.46 | 111.28      | 116.20   |
| 35  | BB    | 2361 | G    | C2-N3-C4    | 5.46  | 114.63      | 111.90   |
| 35  | BB    | 2519 | U    | N3-C4-C5    | -5.46 | 111.32      | 114.60   |
| 45  | BL    | 7    | SER  | CB-CA-C     | -5.46 | 99.72       | 110.10   |
| 52  | BS    | 107  | VAL  | CA-CB-CG1   | -5.46 | 102.71      | 110.90   |
| 1   | AA    | 357  | G    | C4-C5-N7    | 5.46  | 112.98      | 110.80   |
| 1   | AA    | 435  | A    | N1-C2-N3    | -5.46 | 126.57      | 129.30   |
| 1   | AA    | 768  | A    | N3-C4-C5    | -5.46 | 122.98      | 126.80   |
| 1   | AA    | 821  | G    | C8-N9-C4    | -5.46 | 104.22      | 106.40   |
| 1   | AA    | 994  | A    | C5-N7-C8    | 5.46  | 106.63      | 103.90   |
| 1   | AA    | 1202 | U    | C4'-C3'-C2' | -5.46 | 97.14       | 102.60   |
| 35  | BB    | 781  | A    | C6-C5-N7    | -5.46 | 128.48      | 132.30   |
| 35  | BB    | 891  | G    | C5-N7-C8    | -5.46 | 101.57      | 104.30   |
| 35  | BB    | 1064 | C    | C5'-C4'-C3' | -5.46 | 107.26      | 116.00   |
| 35  | BB    | 1204 | A    | C5-C6-N6    | -5.46 | 119.33      | 123.70   |
| 35  | BB    | 1249 | U    | C5-C4-O4    | -5.46 | 122.62      | 125.90   |
| 35  | BB    | 1464 | G    | C5-N7-C8    | 5.46  | 107.03      | 104.30   |
| 35  | BB    | 1795 | C    | C4-C5-C6    | -5.46 | 114.67      | 117.40   |
| 35  | BB    | 2035 | G    | OP1-P-OP2   | -5.46 | 111.41      | 119.60   |
| 35  | BB    | 2108 | A    | C4'-C3'-C2' | -5.46 | 97.14       | 102.60   |
| 35  | BB    | 2182 | U    | C1'-O4'-C4' | 5.46  | 114.27      | 109.90   |
| 35  | BB    | 2359 | C    | P-O5'-C5'   | -5.46 | 112.16      | 120.90   |
| 1   | AA    | 400  | C    | N3-C2-O2    | -5.46 | 118.08      | 121.90   |
| 1   | AA    | 1326 | U    | C1'-O4'-C4' | 5.46  | 114.27      | 109.90   |
| 13  | AM    | 10   | ASP  | CB-CG-OD1   | 5.46  | 123.21      | 118.30   |
| 35  | BB    | 1340 | U    | C5-C6-N1    | 5.46  | 125.43      | 122.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1537 | G    | O4'-C1'-N9  | 5.46  | 112.57      | 108.20   |
| 35  | BB    | 1959 | G    | C2-N3-C4    | -5.46 | 109.17      | 111.90   |
| 1   | AA    | 832  | G    | P-O5'-C5'   | -5.46 | 112.17      | 120.90   |
| 1   | AA    | 952  | U    | C6-N1-C2    | -5.46 | 117.72      | 121.00   |
| 1   | AA    | 1276 | G    | C6-C5-N7    | -5.46 | 127.12      | 130.40   |
| 1   | AA    | 1307 | U    | P-O3'-C3'   | -5.46 | 113.15      | 119.70   |
| 4   | AD    | 31   | CYS  | N-CA-C      | -5.46 | 96.26       | 111.00   |
| 22  | AV    | 41   | C    | N3-C4-N4    | 5.46  | 121.82      | 118.00   |
| 35  | BB    | 179  | C    | C5-C4-N4    | -5.46 | 116.38      | 120.20   |
| 35  | BB    | 300  | A    | N3-C4-C5    | -5.46 | 122.98      | 126.80   |
| 35  | BB    | 793  | A    | C5'-C4'-C3' | -5.46 | 107.27      | 116.00   |
| 35  | BB    | 1018 | U    | N1-C2-O2    | -5.46 | 118.98      | 122.80   |
| 35  | BB    | 1765 | U    | N3-C4-O4    | 5.46  | 123.22      | 119.40   |
| 35  | BB    | 2061 | G    | N7-C8-N9    | 5.46  | 115.83      | 113.10   |
| 35  | BB    | 2144 | G    | N3-C4-C5    | -5.46 | 125.87      | 128.60   |
| 35  | BB    | 2455 | G    | C5-N7-C8    | 5.46  | 107.03      | 104.30   |
| 35  | BB    | 2836 | U    | O4'-C4'-C3' | -5.46 | 98.54       | 104.00   |
| 35  | BB    | 2878 | U    | C4-C5-C6    | 5.46  | 122.98      | 119.70   |
| 1   | AA    | 164  | G    | O4'-C4'-C3' | -5.46 | 98.54       | 104.00   |
| 1   | AA    | 223  | A    | C4-C5-C6    | 5.46  | 119.73      | 117.00   |
| 1   | AA    | 290  | C    | C6-N1-C2    | 5.46  | 122.48      | 120.30   |
| 1   | AA    | 359  | G    | O4'-C1'-N9  | 5.46  | 112.56      | 108.20   |
| 1   | AA    | 576  | C    | N3-C4-N4    | 5.46  | 121.82      | 118.00   |
| 1   | AA    | 1442 | G    | C5-N7-C8    | -5.46 | 101.57      | 104.30   |
| 22  | AV    | 9    | A    | C5-C6-N1    | -5.46 | 114.97      | 117.70   |
| 35  | BB    | 130  | C    | N1-C2-O2    | 5.46  | 122.17      | 118.90   |
| 35  | BB    | 714  | U    | C2-N3-C4    | -5.46 | 123.73      | 127.00   |
| 35  | BB    | 1752 | C    | C4-C5-C6    | 5.46  | 120.13      | 117.40   |
| 35  | BB    | 1788 | C    | C4-C5-C6    | -5.46 | 114.67      | 117.40   |
| 35  | BB    | 2888 | C    | C5-C4-N4    | -5.46 | 116.38      | 120.20   |
| 51  | BR    | 40   | MET  | N-CA-CB     | 5.46  | 120.42      | 110.60   |
| 1   | AA    | 389  | A    | C3'-C2'-C1' | 5.46  | 105.86      | 101.50   |
| 1   | AA    | 557  | G    | N3-C2-N2    | 5.46  | 123.72      | 119.90   |
| 34  | BA    | 61   | G    | C2-N3-C4    | 5.46  | 114.63      | 111.90   |
| 35  | BB    | 229  | C    | N3-C4-N4    | 5.46  | 121.82      | 118.00   |
| 35  | BB    | 655  | A    | P-O3'-C3'   | 5.46  | 126.25      | 119.70   |
| 35  | BB    | 2108 | A    | N3-C4-C5    | -5.46 | 122.98      | 126.80   |
| 35  | BB    | 2728 | U    | C4'-C3'-C2' | -5.46 | 97.14       | 102.60   |
| 1   | AA    | 429  | U    | O4'-C1'-C2' | -5.45 | 100.35      | 105.80   |
| 1   | AA    | 520  | A    | C8-N9-C4    | -5.45 | 103.62      | 105.80   |
| 1   | AA    | 1101 | A    | C6-C5-N7    | -5.45 | 128.48      | 132.30   |
| 1   | AA    | 1399 | C    | O4'-C1'-C2' | -5.45 | 100.35      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 90   | U    | C3'-C2'-C1' | -5.45 | 97.14       | 101.50   |
| 35  | BB    | 768  | G    | C5-C6-N1    | -5.45 | 108.77      | 111.50   |
| 35  | BB    | 780  | G    | C5-C6-O6    | -5.45 | 125.33      | 128.60   |
| 35  | BB    | 1026 | G    | C4-C5-N7    | 5.45  | 112.98      | 110.80   |
| 35  | BB    | 1482 | G    | N3-C4-C5    | -5.45 | 125.87      | 128.60   |
| 35  | BB    | 1623 | G    | OP1-P-OP2   | -5.45 | 111.42      | 119.60   |
| 35  | BB    | 1802 | A    | O4'-C1'-N9  | 5.45  | 112.56      | 108.20   |
| 35  | BB    | 1811 | G    | C1'-O4'-C4' | 5.45  | 114.26      | 109.90   |
| 35  | BB    | 1887 | C    | C5-C4-N4    | -5.45 | 116.38      | 120.20   |
| 35  | BB    | 1911 | U    | N1-C2-O2    | -5.45 | 118.98      | 122.80   |
| 35  | BB    | 2235 | G    | N3-C4-N9    | 5.45  | 129.27      | 126.00   |
| 35  | BB    | 2365 | G    | C4-N9-C1'   | 5.45  | 133.59      | 126.50   |
| 35  | BB    | 2444 | G    | O4'-C1'-N9  | 5.45  | 112.56      | 108.20   |
| 35  | BB    | 2695 | U    | OP1-P-OP2   | -5.45 | 111.42      | 119.60   |
| 1   | AA    | 421  | U    | C2-N3-C4    | -5.45 | 123.73      | 127.00   |
| 1   | AA    | 1127 | G    | C5-C6-O6    | 5.45  | 131.87      | 128.60   |
| 1   | AA    | 196  | A    | C4'-C3'-C2' | -5.45 | 97.15       | 102.60   |
| 1   | AA    | 373  | A    | N3-C4-C5    | -5.45 | 122.98      | 126.80   |
| 1   | AA    | 453  | G    | C6-N1-C2    | -5.45 | 121.83      | 125.10   |
| 1   | AA    | 499  | A    | C4-C5-C6    | 5.45  | 119.72      | 117.00   |
| 1   | AA    | 572  | A    | C5-N7-C8    | 5.45  | 106.62      | 103.90   |
| 1   | AA    | 639  | G    | N9-C1'-C2'  | -5.45 | 106.00      | 112.00   |
| 1   | AA    | 890  | G    | N3-C2-N2    | 5.45  | 123.72      | 119.90   |
| 1   | AA    | 1234 | C    | O4'-C1'-N1  | 5.45  | 112.56      | 108.20   |
| 1   | AA    | 1400 | C    | C5'-C4'-O4' | 5.45  | 115.64      | 109.10   |
| 20  | AT    | 21   | ALA  | N-CA-CB     | 5.45  | 117.73      | 110.10   |
| 35  | BB    | 30   | G    | C3'-C2'-C1' | 5.45  | 105.86      | 101.50   |
| 35  | BB    | 176  | A    | P-O5'-C5'   | 5.45  | 129.62      | 120.90   |
| 35  | BB    | 204  | A    | C3'-C2'-C1' | -5.45 | 97.14       | 101.50   |
| 35  | BB    | 462  | C    | C5-C4-N4    | 5.45  | 124.02      | 120.20   |
| 35  | BB    | 592  | A    | C6-N1-C2    | -5.45 | 115.33      | 118.60   |
| 35  | BB    | 1567 | G    | N1-C6-O6    | 5.45  | 123.17      | 119.90   |
| 35  | BB    | 1694 | C    | C2-N3-C4    | 5.45  | 122.62      | 119.90   |
| 35  | BB    | 1839 | G    | C4-C5-N7    | 5.45  | 112.98      | 110.80   |
| 35  | BB    | 2143 | C    | N1-C2-N3    | 5.45  | 123.02      | 119.20   |
| 35  | BB    | 2281 | A    | C8-N9-C4    | -5.45 | 103.62      | 105.80   |
| 35  | BB    | 2560 | A    | C5-C6-N1    | -5.45 | 114.97      | 117.70   |
| 35  | BB    | 2598 | A    | C6-C5-N7    | -5.45 | 128.49      | 132.30   |
| 35  | BB    | 2712 | C    | C5-C6-N1    | -5.45 | 118.28      | 121.00   |
| 1   | AA    | 11   | G    | N9-C4-C5    | -5.45 | 103.22      | 105.40   |
| 1   | AA    | 588  | G    | C6-N1-C2    | 5.45  | 128.37      | 125.10   |
| 1   | AA    | 1106 | G    | C4-C5-C6    | 5.45  | 122.07      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1174 | G    | C5-C6-N1    | -5.45 | 108.78      | 111.50   |
| 15  | AO    | 62   | ARG  | NE-CZ-NH2   | -5.45 | 117.58      | 120.30   |
| 34  | BA    | 26   | C    | C1'-O4'-C4' | -5.45 | 105.54      | 109.90   |
| 35  | BB    | 235  | U    | N1-C2-N3    | 5.45  | 118.17      | 114.90   |
| 35  | BB    | 362  | A    | C2-N3-C4    | 5.45  | 113.32      | 110.60   |
| 35  | BB    | 388  | G    | N3-C4-C5    | 5.45  | 131.32      | 128.60   |
| 35  | BB    | 819  | A    | C4-C5-N7    | -5.45 | 107.98      | 110.70   |
| 35  | BB    | 1431 | A    | OP2-P-O3'   | 5.45  | 117.19      | 105.20   |
| 35  | BB    | 1461 | C    | C5-C4-N4    | -5.45 | 116.39      | 120.20   |
| 35  | BB    | 1647 | U    | P-O3'-C3'   | -5.45 | 113.16      | 119.70   |
| 35  | BB    | 1684 | G    | N3-C4-C5    | -5.45 | 125.88      | 128.60   |
| 35  | BB    | 1787 | A    | OP1-P-OP2   | -5.45 | 111.43      | 119.60   |
| 35  | BB    | 1800 | C    | C6-N1-C2    | 5.45  | 122.48      | 120.30   |
| 35  | BB    | 2469 | A    | O4'-C1'-N9  | 5.45  | 112.56      | 108.20   |
| 35  | BB    | 2582 | G    | C6-C5-N7    | -5.45 | 127.13      | 130.40   |
| 35  | BB    | 2780 | G    | N1-C2-N3    | -5.45 | 120.63      | 123.90   |
| 48  | BO    | 106  | LEU  | CB-CG-CD1   | 5.45  | 120.26      | 111.00   |
| 1   | AA    | 844  | G    | OP1-P-OP2   | -5.45 | 111.43      | 119.60   |
| 1   | AA    | 906  | A    | C5-N7-C8    | 5.45  | 106.62      | 103.90   |
| 3   | AC    | 159  | ALA  | N-CA-CB     | 5.45  | 117.73      | 110.10   |
| 6   | AF    | 87   | SER  | N-CA-CB     | 5.45  | 118.67      | 110.50   |
| 35  | BB    | 7    | G    | N7-C8-N9    | -5.45 | 110.38      | 113.10   |
| 35  | BB    | 238  | C    | C5-C6-N1    | -5.45 | 118.28      | 121.00   |
| 35  | BB    | 356  | G    | P-O5'-C5'   | -5.45 | 112.19      | 120.90   |
| 35  | BB    | 548  | G    | C8-N9-C1'   | -5.45 | 119.92      | 127.00   |
| 35  | BB    | 2277 | G    | C4-C5-C6    | 5.45  | 122.07      | 118.80   |
| 35  | BB    | 2808 | G    | C2-N3-C4    | 5.45  | 114.62      | 111.90   |
| 1   | AA    | 366  | A    | N3-C4-N9    | -5.45 | 123.04      | 127.40   |
| 1   | AA    | 442  | G    | C4-C5-N7    | -5.45 | 108.62      | 110.80   |
| 1   | AA    | 515  | G    | C8-N9-C1'   | 5.45  | 134.08      | 127.00   |
| 1   | AA    | 1183 | U    | N1-C2-O2    | -5.45 | 118.99      | 122.80   |
| 1   | AA    | 1526 | G    | C8-N9-C4    | -5.45 | 104.22      | 106.40   |
| 35  | BB    | 137  | U    | P-O5'-C5'   | 5.45  | 129.61      | 120.90   |
| 35  | BB    | 187  | G    | N7-C8-N9    | -5.45 | 110.38      | 113.10   |
| 35  | BB    | 278  | A    | C5-C6-N1    | -5.45 | 114.98      | 117.70   |
| 35  | BB    | 452  | G    | C6-C5-N7    | -5.45 | 127.13      | 130.40   |
| 35  | BB    | 468  | G    | O4'-C1'-N9  | 5.45  | 112.56      | 108.20   |
| 35  | BB    | 858  | G    | N3-C2-N2    | 5.45  | 123.71      | 119.90   |
| 35  | BB    | 924  | G    | N9-C4-C5    | -5.45 | 103.22      | 105.40   |
| 35  | BB    | 983  | A    | C4-C5-N7    | -5.45 | 107.98      | 110.70   |
| 35  | BB    | 995  | C    | N1-C2-N3    | 5.45  | 123.01      | 119.20   |
| 35  | BB    | 1040 | A    | N1-C6-N6    | 5.45  | 121.87      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2295 | C    | C4'-C3'-C2' | -5.45 | 97.16       | 102.60   |
| 35  | BB    | 2657 | A    | C8-N9-C4    | 5.45  | 107.98      | 105.80   |
| 36  | BC    | 95   | TYR  | CG-CD1-CE1  | -5.45 | 116.94      | 121.30   |
| 1   | AA    | 763  | G    | C3'-C2'-C1' | 5.44  | 105.86      | 101.50   |
| 35  | BB    | 116  | C    | C2-N1-C1'   | 5.44  | 124.79      | 118.80   |
| 35  | BB    | 468  | G    | O5'-P-OP2   | 5.44  | 117.23      | 110.70   |
| 35  | BB    | 2456 | C    | C2-N3-C4    | -5.44 | 117.18      | 119.90   |
| 1   | AA    | 330  | C    | C1'-O4'-C4' | -5.44 | 105.55      | 109.90   |
| 1   | AA    | 620  | C    | N3-C4-N4    | 5.44  | 121.81      | 118.00   |
| 1   | AA    | 751  | U    | N1-C2-N3    | -5.44 | 111.63      | 114.90   |
| 1   | AA    | 1246 | A    | N1-C6-N6    | 5.44  | 121.87      | 118.60   |
| 1   | AA    | 1505 | G    | N1-C2-N3    | -5.44 | 120.64      | 123.90   |
| 4   | AD    | 124  | VAL  | CA-CB-CG1   | -5.44 | 102.73      | 110.90   |
| 35  | BB    | 68   | G    | OP1-P-OP2   | -5.44 | 111.44      | 119.60   |
| 35  | BB    | 448  | U    | C2-N1-C1'   | 5.44  | 124.23      | 117.70   |
| 35  | BB    | 491  | G    | N1-C2-N2    | 5.44  | 121.10      | 116.20   |
| 35  | BB    | 713  | G    | C6-C5-N7    | -5.44 | 127.13      | 130.40   |
| 35  | BB    | 809  | G    | N7-C8-N9    | 5.44  | 115.82      | 113.10   |
| 35  | BB    | 904  | G    | C4-C5-N7    | -5.44 | 108.62      | 110.80   |
| 35  | BB    | 1383 | A    | C5-C6-N1    | -5.44 | 114.98      | 117.70   |
| 35  | BB    | 1407 | G    | C4-C5-C6    | 5.44  | 122.06      | 118.80   |
| 35  | BB    | 1619 | G    | O4'-C1'-N9  | 5.44  | 112.55      | 108.20   |
| 35  | BB    | 1919 | A    | C5-N7-C8    | 5.44  | 106.62      | 103.90   |
| 35  | BB    | 2095 | A    | O4'-C1'-N9  | 5.44  | 112.55      | 108.20   |
| 35  | BB    | 2172 | U    | N3-C4-O4    | 5.44  | 123.21      | 119.40   |
| 35  | BB    | 2528 | U    | C6-N1-C2    | -5.44 | 117.73      | 121.00   |
| 35  | BB    | 2673 | G    | N3-C2-N2    | 5.44  | 123.71      | 119.90   |
| 1   | AA    | 21   | G    | C6-C5-N7    | -5.44 | 127.14      | 130.40   |
| 1   | AA    | 284  | C    | C5-C4-N4    | -5.44 | 116.39      | 120.20   |
| 1   | AA    | 445  | G    | N3-C2-N2    | 5.44  | 123.71      | 119.90   |
| 1   | AA    | 1288 | A    | O4'-C1'-C2' | 5.44  | 112.50      | 107.60   |
| 1   | AA    | 1352 | C    | N3-C2-O2    | 5.44  | 125.71      | 121.90   |
| 17  | AQ    | 5    | ARG  | NE-CZ-NH1   | 5.44  | 123.02      | 120.30   |
| 35  | BB    | 403  | U    | C5-C6-N1    | 5.44  | 125.42      | 122.70   |
| 35  | BB    | 509  | C    | N1-C2-O2    | -5.44 | 115.64      | 118.90   |
| 35  | BB    | 834  | G    | N9-C4-C5    | -5.44 | 103.22      | 105.40   |
| 35  | BB    | 1568 | G    | O4'-C1'-N9  | 5.44  | 112.55      | 108.20   |
| 35  | BB    | 2265 | U    | O4'-C4'-C3' | -5.44 | 98.56       | 104.00   |
| 35  | BB    | 2664 | G    | C5'-C4'-C3' | -5.44 | 107.30      | 116.00   |
| 1   | AA    | 80   | A    | C2-N3-C4    | 5.44  | 113.32      | 110.60   |
| 1   | AA    | 389  | A    | N3-C4-N9    | 5.44  | 131.75      | 127.40   |
| 1   | AA    | 588  | G    | N3-C2-N2    | 5.44  | 123.71      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | BA    | 108  | A    | N7-C8-N9    | 5.44  | 116.52      | 113.80   |
| 35  | BB    | 2035 | G    | C5-C6-N1    | -5.44 | 108.78      | 111.50   |
| 35  | BB    | 2277 | G    | N3-C4-N9    | 5.44  | 129.26      | 126.00   |
| 35  | BB    | 2414 | G    | C8-N9-C4    | -5.44 | 104.22      | 106.40   |
| 35  | BB    | 2645 | G    | C4-C5-N7    | 5.44  | 112.98      | 110.80   |
| 35  | BB    | 2655 | G    | C5-N7-C8    | 5.44  | 107.02      | 104.30   |
| 1   | AA    | 11   | G    | OP1-P-OP2   | -5.44 | 111.44      | 119.60   |
| 1   | AA    | 372  | C    | C5-C4-N4    | -5.44 | 116.39      | 120.20   |
| 1   | AA    | 452  | A    | C5-C6-N1    | -5.44 | 114.98      | 117.70   |
| 1   | AA    | 808  | C    | N3-C4-N4    | 5.44  | 121.81      | 118.00   |
| 1   | AA    | 1034 | G    | C4-N9-C1'   | 5.44  | 133.57      | 126.50   |
| 1   | AA    | 1340 | A    | C8-N9-C4    | 5.44  | 107.97      | 105.80   |
| 35  | BB    | 1043 | C    | C5-C6-N1    | -5.44 | 118.28      | 121.00   |
| 35  | BB    | 1611 | C    | N1-C2-N3    | -5.44 | 115.39      | 119.20   |
| 35  | BB    | 2411 | A    | C6-N1-C2    | -5.44 | 115.34      | 118.60   |
| 35  | BB    | 2597 | G    | P-O3'-C3'   | 5.44  | 126.23      | 119.70   |
| 35  | BB    | 2681 | C    | C5-C6-N1    | -5.44 | 118.28      | 121.00   |
| 1   | AA    | 76   | G    | C5-N7-C8    | 5.44  | 107.02      | 104.30   |
| 1   | AA    | 501  | C    | N3-C4-N4    | 5.44  | 121.81      | 118.00   |
| 1   | AA    | 663  | A    | N9-C4-C5    | -5.44 | 103.63      | 105.80   |
| 1   | AA    | 1110 | A    | C3'-C2'-C1' | -5.44 | 97.15       | 101.50   |
| 7   | AG    | 4    | ARG  | NE-CZ-NH2   | -5.44 | 117.58      | 120.30   |
| 22  | AV    | 58   | A    | C5-C6-N6    | -5.44 | 119.35      | 123.70   |
| 35  | BB    | 252  | G    | C1'-O4'-C4' | 5.44  | 114.25      | 109.90   |
| 35  | BB    | 448  | U    | OP1-P-OP2   | -5.44 | 111.45      | 119.60   |
| 35  | BB    | 2338 | C    | O5'-C5'-C4' | -5.44 | 101.37      | 111.70   |
| 35  | BB    | 2691 | C    | N3-C4-C5    | -5.44 | 119.72      | 121.90   |
| 44  | BK    | 64   | ARG  | NE-CZ-NH1   | 5.44  | 123.02      | 120.30   |
| 1   | AA    | 986  | U    | C3'-C2'-C1' | 5.43  | 105.85      | 101.50   |
| 1   | AA    | 1133 | G    | N1-C6-O6    | 5.43  | 123.16      | 119.90   |
| 5   | AE    | 49   | TYR  | CG-CD2-CE2  | 5.43  | 125.65      | 121.30   |
| 35  | BB    | 309  | A    | C2-N3-C4    | -5.43 | 107.88      | 110.60   |
| 35  | BB    | 702  | U    | N1-C2-N3    | -5.43 | 111.64      | 114.90   |
| 35  | BB    | 1098 | A    | P-O3'-C3'   | -5.43 | 113.18      | 119.70   |
| 35  | BB    | 1173 | U    | C1'-O4'-C4' | 5.43  | 114.25      | 109.90   |
| 35  | BB    | 1446 | C    | C5-C4-N4    | -5.43 | 116.39      | 120.20   |
| 35  | BB    | 1571 | A    | O4'-C1'-N9  | 5.43  | 112.55      | 108.20   |
| 35  | BB    | 2173 | A    | C4-C5-N7    | -5.43 | 107.98      | 110.70   |
| 35  | BB    | 2309 | A    | C2-N3-C4    | -5.43 | 107.88      | 110.60   |
| 35  | BB    | 2534 | A    | C2-N3-C4    | -5.43 | 107.88      | 110.60   |
| 35  | BB    | 2560 | A    | P-O3'-C3'   | -5.43 | 113.18      | 119.70   |
| 1   | AA    | 1268 | G    | C4-C5-C6    | 5.43  | 122.06      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1305 | G    | N7-C8-N9    | 5.43  | 115.82      | 113.10   |
| 22  | AV    | 62   | C    | N3-C4-C5    | -5.43 | 119.73      | 121.90   |
| 34  | BA    | 103  | U    | O4'-C1'-N1  | 5.43  | 112.55      | 108.20   |
| 35  | BB    | 635  | C    | C1'-O4'-C4' | 5.43  | 114.25      | 109.90   |
| 35  | BB    | 1008 | A    | O3'-P-O5'   | -5.43 | 93.68       | 104.00   |
| 35  | BB    | 1065 | U    | P-O5'-C5'   | 5.43  | 129.59      | 120.90   |
| 35  | BB    | 1610 | A    | C6-N1-C2    | -5.43 | 115.34      | 118.60   |
| 35  | BB    | 1812 | U    | C2-N3-C4    | -5.43 | 123.74      | 127.00   |
| 35  | BB    | 1869 | G    | C4-C5-C6    | 5.43  | 122.06      | 118.80   |
| 35  | BB    | 2490 | G    | O4'-C1'-C2' | 5.43  | 112.49      | 107.60   |
| 35  | BB    | 2516 | A    | C6-C5-N7    | -5.43 | 128.50      | 132.30   |
| 35  | BB    | 2541 | A    | C4-C5-C6    | 5.43  | 119.72      | 117.00   |
| 39  | BF    | 149  | ARG  | C-N-CA      | 5.43  | 133.71      | 122.30   |
| 51  | BR    | 27   | ILE  | N-CA-CB     | 5.43  | 123.30      | 110.80   |
| 1   | AA    | 242  | G    | N7-C8-N9    | 5.43  | 115.81      | 113.10   |
| 1   | AA    | 1141 | C    | C4'-C3'-C2' | -5.43 | 97.17       | 102.60   |
| 15  | AO    | 8    | ALA  | CB-CA-C     | -5.43 | 101.95      | 110.10   |
| 35  | BB    | 26   | G    | C4-C5-C6    | 5.43  | 122.06      | 118.80   |
| 35  | BB    | 617  | G    | N1-C2-N3    | -5.43 | 120.64      | 123.90   |
| 35  | BB    | 1158 | C    | C4-C5-C6    | 5.43  | 120.11      | 117.40   |
| 35  | BB    | 1674 | G    | C5-N7-C8    | 5.43  | 107.02      | 104.30   |
| 35  | BB    | 2046 | G    | C5-C6-O6    | -5.43 | 125.34      | 128.60   |
| 35  | BB    | 2048 | G    | C5-C6-O6    | -5.43 | 125.34      | 128.60   |
| 1   | AA    | 1140 | C    | N3-C4-N4    | 5.43  | 121.80      | 118.00   |
| 8   | AH    | 64   | TYR  | N-CA-CB     | 5.43  | 120.37      | 110.60   |
| 9   | AI    | 11   | ARG  | NE-CZ-NH2   | -5.43 | 117.58      | 120.30   |
| 12  | AL    | 48   | LEU  | CB-CG-CD2   | 5.43  | 120.23      | 111.00   |
| 32  | B7    | 5    | THR  | CA-CB-CG2   | -5.43 | 104.80      | 112.40   |
| 34  | BA    | 64   | G    | C4-C5-C6    | 5.43  | 122.06      | 118.80   |
| 35  | BB    | 1236 | G    | N9-C1'-C2'  | -5.43 | 106.03      | 112.00   |
| 35  | BB    | 1872 | A    | C5'-C4'-C3' | 5.43  | 124.69      | 116.00   |
| 35  | BB    | 1889 | A    | C6-C5-N7    | -5.43 | 128.50      | 132.30   |
| 35  | BB    | 2082 | A    | C5-C6-N1    | -5.43 | 114.98      | 117.70   |
| 35  | BB    | 2116 | G    | P-O3'-C3'   | 5.43  | 126.22      | 119.70   |
| 35  | BB    | 2606 | C    | P-O3'-C3'   | -5.43 | 113.18      | 119.70   |
| 35  | BB    | 2642 | G    | C3'-C2'-C1' | 5.43  | 105.84      | 101.50   |
| 1   | AA    | 1207 | G    | C4'-C3'-C2' | -5.43 | 97.17       | 102.60   |
| 3   | AC    | 5    | HIS  | CA-CB-CG    | 5.43  | 122.83      | 113.60   |
| 6   | AF    | 62   | MET  | N-CA-CB     | 5.43  | 120.37      | 110.60   |
| 34  | BA    | 62   | C    | P-O3'-C3'   | -5.43 | 113.19      | 119.70   |
| 35  | BB    | 742  | A    | O4'-C4'-C3' | -5.43 | 98.57       | 104.00   |
| 35  | BB    | 939  | G    | O4'-C1'-N9  | 5.43  | 112.54      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1177 | G    | C4-C5-C6    | 5.43  | 122.06      | 118.80   |
| 35  | BB    | 2226 | C    | C4-C5-C6    | -5.43 | 114.69      | 117.40   |
| 35  | BB    | 2685 | G    | N3-C2-N2    | 5.43  | 123.70      | 119.90   |
| 1   | AA    | 153  | C    | N1-C2-N3    | -5.43 | 115.40      | 119.20   |
| 1   | AA    | 506  | G    | N1-C2-N3    | -5.43 | 120.64      | 123.90   |
| 1   | AA    | 610  | U    | C2-N3-C4    | 5.43  | 130.25      | 127.00   |
| 1   | AA    | 755  | G    | C1'-O4'-C4' | -5.43 | 105.56      | 109.90   |
| 1   | AA    | 898  | G    | N9-C1'-C2'  | -5.43 | 106.03      | 112.00   |
| 1   | AA    | 954  | G    | O4'-C1'-N9  | 5.43  | 112.54      | 108.20   |
| 3   | AC    | 22   | PHE  | CB-CA-C     | -5.43 | 99.55       | 110.40   |
| 35  | BB    | 95   | A    | O4'-C1'-N9  | 5.43  | 112.54      | 108.20   |
| 35  | BB    | 230  | G    | C5-N7-C8    | -5.43 | 101.59      | 104.30   |
| 35  | BB    | 486  | C    | N3-C4-N4    | 5.43  | 121.80      | 118.00   |
| 35  | BB    | 1041 | G    | P-O3'-C3'   | -5.43 | 113.19      | 119.70   |
| 35  | BB    | 1095 | A    | C5-N7-C8    | 5.43  | 106.61      | 103.90   |
| 35  | BB    | 1173 | U    | O5'-C5'-C4' | -5.43 | 101.39      | 111.70   |
| 35  | BB    | 1514 | G    | N3-C2-N2    | 5.43  | 123.70      | 119.90   |
| 35  | BB    | 1514 | G    | C4-C5-C6    | 5.43  | 122.06      | 118.80   |
| 35  | BB    | 1695 | G    | N7-C8-N9    | 5.43  | 115.81      | 113.10   |
| 35  | BB    | 1970 | A    | C8-N9-C4    | -5.43 | 103.63      | 105.80   |
| 35  | BB    | 2169 | A    | C4-N9-C1'   | 5.43  | 136.07      | 126.30   |
| 35  | BB    | 2600 | A    | C4-C5-N7    | -5.43 | 107.99      | 110.70   |
| 35  | BB    | 2628 | C    | N3-C4-C5    | -5.43 | 119.73      | 121.90   |
| 35  | BB    | 2744 | G    | C1'-O4'-C4' | 5.43  | 114.24      | 109.90   |
| 1   | AA    | 718  | A    | C6-N1-C2    | 5.42  | 121.86      | 118.60   |
| 1   | AA    | 1463 | U    | C2-N3-C4    | 5.42  | 130.25      | 127.00   |
| 1   | AA    | 1511 | G    | C4-C5-C6    | 5.42  | 122.06      | 118.80   |
| 3   | AC    | 21   | TRP  | CE3-CZ3-CH2 | -5.42 | 115.23      | 121.20   |
| 7   | AG    | 25   | PHE  | CG-CD2-CE2  | -5.42 | 114.83      | 120.80   |
| 34  | BA    | 113  | C    | N1-C2-O2    | -5.42 | 115.65      | 118.90   |
| 34  | BA    | 118  | C    | OP1-P-OP2   | -5.42 | 111.46      | 119.60   |
| 35  | BB    | 281  | C    | C5-C4-N4    | -5.42 | 116.40      | 120.20   |
| 35  | BB    | 419  | U    | C2-N1-C1'   | 5.42  | 124.21      | 117.70   |
| 35  | BB    | 918  | A    | C6-C5-N7    | -5.42 | 128.50      | 132.30   |
| 35  | BB    | 2311 | A    | C1'-O4'-C4' | 5.42  | 114.24      | 109.90   |
| 51  | BR    | 79   | ARG  | NE-CZ-NH1   | -5.42 | 117.59      | 120.30   |
| 1   | AA    | 595  | A    | C5-C6-N1    | -5.42 | 114.99      | 117.70   |
| 1   | AA    | 1094 | G    | C2-N3-C4    | 5.42  | 114.61      | 111.90   |
| 34  | BA    | 105  | G    | N1-C6-O6    | 5.42  | 123.15      | 119.90   |
| 35  | BB    | 220  | G    | C8-N9-C4    | 5.42  | 108.57      | 106.40   |
| 35  | BB    | 559  | G    | C5'-C4'-O4' | -5.42 | 102.59      | 109.10   |
| 35  | BB    | 614  | A    | C6-C5-N7    | -5.42 | 128.50      | 132.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2633 | G    | C4-C5-C6    | 5.42  | 122.05      | 118.80   |
| 1   | AA    | 208  | U    | P-O3'-C3'   | -5.42 | 113.19      | 119.70   |
| 1   | AA    | 557  | G    | OP1-P-OP2   | -5.42 | 111.47      | 119.60   |
| 1   | AA    | 636  | U    | N3-C4-O4    | 5.42  | 123.19      | 119.40   |
| 1   | AA    | 640  | A    | C4-C5-N7    | -5.42 | 107.99      | 110.70   |
| 1   | AA    | 885  | G    | C6-C5-N7    | -5.42 | 127.15      | 130.40   |
| 1   | AA    | 1371 | G    | C2-N3-C4    | -5.42 | 109.19      | 111.90   |
| 1   | AA    | 1496 | C    | C5-C6-N1    | 5.42  | 123.71      | 121.00   |
| 34  | BA    | 19   | C    | C5-C4-N4    | 5.42  | 124.00      | 120.20   |
| 35  | BB    | 151  | C    | N1-C2-O2    | -5.42 | 115.65      | 118.90   |
| 35  | BB    | 770  | G    | N7-C8-N9    | 5.42  | 115.81      | 113.10   |
| 35  | BB    | 1023 | U    | P-O3'-C3'   | 5.42  | 126.20      | 119.70   |
| 35  | BB    | 2024 | G    | C6-N1-C2    | 5.42  | 128.35      | 125.10   |
| 38  | BE    | 53   | THR  | CA-CB-CG2   | -5.42 | 104.81      | 112.40   |
| 41  | BH    | 69   | ALA  | CB-CA-C     | -5.42 | 101.97      | 110.10   |
| 46  | BM    | 64   | TRP  | CE3-CZ3-CH2 | -5.42 | 115.24      | 121.20   |
| 1   | AA    | 508  | U    | C5'-C4'-C3' | -5.42 | 107.33      | 116.00   |
| 1   | AA    | 1384 | C    | P-O3'-C3'   | -5.42 | 113.20      | 119.70   |
| 1   | AA    | 1447 | A    | C4-C5-N7    | -5.42 | 107.99      | 110.70   |
| 35  | BB    | 61   | C    | C2-N3-C4    | 5.42  | 122.61      | 119.90   |
| 35  | BB    | 516  | C    | N1-C2-O2    | -5.42 | 115.65      | 118.90   |
| 35  | BB    | 585  | G    | N1-C2-N3    | -5.42 | 120.65      | 123.90   |
| 35  | BB    | 750  | A    | C6-C5-N7    | -5.42 | 128.51      | 132.30   |
| 35  | BB    | 1194 | A    | C5-N7-C8    | 5.42  | 106.61      | 103.90   |
| 35  | BB    | 2152 | G    | C5-N7-C8    | 5.42  | 107.01      | 104.30   |
| 35  | BB    | 2312 | U    | N1-C2-O2    | 5.42  | 126.59      | 122.80   |
| 1   | AA    | 399  | G    | C4-C5-N7    | 5.42  | 112.97      | 110.80   |
| 1   | AA    | 501  | C    | C6-N1-C2    | 5.42  | 122.47      | 120.30   |
| 1   | AA    | 1249 | C    | P-O5'-C5'   | 5.42  | 129.57      | 120.90   |
| 1   | AA    | 1358 | U    | C5-C4-O4    | -5.42 | 122.65      | 125.90   |
| 9   | AI    | 89   | TYR  | CB-CG-CD1   | -5.42 | 117.75      | 121.00   |
| 27  | B2    | 57   | GLU  | N-CA-CB     | 5.42  | 120.35      | 110.60   |
| 34  | BA    | 47   | C    | N3-C2-O2    | -5.42 | 118.11      | 121.90   |
| 35  | BB    | 25   | U    | N3-C4-C5    | -5.42 | 111.35      | 114.60   |
| 35  | BB    | 48   | G    | C4-C5-C6    | -5.42 | 115.55      | 118.80   |
| 35  | BB    | 202  | U    | C5'-C4'-C3' | -5.42 | 107.33      | 116.00   |
| 35  | BB    | 271  | G    | O4'-C1'-N9  | 5.42  | 112.53      | 108.20   |
| 35  | BB    | 609  | A    | C6-N1-C2    | 5.42  | 121.85      | 118.60   |
| 35  | BB    | 1093 | G    | C8-N9-C4    | -5.42 | 104.23      | 106.40   |
| 35  | BB    | 1277 | G    | N1-C2-N3    | -5.42 | 120.65      | 123.90   |
| 35  | BB    | 1414 | C    | C5'-C4'-C3' | -5.42 | 107.33      | 116.00   |
| 35  | BB    | 2153 | C    | C4-C5-C6    | 5.42  | 120.11      | 117.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2215 | C    | N3-C4-C5    | -5.42 | 119.73      | 121.90   |
| 35  | BB    | 2236 | U    | C5-C4-O4    | 5.42  | 129.15      | 125.90   |
| 35  | BB    | 2604 | U    | O5'-P-OP1   | -5.42 | 100.82      | 105.70   |
| 35  | BB    | 2658 | C    | C2-N1-C1'   | -5.42 | 112.84      | 118.80   |
| 54  | BU    | 24   | VAL  | CG1-CB-CG2  | -5.42 | 102.23      | 110.90   |
| 1   | AA    | 104  | G    | C5'-C4'-C3' | -5.42 | 107.33      | 116.00   |
| 1   | AA    | 107  | G    | C4-C5-C6    | 5.42  | 122.05      | 118.80   |
| 1   | AA    | 436  | C    | C6-N1-C2    | -5.42 | 118.13      | 120.30   |
| 1   | AA    | 729  | A    | C5-C6-N1    | -5.42 | 114.99      | 117.70   |
| 1   | AA    | 799  | G    | N1-C2-N2    | -5.42 | 111.33      | 116.20   |
| 1   | AA    | 1141 | C    | O4'-C1'-N1  | 5.42  | 112.53      | 108.20   |
| 1   | AA    | 1221 | G    | C4'-C3'-C2' | -5.42 | 97.18       | 102.60   |
| 1   | AA    | 1279 | G    | C5-N7-C8    | -5.42 | 101.59      | 104.30   |
| 1   | AA    | 1342 | C    | N3-C4-C5    | -5.42 | 119.73      | 121.90   |
| 1   | AA    | 1343 | G    | O4'-C1'-C2' | -5.42 | 100.38      | 105.80   |
| 1   | AA    | 1402 | C    | C6-N1-C2    | -5.42 | 118.13      | 120.30   |
| 1   | AA    | 1407 | C    | P-O3'-C3'   | 5.42  | 126.20      | 119.70   |
| 7   | AG    | 11   | ILE  | N-CA-C      | -5.42 | 96.38       | 111.00   |
| 35  | BB    | 169  | G    | C4-C5-N7    | -5.42 | 108.63      | 110.80   |
| 35  | BB    | 358  | U    | O4'-C1'-N1  | 5.42  | 112.53      | 108.20   |
| 35  | BB    | 723  | C    | C2-N3-C4    | 5.42  | 122.61      | 119.90   |
| 35  | BB    | 1501 | G    | C6-C5-N7    | -5.42 | 127.15      | 130.40   |
| 35  | BB    | 1746 | A    | C4-C5-N7    | -5.42 | 107.99      | 110.70   |
| 35  | BB    | 2012 | G    | N9-C4-C5    | 5.42  | 107.57      | 105.40   |
| 35  | BB    | 2376 | A    | C2'-C3'-O3' | 5.42  | 122.37      | 113.70   |
| 35  | BB    | 2700 | A    | N9-C4-C5    | 5.42  | 107.97      | 105.80   |
| 35  | BB    | 2741 | A    | C5-C6-N6    | -5.42 | 119.37      | 123.70   |
| 35  | BB    | 2763 | G    | C4-C5-C6    | 5.42  | 122.05      | 118.80   |
| 35  | BB    | 2801 | G    | C5-N7-C8    | -5.42 | 101.59      | 104.30   |
| 35  | BB    | 2903 | U    | N3-C4-O4    | 5.42  | 123.19      | 119.40   |
| 1   | AA    | 603  | U    | C5-C6-N1    | -5.42 | 119.99      | 122.70   |
| 1   | AA    | 657  | U    | C4-C5-C6    | 5.42  | 122.95      | 119.70   |
| 1   | AA    | 1499 | A    | C5-C6-N6    | -5.42 | 119.37      | 123.70   |
| 22  | AV    | 48   | C    | N3-C4-C5    | -5.42 | 119.73      | 121.90   |
| 35  | BB    | 1884 | G    | N9-C4-C5    | 5.42  | 107.57      | 105.40   |
| 35  | BB    | 2047 | C    | C2-N1-C1'   | 5.42  | 124.76      | 118.80   |
| 35  | BB    | 2579 | C    | C5-C6-N1    | 5.42  | 123.71      | 121.00   |
| 1   | AA    | 422  | C    | C2-N3-C4    | 5.41  | 122.61      | 119.90   |
| 1   | AA    | 508  | U    | OP1-P-OP2   | -5.41 | 111.48      | 119.60   |
| 1   | AA    | 777  | A    | N3-C4-N9    | -5.41 | 123.07      | 127.40   |
| 5   | AE    | 59   | ILE  | CA-CB-CG1   | 5.41  | 121.29      | 111.00   |
| 17  | AQ    | 14   | ASP  | CB-CG-OD2   | 5.41  | 123.17      | 118.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | BA    | 86   | G    | N9-C1'-C2'  | -5.41 | 106.04      | 112.00   |
| 35  | BB    | 169  | G    | N9-C4-C5    | 5.41  | 107.56      | 105.40   |
| 35  | BB    | 222  | A    | C5-C6-N1    | -5.41 | 114.99      | 117.70   |
| 35  | BB    | 395  | U    | C2-N3-C4    | -5.41 | 123.75      | 127.00   |
| 35  | BB    | 978  | G    | N3-C2-N2    | 5.41  | 123.69      | 119.90   |
| 35  | BB    | 1159 | U    | C4-C5-C6    | 5.41  | 122.95      | 119.70   |
| 35  | BB    | 1347 | A    | C5-N7-C8    | 5.41  | 106.61      | 103.90   |
| 35  | BB    | 1443 | U    | N1-C2-N3    | -5.41 | 111.65      | 114.90   |
| 35  | BB    | 1721 | G    | O5'-C5'-C4' | -5.41 | 101.42      | 111.70   |
| 35  | BB    | 2370 | G    | C4-N9-C1'   | 5.41  | 133.54      | 126.50   |
| 35  | BB    | 2420 | C    | N3-C4-N4    | 5.41  | 121.79      | 118.00   |
| 35  | BB    | 2664 | G    | N9-C4-C5    | -5.41 | 103.23      | 105.40   |
| 35  | BB    | 2852 | G    | C4-C5-C6    | 5.41  | 122.05      | 118.80   |
| 1   | AA    | 578  | C    | O4'-C1'-N1  | 5.41  | 112.53      | 108.20   |
| 1   | AA    | 1184 | G    | C8-N9-C4    | 5.41  | 108.56      | 106.40   |
| 1   | AA    | 598  | U    | P-O5'-C5'   | -5.41 | 112.24      | 120.90   |
| 1   | AA    | 729  | A    | C1'-O4'-C4' | -5.41 | 105.57      | 109.90   |
| 1   | AA    | 948  | C    | C6-N1-C2    | 5.41  | 122.46      | 120.30   |
| 1   | AA    | 1020 | G    | N3-C2-N2    | 5.41  | 123.69      | 119.90   |
| 1   | AA    | 1023 | U    | C3'-C2'-C1' | 5.41  | 105.83      | 101.50   |
| 1   | AA    | 1262 | C    | C6-N1-C1'   | -5.41 | 114.31      | 120.80   |
| 1   | AA    | 1449 | C    | N3-C4-N4    | 5.41  | 121.79      | 118.00   |
| 34  | BA    | 99   | A    | C6-N1-C2    | -5.41 | 115.35      | 118.60   |
| 35  | BB    | 1132 | U    | C5-C6-N1    | -5.41 | 120.00      | 122.70   |
| 35  | BB    | 1188 | U    | O4'-C4'-C3' | -5.41 | 98.59       | 104.00   |
| 35  | BB    | 1196 | C    | C5-C4-N4    | 5.41  | 123.99      | 120.20   |
| 35  | BB    | 1652 | A    | C4-C5-C6    | 5.41  | 119.70      | 117.00   |
| 35  | BB    | 1707 | G    | P-O3'-C3'   | -5.41 | 113.21      | 119.70   |
| 35  | BB    | 1897 | G    | C4-C5-N7    | 5.41  | 112.97      | 110.80   |
| 35  | BB    | 2173 | A    | C2-N3-C4    | -5.41 | 107.89      | 110.60   |
| 35  | BB    | 2697 | G    | P-O3'-C3'   | -5.41 | 113.21      | 119.70   |
| 35  | BB    | 2775 | G    | N9-C1'-C2'  | -5.41 | 106.05      | 112.00   |
| 35  | BB    | 2869 | G    | C4'-C3'-C2' | -5.41 | 97.19       | 102.60   |
| 36  | BC    | 65   | ASP  | CB-CG-OD1   | 5.41  | 123.17      | 118.30   |
| 1   | AA    | 83   | C    | N3-C4-N4    | 5.41  | 121.78      | 118.00   |
| 1   | AA    | 465  | A    | C8-N9-C4    | 5.41  | 107.96      | 105.80   |
| 1   | AA    | 713  | G    | N1-C6-O6    | -5.41 | 116.66      | 119.90   |
| 1   | AA    | 1034 | G    | N3-C2-N2    | -5.41 | 116.11      | 119.90   |
| 1   | AA    | 1078 | U    | C5-C4-O4    | 5.41  | 129.15      | 125.90   |
| 1   | AA    | 1514 | G    | C4'-C3'-C2' | -5.41 | 97.19       | 102.60   |
| 1   | AA    | 1515 | G    | C5'-C4'-O4' | 5.41  | 115.59      | 109.10   |
| 31  | B6    | 42   | LEU  | CB-CA-C     | 5.41  | 120.48      | 110.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 111  | A    | O4'-C1'-N9  | 5.41  | 112.53      | 108.20   |
| 35  | BB    | 667  | U    | N1-C2-N3    | 5.41  | 118.14      | 114.90   |
| 35  | BB    | 1512 | C    | N1-C2-N3    | 5.41  | 122.99      | 119.20   |
| 1   | AA    | 1298 | U    | N3-C4-C5    | -5.41 | 111.36      | 114.60   |
| 1   | AA    | 1485 | U    | C5-C6-N1    | -5.41 | 120.00      | 122.70   |
| 35  | BB    | 907  | G    | C6-N1-C2    | 5.41  | 128.34      | 125.10   |
| 35  | BB    | 2398 | U    | N3-C4-O4    | 5.41  | 123.19      | 119.40   |
| 35  | BB    | 2405 | G    | C1'-O4'-C4' | 5.41  | 114.23      | 109.90   |
| 35  | BB    | 2478 | A    | N7-C8-N9    | -5.41 | 111.10      | 113.80   |
| 1   | AA    | 132  | C    | C2-N3-C4    | 5.41  | 122.60      | 119.90   |
| 1   | AA    | 683  | G    | N7-C8-N9    | 5.41  | 115.80      | 113.10   |
| 1   | AA    | 742  | G    | N9-C4-C5    | -5.41 | 103.24      | 105.40   |
| 1   | AA    | 1224 | U    | P-O3'-C3'   | 5.41  | 126.19      | 119.70   |
| 35  | BB    | 263  | G    | N3-C2-N2    | 5.41  | 123.68      | 119.90   |
| 35  | BB    | 346  | A    | C2-N3-C4    | -5.41 | 107.90      | 110.60   |
| 35  | BB    | 359  | G    | O4'-C4'-C3' | -5.41 | 98.59       | 104.00   |
| 35  | BB    | 438  | G    | C2-N3-C4    | 5.41  | 114.60      | 111.90   |
| 35  | BB    | 986  | C    | N1-C2-O2    | -5.41 | 115.66      | 118.90   |
| 35  | BB    | 1240 | U    | P-O3'-C3'   | 5.41  | 126.19      | 119.70   |
| 35  | BB    | 1240 | U    | C3'-C2'-C1' | 5.41  | 105.83      | 101.50   |
| 35  | BB    | 1343 | G    | C4'-C3'-C2' | 5.41  | 108.01      | 102.60   |
| 35  | BB    | 1353 | A    | O4'-C1'-N9  | 5.41  | 112.52      | 108.20   |
| 35  | BB    | 1413 | A    | C6-C5-N7    | -5.41 | 128.52      | 132.30   |
| 35  | BB    | 1505 | A    | O4'-C1'-N9  | 5.41  | 112.53      | 108.20   |
| 35  | BB    | 1823 | G    | C4-C5-N7    | 5.41  | 112.96      | 110.80   |
| 35  | BB    | 1946 | U    | N1-C2-O2    | 5.41  | 126.58      | 122.80   |
| 35  | BB    | 2162 | G    | N3-C2-N2    | 5.41  | 123.68      | 119.90   |
| 35  | BB    | 2167 | U    | C2-N3-C4    | -5.41 | 123.76      | 127.00   |
| 35  | BB    | 2307 | G    | C8-N9-C1'   | -5.41 | 119.97      | 127.00   |
| 35  | BB    | 2582 | G    | N7-C8-N9    | 5.41  | 115.80      | 113.10   |
| 35  | BB    | 2631 | G    | N3-C2-N2    | 5.41  | 123.68      | 119.90   |
| 35  | BB    | 2708 | G    | N7-C8-N9    | 5.41  | 115.80      | 113.10   |
| 1   | AA    | 754  | C    | C5-C6-N1    | -5.40 | 118.30      | 121.00   |
| 35  | BB    | 929  | U    | O4'-C1'-C2' | 5.40  | 112.46      | 107.60   |
| 35  | BB    | 2260 | C    | O4'-C1'-N1  | 5.40  | 112.52      | 108.20   |
| 1   | AA    | 68   | G    | N9-C4-C5    | -5.40 | 103.24      | 105.40   |
| 1   | AA    | 463  | U    | N1-C2-O2    | -5.40 | 119.02      | 122.80   |
| 1   | AA    | 996  | A    | C4'-C3'-C2' | -5.40 | 97.20       | 102.60   |
| 34  | BA    | 40   | U    | O4'-C1'-N1  | 5.40  | 112.52      | 108.20   |
| 35  | BB    | 20   | C    | C4-C5-C6    | 5.40  | 120.10      | 117.40   |
| 35  | BB    | 367  | G    | N3-C4-C5    | -5.40 | 125.90      | 128.60   |
| 35  | BB    | 811  | U    | N3-C2-O2    | 5.40  | 125.98      | 122.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1069 | A    | O4'-C1'-N9  | 5.40  | 112.52      | 108.20   |
| 35  | BB    | 1093 | G    | C5-N7-C8    | -5.40 | 101.60      | 104.30   |
| 35  | BB    | 1228 | G    | N1-C2-N3    | -5.40 | 120.66      | 123.90   |
| 35  | BB    | 2578 | G    | C6-C5-N7    | -5.40 | 127.16      | 130.40   |
| 1   | AA    | 57   | G    | N1-C6-O6    | 5.40  | 123.14      | 119.90   |
| 1   | AA    | 426  | U    | N3-C2-O2    | 5.40  | 125.98      | 122.20   |
| 1   | AA    | 698  | G    | C4-C5-N7    | 5.40  | 112.96      | 110.80   |
| 1   | AA    | 1213 | A    | C8-N9-C4    | 5.40  | 107.96      | 105.80   |
| 1   | AA    | 1526 | G    | C5-C6-O6    | -5.40 | 125.36      | 128.60   |
| 34  | BA    | 36   | C    | C6-N1-C2    | -5.40 | 118.14      | 120.30   |
| 34  | BA    | 96   | G    | N3-C4-C5    | 5.40  | 131.30      | 128.60   |
| 35  | BB    | 5    | A    | C5-N7-C8    | 5.40  | 106.60      | 103.90   |
| 35  | BB    | 134  | G    | C3'-C2'-C1' | -5.40 | 97.18       | 101.50   |
| 35  | BB    | 1152 | C    | N3-C2-O2    | -5.40 | 118.12      | 121.90   |
| 35  | BB    | 1247 | A    | C5-C6-N6    | -5.40 | 119.38      | 123.70   |
| 35  | BB    | 1553 | A    | C5-N7-C8    | 5.40  | 106.60      | 103.90   |
| 35  | BB    | 1557 | C    | N1-C1'-C2'  | -5.40 | 106.06      | 112.00   |
| 35  | BB    | 1717 | A    | C8-N9-C4    | 5.40  | 107.96      | 105.80   |
| 35  | BB    | 1968 | G    | P-O3'-C3'   | -5.40 | 113.22      | 119.70   |
| 35  | BB    | 2748 | A    | N1-C2-N3    | 5.40  | 132.00      | 129.30   |
| 1   | AA    | 278  | G    | C4'-C3'-C2' | -5.40 | 97.20       | 102.60   |
| 1   | AA    | 389  | A    | C8-N9-C4    | -5.40 | 103.64      | 105.80   |
| 1   | AA    | 825  | A    | N9-C4-C5    | 5.40  | 107.96      | 105.80   |
| 1   | AA    | 1322 | C    | N3-C4-N4    | 5.40  | 121.78      | 118.00   |
| 23  | AX    | 17   | C    | C3'-C2'-C1' | 5.40  | 105.82      | 101.50   |
| 35  | BB    | 230  | G    | C4-N9-C1'   | 5.40  | 133.52      | 126.50   |
| 35  | BB    | 747  | U    | C1'-O4'-C4' | 5.40  | 114.22      | 109.90   |
| 35  | BB    | 1243 | C    | C2-N3-C4    | 5.40  | 122.60      | 119.90   |
| 35  | BB    | 1303 | G    | C5-N7-C8    | 5.40  | 107.00      | 104.30   |
| 35  | BB    | 2293 | G    | N1-C2-N3    | -5.40 | 120.66      | 123.90   |
| 35  | BB    | 2656 | U    | N3-C4-C5    | -5.40 | 111.36      | 114.60   |
| 35  | BB    | 2766 | A    | O4'-C1'-C2' | -5.40 | 100.40      | 105.80   |
| 35  | BB    | 2815 | C    | C6-N1-C2    | -5.40 | 118.14      | 120.30   |
| 1   | AA    | 240  | G    | O5'-P-OP1   | 5.40  | 117.18      | 110.70   |
| 1   | AA    | 449  | G    | N1-C2-N3    | -5.40 | 120.66      | 123.90   |
| 1   | AA    | 660  | C    | OP2-P-O3'   | 5.40  | 117.07      | 105.20   |
| 1   | AA    | 1082 | A    | C5-C6-N6    | -5.40 | 119.38      | 123.70   |
| 1   | AA    | 1227 | A    | C8-N9-C4    | 5.40  | 107.96      | 105.80   |
| 35  | BB    | 290  | U    | C3'-C2'-C1' | 5.40  | 105.82      | 101.50   |
| 35  | BB    | 575  | A    | C6-C5-N7    | -5.40 | 128.52      | 132.30   |
| 35  | BB    | 675  | A    | N9-C4-C5    | 5.40  | 107.96      | 105.80   |
| 35  | BB    | 677  | A    | OP2-P-O3'   | 5.40  | 117.08      | 105.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 876  | C    | C5'-C4'-O4' | 5.40  | 115.58      | 109.10   |
| 35  | BB    | 1247 | A    | N9-C4-C5    | 5.40  | 107.96      | 105.80   |
| 35  | BB    | 1828 | G    | C6-N1-C2    | 5.40  | 128.34      | 125.10   |
| 35  | BB    | 2662 | A    | O4'-C1'-N9  | 5.40  | 112.52      | 108.20   |
| 1   | AA    | 232  | G    | C5-C6-O6    | -5.40 | 125.36      | 128.60   |
| 1   | AA    | 1194 | U    | C5-C4-O4    | -5.40 | 122.66      | 125.90   |
| 29  | B4    | 8    | ILE  | N-CA-C      | -5.40 | 96.43       | 111.00   |
| 35  | BB    | 361  | G    | N9-C4-C5    | 5.40  | 107.56      | 105.40   |
| 35  | BB    | 887  | U    | O4'-C1'-N1  | 5.40  | 112.52      | 108.20   |
| 35  | BB    | 2371 | G    | C5'-C4'-C3' | -5.40 | 107.37      | 116.00   |
| 1   | AA    | 22   | G    | C6-C5-N7    | -5.39 | 127.16      | 130.40   |
| 1   | AA    | 409  | U    | O4'-C1'-N1  | 5.39  | 112.52      | 108.20   |
| 1   | AA    | 1203 | C    | N3-C4-C5    | -5.39 | 119.74      | 121.90   |
| 1   | AA    | 1250 | A    | N1-C2-N3    | 5.39  | 132.00      | 129.30   |
| 1   | AA    | 1504 | G    | C6-C5-N7    | -5.39 | 127.16      | 130.40   |
| 35  | BB    | 497  | A    | N3-C4-C5    | 5.39  | 130.58      | 126.80   |
| 35  | BB    | 627  | A    | N1-C2-N3    | -5.39 | 126.60      | 129.30   |
| 35  | BB    | 858  | G    | O4'-C1'-N9  | 5.39  | 112.52      | 108.20   |
| 35  | BB    | 1761 | C    | C2'-C3'-O3' | 5.39  | 122.33      | 113.70   |
| 35  | BB    | 2012 | G    | N1-C2-N2    | -5.39 | 111.35      | 116.20   |
| 35  | BB    | 2030 | A    | O5'-C5'-C4' | -5.39 | 101.45      | 111.70   |
| 35  | BB    | 2033 | A    | N3-C4-C5    | -5.39 | 123.02      | 126.80   |
| 35  | BB    | 2127 | G    | C5-C6-O6    | -5.39 | 125.36      | 128.60   |
| 35  | BB    | 2361 | G    | N7-C8-N9    | -5.39 | 110.40      | 113.10   |
| 35  | BB    | 2599 | G    | C4-C5-N7    | -5.39 | 108.64      | 110.80   |
| 35  | BB    | 2675 | A    | C6-C5-N7    | -5.39 | 128.52      | 132.30   |
| 35  | BB    | 2825 | G    | C2-N3-C4    | 5.39  | 114.60      | 111.90   |
| 35  | BB    | 2842 | G    | C5-N7-C8    | 5.39  | 107.00      | 104.30   |
| 41  | BH    | 37   | VAL  | N-CA-C      | -5.39 | 96.43       | 111.00   |
| 1   | AA    | 44   | A    | O4'-C1'-N9  | 5.39  | 112.51      | 108.20   |
| 1   | AA    | 84   | U    | O4'-C1'-N1  | 5.39  | 112.51      | 108.20   |
| 1   | AA    | 121  | U    | C6-N1-C1'   | -5.39 | 113.65      | 121.20   |
| 1   | AA    | 543  | U    | P-O5'-C5'   | 5.39  | 129.53      | 120.90   |
| 1   | AA    | 693  | G    | C4-C5-C6    | 5.39  | 122.03      | 118.80   |
| 1   | AA    | 814  | A    | P-O5'-C5'   | -5.39 | 112.27      | 120.90   |
| 1   | AA    | 860  | A    | C4-C5-N7    | -5.39 | 108.00      | 110.70   |
| 1   | AA    | 868  | C    | N1-C2-N3    | 5.39  | 122.97      | 119.20   |
| 1   | AA    | 1081 | A    | O4'-C1'-N9  | 5.39  | 112.52      | 108.20   |
| 1   | AA    | 1284 | C    | C5-C4-N4    | -5.39 | 116.42      | 120.20   |
| 1   | AA    | 1333 | A    | C4-C5-C6    | 5.39  | 119.70      | 117.00   |
| 4   | AD    | 80   | ARG  | NE-CZ-NH2   | -5.39 | 117.60      | 120.30   |
| 5   | AE    | 70   | MET  | CG-SD-CE    | -5.39 | 91.57       | 100.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | AV    | 11   | C    | N3-C4-C5    | -5.39 | 119.74      | 121.90   |
| 35  | BB    | 74   | A    | C5'-C4'-C3' | -5.39 | 107.37      | 116.00   |
| 35  | BB    | 1631 | G    | N3-C2-N2    | 5.39  | 123.67      | 119.90   |
| 35  | BB    | 2040 | G    | O4'-C1'-N9  | 5.39  | 112.52      | 108.20   |
| 35  | BB    | 2345 | G    | C2-N3-C4    | -5.39 | 109.20      | 111.90   |
| 35  | BB    | 2601 | C    | C5-C6-N1    | -5.39 | 118.30      | 121.00   |
| 35  | BB    | 2744 | G    | N3-C4-N9    | 5.39  | 129.24      | 126.00   |
| 1   | AA    | 462  | G    | C4-C5-C6    | 5.39  | 122.03      | 118.80   |
| 1   | AA    | 572  | A    | C5-C6-N1    | -5.39 | 115.00      | 117.70   |
| 1   | AA    | 794  | A    | C5-C6-N6    | -5.39 | 119.39      | 123.70   |
| 1   | AA    | 797  | C    | C2-N1-C1'   | 5.39  | 124.73      | 118.80   |
| 1   | AA    | 1377 | A    | P-O3'-C3'   | -5.39 | 113.23      | 119.70   |
| 1   | AA    | 1493 | A    | C4-C5-N7    | -5.39 | 108.00      | 110.70   |
| 4   | AD    | 162  | GLU  | O-C-N       | -5.39 | 114.07      | 122.70   |
| 35  | BB    | 572  | A    | N1-C2-N3    | -5.39 | 126.60      | 129.30   |
| 35  | BB    | 1151 | A    | C4-C5-N7    | -5.39 | 108.00      | 110.70   |
| 35  | BB    | 1248 | G    | P-O5'-C5'   | 5.39  | 129.53      | 120.90   |
| 35  | BB    | 1426 | G    | C8-N9-C4    | -5.39 | 104.24      | 106.40   |
| 1   | AA    | 739  | C    | P-O3'-C3'   | -5.39 | 113.23      | 119.70   |
| 1   | AA    | 946  | A    | O4'-C1'-N9  | 5.39  | 112.51      | 108.20   |
| 1   | AA    | 1469 | C    | C5-C6-N1    | -5.39 | 118.31      | 121.00   |
| 1   | AA    | 1488 | G    | C8-N9-C4    | -5.39 | 104.24      | 106.40   |
| 16  | AP    | 25   | ARG  | N-CA-CB     | 5.39  | 120.30      | 110.60   |
| 34  | BA    | 78   | A    | C5-N7-C8    | 5.39  | 106.59      | 103.90   |
| 35  | BB    | 48   | G    | C6-C5-N7    | 5.39  | 133.63      | 130.40   |
| 35  | BB    | 294  | A    | O5'-P-OP2   | -5.39 | 100.85      | 105.70   |
| 35  | BB    | 449  | A    | P-O5'-C5'   | 5.39  | 129.52      | 120.90   |
| 35  | BB    | 991  | C    | N3-C4-N4    | 5.39  | 121.77      | 118.00   |
| 35  | BB    | 1359 | A    | C2-N3-C4    | -5.39 | 107.91      | 110.60   |
| 35  | BB    | 2113 | U    | N3-C4-O4    | 5.39  | 123.17      | 119.40   |
| 35  | BB    | 2169 | A    | N3-C4-C5    | -5.39 | 123.03      | 126.80   |
| 35  | BB    | 2819 | G    | O4'-C1'-N9  | 5.39  | 112.51      | 108.20   |
| 1   | AA    | 441  | A    | N7-C8-N9    | 5.39  | 116.49      | 113.80   |
| 1   | AA    | 651  | C    | C6-N1-C2    | 5.39  | 122.45      | 120.30   |
| 1   | AA    | 782  | A    | C4-C5-N7    | -5.39 | 108.01      | 110.70   |
| 15  | AO    | 39   | GLN  | CB-CA-C     | -5.39 | 99.62       | 110.40   |
| 35  | BB    | 125  | A    | C5-C6-N6    | -5.39 | 119.39      | 123.70   |
| 35  | BB    | 506  | G    | N3-C4-N9    | -5.39 | 122.77      | 126.00   |
| 35  | BB    | 676  | A    | N7-C8-N9    | -5.39 | 111.11      | 113.80   |
| 35  | BB    | 749  | A    | N9-C4-C5    | 5.39  | 107.95      | 105.80   |
| 35  | BB    | 945  | A    | O4'-C1'-N9  | 5.39  | 112.51      | 108.20   |
| 35  | BB    | 1127 | A    | N1-C2-N3    | 5.39  | 131.99      | 129.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1384 | A    | C6-C5-N7    | -5.39 | 128.53      | 132.30   |
| 35  | BB    | 1410 | G    | C5-C6-N1    | -5.39 | 108.81      | 111.50   |
| 35  | BB    | 1690 | A    | C5-N7-C8    | 5.39  | 106.59      | 103.90   |
| 1   | AA    | 449  | G    | P-O3'-C3'   | 5.39  | 126.16      | 119.70   |
| 1   | AA    | 827  | U    | C5-C4-O4    | -5.39 | 122.67      | 125.90   |
| 1   | AA    | 1097 | C    | C5-C6-N1    | 5.39  | 123.69      | 121.00   |
| 1   | AA    | 1225 | A    | O4'-C1'-N9  | 5.39  | 112.51      | 108.20   |
| 1   | AA    | 1244 | G    | C5-C6-N1    | -5.39 | 108.81      | 111.50   |
| 1   | AA    | 1428 | A    | C4'-C3'-C2' | -5.39 | 97.21       | 102.60   |
| 35  | BB    | 471  | A    | C4-C5-C6    | 5.39  | 119.69      | 117.00   |
| 35  | BB    | 842  | U    | C5-C6-N1    | -5.39 | 120.01      | 122.70   |
| 35  | BB    | 1771 | C    | N3-C4-C5    | -5.39 | 119.75      | 121.90   |
| 35  | BB    | 2090 | A    | N1-C2-N3    | 5.39  | 131.99      | 129.30   |
| 1   | AA    | 827  | U    | C3'-C2'-C1' | 5.38  | 105.81      | 101.50   |
| 1   | AA    | 1037 | C    | N3-C4-N4    | 5.38  | 121.77      | 118.00   |
| 1   | AA    | 1090 | U    | N1-C1'-C2'  | -5.38 | 106.08      | 112.00   |
| 8   | AH    | 83   | ARG  | CD-NE-CZ    | 5.38  | 131.14      | 123.60   |
| 22  | AV    | 51   | A    | O4'-C1'-N9  | 5.38  | 112.51      | 108.20   |
| 34  | BA    | 66   | A    | C8-N9-C4    | -5.38 | 103.65      | 105.80   |
| 35  | BB    | 718  | A    | O4'-C4'-C3' | -5.38 | 98.62       | 104.00   |
| 35  | BB    | 1028 | A    | N1-C6-N6    | 5.38  | 121.83      | 118.60   |
| 35  | BB    | 1182 | G    | O4'-C4'-C3' | -5.38 | 98.62       | 104.00   |
| 35  | BB    | 1387 | A    | C5-N7-C8    | 5.38  | 106.59      | 103.90   |
| 35  | BB    | 2083 | G    | C6-C5-N7    | -5.38 | 127.17      | 130.40   |
| 35  | BB    | 2094 | A    | C8-N9-C4    | -5.38 | 103.65      | 105.80   |
| 35  | BB    | 2151 | U    | C2-N1-C1'   | -5.38 | 111.24      | 117.70   |
| 35  | BB    | 2257 | U    | N3-C2-O2    | 5.38  | 125.97      | 122.20   |
| 1   | AA    | 107  | G    | N7-C8-N9    | 5.38  | 115.79      | 113.10   |
| 1   | AA    | 320  | A    | N9-C4-C5    | -5.38 | 103.65      | 105.80   |
| 1   | AA    | 1182 | G    | P-O3'-C3'   | 5.38  | 126.16      | 119.70   |
| 1   | AA    | 1317 | C    | N1-C2-O2    | -5.38 | 115.67      | 118.90   |
| 30  | B5    | 51   | ASP  | CA-CB-CG    | -5.38 | 101.56      | 113.40   |
| 35  | BB    | 148  | U    | C5-C4-O4    | 5.38  | 129.13      | 125.90   |
| 35  | BB    | 332  | A    | C2-N3-C4    | 5.38  | 113.29      | 110.60   |
| 35  | BB    | 828  | U    | N1-C1'-C2'  | 5.38  | 121.00      | 114.00   |
| 35  | BB    | 1023 | U    | O4'-C4'-C3' | -5.38 | 98.62       | 104.00   |
| 35  | BB    | 1729 | U    | C4-C5-C6    | 5.38  | 122.93      | 119.70   |
| 35  | BB    | 1843 | C    | C4'-C3'-C2' | -5.38 | 97.22       | 102.60   |
| 35  | BB    | 1845 | G    | C2-N3-C4    | 5.38  | 114.59      | 111.90   |
| 35  | BB    | 2869 | G    | C2-N3-C4    | 5.38  | 114.59      | 111.90   |
| 38  | BE    | 101  | TYR  | CA-CB-CG    | -5.38 | 103.17      | 113.40   |
| 48  | BO    | 2    | ASP  | N-CA-CB     | 5.38  | 120.29      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | BO    | 9    | ARG  | CB-CG-CD    | 5.38  | 125.60      | 111.60   |
| 1   | AA    | 134  | G    | C4-C5-N7    | 5.38  | 112.95      | 110.80   |
| 1   | AA    | 594  | U    | N3-C2-O2    | 5.38  | 125.97      | 122.20   |
| 1   | AA    | 623  | C    | C5-C6-N1    | -5.38 | 118.31      | 121.00   |
| 1   | AA    | 702  | A    | C5-N7-C8    | 5.38  | 106.59      | 103.90   |
| 1   | AA    | 794  | A    | N1-C2-N3    | 5.38  | 131.99      | 129.30   |
| 1   | AA    | 1185 | G    | C2-N3-C4    | 5.38  | 114.59      | 111.90   |
| 22  | AV    | 26   | A    | C5-C6-N1    | -5.38 | 115.01      | 117.70   |
| 27  | B2    | 9    | THR  | N-CA-CB     | 5.38  | 120.52      | 110.30   |
| 35  | BB    | 492  | A    | N3-C4-N9    | 5.38  | 131.71      | 127.40   |
| 35  | BB    | 539  | G    | C6-C5-N7    | -5.38 | 127.17      | 130.40   |
| 35  | BB    | 708  | G    | C8-N9-C4    | 5.38  | 108.55      | 106.40   |
| 35  | BB    | 1039 | A    | C4-C5-N7    | -5.38 | 108.01      | 110.70   |
| 35  | BB    | 1336 | A    | C5-C6-N1    | -5.38 | 115.01      | 117.70   |
| 35  | BB    | 1378 | A    | N1-C6-N6    | 5.38  | 121.83      | 118.60   |
| 35  | BB    | 1423 | G    | N3-C2-N2    | 5.38  | 123.67      | 119.90   |
| 35  | BB    | 1448 | G    | C2-N3-C4    | -5.38 | 109.21      | 111.90   |
| 35  | BB    | 1575 | C    | C2-N3-C4    | 5.38  | 122.59      | 119.90   |
| 35  | BB    | 1665 | A    | N3-C4-C5    | -5.38 | 123.03      | 126.80   |
| 35  | BB    | 1855 | U    | N3-C2-O2    | 5.38  | 125.97      | 122.20   |
| 35  | BB    | 2064 | C    | C4-C5-C6    | -5.38 | 114.71      | 117.40   |
| 35  | BB    | 2123 | G    | P-O5'-C5'   | 5.38  | 129.51      | 120.90   |
| 44  | BK    | 46   | ALA  | N-CA-CB     | 5.38  | 117.64      | 110.10   |
| 1   | AA    | 403  | C    | C6-N1-C2    | -5.38 | 118.15      | 120.30   |
| 1   | AA    | 540  | G    | O4'-C1'-N9  | 5.38  | 112.50      | 108.20   |
| 1   | AA    | 1532 | U    | P-O3'-C3'   | -5.38 | 113.24      | 119.70   |
| 35  | BB    | 411  | G    | N3-C4-N9    | -5.38 | 122.77      | 126.00   |
| 35  | BB    | 925  | A    | C5-N7-C8    | 5.38  | 106.59      | 103.90   |
| 35  | BB    | 1000 | A    | C5-N7-C8    | 5.38  | 106.59      | 103.90   |
| 35  | BB    | 1242 | U    | C5-C4-O4    | 5.38  | 129.13      | 125.90   |
| 35  | BB    | 1504 | A    | C6-C5-N7    | -5.38 | 128.53      | 132.30   |
| 49  | BP    | 99   | LEU  | CB-CG-CD1   | -5.38 | 101.85      | 111.00   |
| 1   | AA    | 371  | A    | C2-N3-C4    | 5.38  | 113.29      | 110.60   |
| 1   | AA    | 1183 | U    | O4'-C4'-C3' | -5.38 | 98.62       | 104.00   |
| 1   | AA    | 1314 | C    | C6-N1-C2    | 5.38  | 122.45      | 120.30   |
| 35  | BB    | 522  | A    | C3'-C2'-C1' | -5.38 | 97.20       | 101.50   |
| 35  | BB    | 757  | G    | N3-C4-N9    | -5.38 | 122.77      | 126.00   |
| 35  | BB    | 877  | A    | C3'-C2'-C1' | -5.38 | 97.20       | 101.50   |
| 35  | BB    | 958  | U    | N1-C2-N3    | -5.38 | 111.67      | 114.90   |
| 35  | BB    | 971  | G    | C2-N3-C4    | 5.38  | 114.59      | 111.90   |
| 35  | BB    | 2219 | U    | P-O5'-C5'   | 5.38  | 129.51      | 120.90   |
| 35  | BB    | 2300 | C    | C5-C6-N1    | 5.38  | 123.69      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2711 | A    | C5-C6-N6    | -5.38 | 119.40      | 123.70   |
| 35  | BB    | 2746 | U    | N1-C2-O2    | -5.38 | 119.03      | 122.80   |
| 1   | AA    | 53   | A    | N9-C1'-C2'  | -5.38 | 106.08      | 112.00   |
| 1   | AA    | 186  | C    | N1-C2-N3    | 5.38  | 122.96      | 119.20   |
| 1   | AA    | 612  | C    | C5-C4-N4    | -5.38 | 116.44      | 120.20   |
| 1   | AA    | 656  | G    | C6-C5-N7    | -5.38 | 127.17      | 130.40   |
| 1   | AA    | 1248 | A    | N7-C8-N9    | -5.38 | 111.11      | 113.80   |
| 22  | AV    | 57   | A    | C5-C6-N1    | -5.38 | 115.01      | 117.70   |
| 35  | BB    | 224  | U    | N1-C1'-C2'  | -5.38 | 106.09      | 112.00   |
| 35  | BB    | 583  | G    | N9-C4-C5    | 5.38  | 107.55      | 105.40   |
| 35  | BB    | 763  | G    | O4'-C1'-N9  | 5.38  | 112.50      | 108.20   |
| 35  | BB    | 824  | U    | O4'-C1'-N1  | 5.38  | 112.50      | 108.20   |
| 35  | BB    | 918  | A    | C5-C6-N1    | -5.38 | 115.01      | 117.70   |
| 35  | BB    | 1223 | G    | N3-C2-N2    | 5.38  | 123.66      | 119.90   |
| 35  | BB    | 1230 | A    | N9-C4-C5    | 5.38  | 107.95      | 105.80   |
| 35  | BB    | 1457 | U    | N1-C1'-C2'  | -5.38 | 106.09      | 112.00   |
| 35  | BB    | 1515 | A    | O4'-C4'-C3' | -5.38 | 98.62       | 104.00   |
| 35  | BB    | 1959 | G    | C4-C5-N7    | 5.38  | 112.95      | 110.80   |
| 35  | BB    | 2160 | C    | P-O3'-C3'   | 5.38  | 126.15      | 119.70   |
| 35  | BB    | 2757 | A    | OP1-P-OP2   | -5.38 | 111.53      | 119.60   |
| 1   | AA    | 333  | U    | N1-C2-O2    | 5.38  | 126.56      | 122.80   |
| 1   | AA    | 818  | G    | N7-C8-N9    | 5.38  | 115.79      | 113.10   |
| 1   | AA    | 1433 | A    | N3-C4-C5    | 5.38  | 130.56      | 126.80   |
| 1   | AA    | 1517 | G    | C4-C5-C6    | 5.38  | 122.03      | 118.80   |
| 34  | BA    | 113  | C    | N1-C2-N3    | 5.38  | 122.96      | 119.20   |
| 35  | BB    | 13   | A    | C6-C5-N7    | -5.38 | 128.54      | 132.30   |
| 35  | BB    | 160  | A    | C5-N7-C8    | 5.38  | 106.59      | 103.90   |
| 35  | BB    | 315  | G    | O4'-C4'-C3' | -5.38 | 98.62       | 104.00   |
| 35  | BB    | 1154 | G    | N7-C8-N9    | 5.38  | 115.79      | 113.10   |
| 35  | BB    | 1192 | G    | N9-C4-C5    | -5.38 | 103.25      | 105.40   |
| 35  | BB    | 1388 | G    | C5'-C4'-C3' | -5.38 | 107.40      | 116.00   |
| 35  | BB    | 1675 | C    | N3-C4-N4    | 5.38  | 121.76      | 118.00   |
| 35  | BB    | 2118 | U    | C1'-O4'-C4' | -5.38 | 105.60      | 109.90   |
| 52  | BS    | 33   | LEU  | N-CA-C      | -5.38 | 96.49       | 111.00   |
| 1   | AA    | 472  | U    | N3-C4-O4    | -5.37 | 115.64      | 119.40   |
| 1   | AA    | 1047 | G    | C6-N1-C2    | 5.37  | 128.32      | 125.10   |
| 35  | BB    | 92   | U    | C4'-C3'-C2' | -5.37 | 97.23       | 102.60   |
| 35  | BB    | 502  | A    | P-O5'-C5'   | -5.37 | 112.30      | 120.90   |
| 35  | BB    | 786  | C    | N3-C4-C5    | -5.37 | 119.75      | 121.90   |
| 35  | BB    | 818  | G    | P-O3'-C3'   | -5.37 | 113.25      | 119.70   |
| 35  | BB    | 1198 | U    | C4'-C3'-C2' | -5.37 | 97.23       | 102.60   |
| 35  | BB    | 1487 | U    | N1-C2-O2    | -5.37 | 119.04      | 122.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1786 | A    | C2-N3-C4    | -5.37 | 107.91      | 110.60   |
| 35  | BB    | 1829 | A    | C6-N1-C2    | -5.37 | 115.38      | 118.60   |
| 35  | BB    | 2124 | G    | C3'-C2'-C1' | -5.37 | 97.20       | 101.50   |
| 35  | BB    | 2226 | C    | C2-N1-C1'   | 5.37  | 124.71      | 118.80   |
| 36  | BC    | 51   | ARG  | NE-CZ-NH2   | -5.37 | 117.61      | 120.30   |
| 1   | AA    | 365  | U    | O4'-C1'-N1  | -5.37 | 103.90      | 108.20   |
| 1   | AA    | 1156 | G    | N9-C4-C5    | 5.37  | 107.55      | 105.40   |
| 7   | AG    | 79   | VAL  | CA-CB-CG1   | -5.37 | 102.84      | 110.90   |
| 35  | BB    | 370  | G    | N9-C4-C5    | -5.37 | 103.25      | 105.40   |
| 35  | BB    | 466  | A    | C6-C5-N7    | -5.37 | 128.54      | 132.30   |
| 35  | BB    | 1217 | U    | C5'-C4'-C3' | -5.37 | 107.41      | 116.00   |
| 35  | BB    | 1240 | U    | P-O5'-C5'   | -5.37 | 112.31      | 120.90   |
| 35  | BB    | 1260 | A    | P-O5'-C5'   | -5.37 | 112.31      | 120.90   |
| 35  | BB    | 1940 | U    | C5-C4-O4    | -5.37 | 122.68      | 125.90   |
| 35  | BB    | 2010 | G    | C5-N7-C8    | 5.37  | 106.98      | 104.30   |
| 35  | BB    | 2023 | C    | C5'-C4'-C3' | -5.37 | 107.41      | 116.00   |
| 35  | BB    | 2202 | U    | N1-C2-N3    | 5.37  | 118.12      | 114.90   |
| 35  | BB    | 2208 | C    | C5-C4-N4    | -5.37 | 116.44      | 120.20   |
| 35  | BB    | 2244 | U    | C6-N1-C1'   | -5.37 | 113.68      | 121.20   |
| 35  | BB    | 2274 | A    | O4'-C1'-N9  | 5.37  | 112.50      | 108.20   |
| 35  | BB    | 2300 | C    | N1-C2-N3    | -5.37 | 115.44      | 119.20   |
| 55  | BW    | 22   | ALA  | CB-CA-C     | -5.37 | 102.04      | 110.10   |
| 55  | BW    | 81   | PRO  | N-CA-CB     | 5.37  | 109.75      | 103.30   |
| 1   | AA    | 376  | G    | C4'-C3'-C2' | -5.37 | 97.23       | 102.60   |
| 1   | AA    | 735  | C    | O4'-C1'-N1  | 5.37  | 112.50      | 108.20   |
| 3   | AC    | 4    | VAL  | C-N-CA      | 5.37  | 135.12      | 121.70   |
| 35  | BB    | 36   | G    | N1-C2-N3    | -5.37 | 120.68      | 123.90   |
| 35  | BB    | 1450 | G    | N3-C2-N2    | 5.37  | 123.66      | 119.90   |
| 35  | BB    | 1570 | A    | P-O3'-C3'   | 5.37  | 126.14      | 119.70   |
| 35  | BB    | 2168 | G    | C8-N9-C4    | 5.37  | 108.55      | 106.40   |
| 35  | BB    | 2201 | G    | C4-C5-N7    | 5.37  | 112.95      | 110.80   |
| 35  | BB    | 2335 | A    | C5-C6-N6    | -5.37 | 119.40      | 123.70   |
| 35  | BB    | 2564 | A    | N9-C4-C5    | 5.37  | 107.95      | 105.80   |
| 35  | BB    | 2756 | U    | C3'-C2'-C1' | -5.37 | 97.20       | 101.50   |
| 1   | AA    | 81   | A    | C6-N1-C2    | -5.37 | 115.38      | 118.60   |
| 1   | AA    | 362  | G    | C3'-C2'-C1' | -5.37 | 97.20       | 101.50   |
| 1   | AA    | 411  | A    | C4-C5-N7    | -5.37 | 108.02      | 110.70   |
| 1   | AA    | 526  | C    | C5-C4-N4    | -5.37 | 116.44      | 120.20   |
| 1   | AA    | 853  | C    | C1'-O4'-C4' | 5.37  | 114.19      | 109.90   |
| 1   | AA    | 923  | A    | N1-C2-N3    | 5.37  | 131.99      | 129.30   |
| 1   | AA    | 1057 | G    | O4'-C1'-N9  | 5.37  | 112.50      | 108.20   |
| 1   | AA    | 1219 | A    | O4'-C1'-N9  | 5.37  | 112.50      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1266 | G    | C3'-C2'-C1' | -5.37 | 97.21       | 101.50   |
| 35  | BB    | 255  | A    | C5-C6-N6    | -5.37 | 119.41      | 123.70   |
| 35  | BB    | 317  | G    | C4-C5-N7    | 5.37  | 112.95      | 110.80   |
| 35  | BB    | 683  | U    | C5-C6-N1    | 5.37  | 125.39      | 122.70   |
| 35  | BB    | 833  | A    | N9-C4-C5    | 5.37  | 107.95      | 105.80   |
| 35  | BB    | 1133 | A    | C5'-C4'-C3' | 5.37  | 124.59      | 116.00   |
| 35  | BB    | 1307 | A    | C6-N1-C2    | -5.37 | 115.38      | 118.60   |
| 35  | BB    | 1583 | A    | C4-C5-C6    | 5.37  | 119.68      | 117.00   |
| 35  | BB    | 2298 | A    | C5-C6-N1    | -5.37 | 115.02      | 117.70   |
| 35  | BB    | 2375 | G    | C8-N9-C4    | -5.37 | 104.25      | 106.40   |
| 1   | AA    | 68   | G    | C2-N3-C4    | -5.37 | 109.22      | 111.90   |
| 1   | AA    | 91   | U    | C5-C6-N1    | 5.37  | 125.38      | 122.70   |
| 1   | AA    | 123  | U    | N3-C2-O2    | 5.37  | 125.96      | 122.20   |
| 35  | BB    | 523  | C    | N1-C2-O2    | 5.37  | 122.12      | 118.90   |
| 35  | BB    | 597  | G    | N1-C2-N3    | -5.37 | 120.68      | 123.90   |
| 35  | BB    | 799  | G    | C8-N9-C1'   | -5.37 | 120.02      | 127.00   |
| 35  | BB    | 878  | A    | N9-C1'-C2'  | -5.37 | 106.10      | 112.00   |
| 35  | BB    | 1275 | A    | O4'-C4'-C3' | -5.37 | 98.63       | 104.00   |
| 35  | BB    | 1950 | G    | N1-C2-N3    | -5.37 | 120.68      | 123.90   |
| 35  | BB    | 2133 | G    | C5-C6-O6    | -5.37 | 125.38      | 128.60   |
| 50  | BQ    | 117  | ALA  | N-CA-CB     | 5.37  | 117.61      | 110.10   |
| 1   | AA    | 35   | G    | OP1-P-OP2   | -5.37 | 111.55      | 119.60   |
| 1   | AA    | 207  | C    | O4'-C4'-C3' | -5.37 | 98.63       | 104.00   |
| 1   | AA    | 441  | A    | C2-N3-C4    | 5.37  | 113.28      | 110.60   |
| 1   | AA    | 512  | U    | N1-C2-N3    | 5.37  | 118.12      | 114.90   |
| 1   | AA    | 600  | A    | C6-C5-N7    | -5.37 | 128.54      | 132.30   |
| 1   | AA    | 723  | U    | C2-N1-C1'   | 5.37  | 124.14      | 117.70   |
| 1   | AA    | 970  | C    | C2-N3-C4    | 5.37  | 122.58      | 119.90   |
| 1   | AA    | 1361 | G    | N3-C2-N2    | 5.37  | 123.66      | 119.90   |
| 22  | AV    | 64   | C    | N3-C4-N4    | 5.37  | 121.76      | 118.00   |
| 22  | AV    | 68   | U    | C1'-O4'-C4' | 5.37  | 114.19      | 109.90   |
| 35  | BB    | 105  | C    | C4-C5-C6    | 5.37  | 120.08      | 117.40   |
| 35  | BB    | 638  | G    | C2-N3-C4    | 5.37  | 114.58      | 111.90   |
| 35  | BB    | 1087 | G    | C2-N3-C4    | 5.37  | 114.58      | 111.90   |
| 35  | BB    | 1230 | A    | C5-N7-C8    | 5.37  | 106.58      | 103.90   |
| 35  | BB    | 1382 | G    | O4'-C4'-C3' | -5.37 | 98.63       | 104.00   |
| 35  | BB    | 1546 | G    | N3-C2-N2    | 5.37  | 123.66      | 119.90   |
| 35  | BB    | 1766 | G    | C4-C5-N7    | -5.37 | 108.65      | 110.80   |
| 35  | BB    | 2201 | G    | C4-C5-C6    | 5.37  | 122.02      | 118.80   |
| 35  | BB    | 2455 | G    | C8-N9-C4    | -5.37 | 104.25      | 106.40   |
| 35  | BB    | 2782 | G    | C6-N1-C2    | -5.37 | 121.88      | 125.10   |
| 1   | AA    | 769  | G    | P-O3'-C3'   | -5.36 | 113.26      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1193 | G    | C5'-C4'-O4' | 5.36  | 115.54      | 109.10   |
| 1   | AA    | 1260 | G    | N3-C4-N9    | 5.36  | 129.22      | 126.00   |
| 1   | AA    | 1297 | G    | C6-C5-N7    | -5.36 | 127.18      | 130.40   |
| 35  | BB    | 70   | G    | P-O3'-C3'   | -5.36 | 113.26      | 119.70   |
| 35  | BB    | 690  | G    | N7-C8-N9    | -5.36 | 110.42      | 113.10   |
| 35  | BB    | 792  | A    | C1'-O4'-C4' | -5.36 | 105.61      | 109.90   |
| 35  | BB    | 1409 | U    | OP1-P-OP2   | -5.36 | 111.55      | 119.60   |
| 35  | BB    | 1569 | A    | N9-C4-C5    | 5.36  | 107.94      | 105.80   |
| 35  | BB    | 1784 | A    | C8-N9-C4    | 5.36  | 107.94      | 105.80   |
| 35  | BB    | 1928 | A    | C8-N9-C4    | -5.36 | 103.66      | 105.80   |
| 35  | BB    | 1988 | G    | N7-C8-N9    | -5.36 | 110.42      | 113.10   |
| 35  | BB    | 2546 | U    | N1-C2-O2    | 5.36  | 126.55      | 122.80   |
| 35  | BB    | 2557 | G    | N7-C8-N9    | -5.36 | 110.42      | 113.10   |
| 35  | BB    | 2806 | C    | C5'-C4'-O4' | -5.36 | 102.67      | 109.10   |
| 38  | BE    | 19   | PHE  | CB-CG-CD2   | -5.36 | 117.05      | 120.80   |
| 51  | BR    | 90   | ARG  | NE-CZ-NH1   | -5.36 | 117.62      | 120.30   |
| 1   | AA    | 255  | G    | C1'-O4'-C4' | -5.36 | 105.61      | 109.90   |
| 22  | AV    | 73   | A    | C2'-C3'-O3' | 5.36  | 122.28      | 113.70   |
| 35  | BB    | 1104 | C    | C6-N1-C2    | -5.36 | 118.16      | 120.30   |
| 35  | BB    | 1265 | A    | C6-C5-N7    | -5.36 | 128.55      | 132.30   |
| 35  | BB    | 2771 | C    | N1-C2-N3    | 5.36  | 122.95      | 119.20   |
| 1   | AA    | 99   | C    | O4'-C1'-N1  | 5.36  | 112.49      | 108.20   |
| 35  | BB    | 59   | U    | N3-C4-C5    | -5.36 | 111.38      | 114.60   |
| 35  | BB    | 208  | C    | C6-N1-C2    | -5.36 | 118.16      | 120.30   |
| 35  | BB    | 663  | G    | C5'-C4'-O4' | -5.36 | 102.67      | 109.10   |
| 35  | BB    | 1189 | A    | C4-C5-C6    | 5.36  | 119.68      | 117.00   |
| 35  | BB    | 1386 | C    | C6-N1-C2    | 5.36  | 122.44      | 120.30   |
| 35  | BB    | 1602 | U    | P-O3'-C3'   | -5.36 | 113.27      | 119.70   |
| 35  | BB    | 1775 | U    | N3-C4-C5    | -5.36 | 111.38      | 114.60   |
| 35  | BB    | 1845 | G    | N9-C1'-C2'  | -5.36 | 106.10      | 112.00   |
| 35  | BB    | 2227 | A    | C5-C6-N6    | -5.36 | 119.41      | 123.70   |
| 35  | BB    | 2290 | G    | C5-N7-C8    | 5.36  | 106.98      | 104.30   |
| 47  | BN    | 94   | TYR  | CB-CG-CD1   | 5.36  | 124.22      | 121.00   |
| 1   | AA    | 1515 | G    | C5-C6-N1    | -5.36 | 108.82      | 111.50   |
| 5   | AE    | 40   | ASP  | CB-CG-OD1   | -5.36 | 113.48      | 118.30   |
| 14  | AN    | 79   | SER  | N-CA-CB     | 5.36  | 118.54      | 110.50   |
| 34  | BA    | 76   | G    | C4-C5-C6    | 5.36  | 122.02      | 118.80   |
| 35  | BB    | 122  | G    | C2-N3-C4    | 5.36  | 114.58      | 111.90   |
| 35  | BB    | 174  | U    | C2-N1-C1'   | 5.36  | 124.13      | 117.70   |
| 35  | BB    | 957  | C    | N3-C4-N4    | 5.36  | 121.75      | 118.00   |
| 35  | BB    | 1985 | C    | C5-C6-N1    | 5.36  | 123.68      | 121.00   |
| 35  | BB    | 2022 | U    | O3'-P-O5'   | -5.36 | 93.82       | 104.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2640 | G    | C3'-C2'-C1' | 5.36  | 105.79      | 101.50   |
| 35  | BB    | 2686 | G    | C8-N9-C1'   | -5.36 | 120.03      | 127.00   |
| 1   | AA    | 530  | G    | O4'-C1'-N9  | 5.36  | 112.49      | 108.20   |
| 1   | AA    | 686  | U    | N3-C4-C5    | -5.36 | 111.39      | 114.60   |
| 1   | AA    | 1198 | G    | N7-C8-N9    | -5.36 | 110.42      | 113.10   |
| 35  | BB    | 121  | G    | C6-N1-C2    | 5.36  | 128.31      | 125.10   |
| 35  | BB    | 366  | C    | C5-C6-N1    | -5.36 | 118.32      | 121.00   |
| 35  | BB    | 426  | C    | C6-N1-C2    | -5.36 | 118.16      | 120.30   |
| 35  | BB    | 633  | A    | C5-C6-N6    | -5.36 | 119.41      | 123.70   |
| 35  | BB    | 875  | G    | C6-C5-N7    | -5.36 | 127.19      | 130.40   |
| 35  | BB    | 927  | A    | C1'-O4'-C4' | -5.36 | 105.61      | 109.90   |
| 35  | BB    | 953  | G    | N3-C4-C5    | 5.36  | 131.28      | 128.60   |
| 35  | BB    | 1485 | U    | N3-C2-O2    | -5.36 | 118.45      | 122.20   |
| 35  | BB    | 1874 | C    | C4'-C3'-C2' | -5.36 | 97.24       | 102.60   |
| 35  | BB    | 2307 | G    | C5'-C4'-O4' | 5.36  | 115.53      | 109.10   |
| 35  | BB    | 2506 | U    | N1-C2-O2    | -5.36 | 119.05      | 122.80   |
| 35  | BB    | 2536 | G    | C4-C5-C6    | 5.36  | 122.02      | 118.80   |
| 35  | BB    | 2635 | A    | C5-C6-N1    | -5.36 | 115.02      | 117.70   |
| 35  | BB    | 2732 | G    | N1-C6-O6    | 5.36  | 123.11      | 119.90   |
| 35  | BB    | 2881 | U    | N3-C4-O4    | 5.36  | 123.15      | 119.40   |
| 53  | BT    | 66   | LYS  | N-CA-C      | -5.36 | 96.53       | 111.00   |
| 1   | AA    | 14   | U    | C1'-O4'-C4' | 5.36  | 114.18      | 109.90   |
| 1   | AA    | 35   | G    | P-O3'-C3'   | -5.36 | 113.27      | 119.70   |
| 1   | AA    | 497  | G    | C6-N1-C2    | 5.36  | 128.31      | 125.10   |
| 1   | AA    | 1394 | A    | C6-N1-C2    | -5.36 | 115.39      | 118.60   |
| 35  | BB    | 52   | A    | C4-N9-C1'   | 5.36  | 135.94      | 126.30   |
| 35  | BB    | 817  | C    | C5-C4-N4    | -5.36 | 116.45      | 120.20   |
| 35  | BB    | 917  | A    | C5-C6-N1    | -5.36 | 115.02      | 117.70   |
| 35  | BB    | 947  | A    | C2-N3-C4    | -5.36 | 107.92      | 110.60   |
| 35  | BB    | 1150 | C    | C5-C6-N1    | 5.36  | 123.68      | 121.00   |
| 35  | BB    | 1268 | A    | C4-C5-C6    | 5.36  | 119.68      | 117.00   |
| 35  | BB    | 1549 | A    | N1-C2-N3    | -5.36 | 126.62      | 129.30   |
| 35  | BB    | 1663 | G    | C8-N9-C4    | -5.36 | 104.26      | 106.40   |
| 35  | BB    | 2357 | G    | O4'-C1'-N9  | 5.36  | 112.48      | 108.20   |
| 35  | BB    | 2801 | G    | C8-N9-C4    | -5.36 | 104.26      | 106.40   |
| 48  | BO    | 33   | ARG  | NE-CZ-NH2   | -5.36 | 117.62      | 120.30   |
| 1   | AA    | 859  | G    | C4-C5-C6    | 5.35  | 122.01      | 118.80   |
| 35  | BB    | 355  | U    | C6-N1-C2    | -5.35 | 117.79      | 121.00   |
| 35  | BB    | 863  | A    | C8-N9-C4    | -5.35 | 103.66      | 105.80   |
| 35  | BB    | 2396 | G    | N3-C2-N2    | 5.35  | 123.65      | 119.90   |
| 35  | BB    | 2586 | U    | C5-C6-N1    | 5.35  | 125.38      | 122.70   |
| 35  | BB    | 2782 | G    | C8-N9-C1'   | -5.35 | 120.04      | 127.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 38   | G    | N3-C2-N2    | 5.35  | 123.65      | 119.90   |
| 1   | AA    | 131  | A    | C5-C6-N6    | -5.35 | 119.42      | 123.70   |
| 1   | AA    | 282  | A    | C4-C5-C6    | 5.35  | 119.68      | 117.00   |
| 1   | AA    | 513  | C    | P-O5'-C5'   | 5.35  | 129.46      | 120.90   |
| 1   | AA    | 643  | C    | N3-C4-C5    | -5.35 | 119.76      | 121.90   |
| 1   | AA    | 1226 | C    | C6-N1-C2    | -5.35 | 118.16      | 120.30   |
| 35  | BB    | 212  | G    | C2-N3-C4    | -5.35 | 109.22      | 111.90   |
| 35  | BB    | 474  | G    | C5'-C4'-O4' | 5.35  | 115.52      | 109.10   |
| 35  | BB    | 868  | U    | C3'-C2'-C1' | 5.35  | 105.78      | 101.50   |
| 35  | BB    | 1110 | G    | P-O3'-C3'   | 5.35  | 126.12      | 119.70   |
| 35  | BB    | 1544 | A    | N1-C2-N3    | 5.35  | 131.98      | 129.30   |
| 35  | BB    | 2045 | C    | C5-C6-N1    | -5.35 | 118.32      | 121.00   |
| 35  | BB    | 2496 | C    | N3-C2-O2    | -5.35 | 118.15      | 121.90   |
| 35  | BB    | 2695 | U    | N3-C4-C5    | -5.35 | 111.39      | 114.60   |
| 1   | AA    | 482  | A    | C4-C5-N7    | -5.35 | 108.02      | 110.70   |
| 1   | AA    | 678  | U    | P-O3'-C3'   | -5.35 | 113.28      | 119.70   |
| 35  | BB    | 686  | U    | C4'-C3'-C2' | -5.35 | 97.25       | 102.60   |
| 35  | BB    | 714  | U    | C5'-C4'-O4' | 5.35  | 115.52      | 109.10   |
| 35  | BB    | 1223 | G    | C4-C5-N7    | -5.35 | 108.66      | 110.80   |
| 35  | BB    | 1372 | U    | C4'-C3'-C2' | -5.35 | 97.25       | 102.60   |
| 35  | BB    | 1863 | G    | C5-N7-C8    | -5.35 | 101.62      | 104.30   |
| 35  | BB    | 2218 | G    | N1-C2-N2    | 5.35  | 121.02      | 116.20   |
| 37  | BD    | 92   | VAL  | CA-CB-CG1   | -5.35 | 102.87      | 110.90   |
| 52  | BS    | 10   | ALA  | CB-CA-C     | 5.35  | 118.13      | 110.10   |
| 1   | AA    | 35   | G    | O4'-C1'-N9  | 5.35  | 112.48      | 108.20   |
| 1   | AA    | 911  | U    | C6-N1-C1'   | -5.35 | 113.71      | 121.20   |
| 1   | AA    | 942  | G    | C8-N9-C4    | 5.35  | 108.54      | 106.40   |
| 1   | AA    | 1122 | U    | N3-C2-O2    | 5.35  | 125.94      | 122.20   |
| 1   | AA    | 1326 | U    | N1-C2-N3    | -5.35 | 111.69      | 114.90   |
| 23  | AX    | 20   | G    | C2-N3-C4    | -5.35 | 109.22      | 111.90   |
| 35  | BB    | 375  | G    | C2-N3-C4    | 5.35  | 114.58      | 111.90   |
| 35  | BB    | 456  | C    | C6-N1-C2    | 5.35  | 122.44      | 120.30   |
| 35  | BB    | 1006 | C    | C2-N1-C1'   | 5.35  | 124.69      | 118.80   |
| 35  | BB    | 1103 | A    | C3'-C2'-C1' | -5.35 | 97.22       | 101.50   |
| 35  | BB    | 1382 | G    | C3'-C2'-C1' | -5.35 | 97.22       | 101.50   |
| 35  | BB    | 1705 | A    | C6-N1-C2    | -5.35 | 115.39      | 118.60   |
| 35  | BB    | 1867 | G    | C4'-C3'-C2' | -5.35 | 97.25       | 102.60   |
| 35  | BB    | 2154 | A    | N9-C4-C5    | 5.35  | 107.94      | 105.80   |
| 47  | BN    | 25   | ALA  | N-CA-CB     | 5.35  | 117.59      | 110.10   |
| 1   | AA    | 216  | U    | P-O3'-C3'   | -5.35 | 113.28      | 119.70   |
| 1   | AA    | 362  | G    | P-O5'-C5'   | 5.35  | 129.46      | 120.90   |
| 35  | BB    | 526  | A    | O4'-C1'-N9  | 5.35  | 112.48      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 661  | A    | C6-C5-N7    | -5.35 | 128.56      | 132.30   |
| 35  | BB    | 749  | A    | N1-C2-N3    | 5.35  | 131.97      | 129.30   |
| 35  | BB    | 943  | A    | C3'-C2'-C1' | -5.35 | 97.22       | 101.50   |
| 35  | BB    | 1228 | G    | C4-N9-C1'   | -5.35 | 119.55      | 126.50   |
| 35  | BB    | 1867 | G    | C2-N3-C4    | 5.35  | 114.57      | 111.90   |
| 35  | BB    | 2165 | C    | C2-N3-C4    | -5.35 | 117.23      | 119.90   |
| 35  | BB    | 2280 | G    | C5-C6-O6    | -5.35 | 125.39      | 128.60   |
| 35  | BB    | 2834 | G    | N7-C8-N9    | 5.35  | 115.77      | 113.10   |
| 41  | BH    | 91   | PHE  | CB-CG-CD2   | -5.35 | 117.06      | 120.80   |
| 1   | AA    | 249  | U    | C2-N1-C1'   | -5.35 | 111.28      | 117.70   |
| 1   | AA    | 282  | A    | N3-C4-N9    | 5.35  | 131.68      | 127.40   |
| 1   | AA    | 595  | A    | C6-C5-N7    | -5.35 | 128.56      | 132.30   |
| 1   | AA    | 1177 | G    | C4-C5-C6    | 5.35  | 122.01      | 118.80   |
| 1   | AA    | 1423 | G    | C6-N1-C2    | 5.35  | 128.31      | 125.10   |
| 35  | BB    | 588  | U    | C4-C5-C6    | -5.35 | 116.49      | 119.70   |
| 35  | BB    | 991  | C    | C5-C4-N4    | -5.35 | 116.46      | 120.20   |
| 35  | BB    | 2172 | U    | C6-N1-C2    | 5.35  | 124.21      | 121.00   |
| 35  | BB    | 2494 | G    | N1-C2-N2    | -5.35 | 111.39      | 116.20   |
| 1   | AA    | 52   | C    | P-O3'-C3'   | 5.34  | 126.11      | 119.70   |
| 1   | AA    | 259  | G    | N3-C2-N2    | 5.34  | 123.64      | 119.90   |
| 1   | AA    | 514  | C    | C5-C4-N4    | -5.34 | 116.46      | 120.20   |
| 1   | AA    | 557  | G    | C1'-O4'-C4' | 5.34  | 114.18      | 109.90   |
| 13  | AM    | 91   | ARG  | CA-CB-CG    | 5.34  | 125.16      | 113.40   |
| 15  | AO    | 4    | THR  | CA-CB-CG2   | -5.34 | 104.92      | 112.40   |
| 35  | BB    | 207  | A    | P-O3'-C3'   | -5.34 | 113.29      | 119.70   |
| 35  | BB    | 217  | A    | C1'-O4'-C4' | -5.34 | 105.62      | 109.90   |
| 35  | BB    | 230  | G    | O5'-C5'-C4' | -5.34 | 101.55      | 111.70   |
| 35  | BB    | 1016 | G    | N9-C1'-C2'  | -5.34 | 106.12      | 112.00   |
| 35  | BB    | 1384 | A    | C4-C5-C6    | 5.34  | 119.67      | 117.00   |
| 35  | BB    | 1490 | A    | N3-C4-N9    | -5.34 | 123.12      | 127.40   |
| 35  | BB    | 1501 | G    | N3-C4-N9    | 5.34  | 129.21      | 126.00   |
| 35  | BB    | 1683 | U    | N3-C4-C5    | -5.34 | 111.39      | 114.60   |
| 35  | BB    | 1957 | C    | N3-C2-O2    | -5.34 | 118.16      | 121.90   |
| 35  | BB    | 2324 | U    | C5'-C4'-C3' | -5.34 | 107.45      | 116.00   |
| 35  | BB    | 2745 | C    | N3-C4-N4    | 5.34  | 121.74      | 118.00   |
| 1   | AA    | 57   | G    | C5-C6-N1    | 5.34  | 114.17      | 111.50   |
| 1   | AA    | 610  | U    | C2-N1-C1'   | 5.34  | 124.11      | 117.70   |
| 1   | AA    | 979  | C    | O4'-C1'-N1  | 5.34  | 112.47      | 108.20   |
| 1   | AA    | 1177 | G    | N1-C2-N3    | 5.34  | 127.11      | 123.90   |
| 1   | AA    | 1416 | G    | O4'-C1'-N9  | 5.34  | 112.47      | 108.20   |
| 35  | BB    | 298  | G    | C1'-O4'-C4' | -5.34 | 105.63      | 109.90   |
| 35  | BB    | 599  | A    | C5-C6-N1    | -5.34 | 115.03      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 873  | C    | N3-C4-N4    | 5.34  | 121.74      | 118.00   |
| 35  | BB    | 973  | A    | C4-C5-C6    | 5.34  | 119.67      | 117.00   |
| 35  | BB    | 981  | A    | O4'-C1'-N9  | 5.34  | 112.47      | 108.20   |
| 35  | BB    | 1259 | G    | N7-C8-N9    | -5.34 | 110.43      | 113.10   |
| 35  | BB    | 1418 | G    | C6-C5-N7    | -5.34 | 127.19      | 130.40   |
| 35  | BB    | 2074 | U    | C2-N1-C1'   | -5.34 | 111.29      | 117.70   |
| 35  | BB    | 2816 | G    | N9-C4-C5    | 5.34  | 107.54      | 105.40   |
| 1   | AA    | 99   | C    | P-O5'-C5'   | -5.34 | 112.36      | 120.90   |
| 1   | AA    | 152  | A    | C5'-C4'-C3' | 5.34  | 124.55      | 116.00   |
| 1   | AA    | 390  | U    | N3-C4-O4    | 5.34  | 123.14      | 119.40   |
| 1   | AA    | 549  | C    | C2'-C3'-O3' | 5.34  | 122.25      | 113.70   |
| 1   | AA    | 586  | C    | C1'-O4'-C4' | -5.34 | 105.63      | 109.90   |
| 1   | AA    | 617  | G    | C8-N9-C4    | 5.34  | 108.54      | 106.40   |
| 22  | AV    | 53   | G    | O4'-C1'-N9  | 5.34  | 112.47      | 108.20   |
| 35  | BB    | 714  | U    | C5-C4-O4    | -5.34 | 122.69      | 125.90   |
| 35  | BB    | 885  | C    | C5-C4-N4    | -5.34 | 116.46      | 120.20   |
| 35  | BB    | 1037 | G    | C6-N1-C2    | 5.34  | 128.31      | 125.10   |
| 35  | BB    | 1220 | G    | C8-N9-C4    | -5.34 | 104.26      | 106.40   |
| 35  | BB    | 1502 | A    | C4-C5-C6    | 5.34  | 119.67      | 117.00   |
| 35  | BB    | 2243 | U    | C2-N3-C4    | -5.34 | 123.80      | 127.00   |
| 35  | BB    | 2290 | G    | C8-N9-C4    | -5.34 | 104.26      | 106.40   |
| 35  | BB    | 2753 | A    | C8-N9-C4    | -5.34 | 103.66      | 105.80   |
| 1   | AA    | 32   | A    | C5-C6-N1    | -5.34 | 115.03      | 117.70   |
| 1   | AA    | 532  | A    | P-O3'-C3'   | 5.34  | 126.11      | 119.70   |
| 1   | AA    | 695  | A    | C4'-C3'-C2' | -5.34 | 97.26       | 102.60   |
| 1   | AA    | 1182 | G    | N1-C6-O6    | 5.34  | 123.10      | 119.90   |
| 19  | AS    | 72   | GLU  | N-CA-CB     | -5.34 | 100.99      | 110.60   |
| 34  | BA    | 54   | G    | C4-C5-N7    | 5.34  | 112.94      | 110.80   |
| 35  | BB    | 192  | C    | N3-C4-C5    | -5.34 | 119.76      | 121.90   |
| 35  | BB    | 412  | A    | O4'-C1'-N9  | 5.34  | 112.47      | 108.20   |
| 35  | BB    | 584  | C    | C6-N1-C1'   | 5.34  | 127.21      | 120.80   |
| 35  | BB    | 1291 | C    | N3-C2-O2    | 5.34  | 125.64      | 121.90   |
| 35  | BB    | 1538 | G    | C8-N9-C4    | 5.34  | 108.54      | 106.40   |
| 35  | BB    | 2101 | A    | C6-C5-N7    | -5.34 | 128.56      | 132.30   |
| 35  | BB    | 2162 | G    | C5-C6-N1    | -5.34 | 108.83      | 111.50   |
| 35  | BB    | 2282 | G    | P-O3'-C3'   | 5.34  | 126.11      | 119.70   |
| 35  | BB    | 2643 | G    | P-O3'-C3'   | -5.34 | 113.29      | 119.70   |
| 35  | BB    | 2779 | U    | C5'-C4'-O4' | 5.34  | 115.51      | 109.10   |
| 1   | AA    | 549  | C    | N3-C4-N4    | 5.34  | 121.74      | 118.00   |
| 1   | AA    | 652  | U    | N3-C4-C5    | 5.34  | 117.80      | 114.60   |
| 1   | AA    | 966  | G    | N1-C2-N3    | -5.34 | 120.70      | 123.90   |
| 34  | BA    | 118  | C    | C4'-C3'-C2' | -5.34 | 97.26       | 102.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 316  | C    | N1-C1'-C2'  | -5.34 | 106.13      | 112.00   |
| 35  | BB    | 616  | A    | C5-N7-C8    | 5.34  | 106.57      | 103.90   |
| 35  | BB    | 1425 | G    | O4'-C1'-N9  | 5.34  | 112.47      | 108.20   |
| 35  | BB    | 2775 | G    | C6-C5-N7    | -5.34 | 127.20      | 130.40   |
| 1   | AA    | 311  | C    | C3'-C2'-C1' | -5.34 | 97.23       | 101.50   |
| 1   | AA    | 428  | G    | N3-C4-N9    | 5.34  | 129.20      | 126.00   |
| 1   | AA    | 652  | U    | C5-C6-N1    | 5.34  | 125.37      | 122.70   |
| 1   | AA    | 670  | G    | N3-C2-N2    | 5.34  | 123.64      | 119.90   |
| 1   | AA    | 1352 | C    | N1-C1'-C2'  | -5.34 | 106.13      | 112.00   |
| 1   | AA    | 1461 | G    | N3-C2-N2    | 5.34  | 123.64      | 119.90   |
| 4   | AD    | 113  | ALA  | N-CA-CB     | 5.34  | 117.57      | 110.10   |
| 15  | AO    | 16   | ARG  | CG-CD-NE    | -5.34 | 100.59      | 111.80   |
| 34  | BA    | 79   | G    | C4-C5-C6    | 5.34  | 122.00      | 118.80   |
| 35  | BB    | 6    | A    | C4-C5-N7    | -5.34 | 108.03      | 110.70   |
| 35  | BB    | 248  | G    | C4-C5-N7    | -5.34 | 108.67      | 110.80   |
| 35  | BB    | 284  | U    | N3-C4-C5    | -5.34 | 111.40      | 114.60   |
| 35  | BB    | 1017 | G    | P-O5'-C5'   | -5.34 | 112.36      | 120.90   |
| 35  | BB    | 1327 | A    | N3-C4-N9    | -5.34 | 123.13      | 127.40   |
| 35  | BB    | 1464 | G    | C1'-O4'-C4' | 5.34  | 114.17      | 109.90   |
| 35  | BB    | 1489 | C    | N3-C4-C5    | -5.34 | 119.77      | 121.90   |
| 35  | BB    | 1509 | A    | C4-C5-C6    | 5.34  | 119.67      | 117.00   |
| 35  | BB    | 1736 | U    | C5-C6-N1    | -5.34 | 120.03      | 122.70   |
| 35  | BB    | 2043 | C    | C2-N1-C1'   | 5.34  | 124.67      | 118.80   |
| 35  | BB    | 2669 | G    | C8-N9-C1'   | 5.34  | 133.94      | 127.00   |
| 35  | BB    | 2852 | G    | C5-C6-N1    | -5.34 | 108.83      | 111.50   |
| 37  | BD    | 167  | ASN  | N-CA-CB     | 5.34  | 120.21      | 110.60   |
| 39  | BF    | 166  | ARG  | NE-CZ-NH2   | -5.34 | 117.63      | 120.30   |
| 1   | AA    | 707  | U    | C5'-C4'-O4' | -5.33 | 102.70      | 109.10   |
| 11  | AK    | 76   | TYR  | CZ-CE2-CD2  | -5.33 | 115.00      | 119.80   |
| 35  | BB    | 459  | U    | C4-C5-C6    | 5.33  | 122.90      | 119.70   |
| 35  | BB    | 676  | A    | O4'-C1'-N9  | 5.33  | 112.47      | 108.20   |
| 35  | BB    | 2183 | A    | C3'-C2'-C1' | -5.33 | 97.23       | 101.50   |
| 35  | BB    | 2531 | A    | N9-C4-C5    | 5.33  | 107.93      | 105.80   |
| 1   | AA    | 69   | G    | C4-C5-C6    | 5.33  | 122.00      | 118.80   |
| 1   | AA    | 561  | U    | N3-C4-C5    | 5.33  | 117.80      | 114.60   |
| 1   | AA    | 1335 | U    | C2-N1-C1'   | 5.33  | 124.10      | 117.70   |
| 35  | BB    | 629  | G    | C4-N9-C1'   | -5.33 | 119.57      | 126.50   |
| 35  | BB    | 951  | C    | C1'-O4'-C4' | -5.33 | 105.63      | 109.90   |
| 35  | BB    | 1019 | U    | N3-C4-O4    | 5.33  | 123.13      | 119.40   |
| 35  | BB    | 1157 | G    | C5'-C4'-C3' | -5.33 | 107.47      | 116.00   |
| 35  | BB    | 1332 | G    | C4-C5-N7    | 5.33  | 112.93      | 110.80   |
| 37  | BD    | 169  | ARG  | NE-CZ-NH1   | -5.33 | 117.63      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 125  | A    | P-O5'-C5'   | -5.33 | 112.37      | 120.90   |
| 35  | BB    | 749  | A    | C6-C5-N7    | -5.33 | 128.57      | 132.30   |
| 35  | BB    | 806  | C    | P-O3'-C3'   | -5.33 | 113.30      | 119.70   |
| 35  | BB    | 822  | G    | N3-C2-N2    | 5.33  | 123.63      | 119.90   |
| 35  | BB    | 1382 | G    | C6-N1-C2    | -5.33 | 121.90      | 125.10   |
| 35  | BB    | 1488 | C    | N3-C4-N4    | 5.33  | 121.73      | 118.00   |
| 35  | BB    | 1699 | G    | C4-C5-N7    | -5.33 | 108.67      | 110.80   |
| 35  | BB    | 2735 | G    | C5-C6-O6    | -5.33 | 125.40      | 128.60   |
| 35  | BB    | 2903 | U    | C5-C4-O4    | -5.33 | 122.70      | 125.90   |
| 1   | AA    | 591  | U    | C4-C5-C6    | -5.33 | 116.50      | 119.70   |
| 1   | AA    | 921  | U    | P-O3'-C3'   | -5.33 | 113.30      | 119.70   |
| 1   | AA    | 1129 | C    | C2-N1-C1'   | 5.33  | 124.66      | 118.80   |
| 34  | BA    | 80   | U    | O3'-P-O5'   | -5.33 | 93.87       | 104.00   |
| 35  | BB    | 962  | G    | N7-C8-N9    | -5.33 | 110.44      | 113.10   |
| 35  | BB    | 1853 | A    | N3-C4-N9    | 5.33  | 131.66      | 127.40   |
| 35  | BB    | 2061 | G    | O3'-P-O5'   | -5.33 | 93.87       | 104.00   |
| 1   | AA    | 77   | A    | C3'-C2'-C1' | -5.33 | 97.24       | 101.50   |
| 1   | AA    | 128  | G    | C5-N7-C8    | 5.33  | 106.96      | 104.30   |
| 1   | AA    | 235  | C    | N3-C4-N4    | 5.33  | 121.73      | 118.00   |
| 1   | AA    | 666  | G    | C5-N7-C8    | 5.33  | 106.96      | 104.30   |
| 1   | AA    | 676  | A    | C2-N3-C4    | 5.33  | 113.26      | 110.60   |
| 1   | AA    | 691  | G    | N3-C2-N2    | 5.33  | 123.63      | 119.90   |
| 1   | AA    | 705  | G    | C4-C5-C6    | 5.33  | 122.00      | 118.80   |
| 1   | AA    | 991  | U    | N3-C4-O4    | 5.33  | 123.13      | 119.40   |
| 1   | AA    | 1156 | G    | C4-C5-C6    | 5.33  | 122.00      | 118.80   |
| 14  | AN    | 52   | ARG  | N-CA-CB     | 5.33  | 120.19      | 110.60   |
| 35  | BB    | 384  | A    | O4'-C1'-N9  | 5.33  | 112.46      | 108.20   |
| 35  | BB    | 937  | C    | C5'-C4'-C3' | -5.33 | 107.47      | 116.00   |
| 35  | BB    | 1270 | C    | C5-C6-N1    | 5.33  | 123.66      | 121.00   |
| 35  | BB    | 1658 | C    | C5-C4-N4    | -5.33 | 116.47      | 120.20   |
| 35  | BB    | 1903 | G    | C4'-C3'-C2' | -5.33 | 97.27       | 102.60   |
| 35  | BB    | 2097 | A    | C4-C5-N7    | 5.33  | 113.36      | 110.70   |
| 35  | BB    | 2372 | U    | O4'-C1'-N1  | 5.33  | 112.46      | 108.20   |
| 35  | BB    | 2708 | G    | N1-C6-O6    | 5.33  | 123.10      | 119.90   |
| 1   | AA    | 1459 | G    | OP1-P-OP2   | -5.33 | 111.61      | 119.60   |
| 35  | BB    | 1350 | C    | O4'-C4'-C3' | -5.33 | 98.67       | 104.00   |
| 35  | BB    | 1905 | C    | C5'-C4'-O4' | 5.33  | 115.49      | 109.10   |
| 35  | BB    | 2325 | G    | N9-C4-C5    | -5.33 | 103.27      | 105.40   |
| 1   | AA    | 100  | G    | N3-C2-N2    | 5.33  | 123.63      | 119.90   |
| 1   | AA    | 373  | A    | N1-C2-N3    | -5.33 | 126.64      | 129.30   |
| 1   | AA    | 1059 | C    | C5'-C4'-C3' | -5.33 | 107.48      | 116.00   |
| 1   | AA    | 1277 | C    | C5-C4-N4    | -5.33 | 116.47      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1454 | G    | N7-C8-N9    | 5.33  | 115.76      | 113.10   |
| 2   | AB    | 73   | ARG  | NE-CZ-NH1   | 5.33  | 122.96      | 120.30   |
| 35  | BB    | 23   | G    | C5'-C4'-O4' | 5.33  | 115.49      | 109.10   |
| 35  | BB    | 564  | C    | N3-C4-C5    | -5.33 | 119.77      | 121.90   |
| 1   | AA    | 153  | C    | P-O3'-C3'   | -5.32 | 113.31      | 119.70   |
| 1   | AA    | 1048 | G    | C8-N9-C4    | -5.32 | 104.27      | 106.40   |
| 1   | AA    | 1150 | A    | O4'-C4'-C3' | -5.32 | 98.68       | 104.00   |
| 35  | BB    | 1438 | U    | C4-C5-C6    | 5.32  | 122.89      | 119.70   |
| 35  | BB    | 1648 | U    | N3-C4-O4    | 5.32  | 123.13      | 119.40   |
| 35  | BB    | 2007 | U    | C2-N3-C4    | -5.32 | 123.81      | 127.00   |
| 35  | BB    | 2259 | U    | C1'-O4'-C4' | 5.32  | 114.16      | 109.90   |
| 35  | BB    | 2310 | C    | N3-C4-N4    | 5.32  | 121.73      | 118.00   |
| 35  | BB    | 2507 | C    | N1-C2-O2    | -5.32 | 115.71      | 118.90   |
| 35  | BB    | 2596 | U    | N1-C2-N3    | -5.32 | 111.71      | 114.90   |
| 35  | BB    | 2684 | U    | C5-C6-N1    | 5.32  | 125.36      | 122.70   |
| 56  | BY    | 34   | SER  | N-CA-CB     | 5.32  | 118.49      | 110.50   |
| 1   | AA    | 361  | G    | N9-C4-C5    | 5.32  | 107.53      | 105.40   |
| 22  | AV    | 59   | A    | C5-C6-N1    | -5.32 | 115.04      | 117.70   |
| 35  | BB    | 757  | G    | C8-N9-C4    | -5.32 | 104.27      | 106.40   |
| 35  | BB    | 2266 | A    | C4-C5-C6    | 5.32  | 119.66      | 117.00   |
| 35  | BB    | 2446 | G    | C5'-C4'-C3' | -5.32 | 107.48      | 116.00   |
| 36  | BC    | 180  | MET  | CB-CA-C     | -5.32 | 99.76       | 110.40   |
| 1   | AA    | 392  | C    | N3-C4-C5    | -5.32 | 119.77      | 121.90   |
| 1   | AA    | 631  | C    | O3'-P-O5'   | -5.32 | 93.89       | 104.00   |
| 1   | AA    | 968  | A    | C8-N9-C4    | -5.32 | 103.67      | 105.80   |
| 1   | AA    | 1168 | U    | OP2-P-O3'   | 5.32  | 116.91      | 105.20   |
| 1   | AA    | 1238 | A    | P-O3'-C3'   | 5.32  | 126.08      | 119.70   |
| 1   | AA    | 1405 | G    | N3-C4-C5    | -5.32 | 125.94      | 128.60   |
| 22  | AV    | 41   | C    | N3-C4-C5    | -5.32 | 119.77      | 121.90   |
| 34  | BA    | 67   | G    | C4'-C3'-C2' | -5.32 | 97.28       | 102.60   |
| 35  | BB    | 143  | C    | C5'-C4'-C3' | 5.32  | 124.51      | 116.00   |
| 35  | BB    | 479  | A    | C5-C6-N6    | -5.32 | 119.44      | 123.70   |
| 35  | BB    | 949  | G    | C6-N1-C2    | 5.32  | 128.29      | 125.10   |
| 35  | BB    | 1121 | C    | P-O3'-C3'   | -5.32 | 113.32      | 119.70   |
| 35  | BB    | 1137 | G    | N9-C4-C5    | 5.32  | 107.53      | 105.40   |
| 35  | BB    | 1169 | A    | C2-N3-C4    | -5.32 | 107.94      | 110.60   |
| 35  | BB    | 1569 | A    | N7-C8-N9    | 5.32  | 116.46      | 113.80   |
| 35  | BB    | 1746 | A    | N1-C2-N3    | 5.32  | 131.96      | 129.30   |
| 35  | BB    | 2049 | G    | O5'-C5'-C4' | -5.32 | 101.59      | 111.70   |
| 35  | BB    | 2657 | A    | C6-C5-N7    | -5.32 | 128.58      | 132.30   |
| 35  | BB    | 2866 | U    | C5-C6-N1    | -5.32 | 120.04      | 122.70   |
| 37  | BD    | 194  | PRO  | N-CD-CG     | 5.32  | 111.18      | 103.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 167  | A    | C6-C5-N7    | -5.32 | 128.58      | 132.30   |
| 1   | AA    | 534  | U    | N1-C2-N3    | -5.32 | 111.71      | 114.90   |
| 1   | AA    | 720  | C    | C5-C4-N4    | -5.32 | 116.48      | 120.20   |
| 1   | AA    | 1089 | G    | C4'-C3'-C2' | -5.32 | 97.28       | 102.60   |
| 1   | AA    | 1191 | A    | P-O5'-C5'   | 5.32  | 129.41      | 120.90   |
| 1   | AA    | 1419 | G    | C5-C6-N1    | -5.32 | 108.84      | 111.50   |
| 35  | BB    | 796  | C    | O4'-C4'-C3' | -5.32 | 98.68       | 104.00   |
| 35  | BB    | 828  | U    | C1'-O4'-C4' | -5.32 | 105.64      | 109.90   |
| 35  | BB    | 1964 | G    | C5'-C4'-O4' | 5.32  | 115.48      | 109.10   |
| 35  | BB    | 2770 | G    | N1-C2-N3    | 5.32  | 127.09      | 123.90   |
| 1   | AA    | 359  | G    | N7-C8-N9    | -5.32 | 110.44      | 113.10   |
| 1   | AA    | 950  | U    | P-O5'-C5'   | 5.32  | 129.41      | 120.90   |
| 1   | AA    | 1252 | A    | C2-N3-C4    | -5.32 | 107.94      | 110.60   |
| 1   | AA    | 1298 | U    | C4-C5-C6    | 5.32  | 122.89      | 119.70   |
| 1   | AA    | 1303 | C    | N1-C2-O2    | -5.32 | 115.71      | 118.90   |
| 2   | AB    | 138  | ARG  | NE-CZ-NH2   | -5.32 | 117.64      | 120.30   |
| 35  | BB    | 415  | A    | C5-C6-N1    | -5.32 | 115.04      | 117.70   |
| 35  | BB    | 469  | G    | C8-N9-C1'   | -5.32 | 120.09      | 127.00   |
| 35  | BB    | 651  | G    | C6-C5-N7    | 5.32  | 133.59      | 130.40   |
| 35  | BB    | 1299 | G    | N1-C6-O6    | 5.32  | 123.09      | 119.90   |
| 35  | BB    | 1618 | A    | N9-C4-C5    | -5.32 | 103.67      | 105.80   |
| 35  | BB    | 1724 | G    | C4-C5-N7    | 5.32  | 112.93      | 110.80   |
| 35  | BB    | 2537 | U    | C5-C6-N1    | 5.32  | 125.36      | 122.70   |
| 39  | BF    | 100  | GLU  | N-CA-C      | -5.32 | 96.64       | 111.00   |
| 52  | BS    | 105  | VAL  | CA-CB-CG2   | -5.32 | 102.92      | 110.90   |
| 1   | AA    | 390  | U    | C5-C6-N1    | 5.32  | 125.36      | 122.70   |
| 1   | AA    | 612  | C    | C4-C5-C6    | 5.32  | 120.06      | 117.40   |
| 1   | AA    | 1026 | G    | C8-N9-C4    | -5.32 | 104.27      | 106.40   |
| 1   | AA    | 1175 | G    | C5-C6-N1    | -5.32 | 108.84      | 111.50   |
| 13  | AM    | 67   | ASP  | N-CA-CB     | 5.32  | 120.17      | 110.60   |
| 35  | BB    | 47   | C    | C4-C5-C6    | -5.32 | 114.74      | 117.40   |
| 35  | BB    | 253  | C    | P-O3'-C3'   | -5.32 | 113.32      | 119.70   |
| 35  | BB    | 474  | G    | N3-C2-N2    | 5.32  | 123.62      | 119.90   |
| 35  | BB    | 914  | G    | C2-N3-C4    | -5.32 | 109.24      | 111.90   |
| 35  | BB    | 1185 | G    | N1-C6-O6    | 5.32  | 123.09      | 119.90   |
| 35  | BB    | 1234 | U    | N1-C2-O2    | 5.32  | 126.52      | 122.80   |
| 35  | BB    | 1321 | A    | N9-C4-C5    | 5.32  | 107.93      | 105.80   |
| 35  | BB    | 1416 | G    | C6-C5-N7    | -5.32 | 127.21      | 130.40   |
| 35  | BB    | 1459 | G    | C5-C6-N1    | 5.32  | 114.16      | 111.50   |
| 35  | BB    | 2654 | A    | O4'-C1'-N9  | 5.32  | 112.45      | 108.20   |
| 35  | BB    | 2714 | G    | C4-C5-N7    | -5.32 | 108.67      | 110.80   |
| 35  | BB    | 2774 | C    | C1'-O4'-C4' | 5.32  | 114.15      | 109.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 50  | BQ    | 90   | ASP  | N-CA-CB     | 5.32  | 120.17      | 110.60   |
| 1   | AA    | 317  | U    | C5'-C4'-C3' | -5.31 | 107.50      | 116.00   |
| 18  | AR    | 56   | ARG  | CD-NE-CZ    | -5.31 | 116.16      | 123.60   |
| 22  | AV    | 31   | C    | N3-C4-C5    | -5.31 | 119.77      | 121.90   |
| 22  | AV    | 64   | C    | N3-C4-C5    | -5.31 | 119.77      | 121.90   |
| 30  | B5    | 163  | TYR  | CG-CD1-CE1  | -5.31 | 117.05      | 121.30   |
| 35  | BB    | 1471 | G    | C5-C6-N1    | -5.31 | 108.84      | 111.50   |
| 35  | BB    | 1915 | U    | N1-C1'-C2'  | -5.31 | 106.16      | 112.00   |
| 35  | BB    | 2151 | U    | C3'-C2'-C1' | -5.31 | 97.25       | 101.50   |
| 35  | BB    | 2823 | A    | C2-N3-C4    | 5.31  | 113.26      | 110.60   |
| 1   | AA    | 672  | U    | C1'-O4'-C4' | 5.31  | 114.15      | 109.90   |
| 1   | AA    | 791  | G    | N1-C6-O6    | 5.31  | 123.09      | 119.90   |
| 1   | AA    | 1263 | C    | C6-N1-C2    | -5.31 | 118.17      | 120.30   |
| 2   | AB    | 116  | LEU  | CB-CG-CD1   | -5.31 | 101.97      | 111.00   |
| 35  | BB    | 14   | A    | C5-C6-N6    | -5.31 | 119.45      | 123.70   |
| 35  | BB    | 340  | A    | C4-C5-N7    | -5.31 | 108.04      | 110.70   |
| 35  | BB    | 974  | G    | N1-C2-N2    | -5.31 | 111.42      | 116.20   |
| 35  | BB    | 1380 | G    | C4-N9-C1'   | 5.31  | 133.41      | 126.50   |
| 35  | BB    | 1393 | A    | C1'-O4'-C4' | -5.31 | 105.65      | 109.90   |
| 35  | BB    | 1749 | A    | C8-N9-C4    | -5.31 | 103.67      | 105.80   |
| 35  | BB    | 1868 | C    | N3-C4-N4    | 5.31  | 121.72      | 118.00   |
| 35  | BB    | 2266 | A    | N1-C6-N6    | 5.31  | 121.79      | 118.60   |
| 35  | BB    | 2735 | G    | C5-N7-C8    | 5.31  | 106.96      | 104.30   |
| 1   | AA    | 413  | G    | C8-N9-C4    | 5.31  | 108.52      | 106.40   |
| 1   | AA    | 765  | G    | C6-N1-C2    | 5.31  | 128.29      | 125.10   |
| 1   | AA    | 1242 | G    | C6-C5-N7    | -5.31 | 127.21      | 130.40   |
| 1   | AA    | 1522 | U    | C4-C5-C6    | -5.31 | 116.51      | 119.70   |
| 35  | BB    | 375  | G    | C5'-C4'-C3' | -5.31 | 107.50      | 116.00   |
| 35  | BB    | 717  | C    | N3-C4-C5    | -5.31 | 119.78      | 121.90   |
| 35  | BB    | 876  | C    | C4-C5-C6    | 5.31  | 120.06      | 117.40   |
| 35  | BB    | 1568 | G    | C4'-C3'-C2' | 5.31  | 107.91      | 102.60   |
| 35  | BB    | 2741 | A    | C4-C5-C6    | 5.31  | 119.66      | 117.00   |
| 1   | AA    | 16   | A    | C6-C5-N7    | -5.31 | 128.58      | 132.30   |
| 1   | AA    | 220  | G    | C6-C5-N7    | -5.31 | 127.21      | 130.40   |
| 1   | AA    | 297  | G    | N1-C6-O6    | 5.31  | 123.08      | 119.90   |
| 1   | AA    | 434  | U    | C6-N1-C2    | -5.31 | 117.81      | 121.00   |
| 1   | AA    | 613  | C    | C5-C4-N4    | -5.31 | 116.48      | 120.20   |
| 1   | AA    | 1226 | C    | N1-C1'-C2'  | 5.31  | 120.90      | 114.00   |
| 1   | AA    | 1385 | G    | N1-C2-N3    | -5.31 | 120.71      | 123.90   |
| 4   | AD    | 46   | ARG  | NE-CZ-NH2   | -5.31 | 117.65      | 120.30   |
| 4   | AD    | 98   | ASP  | CB-CG-OD2   | -5.31 | 113.52      | 118.30   |
| 35  | BB    | 18   | U    | C6-N1-C1'   | -5.31 | 113.77      | 121.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 128  | C    | N3-C4-N4    | 5.31  | 121.72      | 118.00   |
| 35  | BB    | 185  | G    | C5-C6-O6    | -5.31 | 125.41      | 128.60   |
| 35  | BB    | 270  | A    | C4-C5-C6    | 5.31  | 119.65      | 117.00   |
| 35  | BB    | 675  | A    | O4'-C1'-N9  | 5.31  | 112.45      | 108.20   |
| 35  | BB    | 867  | C    | C5-C4-N4    | -5.31 | 116.48      | 120.20   |
| 35  | BB    | 881  | G    | C5'-C4'-O4' | 5.31  | 115.47      | 109.10   |
| 35  | BB    | 1738 | G    | C4-C5-C6    | -5.31 | 115.61      | 118.80   |
| 35  | BB    | 2006 | C    | C4'-C3'-C2' | -5.31 | 97.29       | 102.60   |
| 35  | BB    | 2420 | C    | C6-N1-C2    | 5.31  | 122.42      | 120.30   |
| 35  | BB    | 2856 | A    | C5-C6-N1    | -5.31 | 115.05      | 117.70   |
| 35  | BB    | 2891 | U    | C2-N1-C1'   | 5.31  | 124.07      | 117.70   |
| 1   | AA    | 310  | G    | C4-C5-N7    | -5.31 | 108.68      | 110.80   |
| 1   | AA    | 485  | U    | C6-N1-C1'   | -5.31 | 113.77      | 121.20   |
| 1   | AA    | 821  | G    | P-O3'-C3'   | -5.31 | 113.33      | 119.70   |
| 1   | AA    | 1027 | C    | C5-C6-N1    | 5.31  | 123.65      | 121.00   |
| 1   | AA    | 1133 | G    | N3-C4-N9    | -5.31 | 122.81      | 126.00   |
| 1   | AA    | 1172 | C    | C5'-C4'-C3' | -5.31 | 107.51      | 116.00   |
| 1   | AA    | 1222 | G    | C6-C5-N7    | -5.31 | 127.22      | 130.40   |
| 1   | AA    | 1292 | G    | P-O3'-C3'   | -5.31 | 113.33      | 119.70   |
| 1   | AA    | 1463 | U    | N1-C2-N3    | -5.31 | 111.72      | 114.90   |
| 35  | BB    | 473  | G    | C4-C5-N7    | -5.31 | 108.68      | 110.80   |
| 35  | BB    | 944  | C    | P-O5'-C5'   | -5.31 | 112.41      | 120.90   |
| 35  | BB    | 1019 | U    | C1'-O4'-C4' | 5.31  | 114.14      | 109.90   |
| 35  | BB    | 1313 | U    | C2-N1-C1'   | 5.31  | 124.07      | 117.70   |
| 35  | BB    | 1925 | C    | C5-C6-N1    | -5.31 | 118.35      | 121.00   |
| 35  | BB    | 2414 | G    | O4'-C4'-C3' | -5.31 | 98.69       | 104.00   |
| 1   | AA    | 218  | U    | N3-C4-O4    | -5.31 | 115.69      | 119.40   |
| 1   | AA    | 766  | A    | O4'-C1'-N9  | 5.31  | 112.44      | 108.20   |
| 35  | BB    | 23   | G    | C4-C5-C6    | 5.31  | 121.98      | 118.80   |
| 35  | BB    | 38   | A    | C6-N1-C2    | -5.31 | 115.42      | 118.60   |
| 35  | BB    | 105  | C    | N1-C2-N3    | -5.31 | 115.49      | 119.20   |
| 35  | BB    | 248  | G    | C5-C6-O6    | -5.31 | 125.42      | 128.60   |
| 35  | BB    | 306  | U    | C3'-C2'-C1' | -5.31 | 97.25       | 101.50   |
| 35  | BB    | 1174 | U    | C4'-C3'-C2' | -5.31 | 97.29       | 102.60   |
| 35  | BB    | 2162 | G    | O3'-P-O5'   | -5.31 | 93.92       | 104.00   |
| 35  | BB    | 2578 | G    | C5'-C4'-C3' | -5.31 | 107.51      | 116.00   |
| 49  | BP    | 24   | THR  | O-C-N       | 5.31  | 131.19      | 122.70   |
| 1   | AA    | 97   | G    | N1-C2-N3    | -5.30 | 120.72      | 123.90   |
| 1   | AA    | 332  | G    | N7-C8-N9    | 5.30  | 115.75      | 113.10   |
| 1   | AA    | 707  | U    | N3-C2-O2    | 5.30  | 125.91      | 122.20   |
| 1   | AA    | 889  | A    | C4-C5-C6    | 5.30  | 119.65      | 117.00   |
| 1   | AA    | 1347 | G    | O4'-C1'-N9  | 5.30  | 112.44      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1488 | G    | P-O3'-C3'   | -5.30 | 113.34      | 119.70   |
| 34  | BA    | 74   | U    | N1-C2-N3    | -5.30 | 111.72      | 114.90   |
| 35  | BB    | 321  | U    | C5-C6-N1    | 5.30  | 125.35      | 122.70   |
| 35  | BB    | 586  | A    | P-O3'-C3'   | -5.30 | 113.34      | 119.70   |
| 35  | BB    | 938  | G    | N3-C2-N2    | 5.30  | 123.61      | 119.90   |
| 35  | BB    | 1153 | C    | O4'-C1'-N1  | 5.30  | 112.44      | 108.20   |
| 35  | BB    | 1626 | A    | P-O3'-C3'   | -5.30 | 113.33      | 119.70   |
| 35  | BB    | 2163 | A    | N9-C4-C5    | 5.30  | 107.92      | 105.80   |
| 35  | BB    | 2769 | U    | C5-C4-O4    | -5.30 | 122.72      | 125.90   |
| 1   | AA    | 212  | G    | C6-C5-N7    | -5.30 | 127.22      | 130.40   |
| 1   | AA    | 255  | G    | C4'-C3'-C2' | -5.30 | 97.30       | 102.60   |
| 1   | AA    | 1210 | C    | C5-C4-N4    | -5.30 | 116.49      | 120.20   |
| 35  | BB    | 295  | G    | N7-C8-N9    | 5.30  | 115.75      | 113.10   |
| 35  | BB    | 707  | G    | C5-C6-N1    | -5.30 | 108.85      | 111.50   |
| 35  | BB    | 1458 | U    | O4'-C1'-C2' | -5.30 | 100.50      | 105.80   |
| 35  | BB    | 1492 | G    | O4'-C4'-C3' | -5.30 | 98.70       | 104.00   |
| 35  | BB    | 2009 | A    | N1-C2-N3    | -5.30 | 126.65      | 129.30   |
| 1   | AA    | 196  | A    | C5-N7-C8    | 5.30  | 106.55      | 103.90   |
| 1   | AA    | 1003 | G    | C5-C6-O6    | -5.30 | 125.42      | 128.60   |
| 9   | AI    | 31   | GLN  | N-CA-CB     | 5.30  | 120.14      | 110.60   |
| 34  | BA    | 95   | U    | C3'-C2'-C1' | -5.30 | 97.26       | 101.50   |
| 35  | BB    | 173  | A    | O4'-C1'-N9  | 5.30  | 112.44      | 108.20   |
| 35  | BB    | 241  | A    | C5'-C4'-O4' | 5.30  | 115.46      | 109.10   |
| 35  | BB    | 929  | U    | O4'-C1'-N1  | 5.30  | 112.44      | 108.20   |
| 35  | BB    | 1100 | C    | N1-C2-O2    | -5.30 | 115.72      | 118.90   |
| 35  | BB    | 1139 | G    | N1-C2-N3    | -5.30 | 120.72      | 123.90   |
| 35  | BB    | 1228 | G    | N9-C4-C5    | -5.30 | 103.28      | 105.40   |
| 35  | BB    | 1461 | C    | P-O5'-C5'   | -5.30 | 112.42      | 120.90   |
| 35  | BB    | 1597 | A    | C8-N9-C4    | -5.30 | 103.68      | 105.80   |
| 35  | BB    | 1808 | A    | C6-C5-N7    | -5.30 | 128.59      | 132.30   |
| 35  | BB    | 2207 | C    | C1'-O4'-C4' | -5.30 | 105.66      | 109.90   |
| 35  | BB    | 2407 | A    | N1-C2-N3    | 5.30  | 131.95      | 129.30   |
| 35  | BB    | 2711 | A    | C6-N1-C2    | -5.30 | 115.42      | 118.60   |
| 35  | BB    | 2822 | G    | N7-C8-N9    | -5.30 | 110.45      | 113.10   |
| 35  | BB    | 2837 | A    | N3-C4-N9    | 5.30  | 131.64      | 127.40   |
| 1   | AA    | 162  | A    | C5-C6-N1    | -5.30 | 115.05      | 117.70   |
| 1   | AA    | 253  | A    | C5-C6-N1    | -5.30 | 115.05      | 117.70   |
| 1   | AA    | 380  | G    | P-O3'-C3'   | -5.30 | 113.34      | 119.70   |
| 1   | AA    | 405  | U    | C6-N1-C2    | -5.30 | 117.82      | 121.00   |
| 1   | AA    | 517  | G    | N1-C2-N2    | 5.30  | 120.97      | 116.20   |
| 1   | AA    | 1058 | G    | N1-C2-N3    | -5.30 | 120.72      | 123.90   |
| 3   | AC    | 145  | ALA  | N-CA-CB     | 5.30  | 117.52      | 110.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9   | AI    | 86   | LEU  | N-CA-C      | -5.30 | 96.69       | 111.00   |
| 15  | AO    | 71   | ARG  | NH1-CZ-NH2  | 5.30  | 125.23      | 119.40   |
| 30  | B5    | 216  | THR  | C-N-CA      | 5.30  | 134.95      | 121.70   |
| 35  | BB    | 441  | U    | P-O5'-C5'   | 5.30  | 129.38      | 120.90   |
| 35  | BB    | 958  | U    | C5-C4-O4    | 5.30  | 129.08      | 125.90   |
| 35  | BB    | 1080 | A    | C4-C5-C6    | 5.30  | 119.65      | 117.00   |
| 35  | BB    | 1167 | C    | OP2-P-O3'   | 5.30  | 116.86      | 105.20   |
| 35  | BB    | 1492 | G    | N3-C2-N2    | 5.30  | 123.61      | 119.90   |
| 35  | BB    | 1522 | A    | O4'-C1'-N9  | 5.30  | 112.44      | 108.20   |
| 35  | BB    | 1862 | G    | N9-C4-C5    | 5.30  | 107.52      | 105.40   |
| 35  | BB    | 2189 | U    | O4'-C1'-N1  | 5.30  | 112.44      | 108.20   |
| 35  | BB    | 2285 | C    | C6-N1-C2    | 5.30  | 122.42      | 120.30   |
| 35  | BB    | 2465 | C    | C5-C6-N1    | 5.30  | 123.65      | 121.00   |
| 38  | BE    | 163  | ASN  | CB-CG-OD1   | -5.30 | 111.00      | 121.60   |
| 1   | AA    | 433  | G    | C6-C5-N7    | -5.30 | 127.22      | 130.40   |
| 1   | AA    | 832  | G    | N1-C2-N3    | -5.30 | 120.72      | 123.90   |
| 1   | AA    | 1184 | G    | N9-C4-C5    | -5.30 | 103.28      | 105.40   |
| 1   | AA    | 1432 | G    | N7-C8-N9    | 5.30  | 115.75      | 113.10   |
| 1   | AA    | 1459 | G    | C4-C5-C6    | 5.30  | 121.98      | 118.80   |
| 35  | BB    | 688  | U    | C5-C4-O4    | -5.30 | 122.72      | 125.90   |
| 35  | BB    | 1025 | G    | C2-N3-C4    | -5.30 | 109.25      | 111.90   |
| 35  | BB    | 1070 | A    | C8-N9-C4    | -5.30 | 103.68      | 105.80   |
| 35  | BB    | 1107 | G    | N9-C1'-C2'  | -5.30 | 106.17      | 112.00   |
| 1   | AA    | 203  | G    | C6-C5-N7    | -5.30 | 127.22      | 130.40   |
| 1   | AA    | 555  | U    | O4'-C1'-N1  | 5.30  | 112.44      | 108.20   |
| 1   | AA    | 1379 | G    | N3-C4-C5    | -5.30 | 125.95      | 128.60   |
| 1   | AA    | 1434 | A    | N3-C4-C5    | -5.30 | 123.09      | 126.80   |
| 1   | AA    | 1437 | A    | N1-C2-N3    | -5.30 | 126.65      | 129.30   |
| 1   | AA    | 1445 | U    | C5-C6-N1    | -5.30 | 120.05      | 122.70   |
| 20  | AT    | 58   | ASP  | CB-CG-OD1   | 5.30  | 123.07      | 118.30   |
| 35  | BB    | 14   | A    | O4'-C1'-N9  | 5.30  | 112.44      | 108.20   |
| 35  | BB    | 1003 | G    | C5-C6-O6    | -5.30 | 125.42      | 128.60   |
| 35  | BB    | 1067 | A    | C4'-C3'-C2' | 5.30  | 107.90      | 102.60   |
| 35  | BB    | 1103 | A    | P-O5'-C5'   | 5.30  | 129.37      | 120.90   |
| 35  | BB    | 1158 | C    | P-O5'-C5'   | 5.30  | 129.37      | 120.90   |
| 35  | BB    | 1214 | A    | C4-C5-N7    | 5.30  | 113.35      | 110.70   |
| 35  | BB    | 1451 | C    | P-O3'-C3'   | -5.30 | 113.34      | 119.70   |
| 35  | BB    | 1711 | A    | C5-N7-C8    | 5.30  | 106.55      | 103.90   |
| 35  | BB    | 1734 | G    | C5-N7-C8    | 5.30  | 106.95      | 104.30   |
| 35  | BB    | 2184 | A    | N9-C4-C5    | -5.30 | 103.68      | 105.80   |
| 35  | BB    | 2674 | G    | C6-C5-N7    | -5.30 | 127.22      | 130.40   |
| 35  | BB    | 2869 | G    | C6-N1-C2    | -5.30 | 121.92      | 125.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 461  | A    | N7-C8-N9    | -5.29 | 111.15      | 113.80   |
| 35  | BB    | 812  | C    | C6-N1-C2    | 5.29  | 122.42      | 120.30   |
| 35  | BB    | 1428 | C    | C2-N3-C4    | 5.29  | 122.55      | 119.90   |
| 35  | BB    | 1492 | G    | C1'-O4'-C4' | 5.29  | 114.14      | 109.90   |
| 35  | BB    | 1681 | G    | C3'-C2'-C1' | -5.29 | 97.26       | 101.50   |
| 35  | BB    | 2057 | G    | C6-C5-N7    | -5.29 | 127.22      | 130.40   |
| 35  | BB    | 2896 | C    | C6-N1-C2    | -5.29 | 118.18      | 120.30   |
| 1   | AA    | 389  | A    | C6-C5-N7    | -5.29 | 128.59      | 132.30   |
| 1   | AA    | 710  | G    | P-O5'-C5'   | -5.29 | 112.43      | 120.90   |
| 1   | AA    | 1055 | A    | P-O5'-C5'   | -5.29 | 112.43      | 120.90   |
| 1   | AA    | 1239 | A    | C5'-C4'-O4' | 5.29  | 115.45      | 109.10   |
| 1   | AA    | 1289 | A    | C5'-C4'-O4' | 5.29  | 115.45      | 109.10   |
| 1   | AA    | 1347 | G    | P-O3'-C3'   | 5.29  | 126.05      | 119.70   |
| 1   | AA    | 1504 | G    | N1-C2-N3    | -5.29 | 120.72      | 123.90   |
| 15  | AO    | 74   | VAL  | CA-CB-CG2   | -5.29 | 102.96      | 110.90   |
| 35  | BB    | 400  | G    | C5-N7-C8    | 5.29  | 106.95      | 104.30   |
| 35  | BB    | 905  | A    | C4-C5-C6    | 5.29  | 119.65      | 117.00   |
| 35  | BB    | 952  | G    | C3'-C2'-C1' | -5.29 | 97.27       | 101.50   |
| 35  | BB    | 1300 | G    | N9-C4-C5    | -5.29 | 103.28      | 105.40   |
| 35  | BB    | 1545 | A    | C3'-C2'-C1' | -5.29 | 97.27       | 101.50   |
| 35  | BB    | 1886 | U    | N1-C2-O2    | 5.29  | 126.50      | 122.80   |
| 35  | BB    | 2172 | U    | C3'-C2'-C1' | -5.29 | 97.27       | 101.50   |
| 35  | BB    | 2464 | G    | N1-C2-N3    | -5.29 | 120.72      | 123.90   |
| 35  | BB    | 2616 | C    | C2-N3-C4    | 5.29  | 122.55      | 119.90   |
| 1   | AA    | 154  | U    | C4'-C3'-C2' | -5.29 | 97.31       | 102.60   |
| 1   | AA    | 155  | A    | C4-C5-N7    | 5.29  | 113.35      | 110.70   |
| 1   | AA    | 274  | A    | C4-C5-C6    | 5.29  | 119.65      | 117.00   |
| 1   | AA    | 1423 | G    | C5-C6-O6    | -5.29 | 125.42      | 128.60   |
| 22  | AV    | 15   | G    | O4'-C1'-N9  | 5.29  | 112.43      | 108.20   |
| 24  | AZ    | 24   | ALA  | CA-C-O      | -5.29 | 108.99      | 120.10   |
| 34  | BA    | 23   | G    | N9-C4-C5    | -5.29 | 103.28      | 105.40   |
| 35  | BB    | 145  | C    | C6-N1-C2    | -5.29 | 118.18      | 120.30   |
| 35  | BB    | 169  | G    | N3-C2-N2    | 5.29  | 123.60      | 119.90   |
| 35  | BB    | 755  | U    | C5-C4-O4    | -5.29 | 122.72      | 125.90   |
| 35  | BB    | 1169 | A    | C4-C5-C6    | 5.29  | 119.65      | 117.00   |
| 35  | BB    | 1967 | C    | C5-C4-N4    | -5.29 | 116.50      | 120.20   |
| 35  | BB    | 1977 | A    | C4'-C3'-C2' | -5.29 | 97.31       | 102.60   |
| 37  | BD    | 46   | ARG  | N-CA-C      | -5.29 | 96.71       | 111.00   |
| 1   | AA    | 117  | G    | N3-C2-N2    | 5.29  | 123.60      | 119.90   |
| 1   | AA    | 217  | C    | C5-C4-N4    | -5.29 | 116.50      | 120.20   |
| 1   | AA    | 1440 | U    | N3-C2-O2    | 5.29  | 125.90      | 122.20   |
| 1   | AA    | 1520 | C    | C5'-C4'-O4' | 5.29  | 115.45      | 109.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 891  | G    | P-O5'-C5'   | 5.29  | 129.36      | 120.90   |
| 35  | BB    | 1461 | C    | C2-N3-C4    | 5.29  | 122.55      | 119.90   |
| 35  | BB    | 2033 | A    | N3-C4-N9    | 5.29  | 131.63      | 127.40   |
| 35  | BB    | 2445 | G    | N3-C4-N9    | -5.29 | 122.83      | 126.00   |
| 1   | AA    | 116  | A    | C6-C5-N7    | -5.29 | 128.60      | 132.30   |
| 1   | AA    | 602  | A    | P-O3'-C3'   | -5.29 | 113.35      | 119.70   |
| 1   | AA    | 725  | G    | C6-C5-N7    | -5.29 | 127.23      | 130.40   |
| 1   | AA    | 947  | G    | C5-N7-C8    | -5.29 | 101.66      | 104.30   |
| 1   | AA    | 1407 | C    | N1-C2-N3    | -5.29 | 115.50      | 119.20   |
| 2   | AB    | 8    | MET  | CA-CB-CG    | 5.29  | 122.29      | 113.30   |
| 22  | AV    | 13   | C    | C1'-O4'-C4' | -5.29 | 105.67      | 109.90   |
| 34  | BA    | 34   | A    | N9-C4-C5    | 5.29  | 107.92      | 105.80   |
| 35  | BB    | 253  | C    | C6-N1-C2    | -5.29 | 118.18      | 120.30   |
| 35  | BB    | 448  | U    | N3-C2-O2    | -5.29 | 118.50      | 122.20   |
| 35  | BB    | 915  | C    | O5'-P-OP1   | -5.29 | 100.94      | 105.70   |
| 35  | BB    | 1024 | G    | P-O3'-C3'   | 5.29  | 126.05      | 119.70   |
| 35  | BB    | 1245 | G    | N1-C2-N2    | -5.29 | 111.44      | 116.20   |
| 35  | BB    | 1546 | G    | C2-N3-C4    | 5.29  | 114.54      | 111.90   |
| 35  | BB    | 1562 | U    | P-O5'-C5'   | 5.29  | 129.36      | 120.90   |
| 35  | BB    | 1669 | A    | C8-N9-C4    | -5.29 | 103.69      | 105.80   |
| 35  | BB    | 2049 | G    | N1-C2-N3    | -5.29 | 120.73      | 123.90   |
| 35  | BB    | 2184 | A    | C4-C5-C6    | 5.29  | 119.64      | 117.00   |
| 35  | BB    | 2558 | C    | C5-C6-N1    | 5.29  | 123.64      | 121.00   |
| 35  | BB    | 2665 | A    | C4'-C3'-C2' | -5.29 | 97.31       | 102.60   |
| 36  | BC    | 102  | TYR  | CG-CD2-CE2  | 5.29  | 125.53      | 121.30   |
| 1   | AA    | 43   | C    | P-O3'-C3'   | 5.29  | 126.04      | 119.70   |
| 1   | AA    | 517  | G    | N9-C4-C5    | 5.29  | 107.52      | 105.40   |
| 1   | AA    | 1292 | G    | C4-C5-C6    | 5.29  | 121.97      | 118.80   |
| 2   | AB    | 146  | SER  | CB-CA-C     | -5.29 | 100.06      | 110.10   |
| 22  | AV    | 59   | A    | C5-C6-N6    | -5.29 | 119.47      | 123.70   |
| 35  | BB    | 127  | A    | C4-C5-C6    | 5.29  | 119.64      | 117.00   |
| 35  | BB    | 1049 | C    | C2-N3-C4    | 5.29  | 122.54      | 119.90   |
| 35  | BB    | 1102 | C    | N3-C4-N4    | 5.29  | 121.70      | 118.00   |
| 35  | BB    | 1897 | G    | C8-N9-C4    | 5.29  | 108.52      | 106.40   |
| 35  | BB    | 2556 | C    | O4'-C4'-C3' | -5.29 | 98.71       | 104.00   |
| 1   | AA    | 573  | A    | C8-N9-C4    | -5.29 | 103.69      | 105.80   |
| 1   | AA    | 586  | C    | C5-C4-N4    | -5.29 | 116.50      | 120.20   |
| 1   | AA    | 682  | G    | N1-C2-N3    | 5.29  | 127.07      | 123.90   |
| 1   | AA    | 812  | G    | N3-C4-C5    | -5.29 | 125.96      | 128.60   |
| 1   | AA    | 851  | G    | C4-C5-N7    | 5.29  | 112.91      | 110.80   |
| 1   | AA    | 942  | G    | P-O5'-C5'   | 5.29  | 129.36      | 120.90   |
| 1   | AA    | 997  | U    | O4'-C1'-C2' | -5.29 | 100.51      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1124 | G    | C6-N1-C2    | 5.29  | 128.27      | 125.10   |
| 1   | AA    | 1303 | C    | C3'-C2'-C1' | -5.29 | 97.27       | 101.50   |
| 1   | AA    | 1430 | A    | C4-C5-N7    | -5.29 | 108.06      | 110.70   |
| 2   | AB    | 195  | VAL  | CA-CB-CG2   | -5.29 | 102.97      | 110.90   |
| 12  | AL    | 60   | PHE  | N-CA-CB     | 5.29  | 120.11      | 110.60   |
| 27  | B2    | 28   | LEU  | CB-CG-CD2   | 5.29  | 119.98      | 111.00   |
| 34  | BA    | 4    | C    | N1-C2-O2    | 5.29  | 122.07      | 118.90   |
| 35  | BB    | 302  | C    | P-O3'-C3'   | -5.29 | 113.36      | 119.70   |
| 35  | BB    | 320  | A    | OP1-P-O3'   | 5.29  | 116.83      | 105.20   |
| 35  | BB    | 324  | A    | C2-N3-C4    | 5.29  | 113.24      | 110.60   |
| 35  | BB    | 830  | G    | N1-C6-O6    | 5.29  | 123.07      | 119.90   |
| 35  | BB    | 1122 | G    | C6-N1-C2    | 5.29  | 128.27      | 125.10   |
| 35  | BB    | 1445 | G    | N3-C4-N9    | 5.29  | 129.17      | 126.00   |
| 35  | BB    | 1848 | A    | C4-C5-C6    | 5.29  | 119.64      | 117.00   |
| 35  | BB    | 2077 | A    | C5-C6-N6    | -5.29 | 119.47      | 123.70   |
| 35  | BB    | 2343 | U    | C1'-O4'-C4' | 5.29  | 114.13      | 109.90   |
| 35  | BB    | 2485 | G    | C4'-C3'-C2' | -5.29 | 97.31       | 102.60   |
| 35  | BB    | 2874 | C    | C2-N3-C4    | -5.29 | 117.26      | 119.90   |
| 44  | BK    | 32   | TYR  | CD1-CE1-CZ  | -5.29 | 115.04      | 119.80   |
| 1   | AA    | 325  | A    | N9-C4-C5    | 5.28  | 107.91      | 105.80   |
| 1   | AA    | 326  | G    | C4'-C3'-C2' | 5.28  | 107.88      | 102.60   |
| 1   | AA    | 799  | G    | C4-C5-N7    | -5.28 | 108.69      | 110.80   |
| 1   | AA    | 933  | G    | C4-N9-C1'   | -5.28 | 119.63      | 126.50   |
| 14  | AN    | 16   | ALA  | N-CA-CB     | 5.28  | 117.50      | 110.10   |
| 35  | BB    | 685  | A    | C8-N9-C4    | 5.28  | 107.91      | 105.80   |
| 35  | BB    | 735  | A    | C8-N9-C4    | -5.28 | 103.69      | 105.80   |
| 35  | BB    | 1086 | A    | OP1-P-OP2   | -5.28 | 111.67      | 119.60   |
| 35  | BB    | 1167 | C    | C5'-C4'-C3' | 5.28  | 124.45      | 116.00   |
| 35  | BB    | 1490 | A    | C4-C5-N7    | -5.28 | 108.06      | 110.70   |
| 35  | BB    | 2197 | U    | N1-C1'-C2'  | -5.28 | 106.19      | 112.00   |
| 35  | BB    | 2637 | U    | N1-C2-O2    | 5.28  | 126.50      | 122.80   |
| 35  | BB    | 2862 | G    | N1-C2-N3    | -5.28 | 120.73      | 123.90   |
| 35  | BB    | 2862 | G    | N3-C2-N2    | -5.28 | 116.20      | 119.90   |
| 1   | AA    | 111  | G    | N1-C2-N3    | -5.28 | 120.73      | 123.90   |
| 1   | AA    | 462  | G    | C3'-C2'-C1' | 5.28  | 105.72      | 101.50   |
| 1   | AA    | 1044 | A    | C6-N1-C2    | -5.28 | 115.43      | 118.60   |
| 34  | BA    | 56   | G    | O4'-C1'-N9  | 5.28  | 112.42      | 108.20   |
| 35  | BB    | 25   | U    | C5-C4-O4    | -5.28 | 122.73      | 125.90   |
| 35  | BB    | 207  | A    | C5'-C4'-C3' | -5.28 | 107.55      | 116.00   |
| 35  | BB    | 775  | G    | O4'-C1'-N9  | 5.28  | 112.43      | 108.20   |
| 35  | BB    | 1369 | G    | O4'-C1'-N9  | 5.28  | 112.43      | 108.20   |
| 35  | BB    | 1370 | C    | P-O3'-C3'   | -5.28 | 113.36      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1374 | G    | C5-N7-C8    | -5.28 | 101.66      | 104.30   |
| 35  | BB    | 1801 | A    | N1-C6-N6    | 5.28  | 121.77      | 118.60   |
| 35  | BB    | 2360 | G    | C5-C6-N1    | 5.28  | 114.14      | 111.50   |
| 51  | BR    | 2    | TYR  | CB-CA-C     | -5.28 | 99.84       | 110.40   |
| 1   | AA    | 60   | A    | C5-C6-N1    | -5.28 | 115.06      | 117.70   |
| 1   | AA    | 230  | G    | C8-N9-C1'   | 5.28  | 133.86      | 127.00   |
| 1   | AA    | 294  | U    | N3-C4-O4    | 5.28  | 123.10      | 119.40   |
| 1   | AA    | 1033 | G    | C5'-C4'-C3' | 5.28  | 124.45      | 116.00   |
| 1   | AA    | 1144 | G    | C5'-C4'-O4' | 5.28  | 115.44      | 109.10   |
| 34  | BA    | 102  | G    | N1-C2-N3    | 5.28  | 127.07      | 123.90   |
| 35  | BB    | 395  | U    | N1-C1'-C2'  | -5.28 | 106.19      | 112.00   |
| 35  | BB    | 402  | A    | C6-N1-C2    | -5.28 | 115.43      | 118.60   |
| 35  | BB    | 764  | A    | P-O3'-C3'   | -5.28 | 113.36      | 119.70   |
| 35  | BB    | 1036 | G    | N1-C6-O6    | 5.28  | 123.07      | 119.90   |
| 35  | BB    | 1387 | A    | P-O3'-C3'   | 5.28  | 126.04      | 119.70   |
| 35  | BB    | 1684 | G    | C2-N3-C4    | 5.28  | 114.54      | 111.90   |
| 35  | BB    | 1705 | A    | C8-N9-C4    | 5.28  | 107.91      | 105.80   |
| 35  | BB    | 1723 | G    | P-O3'-C3'   | -5.28 | 113.36      | 119.70   |
| 35  | BB    | 2116 | G    | N1-C2-N3    | -5.28 | 120.73      | 123.90   |
| 35  | BB    | 2335 | A    | C5-N7-C8    | 5.28  | 106.54      | 103.90   |
| 35  | BB    | 2489 | U    | N1-C2-N3    | -5.28 | 111.73      | 114.90   |
| 35  | BB    | 2582 | G    | C8-N9-C4    | -5.28 | 104.29      | 106.40   |
| 43  | BJ    | 30   | THR  | CA-CB-CG2   | -5.28 | 105.01      | 112.40   |
| 47  | BN    | 38   | LEU  | CB-CG-CD1   | -5.28 | 102.02      | 111.00   |
| 1   | AA    | 886  | G    | N3-C2-N2    | 5.28  | 123.60      | 119.90   |
| 35  | BB    | 1397 | U    | C6-N1-C2    | -5.28 | 117.83      | 121.00   |
| 35  | BB    | 2279 | G    | C4'-C3'-C2' | -5.28 | 97.32       | 102.60   |
| 35  | BB    | 2397 | G    | C5-C6-O6    | -5.28 | 125.43      | 128.60   |
| 35  | BB    | 2608 | G    | P-O3'-C3'   | 5.28  | 126.03      | 119.70   |
| 1   | AA    | 236  | A    | C4-C5-N7    | -5.28 | 108.06      | 110.70   |
| 1   | AA    | 238  | A    | C3'-C2'-C1' | -5.28 | 97.28       | 101.50   |
| 1   | AA    | 302  | G    | N1-C6-O6    | 5.28  | 123.07      | 119.90   |
| 1   | AA    | 346  | G    | N3-C4-C5    | -5.28 | 125.96      | 128.60   |
| 1   | AA    | 779  | C    | C5-C6-N1    | 5.28  | 123.64      | 121.00   |
| 1   | AA    | 831  | A    | C8-N9-C4    | -5.28 | 103.69      | 105.80   |
| 1   | AA    | 930  | C    | C4'-C3'-C2' | -5.28 | 97.32       | 102.60   |
| 1   | AA    | 1434 | A    | C5-C6-N6    | -5.28 | 119.48      | 123.70   |
| 35  | BB    | 178  | G    | N1-C2-N3    | -5.28 | 120.73      | 123.90   |
| 35  | BB    | 898  | C    | C6-N1-C2    | -5.28 | 118.19      | 120.30   |
| 35  | BB    | 912  | C    | P-O3'-C3'   | 5.28  | 126.03      | 119.70   |
| 35  | BB    | 994  | C    | C5-C4-N4    | -5.28 | 116.51      | 120.20   |
| 35  | BB    | 1577 | C    | C2-N1-C1'   | 5.28  | 124.61      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2403 | C    | OP1-P-O3'   | 5.28  | 116.81      | 105.20   |
| 35  | BB    | 2649 | C    | C1'-O4'-C4' | 5.28  | 114.12      | 109.90   |
| 35  | BB    | 2669 | G    | C4-C5-N7    | 5.28  | 112.91      | 110.80   |
| 35  | BB    | 2806 | C    | N3-C4-C5    | -5.28 | 119.79      | 121.90   |
| 46  | BM    | 38   | ARG  | NE-CZ-NH1   | 5.28  | 122.94      | 120.30   |
| 1   | AA    | 710  | G    | N3-C4-C5    | -5.28 | 125.96      | 128.60   |
| 1   | AA    | 805  | C    | N3-C4-N4    | 5.28  | 121.69      | 118.00   |
| 1   | AA    | 1374 | A    | C5-N7-C8    | 5.28  | 106.54      | 103.90   |
| 1   | AA    | 1495 | U    | C1'-O4'-C4' | 5.28  | 114.12      | 109.90   |
| 30  | B5    | 13   | GLU  | N-CA-CB     | -5.28 | 101.11      | 110.60   |
| 35  | BB    | 705  | A    | C6-C5-N7    | -5.28 | 128.61      | 132.30   |
| 35  | BB    | 830  | G    | O3'-P-O5'   | -5.28 | 93.98       | 104.00   |
| 35  | BB    | 890  | C    | C5'-C4'-O4' | 5.28  | 115.43      | 109.10   |
| 35  | BB    | 1138 | G    | N7-C8-N9    | -5.28 | 110.46      | 113.10   |
| 35  | BB    | 1147 | A    | N7-C8-N9    | 5.28  | 116.44      | 113.80   |
| 35  | BB    | 1826 | G    | C5-C6-O6    | -5.28 | 125.43      | 128.60   |
| 35  | BB    | 2194 | U    | C5'-C4'-C3' | 5.28  | 124.44      | 116.00   |
| 35  | BB    | 2284 | A    | C5'-C4'-C3' | 5.28  | 124.44      | 116.00   |
| 35  | BB    | 2393 | U    | C4-C5-C6    | -5.28 | 116.53      | 119.70   |
| 35  | BB    | 2425 | A    | C2'-C3'-O3' | 5.28  | 122.14      | 113.70   |
| 35  | BB    | 2692 | G    | N9-C1'-C2'  | -5.28 | 106.20      | 112.00   |
| 36  | BC    | 82   | TYR  | CD1-CE1-CZ  | 5.28  | 124.55      | 119.80   |
| 1   | AA    | 281  | G    | P-O5'-C5'   | 5.27  | 129.34      | 120.90   |
| 1   | AA    | 401  | C    | C2-N3-C4    | -5.27 | 117.26      | 119.90   |
| 1   | AA    | 1393 | U    | N1-C2-N3    | -5.27 | 111.73      | 114.90   |
| 1   | AA    | 1518 | A    | C4-C5-N7    | -5.27 | 108.06      | 110.70   |
| 35  | BB    | 236  | C    | C2-N1-C1'   | 5.27  | 124.60      | 118.80   |
| 35  | BB    | 1557 | C    | C2-N3-C4    | 5.27  | 122.54      | 119.90   |
| 35  | BB    | 1885 | A    | C5-N7-C8    | 5.27  | 106.54      | 103.90   |
| 35  | BB    | 2055 | C    | C2-N1-C1'   | 5.27  | 124.60      | 118.80   |
| 35  | BB    | 2436 | G    | C4-C5-C6    | 5.27  | 121.96      | 118.80   |
| 1   | AA    | 137  | U    | O4'-C1'-N1  | 5.27  | 112.42      | 108.20   |
| 1   | AA    | 318  | G    | C8-N9-C1'   | 5.27  | 133.85      | 127.00   |
| 1   | AA    | 552  | U    | N1-C2-O2    | -5.27 | 119.11      | 122.80   |
| 1   | AA    | 715  | A    | N1-C2-N3    | 5.27  | 131.94      | 129.30   |
| 1   | AA    | 785  | G    | C1'-O4'-C4' | 5.27  | 114.12      | 109.90   |
| 1   | AA    | 994  | A    | N7-C8-N9    | -5.27 | 111.16      | 113.80   |
| 1   | AA    | 1065 | U    | N1-C2-N3    | 5.27  | 118.06      | 114.90   |
| 19  | AS    | 79   | TYR  | CD1-CG-CD2  | 5.27  | 123.70      | 117.90   |
| 35  | BB    | 279  | A    | C4-C5-N7    | 5.27  | 113.34      | 110.70   |
| 35  | BB    | 465  | G    | C8-N9-C4    | -5.27 | 104.29      | 106.40   |
| 35  | BB    | 536  | G    | O4'-C1'-N9  | 5.27  | 112.42      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 665  | U    | C5-C6-N1    | 5.27  | 125.34      | 122.70   |
| 35  | BB    | 712  | G    | N9-C4-C5    | 5.27  | 107.51      | 105.40   |
| 35  | BB    | 1012 | U    | C2-N3-C4    | -5.27 | 123.84      | 127.00   |
| 35  | BB    | 1075 | C    | C6-N1-C2    | 5.27  | 122.41      | 120.30   |
| 35  | BB    | 1219 | U    | C5-C4-O4    | -5.27 | 122.74      | 125.90   |
| 35  | BB    | 1246 | A    | C4-C5-C6    | 5.27  | 119.64      | 117.00   |
| 35  | BB    | 1612 | C    | O4'-C1'-N1  | 5.27  | 112.42      | 108.20   |
| 35  | BB    | 1688 | U    | C5-C4-O4    | -5.27 | 122.74      | 125.90   |
| 35  | BB    | 1985 | C    | C4-C5-C6    | 5.27  | 120.04      | 117.40   |
| 35  | BB    | 2122 | U    | C4'-C3'-C2' | -5.27 | 97.33       | 102.60   |
| 35  | BB    | 2152 | G    | C4-C5-C6    | 5.27  | 121.96      | 118.80   |
| 36  | BC    | 173  | LEU  | CB-CG-CD2   | 5.27  | 119.96      | 111.00   |
| 56  | BY    | 34   | SER  | N-CA-C      | -5.27 | 96.76       | 111.00   |
| 1   | AA    | 81   | A    | C5-C6-N1    | 5.27  | 120.33      | 117.70   |
| 1   | AA    | 423  | G    | C4'-C3'-C2' | -5.27 | 97.33       | 102.60   |
| 1   | AA    | 667  | G    | C5-N7-C8    | 5.27  | 106.94      | 104.30   |
| 35  | BB    | 713  | G    | C4'-C3'-C2' | -5.27 | 97.33       | 102.60   |
| 35  | BB    | 1584 | U    | N3-C2-O2    | 5.27  | 125.89      | 122.20   |
| 35  | BB    | 1750 | G    | C6-N1-C2    | -5.27 | 121.94      | 125.10   |
| 35  | BB    | 2140 | G    | N1-C2-N3    | -5.27 | 120.74      | 123.90   |
| 1   | AA    | 495  | A    | O4'-C1'-N9  | 5.27  | 112.42      | 108.20   |
| 1   | AA    | 645  | G    | C4-C5-C6    | 5.27  | 121.96      | 118.80   |
| 1   | AA    | 826  | C    | N1-C2-O2    | 5.27  | 122.06      | 118.90   |
| 1   | AA    | 1453 | G    | O5'-C5'-C4' | -5.27 | 101.69      | 111.70   |
| 32  | B7    | 16   | THR  | N-CA-CB     | 5.27  | 120.31      | 110.30   |
| 35  | BB    | 256  | A    | C4-C5-C6    | 5.27  | 119.63      | 117.00   |
| 35  | BB    | 446  | G    | C8-N9-C4    | 5.27  | 108.51      | 106.40   |
| 35  | BB    | 988  | A    | N9-C1'-C2'  | -5.27 | 106.20      | 112.00   |
| 35  | BB    | 1099 | G    | C5-N7-C8    | -5.27 | 101.67      | 104.30   |
| 35  | BB    | 1122 | G    | N1-C2-N3    | -5.27 | 120.74      | 123.90   |
| 35  | BB    | 1202 | G    | C6-C5-N7    | -5.27 | 127.24      | 130.40   |
| 35  | BB    | 1454 | C    | O3'-P-O5'   | -5.27 | 93.99       | 104.00   |
| 35  | BB    | 1668 | A    | O4'-C1'-N9  | 5.27  | 112.42      | 108.20   |
| 35  | BB    | 2273 | A    | C2-N3-C4    | 5.27  | 113.23      | 110.60   |
| 35  | BB    | 2548 | U    | N3-C4-C5    | -5.27 | 111.44      | 114.60   |
| 42  | BI    | 141  | ASP  | CA-C-O      | -5.27 | 109.03      | 120.10   |
| 1   | AA    | 538  | G    | C6-C5-N7    | -5.27 | 127.24      | 130.40   |
| 1   | AA    | 610  | U    | C4-C5-C6    | 5.27  | 122.86      | 119.70   |
| 1   | AA    | 708  | C    | O3'-P-O5'   | -5.27 | 93.99       | 104.00   |
| 1   | AA    | 1145 | A    | C5'-C4'-C3' | -5.27 | 107.57      | 116.00   |
| 35  | BB    | 123  | G    | C5'-C4'-O4' | 5.27  | 115.42      | 109.10   |
| 35  | BB    | 355  | U    | N1-C2-O2    | 5.27  | 126.49      | 122.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 912  | C    | C5-C6-N1    | 5.27  | 123.63      | 121.00   |
| 35  | BB    | 990  | A    | C6-N1-C2    | 5.27  | 121.76      | 118.60   |
| 35  | BB    | 1100 | C    | N3-C4-C5    | -5.27 | 119.79      | 121.90   |
| 35  | BB    | 1247 | A    | C6-C5-N7    | -5.27 | 128.61      | 132.30   |
| 35  | BB    | 2075 | U    | C1'-O4'-C4' | -5.27 | 105.69      | 109.90   |
| 35  | BB    | 2085 | U    | N1-C2-N3    | -5.27 | 111.74      | 114.90   |
| 35  | BB    | 2263 | C    | N1-C2-O2    | -5.27 | 115.74      | 118.90   |
| 35  | BB    | 2410 | G    | C3'-C2'-C1' | -5.27 | 97.29       | 101.50   |
| 35  | BB    | 2583 | G    | C6-C5-N7    | -5.27 | 127.24      | 130.40   |
| 35  | BB    | 2597 | G    | C8-N9-C4    | 5.27  | 108.51      | 106.40   |
| 35  | BB    | 2797 | U    | C6-N1-C1'   | -5.27 | 113.83      | 121.20   |
| 1   | AA    | 25   | C    | N1-C2-O2    | -5.27 | 115.74      | 118.90   |
| 1   | AA    | 600  | A    | N9-C4-C5    | -5.27 | 103.69      | 105.80   |
| 1   | AA    | 790  | A    | C5-C6-N6    | -5.27 | 119.49      | 123.70   |
| 35  | BB    | 199  | A    | C4-N9-C1'   | -5.27 | 116.82      | 126.30   |
| 35  | BB    | 213  | A    | C5-C6-N6    | -5.27 | 119.49      | 123.70   |
| 35  | BB    | 785  | G    | P-O5'-C5'   | -5.27 | 112.47      | 120.90   |
| 35  | BB    | 1321 | A    | N3-C4-C5    | -5.27 | 123.11      | 126.80   |
| 1   | AA    | 160  | A    | N9-C4-C5    | 5.26  | 107.91      | 105.80   |
| 1   | AA    | 527  | G    | N1-C2-N3    | 5.26  | 127.06      | 123.90   |
| 1   | AA    | 921  | U    | C4'-C3'-C2' | -5.26 | 97.34       | 102.60   |
| 1   | AA    | 1027 | C    | O4'-C1'-N1  | 5.26  | 112.41      | 108.20   |
| 1   | AA    | 1144 | G    | N3-C4-C5    | -5.26 | 125.97      | 128.60   |
| 1   | AA    | 1497 | G    | C4-C5-C6    | 5.26  | 121.96      | 118.80   |
| 34  | BA    | 31   | C    | C5-C6-N1    | 5.26  | 123.63      | 121.00   |
| 35  | BB    | 119  | A    | P-O3'-C3'   | 5.26  | 126.02      | 119.70   |
| 35  | BB    | 217  | A    | C8-N9-C1'   | 5.26  | 137.18      | 127.70   |
| 35  | BB    | 310  | A    | C4-C5-N7    | -5.26 | 108.07      | 110.70   |
| 35  | BB    | 585  | G    | O4'-C1'-N9  | 5.26  | 112.41      | 108.20   |
| 35  | BB    | 607  | U    | C6-N1-C2    | -5.26 | 117.84      | 121.00   |
| 35  | BB    | 719  | C    | C2-N1-C1'   | 5.26  | 124.59      | 118.80   |
| 35  | BB    | 876  | C    | C3'-C2'-C1' | -5.26 | 97.29       | 101.50   |
| 35  | BB    | 903  | C    | C4-C5-C6    | -5.26 | 114.77      | 117.40   |
| 35  | BB    | 1039 | A    | P-O3'-C3'   | -5.26 | 113.38      | 119.70   |
| 35  | BB    | 1177 | G    | P-O5'-C5'   | 5.26  | 129.32      | 120.90   |
| 35  | BB    | 1377 | G    | C8-N9-C4    | -5.26 | 104.29      | 106.40   |
| 35  | BB    | 1754 | A    | C2-N3-C4    | 5.26  | 113.23      | 110.60   |
| 35  | BB    | 2029 | G    | O4'-C1'-N9  | 5.26  | 112.41      | 108.20   |
| 35  | BB    | 2283 | C    | O4'-C1'-C2' | -5.26 | 100.53      | 105.80   |
| 35  | BB    | 2663 | G    | C2-N3-C4    | -5.26 | 109.27      | 111.90   |
| 35  | BB    | 2852 | G    | C6-C5-N7    | -5.26 | 127.24      | 130.40   |
| 35  | BB    | 2886 | A    | C2-N3-C4    | -5.26 | 107.97      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 38  | BE    | 124  | PHE  | CB-CG-CD2   | 5.26  | 124.49      | 120.80   |
| 1   | AA    | 80   | A    | O4'-C1'-N9  | 5.26  | 112.41      | 108.20   |
| 1   | AA    | 255  | G    | N7-C8-N9    | -5.26 | 110.47      | 113.10   |
| 1   | AA    | 380  | G    | N3-C4-N9    | 5.26  | 129.16      | 126.00   |
| 4   | AD    | 114  | ARG  | NE-CZ-NH2   | 5.26  | 122.93      | 120.30   |
| 22  | AV    | 70   | C    | N3-C4-C5    | 5.26  | 124.00      | 121.90   |
| 35  | BB    | 1114 | C    | N3-C4-N4    | 5.26  | 121.68      | 118.00   |
| 35  | BB    | 1185 | G    | O4'-C1'-N9  | 5.26  | 112.41      | 108.20   |
| 35  | BB    | 1841 | U    | C6-N1-C2    | -5.26 | 117.84      | 121.00   |
| 35  | BB    | 1858 | A    | N7-C8-N9    | -5.26 | 111.17      | 113.80   |
| 35  | BB    | 2343 | U    | C4'-C3'-C2' | 5.26  | 107.86      | 102.60   |
| 35  | BB    | 2602 | A    | C8-N9-C1'   | 5.26  | 137.17      | 127.70   |
| 48  | BO    | 79   | ALA  | N-CA-CB     | 5.26  | 117.47      | 110.10   |
| 1   | AA    | 51   | A    | C2'-C3'-O3' | 5.26  | 122.12      | 113.70   |
| 1   | AA    | 119  | A    | C3'-C2'-C1' | -5.26 | 97.29       | 101.50   |
| 1   | AA    | 850  | U    | C3'-C2'-C1' | 5.26  | 105.71      | 101.50   |
| 7   | AG    | 118  | ARG  | C-N-CA      | 5.26  | 134.86      | 121.70   |
| 32  | B7    | 39   | ARG  | NE-CZ-NH1   | -5.26 | 117.67      | 120.30   |
| 35  | BB    | 296  | U    | N3-C4-C5    | -5.26 | 111.44      | 114.60   |
| 35  | BB    | 443  | A    | C6-C5-N7    | -5.26 | 128.62      | 132.30   |
| 35  | BB    | 464  | U    | P-O5'-C5'   | -5.26 | 112.48      | 120.90   |
| 35  | BB    | 661  | A    | N9-C4-C5    | 5.26  | 107.91      | 105.80   |
| 35  | BB    | 1833 | C    | C3'-C2'-C1' | 5.26  | 105.71      | 101.50   |
| 35  | BB    | 2165 | C    | C5-C4-N4    | -5.26 | 116.52      | 120.20   |
| 35  | BB    | 2345 | G    | P-O3'-C3'   | 5.26  | 126.02      | 119.70   |
| 35  | BB    | 2392 | A    | C4-C5-C6    | 5.26  | 119.63      | 117.00   |
| 35  | BB    | 2544 | G    | N7-C8-N9    | 5.26  | 115.73      | 113.10   |
| 52  | BS    | 81   | SER  | N-CA-CB     | 5.26  | 118.39      | 110.50   |
| 56  | BY    | 10   | ARG  | N-CA-C      | -5.26 | 96.79       | 111.00   |
| 1   | AA    | 107  | G    | C5-C6-O6    | 5.26  | 131.76      | 128.60   |
| 1   | AA    | 367  | U    | O4'-C1'-N1  | 5.26  | 112.41      | 108.20   |
| 1   | AA    | 692  | U    | O4'-C1'-N1  | 5.26  | 112.41      | 108.20   |
| 1   | AA    | 889  | A    | N9-C4-C5    | 5.26  | 107.90      | 105.80   |
| 1   | AA    | 1044 | A    | C2-N3-C4    | -5.26 | 107.97      | 110.60   |
| 1   | AA    | 1222 | G    | P-O3'-C3'   | -5.26 | 113.39      | 119.70   |
| 7   | AG    | 9    | ARG  | NE-CZ-NH2   | -5.26 | 117.67      | 120.30   |
| 34  | BA    | 53   | A    | N3-C4-C5    | -5.26 | 123.12      | 126.80   |
| 35  | BB    | 350  | G    | P-O3'-C3'   | 5.26  | 126.01      | 119.70   |
| 35  | BB    | 536  | G    | C1'-O4'-C4' | 5.26  | 114.11      | 109.90   |
| 35  | BB    | 572  | A    | C2-N3-C4    | 5.26  | 113.23      | 110.60   |
| 35  | BB    | 770  | G    | C4'-C3'-C2' | -5.26 | 97.34       | 102.60   |
| 35  | BB    | 784  | G    | C5-N7-C8    | 5.26  | 106.93      | 104.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1043 | C    | C6-N1-C2    | 5.26  | 122.40      | 120.30   |
| 35  | BB    | 1112 | G    | C6-C5-N7    | -5.26 | 127.24      | 130.40   |
| 35  | BB    | 1429 | G    | OP1-P-OP2   | -5.26 | 111.71      | 119.60   |
| 35  | BB    | 1743 | G    | C2-N3-C4    | -5.26 | 109.27      | 111.90   |
| 35  | BB    | 1792 | G    | C8-N9-C4    | 5.26  | 108.50      | 106.40   |
| 35  | BB    | 2501 | C    | N3-C4-N4    | 5.26  | 121.68      | 118.00   |
| 35  | BB    | 2792 | A    | N7-C8-N9    | 5.26  | 116.43      | 113.80   |
| 1   | AA    | 300  | A    | N1-C2-N3    | 5.26  | 131.93      | 129.30   |
| 34  | BA    | 92   | C    | O4'-C4'-C3' | -5.26 | 98.74       | 104.00   |
| 35  | BB    | 111  | A    | N9-C4-C5    | 5.26  | 107.90      | 105.80   |
| 35  | BB    | 2082 | A    | P-O3'-C3'   | -5.26 | 113.39      | 119.70   |
| 35  | BB    | 2411 | A    | C5-C6-N1    | -5.26 | 115.07      | 117.70   |
| 48  | BO    | 24   | THR  | N-CA-C      | -5.26 | 96.80       | 111.00   |
| 1   | AA    | 38   | G    | C2-N3-C4    | -5.26 | 109.27      | 111.90   |
| 1   | AA    | 95   | C    | N3-C4-N4    | 5.26  | 121.68      | 118.00   |
| 1   | AA    | 182  | A    | C1'-O4'-C4' | 5.26  | 114.11      | 109.90   |
| 1   | AA    | 649  | A    | O5'-C5'-C4' | -5.26 | 101.71      | 111.70   |
| 1   | AA    | 1195 | C    | C4-C5-C6    | -5.26 | 114.77      | 117.40   |
| 1   | AA    | 1285 | A    | C5'-C4'-C3' | -5.26 | 107.59      | 116.00   |
| 25  | B0    | 77   | TYR  | CZ-CE2-CD2  | 5.26  | 124.53      | 119.80   |
| 34  | BA    | 24   | G    | C8-N9-C1'   | 5.26  | 133.83      | 127.00   |
| 35  | BB    | 154  | U    | P-O3'-C3'   | -5.26 | 113.39      | 119.70   |
| 35  | BB    | 675  | A    | C3'-C2'-C1' | 5.26  | 105.70      | 101.50   |
| 35  | BB    | 810  | U    | P-O3'-C3'   | 5.26  | 126.01      | 119.70   |
| 35  | BB    | 943  | A    | N7-C8-N9    | 5.26  | 116.43      | 113.80   |
| 35  | BB    | 1062 | G    | N3-C4-C5    | -5.26 | 125.97      | 128.60   |
| 35  | BB    | 1134 | A    | C5-C6-N6    | -5.26 | 119.50      | 123.70   |
| 35  | BB    | 1618 | A    | C1'-O4'-C4' | -5.26 | 105.69      | 109.90   |
| 35  | BB    | 1905 | C    | N3-C4-C5    | -5.26 | 119.80      | 121.90   |
| 35  | BB    | 1925 | C    | N1-C2-O2    | -5.26 | 115.75      | 118.90   |
| 35  | BB    | 2150 | C    | OP2-P-O3'   | 5.26  | 116.76      | 105.20   |
| 35  | BB    | 2205 | A    | P-O3'-C3'   | 5.26  | 126.01      | 119.70   |
| 35  | BB    | 2305 | U    | C5-C6-N1    | 5.26  | 125.33      | 122.70   |
| 35  | BB    | 2541 | A    | C5-C6-N1    | -5.26 | 115.07      | 117.70   |
| 35  | BB    | 2659 | G    | C4-C5-C6    | 5.26  | 121.95      | 118.80   |
| 52  | BS    | 94   | ASP  | CB-CG-OD2   | -5.26 | 113.57      | 118.30   |
| 1   | AA    | 450  | G    | C8-N9-C4    | -5.25 | 104.30      | 106.40   |
| 1   | AA    | 993  | G    | N3-C4-N9    | 5.25  | 129.15      | 126.00   |
| 35  | BB    | 223  | A    | C1'-O4'-C4' | 5.25  | 114.10      | 109.90   |
| 35  | BB    | 635  | C    | C5-C4-N4    | -5.25 | 116.52      | 120.20   |
| 35  | BB    | 1160 | G    | N3-C2-N2    | 5.25  | 123.58      | 119.90   |
| 35  | BB    | 1987 | A    | C4-C5-C6    | 5.25  | 119.63      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2822 | G    | O4'-C1'-N9  | 5.25  | 112.40      | 108.20   |
| 41  | BH    | 123  | ARG  | NE-CZ-NH2   | -5.25 | 117.67      | 120.30   |
| 45  | BL    | 116  | VAL  | CB-CA-C     | 5.25  | 121.39      | 111.40   |
| 1   | AA    | 94   | G    | C2-N3-C4    | -5.25 | 109.27      | 111.90   |
| 1   | AA    | 147  | G    | C3'-C2'-C1' | 5.25  | 105.70      | 101.50   |
| 1   | AA    | 453  | G    | N7-C8-N9    | -5.25 | 110.47      | 113.10   |
| 1   | AA    | 468  | A    | O4'-C1'-N9  | 5.25  | 112.40      | 108.20   |
| 1   | AA    | 560  | A    | C5'-C4'-C3' | -5.25 | 107.59      | 116.00   |
| 1   | AA    | 763  | G    | N9-C4-C5    | 5.25  | 107.50      | 105.40   |
| 1   | AA    | 1034 | G    | N1-C2-N2    | 5.25  | 120.93      | 116.20   |
| 1   | AA    | 1154 | G    | N9-C4-C5    | 5.25  | 107.50      | 105.40   |
| 1   | AA    | 1183 | U    | O4'-C1'-N1  | 5.25  | 112.40      | 108.20   |
| 1   | AA    | 1275 | A    | C5-N7-C8    | 5.25  | 106.53      | 103.90   |
| 35  | BB    | 887  | U    | O4'-C4'-C3' | -5.25 | 98.75       | 104.00   |
| 35  | BB    | 1361 | G    | N3-C4-N9    | 5.25  | 129.15      | 126.00   |
| 35  | BB    | 1681 | G    | C5'-C4'-C3' | -5.25 | 107.59      | 116.00   |
| 35  | BB    | 2223 | G    | C5-C6-O6    | -5.25 | 125.45      | 128.60   |
| 35  | BB    | 2286 | G    | C4-C5-C6    | 5.25  | 121.95      | 118.80   |
| 35  | BB    | 2525 | G    | C8-N9-C1'   | 5.25  | 133.83      | 127.00   |
| 35  | BB    | 2647 | U    | C4-C5-C6    | 5.25  | 122.85      | 119.70   |
| 35  | BB    | 2734 | A    | O4'-C1'-N9  | 5.25  | 112.40      | 108.20   |
| 35  | BB    | 2816 | G    | C8-N9-C4    | -5.25 | 104.30      | 106.40   |
| 43  | BJ    | 134  | ALA  | CB-CA-C     | -5.25 | 102.22      | 110.10   |
| 1   | AA    | 18   | C    | N3-C2-O2    | 5.25  | 125.58      | 121.90   |
| 1   | AA    | 56   | U    | N1-C2-N3    | -5.25 | 111.75      | 114.90   |
| 1   | AA    | 148  | G    | C5-N7-C8    | -5.25 | 101.67      | 104.30   |
| 1   | AA    | 155  | A    | C5-C6-N6    | -5.25 | 119.50      | 123.70   |
| 1   | AA    | 177  | G    | N3-C4-C5    | -5.25 | 125.97      | 128.60   |
| 1   | AA    | 215  | C    | C2-N3-C4    | -5.25 | 117.27      | 119.90   |
| 1   | AA    | 836  | G    | N3-C2-N2    | 5.25  | 123.58      | 119.90   |
| 1   | AA    | 860  | A    | C3'-C2'-C1' | -5.25 | 97.30       | 101.50   |
| 1   | AA    | 1056 | U    | C6-N1-C2    | 5.25  | 124.15      | 121.00   |
| 1   | AA    | 1240 | U    | C3'-C2'-C1' | 5.25  | 105.70      | 101.50   |
| 1   | AA    | 1522 | U    | C1'-O4'-C4' | -5.25 | 105.70      | 109.90   |
| 28  | B3    | 3    | GLN  | N-CA-CB     | 5.25  | 120.05      | 110.60   |
| 35  | BB    | 558  | U    | O4'-C1'-C2' | -5.25 | 100.55      | 105.80   |
| 35  | BB    | 1060 | U    | C2-N1-C1'   | 5.25  | 124.00      | 117.70   |
| 35  | BB    | 1098 | A    | C6-C5-N7    | -5.25 | 128.62      | 132.30   |
| 35  | BB    | 1398 | C    | OP1-P-OP2   | -5.25 | 111.72      | 119.60   |
| 35  | BB    | 1621 | U    | OP1-P-O3'   | 5.25  | 116.75      | 105.20   |
| 35  | BB    | 1799 | G    | N3-C2-N2    | 5.25  | 123.58      | 119.90   |
| 35  | BB    | 2385 | C    | C3'-C2'-C1' | 5.25  | 105.70      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2397 | G    | P-O3'-C3'   | -5.25 | 113.40      | 119.70   |
| 35  | BB    | 2461 | A    | C6-C5-N7    | -5.25 | 128.62      | 132.30   |
| 38  | BE    | 106  | LYS  | N-CA-C      | -5.25 | 96.82       | 111.00   |
| 1   | AA    | 380  | G    | C1'-O4'-C4' | -5.25 | 105.70      | 109.90   |
| 1   | AA    | 632  | U    | C6-N1-C2    | -5.25 | 117.85      | 121.00   |
| 1   | AA    | 935  | A    | N9-C4-C5    | 5.25  | 107.90      | 105.80   |
| 1   | AA    | 1444 | U    | N1-C2-O2    | 5.25  | 126.47      | 122.80   |
| 1   | AA    | 1504 | G    | C4-C5-N7    | 5.25  | 112.90      | 110.80   |
| 35  | BB    | 1665 | A    | N3-C4-N9    | 5.25  | 131.60      | 127.40   |
| 35  | BB    | 1911 | U    | N3-C2-O2    | 5.25  | 125.88      | 122.20   |
| 35  | BB    | 2382 | G    | O4'-C1'-N9  | 5.25  | 112.40      | 108.20   |
| 45  | BL    | 33   | ARG  | NE-CZ-NH1   | -5.25 | 117.67      | 120.30   |
| 45  | BL    | 127  | VAL  | CG1-CB-CG2  | 5.25  | 119.30      | 110.90   |
| 1   | AA    | 1155 | A    | C5-C6-N1    | -5.25 | 115.08      | 117.70   |
| 34  | BA    | 75   | G    | N1-C6-O6    | 5.25  | 123.05      | 119.90   |
| 35  | BB    | 649  | G    | N1-C2-N3    | -5.25 | 120.75      | 123.90   |
| 35  | BB    | 726  | G    | P-O3'-C3'   | 5.25  | 126.00      | 119.70   |
| 35  | BB    | 769  | U    | OP1-P-OP2   | -5.25 | 111.73      | 119.60   |
| 35  | BB    | 979  | A    | N9-C1'-C2'  | -5.25 | 106.23      | 112.00   |
| 35  | BB    | 1001 | A    | C5-C6-N6    | -5.25 | 119.50      | 123.70   |
| 35  | BB    | 1086 | A    | C5-N7-C8    | -5.25 | 101.28      | 103.90   |
| 1   | AA    | 486  | U    | N1-C2-N3    | 5.25  | 118.05      | 114.90   |
| 1   | AA    | 611  | C    | C6-N1-C2    | -5.25 | 118.20      | 120.30   |
| 1   | AA    | 763  | G    | C6-N1-C2    | -5.25 | 121.95      | 125.10   |
| 1   | AA    | 785  | G    | O4'-C1'-N9  | 5.25  | 112.40      | 108.20   |
| 1   | AA    | 1335 | U    | C6-N1-C1'   | -5.25 | 113.85      | 121.20   |
| 3   | AC    | 38   | VAL  | CG1-CB-CG2  | -5.25 | 102.50      | 110.90   |
| 34  | BA    | 107  | G    | N1-C6-O6    | 5.25  | 123.05      | 119.90   |
| 35  | BB    | 186  | G    | C4-C5-C6    | 5.25  | 121.95      | 118.80   |
| 35  | BB    | 303  | G    | N7-C8-N9    | -5.25 | 110.48      | 113.10   |
| 35  | BB    | 561  | G    | C5-C6-N1    | -5.25 | 108.88      | 111.50   |
| 35  | BB    | 584  | C    | N3-C4-C5    | -5.25 | 119.80      | 121.90   |
| 35  | BB    | 633  | A    | N9-C4-C5    | -5.25 | 103.70      | 105.80   |
| 35  | BB    | 654  | A    | N3-C4-C5    | -5.25 | 123.13      | 126.80   |
| 35  | BB    | 1063 | G    | C5-C6-O6    | -5.25 | 125.45      | 128.60   |
| 35  | BB    | 1337 | G    | O4'-C1'-N9  | 5.25  | 112.40      | 108.20   |
| 35  | BB    | 1373 | A    | C4-C5-C6    | 5.25  | 119.62      | 117.00   |
| 35  | BB    | 2243 | U    | N1-C2-O2    | -5.25 | 119.13      | 122.80   |
| 38  | BE    | 21   | ARG  | NE-CZ-NH2   | -5.25 | 117.68      | 120.30   |
| 54  | BU    | 70   | ALA  | N-CA-CB     | 5.25  | 117.44      | 110.10   |
| 1   | AA    | 123  | U    | N3-C4-C5    | -5.25 | 111.45      | 114.60   |
| 1   | AA    | 584  | G    | C6-N1-C2    | 5.25  | 128.25      | 125.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 977  | A    | OP2-P-O3'   | 5.25  | 116.74      | 105.20   |
| 1   | AA    | 1133 | G    | P-O3'-C3'   | 5.25  | 125.99      | 119.70   |
| 1   | AA    | 1249 | C    | C6-N1-C1'   | -5.25 | 114.51      | 120.80   |
| 35  | BB    | 1068 | G    | N1-C2-N3    | -5.25 | 120.75      | 123.90   |
| 35  | BB    | 1915 | U    | C1'-O4'-C4' | -5.25 | 105.70      | 109.90   |
| 35  | BB    | 1998 | A    | N9-C4-C5    | 5.25  | 107.90      | 105.80   |
| 35  | BB    | 2734 | A    | C5'-C4'-O4' | 5.25  | 115.39      | 109.10   |
| 1   | AA    | 579  | A    | N7-C8-N9    | 5.24  | 116.42      | 113.80   |
| 1   | AA    | 1012 | A    | P-O3'-C3'   | -5.24 | 113.41      | 119.70   |
| 1   | AA    | 1280 | A    | C5-C6-N1    | -5.24 | 115.08      | 117.70   |
| 17  | AQ    | 49   | ASN  | N-CA-C      | -5.24 | 96.84       | 111.00   |
| 22  | AV    | 17   | C    | N3-C4-C5    | -5.24 | 119.80      | 121.90   |
| 35  | BB    | 171  | U    | O4'-C1'-N1  | 5.24  | 112.39      | 108.20   |
| 35  | BB    | 321  | U    | C6-N1-C2    | -5.24 | 117.85      | 121.00   |
| 35  | BB    | 905  | A    | C5-C6-N6    | -5.24 | 119.50      | 123.70   |
| 35  | BB    | 1958 | C    | O4'-C1'-N1  | 5.24  | 112.39      | 108.20   |
| 35  | BB    | 2306 | C    | C4-C5-C6    | -5.24 | 114.78      | 117.40   |
| 35  | BB    | 2662 | A    | C5-N7-C8    | 5.24  | 106.52      | 103.90   |
| 35  | BB    | 2903 | U    | C2-N3-C4    | -5.24 | 123.85      | 127.00   |
| 38  | BE    | 101  | TYR  | CZ-CE2-CD2  | 5.24  | 124.52      | 119.80   |
| 54  | BU    | 16   | LYS  | N-CA-CB     | 5.24  | 120.04      | 110.60   |
| 1   | AA    | 34   | C    | C2-N3-C4    | 5.24  | 122.52      | 119.90   |
| 1   | AA    | 346  | G    | N3-C2-N2    | 5.24  | 123.57      | 119.90   |
| 15  | AO    | 68   | TYR  | CD1-CG-CD2  | 5.24  | 123.67      | 117.90   |
| 34  | BA    | 116  | G    | C6-C5-N7    | -5.24 | 127.25      | 130.40   |
| 35  | BB    | 772  | C    | N1-C2-N3    | -5.24 | 115.53      | 119.20   |
| 35  | BB    | 1064 | C    | C5'-C4'-O4' | 5.24  | 115.39      | 109.10   |
| 35  | BB    | 1693 | U    | C4-C5-C6    | 5.24  | 122.84      | 119.70   |
| 35  | BB    | 1761 | C    | P-O3'-C3'   | 5.24  | 125.99      | 119.70   |
| 35  | BB    | 2311 | A    | C5-C6-N1    | -5.24 | 115.08      | 117.70   |
| 35  | BB    | 2765 | A    | OP1-P-OP2   | -5.24 | 111.74      | 119.60   |
| 1   | AA    | 209  | U    | C3'-C2'-C1' | -5.24 | 97.31       | 101.50   |
| 1   | AA    | 812  | G    | OP2-P-O3'   | 5.24  | 116.73      | 105.20   |
| 1   | AA    | 1501 | C    | O4'-C1'-N1  | 5.24  | 112.39      | 108.20   |
| 6   | AF    | 44   | ARG  | NE-CZ-NH2   | -5.24 | 117.68      | 120.30   |
| 21  | AU    | 36   | PHE  | CB-CA-C     | -5.24 | 99.92       | 110.40   |
| 35  | BB    | 588  | U    | N1-C2-N3    | -5.24 | 111.76      | 114.90   |
| 35  | BB    | 645  | C    | C4'-C3'-C2' | -5.24 | 97.36       | 102.60   |
| 35  | BB    | 914  | G    | O4'-C1'-N9  | 5.24  | 112.39      | 108.20   |
| 35  | BB    | 2027 | G    | C5-C6-N1    | -5.24 | 108.88      | 111.50   |
| 35  | BB    | 2055 | C    | C6-N1-C2    | -5.24 | 118.20      | 120.30   |
| 35  | BB    | 2367 | G    | C6-C5-N7    | -5.24 | 127.25      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2513 | A    | C5'-C4'-C3' | 5.24  | 124.38      | 116.00   |
| 35  | BB    | 2569 | G    | N1-C2-N3    | -5.24 | 120.76      | 123.90   |
| 35  | BB    | 2609 | U    | P-O5'-C5'   | -5.24 | 112.52      | 120.90   |
| 35  | BB    | 2625 | G    | C8-N9-C4    | -5.24 | 104.30      | 106.40   |
| 35  | BB    | 2791 | G    | N1-C2-N2    | -5.24 | 111.48      | 116.20   |
| 1   | AA    | 270  | A    | C5-C6-N6    | -5.24 | 119.51      | 123.70   |
| 1   | AA    | 321  | A    | N3-C4-C5    | -5.24 | 123.13      | 126.80   |
| 1   | AA    | 327  | A    | C2-N3-C4    | 5.24  | 113.22      | 110.60   |
| 1   | AA    | 529  | G    | C4-C5-C6    | -5.24 | 115.66      | 118.80   |
| 1   | AA    | 824  | G    | C5-C6-O6    | -5.24 | 125.46      | 128.60   |
| 1   | AA    | 912  | C    | P-O3'-C3'   | 5.24  | 125.98      | 119.70   |
| 1   | AA    | 1150 | A    | N3-C4-C5    | -5.24 | 123.13      | 126.80   |
| 1   | AA    | 1177 | G    | C3'-C2'-C1' | 5.24  | 105.69      | 101.50   |
| 1   | AA    | 1317 | C    | C5-C6-N1    | 5.24  | 123.62      | 121.00   |
| 1   | AA    | 1398 | A    | N9-C4-C5    | 5.24  | 107.89      | 105.80   |
| 1   | AA    | 1497 | G    | C6-C5-N7    | -5.24 | 127.26      | 130.40   |
| 35  | BB    | 120  | U    | C6-N1-C2    | -5.24 | 117.86      | 121.00   |
| 35  | BB    | 239  | C    | C2-N3-C4    | 5.24  | 122.52      | 119.90   |
| 35  | BB    | 448  | U    | C5-C6-N1    | 5.24  | 125.32      | 122.70   |
| 35  | BB    | 469  | G    | C4-C5-C6    | 5.24  | 121.94      | 118.80   |
| 35  | BB    | 812  | C    | P-O3'-C3'   | -5.24 | 113.41      | 119.70   |
| 35  | BB    | 1111 | A    | C3'-C2'-C1' | -5.24 | 97.31       | 101.50   |
| 35  | BB    | 1197 | G    | C8-N9-C4    | 5.24  | 108.50      | 106.40   |
| 35  | BB    | 1454 | C    | C6-N1-C1'   | -5.24 | 114.51      | 120.80   |
| 35  | BB    | 1466 | U    | C6-N1-C2    | -5.24 | 117.86      | 121.00   |
| 35  | BB    | 1766 | G    | OP1-P-O3'   | 5.24  | 116.72      | 105.20   |
| 35  | BB    | 1987 | A    | C4'-C3'-C2' | -5.24 | 97.36       | 102.60   |
| 35  | BB    | 2653 | U    | C6-N1-C2    | 5.24  | 124.14      | 121.00   |
| 35  | BB    | 2713 | U    | OP2-P-O3'   | 5.24  | 116.72      | 105.20   |
| 43  | BJ    | 29   | ALA  | N-CA-CB     | 5.24  | 117.44      | 110.10   |
| 1   | AA    | 565  | U    | C5-C6-N1    | 5.24  | 125.32      | 122.70   |
| 1   | AA    | 912  | C    | C2-N1-C1'   | 5.24  | 124.56      | 118.80   |
| 1   | AA    | 1080 | A    | N3-C4-N9    | 5.24  | 131.59      | 127.40   |
| 35  | BB    | 667  | U    | C2-N3-C4    | -5.24 | 123.86      | 127.00   |
| 35  | BB    | 1600 | C    | N3-C4-N4    | 5.24  | 121.67      | 118.00   |
| 35  | BB    | 1619 | G    | C8-N9-C4    | -5.24 | 104.31      | 106.40   |
| 35  | BB    | 2404 | U    | C4'-C3'-C2' | 5.24  | 107.84      | 102.60   |
| 35  | BB    | 2535 | G    | N1-C2-N3    | -5.24 | 120.76      | 123.90   |
| 1   | AA    | 63   | C    | N1-C2-O2    | -5.24 | 115.76      | 118.90   |
| 1   | AA    | 163  | C    | C5-C4-N4    | -5.24 | 116.54      | 120.20   |
| 1   | AA    | 903  | G    | O4'-C1'-C2' | 5.24  | 112.31      | 107.60   |
| 1   | AA    | 1226 | C    | C3'-C2'-C1' | -5.24 | 97.31       | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | AV    | 56   | C    | N3-C4-C5    | -5.24 | 119.81      | 121.90   |
| 34  | BA    | 81   | G    | C4-C5-N7    | 5.24  | 112.89      | 110.80   |
| 35  | BB    | 477  | A    | P-O5'-C5'   | -5.24 | 112.52      | 120.90   |
| 35  | BB    | 662  | G    | O5'-P-OP2   | -5.24 | 100.99      | 105.70   |
| 35  | BB    | 866  | A    | C4-C5-C6    | 5.24  | 119.62      | 117.00   |
| 35  | BB    | 956  | G    | OP1-P-OP2   | -5.24 | 111.75      | 119.60   |
| 35  | BB    | 1124 | G    | OP1-P-OP2   | -5.24 | 111.75      | 119.60   |
| 35  | BB    | 1239 | G    | N1-C2-N3    | -5.24 | 120.76      | 123.90   |
| 35  | BB    | 1478 | G    | P-O3'-C3'   | 5.24  | 125.98      | 119.70   |
| 35  | BB    | 1478 | G    | C5-N7-C8    | 5.24  | 106.92      | 104.30   |
| 35  | BB    | 2487 | G    | N7-C8-N9    | -5.24 | 110.48      | 113.10   |
| 35  | BB    | 2532 | G    | C5-C6-N1    | -5.24 | 108.88      | 111.50   |
| 1   | AA    | 5    | U    | C3'-C2'-C1' | -5.23 | 97.31       | 101.50   |
| 1   | AA    | 671  | G    | N7-C8-N9    | 5.23  | 115.72      | 113.10   |
| 1   | AA    | 778  | G    | C2-N3-C4    | 5.23  | 114.52      | 111.90   |
| 1   | AA    | 809  | G    | N3-C2-N2    | -5.23 | 116.24      | 119.90   |
| 1   | AA    | 1480 | A    | C4'-C3'-C2' | -5.23 | 97.37       | 102.60   |
| 35  | BB    | 434  | U    | C5'-C4'-O4' | -5.23 | 102.82      | 109.10   |
| 35  | BB    | 878  | A    | C5'-C4'-C3' | 5.23  | 124.38      | 116.00   |
| 35  | BB    | 942  | G    | N3-C4-C5    | -5.23 | 125.98      | 128.60   |
| 35  | BB    | 2461 | A    | N1-C2-N3    | 5.23  | 131.92      | 129.30   |
| 1   | AA    | 35   | G    | N3-C4-C5    | 5.23  | 131.22      | 128.60   |
| 1   | AA    | 203  | G    | O4'-C4'-C3' | -5.23 | 98.77       | 104.00   |
| 1   | AA    | 239  | U    | N3-C4-C5    | -5.23 | 111.46      | 114.60   |
| 1   | AA    | 824  | G    | N1-C2-N2    | 5.23  | 120.91      | 116.20   |
| 1   | AA    | 918  | A    | N3-C4-C5    | -5.23 | 123.14      | 126.80   |
| 1   | AA    | 1063 | C    | N3-C4-C5    | -5.23 | 119.81      | 121.90   |
| 1   | AA    | 1360 | A    | N3-C4-N9    | 5.23  | 131.59      | 127.40   |
| 1   | AA    | 1532 | U    | N1-C2-O2    | -5.23 | 119.14      | 122.80   |
| 35  | BB    | 68   | G    | N7-C8-N9    | -5.23 | 110.48      | 113.10   |
| 35  | BB    | 70   | G    | C5-C6-N1    | -5.23 | 108.88      | 111.50   |
| 35  | BB    | 164  | C    | N3-C4-N4    | 5.23  | 121.66      | 118.00   |
| 35  | BB    | 237  | C    | C5-C4-N4    | -5.23 | 116.54      | 120.20   |
| 35  | BB    | 840  | C    | C6-N1-C1'   | -5.23 | 114.52      | 120.80   |
| 35  | BB    | 1723 | G    | N1-C2-N2    | -5.23 | 111.49      | 116.20   |
| 35  | BB    | 1846 | G    | C6-C5-N7    | -5.23 | 127.26      | 130.40   |
| 35  | BB    | 1978 | A    | O4'-C1'-N9  | 5.23  | 112.39      | 108.20   |
| 35  | BB    | 2037 | A    | C4'-C3'-C2' | -5.23 | 97.37       | 102.60   |
| 35  | BB    | 2289 | G    | C6-C5-N7    | -5.23 | 127.26      | 130.40   |
| 35  | BB    | 2322 | A    | C3'-C2'-C1' | 5.23  | 105.69      | 101.50   |
| 35  | BB    | 2902 | C    | C4-C5-C6    | 5.23  | 120.02      | 117.40   |
| 46  | BM    | 9    | PHE  | CB-CG-CD2   | 5.23  | 124.46      | 120.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 159  | G    | P-O5'-C5'   | -5.23 | 112.53      | 120.90   |
| 1   | AA    | 192  | A    | O4'-C1'-N9  | 5.23  | 112.38      | 108.20   |
| 1   | AA    | 531  | U    | N3-C4-O4    | 5.23  | 123.06      | 119.40   |
| 1   | AA    | 755  | G    | C5-C6-O6    | -5.23 | 125.46      | 128.60   |
| 1   | AA    | 998  | C    | P-O3'-C3'   | -5.23 | 113.42      | 119.70   |
| 1   | AA    | 1165 | U    | O4'-C1'-N1  | 5.23  | 112.38      | 108.20   |
| 1   | AA    | 1476 | A    | P-O5'-C5'   | 5.23  | 129.27      | 120.90   |
| 28  | B3    | 12   | ARG  | NE-CZ-NH1   | 5.23  | 122.92      | 120.30   |
| 34  | BA    | 73   | A    | N1-C2-N3    | -5.23 | 126.68      | 129.30   |
| 35  | BB    | 130  | C    | O4'-C1'-N1  | 5.23  | 112.38      | 108.20   |
| 35  | BB    | 1026 | G    | C5-C6-O6    | -5.23 | 125.46      | 128.60   |
| 35  | BB    | 1067 | A    | C6-N1-C2    | 5.23  | 121.74      | 118.60   |
| 35  | BB    | 1521 | G    | C8-N9-C4    | -5.23 | 104.31      | 106.40   |
| 35  | BB    | 1848 | A    | N3-C4-C5    | -5.23 | 123.14      | 126.80   |
| 35  | BB    | 1855 | U    | N3-C4-C5    | -5.23 | 111.46      | 114.60   |
| 35  | BB    | 2077 | A    | C4-C5-N7    | -5.23 | 108.08      | 110.70   |
| 35  | BB    | 2305 | U    | N3-C2-O2    | -5.23 | 118.54      | 122.20   |
| 35  | BB    | 2327 | A    | C4-N9-C1'   | 5.23  | 135.72      | 126.30   |
| 49  | BP    | 15   | ASP  | CB-CG-OD2   | -5.23 | 113.59      | 118.30   |
| 1   | AA    | 462  | G    | C5-N7-C8    | 5.23  | 106.92      | 104.30   |
| 24  | AZ    | 5    | ALA  | O-C-N       | -5.23 | 114.33      | 122.70   |
| 35  | BB    | 34   | U    | C5'-C4'-O4' | 5.23  | 115.38      | 109.10   |
| 35  | BB    | 1496 | A    | C5'-C4'-O4' | 5.23  | 115.37      | 109.10   |
| 35  | BB    | 1539 | U    | N3-C4-C5    | -5.23 | 111.46      | 114.60   |
| 35  | BB    | 1718 | G    | C1'-O4'-C4' | 5.23  | 114.08      | 109.90   |
| 46  | BM    | 54   | THR  | N-CA-CB     | 5.23  | 120.23      | 110.30   |
| 1   | AA    | 296  | U    | N1-C2-N3    | 5.23  | 118.04      | 114.90   |
| 1   | AA    | 754  | C    | C3'-C2'-C1' | 5.23  | 105.68      | 101.50   |
| 1   | AA    | 1215 | G    | N1-C2-N2    | 5.23  | 120.91      | 116.20   |
| 12  | AL    | 49   | ARG  | NE-CZ-NH1   | 5.23  | 122.91      | 120.30   |
| 35  | BB    | 34   | U    | N3-C4-C5    | -5.23 | 111.46      | 114.60   |
| 35  | BB    | 155  | A    | C6-C5-N7    | -5.23 | 128.64      | 132.30   |
| 35  | BB    | 417  | C    | N1-C2-O2    | 5.23  | 122.04      | 118.90   |
| 35  | BB    | 495  | G    | C8-N9-C4    | -5.23 | 104.31      | 106.40   |
| 35  | BB    | 794  | A    | P-O5'-C5'   | -5.23 | 112.54      | 120.90   |
| 35  | BB    | 937  | C    | C1'-O4'-C4' | -5.23 | 105.72      | 109.90   |
| 35  | BB    | 966  | G    | N1-C6-O6    | 5.23  | 123.04      | 119.90   |
| 35  | BB    | 983  | A    | P-O3'-C3'   | 5.23  | 125.97      | 119.70   |
| 35  | BB    | 1104 | C    | C5-C4-N4    | -5.23 | 116.54      | 120.20   |
| 35  | BB    | 1252 | G    | N3-C4-C5    | -5.23 | 125.99      | 128.60   |
| 35  | BB    | 1337 | G    | C3'-C2'-C1' | 5.23  | 105.68      | 101.50   |
| 35  | BB    | 1529 | G    | N3-C4-N9    | -5.23 | 122.86      | 126.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1627 | G    | C2-N3-C4    | 5.23  | 114.51      | 111.90   |
| 35  | BB    | 2371 | G    | C5-C6-N1    | -5.23 | 108.89      | 111.50   |
| 35  | BB    | 2646 | C    | C1'-O4'-C4' | -5.23 | 105.72      | 109.90   |
| 35  | BB    | 2844 | G    | C2-N3-C4    | -5.23 | 109.29      | 111.90   |
| 47  | BN    | 99   | LYS  | N-CA-CB     | 5.23  | 120.01      | 110.60   |
| 1   | AA    | 481  | G    | O4'-C1'-N9  | 5.23  | 112.38      | 108.20   |
| 1   | AA    | 1533 | C    | P-O3'-C3'   | 5.23  | 125.97      | 119.70   |
| 22  | AV    | 9    | A    | O4'-C1'-N9  | 5.23  | 112.38      | 108.20   |
| 35  | BB    | 528  | A    | C5-C6-N6    | -5.23 | 119.52      | 123.70   |
| 35  | BB    | 725  | G    | C5'-C4'-C3' | 5.23  | 124.36      | 116.00   |
| 35  | BB    | 942  | G    | N9-C4-C5    | 5.23  | 107.49      | 105.40   |
| 35  | BB    | 1025 | G    | C5-C6-O6    | 5.23  | 131.74      | 128.60   |
| 35  | BB    | 1497 | U    | C4-C5-C6    | 5.23  | 122.84      | 119.70   |
| 35  | BB    | 2634 | A    | O4'-C4'-C3' | -5.23 | 98.77       | 104.00   |
| 35  | BB    | 2642 | G    | P-O3'-C3'   | -5.23 | 113.43      | 119.70   |
| 35  | BB    | 2803 | G    | C5-C6-N1    | -5.23 | 108.89      | 111.50   |
| 45  | BL    | 106  | GLU  | N-CA-CB     | 5.23  | 120.01      | 110.60   |
| 53  | BT    | 66   | LYS  | O-C-N       | -5.23 | 114.34      | 122.70   |
| 1   | AA    | 122  | G    | C5-C6-N1    | -5.22 | 108.89      | 111.50   |
| 1   | AA    | 190  | A    | C8-N9-C4    | -5.22 | 103.71      | 105.80   |
| 1   | AA    | 332  | G    | N3-C4-N9    | 5.22  | 129.13      | 126.00   |
| 1   | AA    | 597  | G    | N1-C6-O6    | 5.22  | 123.03      | 119.90   |
| 1   | AA    | 1073 | U    | O4'-C1'-N1  | 5.22  | 112.38      | 108.20   |
| 1   | AA    | 1344 | C    | C5-C4-N4    | 5.22  | 123.86      | 120.20   |
| 3   | AC    | 146  | LYS  | N-CA-C      | -5.22 | 96.90       | 111.00   |
| 10  | AJ    | 65   | TYR  | CB-CG-CD1   | 5.22  | 124.14      | 121.00   |
| 35  | BB    | 25   | U    | N1-C2-N3    | 5.22  | 118.03      | 114.90   |
| 35  | BB    | 265  | A    | C5-C6-N1    | -5.22 | 115.09      | 117.70   |
| 35  | BB    | 419  | U    | N3-C4-O4    | 5.22  | 123.06      | 119.40   |
| 35  | BB    | 662  | G    | C6-N1-C2    | 5.22  | 128.23      | 125.10   |
| 35  | BB    | 669  | G    | N3-C2-N2    | 5.22  | 123.56      | 119.90   |
| 35  | BB    | 814  | C    | P-O3'-C3'   | -5.22 | 113.43      | 119.70   |
| 35  | BB    | 2303 | G    | O5'-C5'-C4' | -5.22 | 101.77      | 111.70   |
| 35  | BB    | 2322 | A    | C5-N7-C8    | 5.22  | 106.51      | 103.90   |
| 35  | BB    | 2383 | G    | C4-C5-C6    | 5.22  | 121.94      | 118.80   |
| 35  | BB    | 2434 | A    | C3'-C2'-C1' | 5.22  | 105.68      | 101.50   |
| 35  | BB    | 2696 | U    | C4'-C3'-C2' | -5.22 | 97.38       | 102.60   |
| 35  | BB    | 2840 | C    | C2-N1-C1'   | 5.22  | 124.55      | 118.80   |
| 38  | BE    | 35   | TYR  | CZ-CE2-CD2  | -5.22 | 115.10      | 119.80   |
| 47  | BN    | 67   | PHE  | CB-CG-CD2   | -5.22 | 117.14      | 120.80   |
| 1   | AA    | 100  | G    | N1-C2-N3    | -5.22 | 120.77      | 123.90   |
| 1   | AA    | 1182 | G    | N3-C2-N2    | 5.22  | 123.56      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 738  | G    | N9-C4-C5    | 5.22  | 107.49      | 105.40   |
| 35  | BB    | 874  | G    | C8-N9-C1'   | -5.22 | 120.21      | 127.00   |
| 35  | BB    | 1017 | G    | N1-C2-N3    | -5.22 | 120.77      | 123.90   |
| 35  | BB    | 1214 | A    | N7-C8-N9    | -5.22 | 111.19      | 113.80   |
| 35  | BB    | 1289 | C    | C6-N1-C2    | -5.22 | 118.21      | 120.30   |
| 35  | BB    | 1523 | U    | N1-C2-O2    | 5.22  | 126.46      | 122.80   |
| 35  | BB    | 1834 | U    | N3-C2-O2    | 5.22  | 125.86      | 122.20   |
| 35  | BB    | 1846 | G    | C2-N3-C4    | 5.22  | 114.51      | 111.90   |
| 35  | BB    | 2204 | G    | C6-N1-C2    | -5.22 | 121.97      | 125.10   |
| 35  | BB    | 2416 | C    | O4'-C1'-C2' | 5.22  | 112.30      | 107.60   |
| 38  | BE    | 164  | LEU  | N-CA-CB     | 5.22  | 120.84      | 110.40   |
| 51  | BR    | 77   | PHE  | CG-CD2-CE2  | -5.22 | 115.06      | 120.80   |
| 1   | AA    | 1213 | A    | P-O3'-C3'   | 5.22  | 125.97      | 119.70   |
| 35  | BB    | 1168 | G    | C4-N9-C1'   | -5.22 | 119.71      | 126.50   |
| 35  | BB    | 1578 | U    | O4'-C1'-C2' | -5.22 | 100.58      | 105.80   |
| 1   | AA    | 141  | G    | N3-C4-N9    | 5.22  | 129.13      | 126.00   |
| 1   | AA    | 745  | G    | C6-C5-N7    | -5.22 | 127.27      | 130.40   |
| 1   | AA    | 778  | G    | P-O3'-C3'   | 5.22  | 125.96      | 119.70   |
| 1   | AA    | 797  | C    | C2-N3-C4    | 5.22  | 122.51      | 119.90   |
| 23  | AX    | 12   | A    | N1-C6-N6    | -5.22 | 115.47      | 118.60   |
| 35  | BB    | 47   | C    | P-O5'-C5'   | 5.22  | 129.25      | 120.90   |
| 35  | BB    | 190  | A    | C8-N9-C4    | -5.22 | 103.71      | 105.80   |
| 35  | BB    | 517  | C    | C5-C6-N1    | -5.22 | 118.39      | 121.00   |
| 35  | BB    | 1666 | G    | C8-N9-C1'   | 5.22  | 133.79      | 127.00   |
| 35  | BB    | 1736 | U    | P-O5'-C5'   | 5.22  | 129.25      | 120.90   |
| 35  | BB    | 2102 | G    | C5-C6-N1    | -5.22 | 108.89      | 111.50   |
| 35  | BB    | 2276 | G    | C1'-O4'-C4' | -5.22 | 105.72      | 109.90   |
| 35  | BB    | 2663 | G    | C8-N9-C4    | -5.22 | 104.31      | 106.40   |
| 1   | AA    | 120  | A    | C8-N9-C4    | -5.22 | 103.71      | 105.80   |
| 1   | AA    | 890  | G    | C2-N3-C4    | 5.22  | 114.51      | 111.90   |
| 35  | BB    | 31   | C    | O4'-C1'-N1  | 5.22  | 112.37      | 108.20   |
| 35  | BB    | 282  | A    | C4-C5-C6    | 5.22  | 119.61      | 117.00   |
| 35  | BB    | 745  | G    | C8-N9-C4    | -5.22 | 104.31      | 106.40   |
| 35  | BB    | 761  | A    | C8-N9-C4    | -5.22 | 103.71      | 105.80   |
| 35  | BB    | 1580 | A    | N9-C1'-C2'  | -5.22 | 106.26      | 112.00   |
| 35  | BB    | 2764 | A    | OP2-P-O3'   | 5.22  | 116.68      | 105.20   |
| 1   | AA    | 269  | C    | C6-N1-C2    | 5.22  | 122.39      | 120.30   |
| 1   | AA    | 291  | U    | N1-C2-N3    | -5.22 | 111.77      | 114.90   |
| 1   | AA    | 505  | G    | N7-C8-N9    | 5.22  | 115.71      | 113.10   |
| 1   | AA    | 628  | G    | C5-C6-N1    | -5.22 | 108.89      | 111.50   |
| 1   | AA    | 972  | C    | OP2-P-O3'   | 5.22  | 116.68      | 105.20   |
| 22  | AV    | 10   | G    | O4'-C1'-N9  | 5.22  | 112.37      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 187  | G    | N3-C2-N2    | 5.22  | 123.55      | 119.90   |
| 35  | BB    | 851  | C    | N3-C4-C5    | -5.22 | 119.81      | 121.90   |
| 35  | BB    | 1087 | G    | O4'-C1'-N9  | 5.22  | 112.37      | 108.20   |
| 35  | BB    | 1541 | C    | C5-C6-N1    | 5.22  | 123.61      | 121.00   |
| 35  | BB    | 1998 | A    | P-O5'-C5'   | 5.22  | 129.25      | 120.90   |
| 35  | BB    | 2337 | G    | C4-N9-C1'   | 5.22  | 133.28      | 126.50   |
| 35  | BB    | 2536 | G    | C5-N7-C8    | -5.22 | 101.69      | 104.30   |
| 35  | BB    | 2641 | G    | P-O3'-C3'   | -5.22 | 113.44      | 119.70   |
| 35  | BB    | 2748 | A    | C4-N9-C1'   | -5.22 | 116.91      | 126.30   |
| 35  | BB    | 2803 | G    | C6-C5-N7    | -5.22 | 127.27      | 130.40   |
| 1   | AA    | 192  | A    | N9-C4-C5    | -5.21 | 103.71      | 105.80   |
| 1   | AA    | 371  | A    | N9-C4-C5    | 5.21  | 107.89      | 105.80   |
| 1   | AA    | 1398 | A    | C8-N9-C4    | -5.21 | 103.71      | 105.80   |
| 1   | AA    | 1487 | G    | C5-N7-C8    | 5.21  | 106.91      | 104.30   |
| 34  | BA    | 24   | G    | N7-C8-N9    | 5.21  | 115.71      | 113.10   |
| 35  | BB    | 137  | U    | C4-C5-C6    | 5.21  | 122.83      | 119.70   |
| 35  | BB    | 320  | A    | C6-N1-C2    | 5.21  | 121.73      | 118.60   |
| 35  | BB    | 715  | A    | C4'-C3'-C2' | -5.21 | 97.39       | 102.60   |
| 35  | BB    | 836  | G    | C5-C6-O6    | -5.21 | 125.47      | 128.60   |
| 35  | BB    | 1128 | G    | N7-C8-N9    | -5.21 | 110.49      | 113.10   |
| 35  | BB    | 1138 | G    | OP1-P-OP2   | -5.21 | 111.78      | 119.60   |
| 35  | BB    | 1156 | A    | P-O5'-C5'   | -5.21 | 112.56      | 120.90   |
| 35  | BB    | 1595 | C    | C6-N1-C1'   | 5.21  | 127.06      | 120.80   |
| 35  | BB    | 1667 | G    | C3'-C2'-C1' | -5.21 | 97.33       | 101.50   |
| 35  | BB    | 1953 | A    | P-O5'-C5'   | -5.21 | 112.56      | 120.90   |
| 35  | BB    | 2885 | G    | C4-C5-N7    | 5.21  | 112.89      | 110.80   |
| 56  | BY    | 76   | ARG  | NE-CZ-NH2   | -5.21 | 117.69      | 120.30   |
| 1   | AA    | 33   | A    | C6-N1-C2    | -5.21 | 115.47      | 118.60   |
| 1   | AA    | 1127 | G    | N1-C2-N3    | -5.21 | 120.77      | 123.90   |
| 22  | AV    | 6    | C    | N3-C4-C5    | -5.21 | 119.81      | 121.90   |
| 34  | BA    | 14   | U    | N1-C2-N3    | 5.21  | 118.03      | 114.90   |
| 35  | BB    | 869  | G    | O4'-C1'-N9  | 5.21  | 112.37      | 108.20   |
| 35  | BB    | 914  | G    | C5'-C4'-O4' | 5.21  | 115.36      | 109.10   |
| 35  | BB    | 2010 | G    | C4'-C3'-C2' | -5.21 | 97.39       | 102.60   |
| 35  | BB    | 2118 | U    | P-O3'-C3'   | -5.21 | 113.44      | 119.70   |
| 1   | AA    | 80   | A    | C1'-O4'-C4' | -5.21 | 105.73      | 109.90   |
| 1   | AA    | 532  | A    | C4-C5-N7    | -5.21 | 108.09      | 110.70   |
| 1   | AA    | 1387 | G    | N1-C6-O6    | 5.21  | 123.03      | 119.90   |
| 9   | AI    | 106  | ASP  | CB-CG-OD2   | -5.21 | 113.61      | 118.30   |
| 22  | AV    | 51   | A    | C5-C6-N1    | -5.21 | 115.09      | 117.70   |
| 22  | AV    | 61   | C    | N3-C4-C5    | -5.21 | 119.81      | 121.90   |
| 35  | BB    | 582  | A    | C2-N3-C4    | -5.21 | 108.00      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 950  | G    | N3-C2-N2    | 5.21  | 123.55      | 119.90   |
| 35  | BB    | 1567 | G    | P-O5'-C5'   | -5.21 | 112.56      | 120.90   |
| 35  | BB    | 2437 | G    | N3-C4-C5    | -5.21 | 125.99      | 128.60   |
| 35  | BB    | 2801 | G    | N7-C8-N9    | 5.21  | 115.71      | 113.10   |
| 1   | AA    | 1216 | A    | P-O3'-C3'   | -5.21 | 113.45      | 119.70   |
| 1   | AA    | 1267 | C    | N1-C2-O2    | 5.21  | 122.03      | 118.90   |
| 1   | AA    | 1415 | G    | C2-N3-C4    | 5.21  | 114.50      | 111.90   |
| 1   | AA    | 1462 | C    | P-O3'-C3'   | -5.21 | 113.45      | 119.70   |
| 10  | AJ    | 50   | THR  | N-CA-CB     | 5.21  | 120.20      | 110.30   |
| 35  | BB    | 945  | A    | N9-C1'-C2'  | -5.21 | 106.27      | 112.00   |
| 35  | BB    | 1162 | G    | N3-C4-N9    | -5.21 | 122.87      | 126.00   |
| 35  | BB    | 1296 | G    | N3-C4-C5    | -5.21 | 126.00      | 128.60   |
| 35  | BB    | 1600 | C    | N1-C2-N3    | -5.21 | 115.55      | 119.20   |
| 35  | BB    | 2065 | C    | P-O5'-C5'   | 5.21  | 129.24      | 120.90   |
| 38  | BE    | 68   | ALA  | N-CA-CB     | 5.21  | 117.39      | 110.10   |
| 1   | AA    | 24   | U    | N1-C2-N3    | 5.21  | 118.03      | 114.90   |
| 1   | AA    | 120  | A    | C2-N3-C4    | -5.21 | 108.00      | 110.60   |
| 1   | AA    | 592  | G    | C8-N9-C4    | -5.21 | 104.32      | 106.40   |
| 1   | AA    | 1254 | A    | C4-C5-C6    | 5.21  | 119.60      | 117.00   |
| 1   | AA    | 1334 | G    | N3-C2-N2    | 5.21  | 123.55      | 119.90   |
| 6   | AF    | 95   | ALA  | CB-CA-C     | -5.21 | 102.29      | 110.10   |
| 22  | AV    | 7    | G    | N7-C8-N9    | -5.21 | 110.50      | 113.10   |
| 23  | AX    | 19   | A    | P-O3'-C3'   | -5.21 | 113.45      | 119.70   |
| 35  | BB    | 128  | C    | C4'-C3'-C2' | -5.21 | 97.39       | 102.60   |
| 35  | BB    | 336  | C    | C1'-O4'-C4' | -5.21 | 105.73      | 109.90   |
| 35  | BB    | 413  | C    | C1'-O4'-C4' | 5.21  | 114.07      | 109.90   |
| 35  | BB    | 493  | G    | N9-C1'-C2'  | -5.21 | 106.27      | 112.00   |
| 35  | BB    | 499  | U    | C4-C5-C6    | 5.21  | 122.83      | 119.70   |
| 35  | BB    | 1224 | U    | O4'-C1'-N1  | 5.21  | 112.37      | 108.20   |
| 35  | BB    | 1227 | G    | C5-C6-N1    | -5.21 | 108.90      | 111.50   |
| 35  | BB    | 1307 | A    | N1-C2-N3    | 5.21  | 131.91      | 129.30   |
| 35  | BB    | 1578 | U    | C3'-C2'-C1' | 5.21  | 105.67      | 101.50   |
| 35  | BB    | 1826 | G    | N3-C4-C5    | -5.21 | 126.00      | 128.60   |
| 35  | BB    | 2279 | G    | O4'-C1'-N9  | 5.21  | 112.37      | 108.20   |
| 1   | AA    | 1456 | A    | C4-C5-C6    | 5.21  | 119.60      | 117.00   |
| 8   | AH    | 40   | LYS  | CD-CE-NZ    | -5.21 | 99.73       | 111.70   |
| 34  | BA    | 12   | C    | C4-C5-C6    | -5.21 | 114.80      | 117.40   |
| 35  | BB    | 375  | G    | N3-C2-N2    | 5.21  | 123.55      | 119.90   |
| 35  | BB    | 743  | A    | C5-C6-N6    | -5.21 | 119.53      | 123.70   |
| 35  | BB    | 800  | A    | C3'-C2'-C1' | -5.21 | 97.33       | 101.50   |
| 35  | BB    | 847  | U    | N3-C4-O4    | 5.21  | 123.05      | 119.40   |
| 35  | BB    | 1347 | A    | N3-C4-C5    | -5.21 | 123.16      | 126.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1921 | G    | C5-N7-C8    | 5.21  | 106.90      | 104.30   |
| 35  | BB    | 2518 | A    | C5-C6-N1    | -5.21 | 115.10      | 117.70   |
| 35  | BB    | 2562 | U    | O4'-C1'-N1  | 5.21  | 112.36      | 108.20   |
| 1   | AA    | 272  | C    | C5-C6-N1    | 5.21  | 123.60      | 121.00   |
| 1   | AA    | 526  | C    | C5-C6-N1    | 5.21  | 123.60      | 121.00   |
| 1   | AA    | 973  | G    | O5'-P-OP2   | -5.21 | 101.02      | 105.70   |
| 1   | AA    | 1048 | G    | C2-N3-C4    | -5.21 | 109.30      | 111.90   |
| 1   | AA    | 1373 | G    | C2-N3-C4    | 5.21  | 114.50      | 111.90   |
| 35  | BB    | 126  | A    | O4'-C1'-N9  | 5.21  | 112.36      | 108.20   |
| 35  | BB    | 1136 | G    | C4-C5-C6    | 5.21  | 121.92      | 118.80   |
| 35  | BB    | 1567 | G    | C3'-C2'-C1' | -5.21 | 97.34       | 101.50   |
| 1   | AA    | 431  | A    | C8-N9-C4    | -5.20 | 103.72      | 105.80   |
| 1   | AA    | 1195 | C    | N3-C2-O2    | -5.20 | 118.26      | 121.90   |
| 1   | AA    | 1277 | C    | C2-N1-C1'   | -5.20 | 113.08      | 118.80   |
| 1   | AA    | 1303 | C    | N3-C4-N4    | 5.20  | 121.64      | 118.00   |
| 1   | AA    | 1377 | A    | C5-C6-N6    | -5.20 | 119.54      | 123.70   |
| 1   | AA    | 1447 | A    | N3-C4-C5    | -5.20 | 123.16      | 126.80   |
| 35  | BB    | 17   | G    | P-O3'-C3'   | -5.20 | 113.46      | 119.70   |
| 35  | BB    | 30   | G    | OP1-P-OP2   | -5.20 | 111.79      | 119.60   |
| 35  | BB    | 537  | G    | C8-N9-C4    | -5.20 | 104.32      | 106.40   |
| 35  | BB    | 565  | C    | N3-C4-N4    | 5.20  | 121.64      | 118.00   |
| 35  | BB    | 639  | U    | N3-C4-O4    | 5.20  | 123.04      | 119.40   |
| 35  | BB    | 864  | G    | OP1-P-O3'   | 5.20  | 116.65      | 105.20   |
| 35  | BB    | 1009 | A    | C5-C6-N6    | -5.20 | 119.54      | 123.70   |
| 35  | BB    | 1454 | C    | C5-C4-N4    | -5.20 | 116.56      | 120.20   |
| 35  | BB    | 1569 | A    | N3-C4-C5    | -5.20 | 123.16      | 126.80   |
| 35  | BB    | 2114 | A    | C4-C5-N7    | -5.20 | 108.10      | 110.70   |
| 35  | BB    | 2345 | G    | N3-C2-N2    | 5.20  | 123.54      | 119.90   |
| 35  | BB    | 2472 | G    | C5-N7-C8    | -5.20 | 101.70      | 104.30   |
| 35  | BB    | 2540 | C    | C2-N1-C1'   | -5.20 | 113.08      | 118.80   |
| 40  | BG    | 69   | ALA  | N-CA-CB     | 5.20  | 117.39      | 110.10   |
| 51  | BR    | 13   | ARG  | O-C-N       | 5.20  | 131.02      | 122.70   |
| 1   | AA    | 172  | A    | C8-N9-C4    | -5.20 | 103.72      | 105.80   |
| 1   | AA    | 275  | G    | N1-C2-N3    | -5.20 | 120.78      | 123.90   |
| 1   | AA    | 383  | A    | N1-C6-N6    | 5.20  | 121.72      | 118.60   |
| 1   | AA    | 428  | G    | N1-C2-N2    | -5.20 | 111.52      | 116.20   |
| 1   | AA    | 1475 | G    | C4-C5-N7    | -5.20 | 108.72      | 110.80   |
| 35  | BB    | 119  | A    | C5'-C4'-O4' | 5.20  | 115.34      | 109.10   |
| 35  | BB    | 1025 | G    | C6-C5-N7    | -5.20 | 127.28      | 130.40   |
| 35  | BB    | 1823 | G    | OP1-P-OP2   | -5.20 | 111.80      | 119.60   |
| 35  | BB    | 2102 | G    | N7-C8-N9    | -5.20 | 110.50      | 113.10   |
| 35  | BB    | 2834 | G    | C2-N3-C4    | -5.20 | 109.30      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 16   | A    | C5-N7-C8    | 5.20  | 106.50      | 103.90   |
| 1   | AA    | 252  | U    | C5-C6-N1    | 5.20  | 125.30      | 122.70   |
| 1   | AA    | 342  | C    | N1-C2-O2    | -5.20 | 115.78      | 118.90   |
| 1   | AA    | 571  | U    | C2-N3-C4    | -5.20 | 123.88      | 127.00   |
| 1   | AA    | 1510 | C    | O5'-C5'-C4' | -5.20 | 101.82      | 111.70   |
| 5   | AE    | 64   | GLU  | OE1-CD-OE2  | 5.20  | 129.54      | 123.30   |
| 34  | BA    | 110  | C    | P-O5'-C5'   | 5.20  | 129.22      | 120.90   |
| 35  | BB    | 46   | G    | C6-C5-N7    | -5.20 | 127.28      | 130.40   |
| 35  | BB    | 590  | A    | OP1-P-OP2   | -5.20 | 111.80      | 119.60   |
| 35  | BB    | 1134 | A    | C6-C5-N7    | -5.20 | 128.66      | 132.30   |
| 35  | BB    | 1483 | G    | N9-C4-C5    | -5.20 | 103.32      | 105.40   |
| 35  | BB    | 1715 | G    | N3-C4-C5    | -5.20 | 126.00      | 128.60   |
| 35  | BB    | 2290 | G    | P-O3'-C3'   | -5.20 | 113.46      | 119.70   |
| 35  | BB    | 2625 | G    | C2-N3-C4    | 5.20  | 114.50      | 111.90   |
| 35  | BB    | 2814 | A    | OP2-P-O3'   | 5.20  | 116.64      | 105.20   |
| 1   | AA    | 341  | C    | C2-N1-C1'   | 5.20  | 124.52      | 118.80   |
| 1   | AA    | 681  | A    | P-O3'-C3'   | -5.20 | 113.46      | 119.70   |
| 17  | AQ    | 14   | ASP  | CB-CG-OD1   | -5.20 | 113.62      | 118.30   |
| 34  | BA    | 25   | U    | N3-C2-O2    | 5.20  | 125.84      | 122.20   |
| 34  | BA    | 59   | A    | N9-C4-C5    | 5.20  | 107.88      | 105.80   |
| 35  | BB    | 35   | G    | N1-C2-N3    | -5.20 | 120.78      | 123.90   |
| 35  | BB    | 457  | A    | N7-C8-N9    | -5.20 | 111.20      | 113.80   |
| 35  | BB    | 569  | U    | N1-C2-O2    | -5.20 | 119.16      | 122.80   |
| 35  | BB    | 718  | A    | N9-C1'-C2'  | -5.20 | 106.28      | 112.00   |
| 35  | BB    | 914  | G    | N1-C6-O6    | 5.20  | 123.02      | 119.90   |
| 35  | BB    | 949  | G    | O4'-C1'-N9  | 5.20  | 112.36      | 108.20   |
| 35  | BB    | 1867 | G    | C4-C5-N7    | 5.20  | 112.88      | 110.80   |
| 35  | BB    | 1981 | A    | N3-C4-C5    | -5.20 | 123.16      | 126.80   |
| 35  | BB    | 2046 | G    | C2-N3-C4    | 5.20  | 114.50      | 111.90   |
| 35  | BB    | 2364 | C    | C2-N1-C1'   | 5.20  | 124.52      | 118.80   |
| 35  | BB    | 2502 | G    | N3-C4-C5    | -5.20 | 126.00      | 128.60   |
| 35  | BB    | 2536 | G    | C5-C6-N1    | -5.20 | 108.90      | 111.50   |
| 1   | AA    | 726  | C    | C6-N1-C2    | -5.20 | 118.22      | 120.30   |
| 1   | AA    | 1184 | G    | C6-N1-C2    | 5.20  | 128.22      | 125.10   |
| 1   | AA    | 1409 | C    | P-O3'-C3'   | -5.20 | 113.46      | 119.70   |
| 34  | BA    | 73   | A    | O4'-C1'-N9  | 5.20  | 112.36      | 108.20   |
| 35  | BB    | 207  | A    | C5-N7-C8    | -5.20 | 101.30      | 103.90   |
| 35  | BB    | 384  | A    | C6-N1-C2    | 5.20  | 121.72      | 118.60   |
| 35  | BB    | 2282 | G    | N1-C6-O6    | 5.20  | 123.02      | 119.90   |
| 35  | BB    | 2570 | G    | C4'-C3'-C2' | -5.20 | 97.40       | 102.60   |
| 35  | BB    | 2632 | A    | C8-N9-C4    | -5.20 | 103.72      | 105.80   |
| 35  | BB    | 2769 | U    | N1-C2-O2    | -5.20 | 119.16      | 122.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | BU    | 2    | ALA  | N-CA-CB     | 5.20  | 117.38      | 110.10   |
| 1   | AA    | 85   | U    | O4'-C1'-N1  | 5.20  | 112.36      | 108.20   |
| 1   | AA    | 177  | G    | N1-C6-O6    | 5.20  | 123.02      | 119.90   |
| 1   | AA    | 888  | G    | C8-N9-C1'   | 5.20  | 133.75      | 127.00   |
| 1   | AA    | 1329 | A    | C5'-C4'-C3' | 5.20  | 124.31      | 116.00   |
| 1   | AA    | 1509 | C    | N1-C2-O2    | -5.20 | 115.78      | 118.90   |
| 22  | AV    | 24   | G    | O4'-C1'-N9  | 5.20  | 112.36      | 108.20   |
| 30  | B5    | 53   | ARG  | CG-CD-NE    | -5.20 | 100.89      | 111.80   |
| 34  | BA    | 100  | G    | N3-C2-N2    | 5.20  | 123.54      | 119.90   |
| 35  | BB    | 87   | U    | C1'-O4'-C4' | 5.20  | 114.06      | 109.90   |
| 35  | BB    | 433  | C    | N3-C4-C5    | -5.20 | 119.82      | 121.90   |
| 35  | BB    | 558  | U    | C2-N3-C4    | -5.20 | 123.88      | 127.00   |
| 35  | BB    | 945  | A    | C4-C5-N7    | -5.20 | 108.10      | 110.70   |
| 35  | BB    | 1423 | G    | O4'-C1'-N9  | 5.20  | 112.36      | 108.20   |
| 35  | BB    | 1615 | C    | C5-C4-N4    | -5.20 | 116.56      | 120.20   |
| 35  | BB    | 1752 | C    | C6-N1-C2    | -5.20 | 118.22      | 120.30   |
| 35  | BB    | 1857 | G    | C5-N7-C8    | -5.20 | 101.70      | 104.30   |
| 35  | BB    | 2141 | G    | C1'-O4'-C4' | 5.20  | 114.06      | 109.90   |
| 35  | BB    | 2437 | G    | C4-C5-N7    | -5.20 | 108.72      | 110.80   |
| 35  | BB    | 2512 | C    | N3-C4-C5    | -5.20 | 119.82      | 121.90   |
| 35  | BB    | 2722 | G    | C4-C5-C6    | 5.20  | 121.92      | 118.80   |
| 41  | BH    | 144  | VAL  | O-C-N       | 5.20  | 131.01      | 122.70   |
| 1   | AA    | 1038 | C    | C4-C5-C6    | -5.19 | 114.80      | 117.40   |
| 1   | AA    | 1283 | U    | C5-C4-O4    | -5.19 | 122.78      | 125.90   |
| 35  | BB    | 425  | G    | C2-N3-C4    | 5.19  | 114.50      | 111.90   |
| 35  | BB    | 741  | U    | C1'-O4'-C4' | 5.19  | 114.06      | 109.90   |
| 35  | BB    | 2409 | G    | N9-C4-C5    | -5.19 | 103.32      | 105.40   |
| 35  | BB    | 2776 | A    | C1'-O4'-C4' | -5.19 | 105.75      | 109.90   |
| 1   | AA    | 55   | A    | O4'-C1'-C2' | -5.19 | 100.61      | 105.80   |
| 1   | AA    | 619  | U    | C2-N3-C4    | 5.19  | 130.12      | 127.00   |
| 1   | AA    | 1206 | G    | N3-C4-C5    | 5.19  | 131.20      | 128.60   |
| 1   | AA    | 1276 | G    | C3'-C2'-C1' | 5.19  | 105.65      | 101.50   |
| 1   | AA    | 1323 | G    | O4'-C1'-N9  | 5.19  | 112.35      | 108.20   |
| 35  | BB    | 285  | G    | N3-C2-N2    | 5.19  | 123.53      | 119.90   |
| 35  | BB    | 413  | C    | N3-C4-C5    | -5.19 | 119.82      | 121.90   |
| 35  | BB    | 614  | A    | N9-C4-C5    | 5.19  | 107.88      | 105.80   |
| 35  | BB    | 862  | G    | C6-C5-N7    | -5.19 | 127.28      | 130.40   |
| 35  | BB    | 1128 | G    | N1-C2-N3    | -5.19 | 120.78      | 123.90   |
| 35  | BB    | 1184 | U    | C6-N1-C2    | 5.19  | 124.11      | 121.00   |
| 35  | BB    | 1340 | U    | C6-N1-C2    | -5.19 | 117.89      | 121.00   |
| 35  | BB    | 1597 | A    | C4'-C3'-C2' | -5.19 | 97.41       | 102.60   |
| 35  | BB    | 1658 | C    | O5'-C5'-C4' | -5.19 | 101.83      | 111.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1894 | C    | C4-C5-C6    | -5.19 | 114.80      | 117.40   |
| 35  | BB    | 1937 | A    | C5-C6-N6    | -5.19 | 119.55      | 123.70   |
| 35  | BB    | 2114 | A    | C5-C6-N1    | -5.19 | 115.10      | 117.70   |
| 35  | BB    | 2216 | G    | C6-C5-N7    | -5.19 | 127.28      | 130.40   |
| 35  | BB    | 2219 | U    | C5-C6-N1    | -5.19 | 120.10      | 122.70   |
| 35  | BB    | 2645 | G    | O4'-C1'-N9  | 5.19  | 112.35      | 108.20   |
| 35  | BB    | 2668 | G    | C4-C5-N7    | -5.19 | 108.72      | 110.80   |
| 35  | BB    | 2747 | G    | C5-C6-N1    | -5.19 | 108.90      | 111.50   |
| 35  | BB    | 2788 | C    | C4'-C3'-C2' | -5.19 | 97.41       | 102.60   |
| 1   | AA    | 146  | G    | N7-C8-N9    | -5.19 | 110.50      | 113.10   |
| 1   | AA    | 518  | C    | C1'-O4'-C4' | 5.19  | 114.05      | 109.90   |
| 1   | AA    | 596  | A    | N3-C4-C5    | -5.19 | 123.17      | 126.80   |
| 1   | AA    | 631  | C    | N1-C2-O2    | 5.19  | 122.02      | 118.90   |
| 1   | AA    | 633  | G    | C6-N1-C2    | 5.19  | 128.21      | 125.10   |
| 18  | AR    | 56   | ARG  | NH1-CZ-NH2  | -5.19 | 113.69      | 119.40   |
| 35  | BB    | 1326 | U    | C4-C5-C6    | 5.19  | 122.81      | 119.70   |
| 35  | BB    | 1949 | G    | N1-C6-O6    | 5.19  | 123.02      | 119.90   |
| 35  | BB    | 2031 | A    | C5'-C4'-O4' | 5.19  | 115.33      | 109.10   |
| 35  | BB    | 2164 | C    | N1-C2-O2    | 5.19  | 122.02      | 118.90   |
| 35  | BB    | 2369 | A    | O5'-C5'-C4' | -5.19 | 101.84      | 111.70   |
| 35  | BB    | 2395 | C    | C5-C4-N4    | -5.19 | 116.57      | 120.20   |
| 35  | BB    | 2507 | C    | C3'-C2'-C1' | 5.19  | 105.65      | 101.50   |
| 35  | BB    | 2758 | A    | N7-C8-N9    | -5.19 | 111.20      | 113.80   |
| 36  | BC    | 170  | TYR  | N-CA-CB     | 5.19  | 119.94      | 110.60   |
| 36  | BC    | 200  | MET  | CA-CB-CG    | 5.19  | 122.12      | 113.30   |
| 1   | AA    | 18   | C    | C5-C4-N4    | -5.19 | 116.57      | 120.20   |
| 1   | AA    | 347  | G    | C4-C5-C6    | 5.19  | 121.91      | 118.80   |
| 1   | AA    | 417  | G    | N3-C4-N9    | 5.19  | 129.11      | 126.00   |
| 1   | AA    | 521  | G    | C4'-C3'-C2' | -5.19 | 97.41       | 102.60   |
| 1   | AA    | 1180 | A    | C1'-O4'-C4' | -5.19 | 105.75      | 109.90   |
| 1   | AA    | 1238 | A    | C5-C6-N1    | -5.19 | 115.11      | 117.70   |
| 1   | AA    | 1369 | C    | N1-C2-O2    | 5.19  | 122.01      | 118.90   |
| 1   | AA    | 1489 | G    | C8-N9-C4    | 5.19  | 108.48      | 106.40   |
| 2   | AB    | 217  | ALA  | N-CA-CB     | -5.19 | 102.84      | 110.10   |
| 12  | AL    | 65   | TYR  | CD1-CE1-CZ  | 5.19  | 124.47      | 119.80   |
| 35  | BB    | 1360 | G    | C4'-C3'-C2' | -5.19 | 97.41       | 102.60   |
| 35  | BB    | 1726 | C    | C5-C4-N4    | -5.19 | 116.57      | 120.20   |
| 35  | BB    | 2003 | A    | N7-C8-N9    | -5.19 | 111.21      | 113.80   |
| 35  | BB    | 2628 | C    | N3-C4-N4    | 5.19  | 121.63      | 118.00   |
| 1   | AA    | 158  | G    | C2-N3-C4    | 5.19  | 114.49      | 111.90   |
| 1   | AA    | 195  | A    | N1-C6-N6    | 5.19  | 121.71      | 118.60   |
| 1   | AA    | 317  | U    | O4'-C1'-N1  | 5.19  | 112.35      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 325  | A    | C5'-C4'-C3' | 5.19  | 124.30      | 116.00   |
| 1   | AA    | 493  | A    | C4-C5-C6    | 5.19  | 119.59      | 117.00   |
| 1   | AA    | 1076 | U    | O5'-C5'-C4' | -5.19 | 101.84      | 111.70   |
| 1   | AA    | 1148 | U    | N3-C4-O4    | 5.19  | 123.03      | 119.40   |
| 1   | AA    | 1159 | U    | O4'-C1'-C2' | -5.19 | 100.61      | 105.80   |
| 1   | AA    | 1216 | A    | C5-N7-C8    | 5.19  | 106.49      | 103.90   |
| 1   | AA    | 1221 | G    | P-O3'-C3'   | -5.19 | 113.47      | 119.70   |
| 1   | AA    | 1251 | A    | C4-C5-N7    | 5.19  | 113.29      | 110.70   |
| 1   | AA    | 1507 | A    | C4-C5-C6    | 5.19  | 119.59      | 117.00   |
| 35  | BB    | 230  | G    | N1-C6-O6    | 5.19  | 123.01      | 119.90   |
| 35  | BB    | 744  | U    | C5-C6-N1    | 5.19  | 125.29      | 122.70   |
| 35  | BB    | 1681 | G    | P-O5'-C5'   | 5.19  | 129.20      | 120.90   |
| 35  | BB    | 1956 | U    | P-O3'-C3'   | -5.19 | 113.48      | 119.70   |
| 35  | BB    | 2669 | G    | C4'-C3'-C2' | -5.19 | 97.41       | 102.60   |
| 36  | BC    | 161  | VAL  | CG1-CB-CG2  | -5.19 | 102.60      | 110.90   |
| 1   | AA    | 121  | U    | C3'-C2'-C1' | 5.19  | 105.65      | 101.50   |
| 1   | AA    | 1486 | G    | C4-C5-N7    | -5.19 | 108.73      | 110.80   |
| 9   | AI    | 18   | VAL  | CA-CB-CG1   | 5.19  | 118.68      | 110.90   |
| 35  | BB    | 671  | C    | C6-N1-C2    | -5.19 | 118.23      | 120.30   |
| 35  | BB    | 672  | C    | C6-N1-C2    | 5.19  | 122.37      | 120.30   |
| 35  | BB    | 1085 | A    | OP2-P-O3'   | 5.19  | 116.61      | 105.20   |
| 35  | BB    | 1254 | A    | C4-C5-C6    | 5.19  | 119.59      | 117.00   |
| 35  | BB    | 1475 | G    | P-O3'-C3'   | 5.19  | 125.92      | 119.70   |
| 35  | BB    | 1530 | G    | N9-C4-C5    | -5.19 | 103.33      | 105.40   |
| 35  | BB    | 2314 | A    | O4'-C1'-N9  | 5.19  | 112.35      | 108.20   |
| 1   | AA    | 124  | C    | C6-N1-C2    | 5.18  | 122.37      | 120.30   |
| 1   | AA    | 608  | A    | C4-C5-C6    | 5.18  | 119.59      | 117.00   |
| 1   | AA    | 1017 | U    | C5-C4-O4    | -5.18 | 122.79      | 125.90   |
| 1   | AA    | 1082 | A    | O4'-C1'-N9  | 5.18  | 112.35      | 108.20   |
| 1   | AA    | 1288 | A    | C5-C6-N1    | -5.18 | 115.11      | 117.70   |
| 2   | AB    | 152  | ASP  | N-CA-CB     | 5.18  | 119.93      | 110.60   |
| 34  | BA    | 30   | C    | C5-C6-N1    | 5.18  | 123.59      | 121.00   |
| 35  | BB    | 55   | G    | O4'-C1'-N9  | 5.18  | 112.35      | 108.20   |
| 35  | BB    | 1660 | G    | N3-C4-N9    | 5.18  | 129.11      | 126.00   |
| 35  | BB    | 1896 | G    | O4'-C1'-C2' | 5.18  | 112.27      | 107.60   |
| 35  | BB    | 2072 | C    | C2-N3-C4    | 5.18  | 122.49      | 119.90   |
| 35  | BB    | 2836 | U    | C5-C4-O4    | -5.18 | 122.79      | 125.90   |
| 37  | BD    | 86   | GLU  | N-CA-C      | -5.18 | 97.00       | 111.00   |
| 55  | BW    | 57   | TYR  | CD1-CG-CD2  | 5.18  | 123.60      | 117.90   |
| 1   | AA    | 872  | A    | N1-C6-N6    | 5.18  | 121.71      | 118.60   |
| 1   | AA    | 881  | G    | C3'-C2'-C1' | 5.18  | 105.65      | 101.50   |
| 1   | AA    | 1034 | G    | C4-C5-C6    | 5.18  | 121.91      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 63   | A    | O4'-C1'-N9  | 5.18  | 112.35      | 108.20   |
| 35  | BB    | 579  | G    | P-O5'-C5'   | -5.18 | 112.61      | 120.90   |
| 35  | BB    | 773  | U    | C5'-C4'-C3' | -5.18 | 107.71      | 116.00   |
| 35  | BB    | 939  | G    | C4-C5-C6    | 5.18  | 121.91      | 118.80   |
| 35  | BB    | 944  | C    | C4-C5-C6    | -5.18 | 114.81      | 117.40   |
| 35  | BB    | 1042 | G    | N7-C8-N9    | -5.18 | 110.51      | 113.10   |
| 35  | BB    | 1245 | G    | N1-C6-O6    | 5.18  | 123.01      | 119.90   |
| 35  | BB    | 1888 | G    | C8-N9-C4    | 5.18  | 108.47      | 106.40   |
| 35  | BB    | 1948 | G    | N3-C2-N2    | -5.18 | 116.27      | 119.90   |
| 1   | AA    | 115  | G    | P-O5'-C5'   | -5.18 | 112.61      | 120.90   |
| 1   | AA    | 220  | G    | N1-C2-N2    | -5.18 | 111.54      | 116.20   |
| 1   | AA    | 957  | U    | C4-C5-C6    | -5.18 | 116.59      | 119.70   |
| 34  | BA    | 100  | G    | C6-C5-N7    | -5.18 | 127.29      | 130.40   |
| 35  | BB    | 424  | G    | P-O5'-C5'   | 5.18  | 129.19      | 120.90   |
| 35  | BB    | 1548 | A    | C8-N9-C4    | 5.18  | 107.87      | 105.80   |
| 35  | BB    | 1761 | C    | C4'-C3'-C2' | -5.18 | 97.42       | 102.60   |
| 35  | BB    | 2446 | G    | N1-C2-N2    | -5.18 | 111.54      | 116.20   |
| 35  | BB    | 2503 | A    | O5'-C5'-C4' | -5.18 | 101.86      | 111.70   |
| 39  | BF    | 137  | PHE  | CB-CA-C     | -5.18 | 100.04      | 110.40   |
| 1   | AA    | 178  | C    | C5-C4-N4    | 5.18  | 123.83      | 120.20   |
| 1   | AA    | 265  | G    | N7-C8-N9    | -5.18 | 110.51      | 113.10   |
| 1   | AA    | 283  | U    | C4-C5-C6    | -5.18 | 116.59      | 119.70   |
| 1   | AA    | 296  | U    | C6-N1-C2    | -5.18 | 117.89      | 121.00   |
| 1   | AA    | 384  | G    | C4-C5-N7    | 5.18  | 112.87      | 110.80   |
| 1   | AA    | 553  | A    | C6-C5-N7    | -5.18 | 128.67      | 132.30   |
| 1   | AA    | 1196 | A    | P-O3'-C3'   | -5.18 | 113.48      | 119.70   |
| 1   | AA    | 1431 | A    | O4'-C1'-N9  | 5.18  | 112.34      | 108.20   |
| 7   | AG    | 118  | ARG  | NE-CZ-NH2   | -5.18 | 117.71      | 120.30   |
| 20  | AT    | 10   | ALA  | CB-CA-C     | -5.18 | 102.33      | 110.10   |
| 34  | BA    | 28   | C    | O4'-C1'-N1  | 5.18  | 112.34      | 108.20   |
| 34  | BA    | 98   | G    | C5-N7-C8    | -5.18 | 101.71      | 104.30   |
| 34  | BA    | 110  | C    | C5-C6-N1    | 5.18  | 123.59      | 121.00   |
| 35  | BB    | 879  | G    | P-O3'-C3'   | -5.18 | 113.48      | 119.70   |
| 35  | BB    | 1093 | G    | O4'-C1'-N9  | 5.18  | 112.34      | 108.20   |
| 35  | BB    | 1127 | A    | O4'-C1'-N9  | 5.18  | 112.34      | 108.20   |
| 35  | BB    | 1202 | G    | C4'-C3'-C2' | -5.18 | 97.42       | 102.60   |
| 35  | BB    | 1267 | U    | C1'-O4'-C4' | 5.18  | 114.04      | 109.90   |
| 35  | BB    | 1629 | U    | C4-C5-C6    | -5.18 | 116.59      | 119.70   |
| 35  | BB    | 1896 | G    | C5-C6-O6    | -5.18 | 125.49      | 128.60   |
| 35  | BB    | 2418 | A    | N9-C4-C5    | 5.18  | 107.87      | 105.80   |
| 1   | AA    | 433  | G    | C5-C6-O6    | -5.18 | 125.49      | 128.60   |
| 1   | AA    | 1212 | U    | C6-N1-C1'   | -5.18 | 113.95      | 121.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 837  | C    | C1'-O4'-C4' | 5.18  | 114.04      | 109.90   |
| 35  | BB    | 891  | G    | P-O3'-C3'   | 5.18  | 125.91      | 119.70   |
| 35  | BB    | 1272 | A    | C5-C6-N1    | -5.18 | 115.11      | 117.70   |
| 35  | BB    | 2616 | C    | C4'-C3'-C2' | -5.18 | 97.42       | 102.60   |
| 36  | BC    | 16   | VAL  | N-CA-C      | -5.18 | 97.02       | 111.00   |
| 36  | BC    | 269  | ARG  | N-CA-CB     | 5.18  | 119.92      | 110.60   |
| 41  | BH    | 86   | ASP  | CB-CG-OD2   | -5.18 | 113.64      | 118.30   |
| 1   | AA    | 9    | G    | N7-C8-N9    | -5.18 | 110.51      | 113.10   |
| 1   | AA    | 145  | G    | C2-N3-C4    | 5.18  | 114.49      | 111.90   |
| 1   | AA    | 215  | C    | N3-C2-O2    | -5.18 | 118.28      | 121.90   |
| 1   | AA    | 257  | G    | N1-C2-N2    | -5.18 | 111.54      | 116.20   |
| 1   | AA    | 428  | G    | N7-C8-N9    | 5.18  | 115.69      | 113.10   |
| 1   | AA    | 648  | A    | C1'-O4'-C4' | 5.18  | 114.04      | 109.90   |
| 1   | AA    | 955  | U    | N3-C4-C5    | -5.18 | 111.49      | 114.60   |
| 1   | AA    | 1447 | A    | C6-N1-C2    | 5.18  | 121.71      | 118.60   |
| 35  | BB    | 216  | A    | N7-C8-N9    | 5.18  | 116.39      | 113.80   |
| 35  | BB    | 343  | C    | C2-N3-C4    | 5.18  | 122.49      | 119.90   |
| 35  | BB    | 359  | G    | C6-C5-N7    | -5.18 | 127.29      | 130.40   |
| 35  | BB    | 897  | C    | N1-C2-N3    | -5.18 | 115.58      | 119.20   |
| 35  | BB    | 1742 | U    | C6-N1-C2    | 5.18  | 124.11      | 121.00   |
| 35  | BB    | 1758 | U    | N3-C4-O4    | 5.18  | 123.02      | 119.40   |
| 35  | BB    | 2566 | A    | C5-C6-N1    | -5.18 | 115.11      | 117.70   |
| 35  | BB    | 2743 | U    | C2-N1-C1'   | 5.18  | 123.91      | 117.70   |
| 48  | BO    | 93   | ASP  | CB-CG-OD2   | 5.18  | 122.96      | 118.30   |
| 1   | AA    | 501  | C    | P-O3'-C3'   | -5.17 | 113.49      | 119.70   |
| 1   | AA    | 1314 | C    | C4'-C3'-C2' | -5.17 | 97.43       | 102.60   |
| 1   | AA    | 1492 | A    | C4-C5-N7    | -5.17 | 108.11      | 110.70   |
| 35  | BB    | 168  | G    | C8-N9-C4    | -5.17 | 104.33      | 106.40   |
| 35  | BB    | 658  | U    | C4-C5-C6    | -5.17 | 116.59      | 119.70   |
| 35  | BB    | 873  | C    | C6-N1-C2    | 5.17  | 122.37      | 120.30   |
| 35  | BB    | 962  | G    | C3'-C2'-C1' | 5.17  | 105.64      | 101.50   |
| 35  | BB    | 1593 | A    | C6-C5-N7    | 5.17  | 135.92      | 132.30   |
| 35  | BB    | 2540 | C    | C5-C4-N4    | -5.17 | 116.58      | 120.20   |
| 35  | BB    | 2886 | A    | C3'-C2'-C1' | -5.17 | 97.36       | 101.50   |
| 1   | AA    | 645  | G    | C4'-C3'-C2' | -5.17 | 97.43       | 102.60   |
| 13  | AM    | 50   | GLY  | N-CA-C      | -5.17 | 100.17      | 113.10   |
| 35  | BB    | 59   | U    | N1-C2-N3    | -5.17 | 111.80      | 114.90   |
| 35  | BB    | 141  | G    | C1'-O4'-C4' | -5.17 | 105.76      | 109.90   |
| 35  | BB    | 216  | A    | C6-C5-N7    | -5.17 | 128.68      | 132.30   |
| 35  | BB    | 867  | C    | N3-C4-C5    | -5.17 | 119.83      | 121.90   |
| 35  | BB    | 944  | C    | C5'-C4'-C3' | -5.17 | 107.72      | 116.00   |
| 35  | BB    | 2110 | G    | C4-C5-C6    | -5.17 | 115.70      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2138 | G    | O5'-P-OP2   | 5.17  | 116.91      | 110.70   |
| 35  | BB    | 2141 | G    | C6-C5-N7    | -5.17 | 127.30      | 130.40   |
| 35  | BB    | 2216 | G    | C2-N3-C4    | 5.17  | 114.49      | 111.90   |
| 35  | BB    | 2298 | A    | OP1-P-OP2   | -5.17 | 111.84      | 119.60   |
| 35  | BB    | 2378 | A    | OP1-P-OP2   | -5.17 | 111.84      | 119.60   |
| 37  | BD    | 121  | THR  | CA-CB-CG2   | -5.17 | 105.16      | 112.40   |
| 1   | AA    | 37   | U    | N1-C1'-C2'  | -5.17 | 106.31      | 112.00   |
| 1   | AA    | 147  | G    | O4'-C1'-N9  | 5.17  | 112.34      | 108.20   |
| 1   | AA    | 359  | G    | N1-C2-N2    | 5.17  | 120.85      | 116.20   |
| 1   | AA    | 456  | A    | N9-C4-C5    | 5.17  | 107.87      | 105.80   |
| 1   | AA    | 949  | A    | C4'-C3'-C2' | -5.17 | 97.43       | 102.60   |
| 1   | AA    | 1033 | G    | OP1-P-OP2   | -5.17 | 111.84      | 119.60   |
| 1   | AA    | 1067 | A    | P-O3'-C3'   | 5.17  | 125.91      | 119.70   |
| 1   | AA    | 1271 | A    | P-O3'-C3'   | -5.17 | 113.50      | 119.70   |
| 1   | AA    | 1295 | U    | N1-C2-O2    | -5.17 | 119.18      | 122.80   |
| 9   | AI    | 129  | ARG  | NE-CZ-NH1   | 5.17  | 122.89      | 120.30   |
| 22  | AV    | 7    | G    | C2-N3-C4    | 5.17  | 114.49      | 111.90   |
| 35  | BB    | 549  | G    | C6-N1-C2    | 5.17  | 128.20      | 125.10   |
| 35  | BB    | 876  | C    | N3-C4-C5    | -5.17 | 119.83      | 121.90   |
| 35  | BB    | 958  | U    | C1'-O4'-C4' | -5.17 | 105.76      | 109.90   |
| 35  | BB    | 1099 | G    | OP1-P-OP2   | -5.17 | 111.84      | 119.60   |
| 35  | BB    | 1214 | A    | C6-N1-C2    | 5.17  | 121.70      | 118.60   |
| 35  | BB    | 1304 | A    | C2-N3-C4    | -5.17 | 108.01      | 110.60   |
| 35  | BB    | 1473 | G    | C6-N1-C2    | -5.17 | 122.00      | 125.10   |
| 35  | BB    | 1745 | A    | N7-C8-N9    | 5.17  | 116.39      | 113.80   |
| 35  | BB    | 1792 | G    | C5-N7-C8    | 5.17  | 106.89      | 104.30   |
| 35  | BB    | 2574 | G    | P-O3'-C3'   | 5.17  | 125.91      | 119.70   |
| 35  | BB    | 2664 | G    | C4-C5-N7    | 5.17  | 112.87      | 110.80   |
| 46  | BM    | 92   | TRP  | CD1-CG-CD2  | 5.17  | 110.44      | 106.30   |
| 1   | AA    | 206  | C    | C4-C5-C6    | 5.17  | 119.98      | 117.40   |
| 1   | AA    | 1197 | A    | P-O5'-C5'   | 5.17  | 129.17      | 120.90   |
| 11  | AK    | 28   | ASN  | O-C-N       | -5.17 | 114.43      | 122.70   |
| 35  | BB    | 1444 | G    | N1-C2-N2    | -5.17 | 111.55      | 116.20   |
| 35  | BB    | 1818 | U    | N3-C4-O4    | 5.17  | 123.02      | 119.40   |
| 35  | BB    | 1846 | G    | C1'-O4'-C4' | -5.17 | 105.76      | 109.90   |
| 35  | BB    | 2153 | C    | N3-C4-N4    | 5.17  | 121.62      | 118.00   |
| 1   | AA    | 16   | A    | C5-C6-N6    | -5.17 | 119.57      | 123.70   |
| 1   | AA    | 90   | C    | C4-C5-C6    | 5.17  | 119.98      | 117.40   |
| 1   | AA    | 380  | G    | C4'-C3'-C2' | -5.17 | 97.43       | 102.60   |
| 1   | AA    | 622  | A    | C8-N9-C4    | -5.17 | 103.73      | 105.80   |
| 1   | AA    | 1202 | U    | O4'-C1'-N1  | 5.17  | 112.33      | 108.20   |
| 1   | AA    | 1348 | U    | C1'-O4'-C4' | 5.17  | 114.03      | 109.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | BA    | 64   | G    | N3-C4-C5    | -5.17 | 126.02      | 128.60   |
| 35  | BB    | 500  | G    | N1-C2-N2    | -5.17 | 111.55      | 116.20   |
| 35  | BB    | 668  | A    | C5-C6-N1    | -5.17 | 115.12      | 117.70   |
| 35  | BB    | 837  | C    | C6-N1-C1'   | -5.17 | 114.60      | 120.80   |
| 35  | BB    | 1538 | G    | N1-C2-N3    | -5.17 | 120.80      | 123.90   |
| 35  | BB    | 1578 | U    | O4'-C1'-N1  | 5.17  | 112.33      | 108.20   |
| 35  | BB    | 1840 | G    | C8-N9-C4    | 5.17  | 108.47      | 106.40   |
| 35  | BB    | 2751 | G    | C8-N9-C1'   | -5.17 | 120.28      | 127.00   |
| 1   | AA    | 146  | G    | O4'-C1'-C2' | -5.17 | 100.63      | 105.80   |
| 1   | AA    | 399  | G    | C6-N1-C2    | -5.17 | 122.00      | 125.10   |
| 1   | AA    | 417  | G    | N9-C4-C5    | -5.17 | 103.33      | 105.40   |
| 1   | AA    | 456  | A    | C4-C5-N7    | -5.17 | 108.12      | 110.70   |
| 1   | AA    | 640  | A    | N9-C4-C5    | 5.17  | 107.87      | 105.80   |
| 1   | AA    | 1011 | C    | C4'-C3'-C2' | 5.17  | 107.77      | 102.60   |
| 1   | AA    | 1338 | G    | C5-N7-C8    | 5.17  | 106.88      | 104.30   |
| 15  | AO    | 38   | LEU  | N-CA-CB     | 5.17  | 120.73      | 110.40   |
| 20  | AT    | 77   | ASN  | CB-CA-C     | -5.17 | 100.07      | 110.40   |
| 22  | AV    | 38   | U    | N3-C2-O2    | 5.17  | 125.82      | 122.20   |
| 31  | B6    | 26   | ASN  | C-N-CA      | 5.17  | 133.15      | 122.30   |
| 34  | BA    | 16   | G    | C4-C5-N7    | 5.17  | 112.87      | 110.80   |
| 35  | BB    | 7    | G    | N1-C6-O6    | 5.17  | 123.00      | 119.90   |
| 35  | BB    | 294  | A    | C6-N1-C2    | -5.17 | 115.50      | 118.60   |
| 35  | BB    | 487  | C    | C3'-C2'-C1' | 5.17  | 105.63      | 101.50   |
| 35  | BB    | 852  | U    | N1-C2-N3    | -5.17 | 111.80      | 114.90   |
| 35  | BB    | 908  | C    | OP1-P-OP2   | -5.17 | 111.85      | 119.60   |
| 35  | BB    | 1673 | G    | OP2-P-O3'   | 5.17  | 116.57      | 105.20   |
| 35  | BB    | 1721 | G    | C6-C5-N7    | -5.17 | 127.30      | 130.40   |
| 35  | BB    | 2003 | A    | C2-N3-C4    | -5.17 | 108.02      | 110.60   |
| 35  | BB    | 2190 | G    | C8-N9-C4    | 5.17  | 108.47      | 106.40   |
| 35  | BB    | 2378 | A    | C6-C5-N7    | -5.17 | 128.68      | 132.30   |
| 35  | BB    | 2704 | C    | O5'-P-OP1   | 5.17  | 116.90      | 110.70   |
| 51  | BR    | 42   | ALA  | CB-CA-C     | -5.17 | 102.35      | 110.10   |
| 1   | AA    | 169  | C    | O4'-C4'-C3' | -5.17 | 98.83       | 104.00   |
| 1   | AA    | 629  | A    | C6-N1-C2    | -5.17 | 115.50      | 118.60   |
| 1   | AA    | 1018 | G    | P-O3'-C3'   | -5.17 | 113.50      | 119.70   |
| 1   | AA    | 1023 | U    | C5'-C4'-C3' | 5.17  | 124.26      | 116.00   |
| 1   | AA    | 1527 | U    | N3-C4-C5    | 5.17  | 117.70      | 114.60   |
| 35  | BB    | 89   | A    | C4-C5-N7    | -5.17 | 108.12      | 110.70   |
| 35  | BB    | 412  | A    | C4-C5-N7    | -5.17 | 108.12      | 110.70   |
| 35  | BB    | 641  | U    | OP1-P-OP2   | -5.17 | 111.85      | 119.60   |
| 35  | BB    | 1530 | G    | N3-C4-N9    | 5.17  | 129.10      | 126.00   |
| 35  | BB    | 1909 | C    | P-O3'-C3'   | -5.17 | 113.50      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 43  | BJ    | 44   | TYR  | CZ-CE2-CD2  | -5.17 | 115.15      | 119.80   |
| 44  | BK    | 9    | ASN  | O-C-N       | -5.17 | 114.44      | 122.70   |
| 1   | AA    | 66   | A    | C6-C5-N7    | -5.16 | 128.69      | 132.30   |
| 1   | AA    | 131  | A    | P-O5'-C5'   | -5.16 | 112.64      | 120.90   |
| 1   | AA    | 402  | G    | N9-C4-C5    | 5.16  | 107.47      | 105.40   |
| 1   | AA    | 421  | U    | C4-C5-C6    | 5.16  | 122.80      | 119.70   |
| 1   | AA    | 563  | A    | C2-N3-C4    | 5.16  | 113.18      | 110.60   |
| 1   | AA    | 884  | U    | C6-N1-C2    | 5.16  | 124.10      | 121.00   |
| 1   | AA    | 1302 | C    | C5-C4-N4    | -5.16 | 116.59      | 120.20   |
| 22  | AV    | 21   | A    | C5-C6-N1    | -5.16 | 115.12      | 117.70   |
| 22  | AV    | 56   | C    | N3-C4-N4    | 5.16  | 121.61      | 118.00   |
| 35  | BB    | 336  | C    | P-O5'-C5'   | -5.16 | 112.64      | 120.90   |
| 35  | BB    | 2378 | A    | O4'-C1'-N9  | 5.16  | 112.33      | 108.20   |
| 35  | BB    | 2426 | A    | N1-C2-N3    | 5.16  | 131.88      | 129.30   |
| 35  | BB    | 2797 | U    | O4'-C4'-C3' | -5.16 | 98.84       | 104.00   |
| 35  | BB    | 2798 | U    | N1-C2-O2    | -5.16 | 119.19      | 122.80   |
| 35  | BB    | 2887 | A    | N1-C6-N6    | 5.16  | 121.70      | 118.60   |
| 54  | BU    | 2    | ALA  | N-CA-C      | -5.16 | 97.06       | 111.00   |
| 1   | AA    | 1073 | U    | C5-C4-O4    | -5.16 | 122.80      | 125.90   |
| 1   | AA    | 1431 | A    | O4'-C1'-C2' | 5.16  | 112.25      | 107.60   |
| 34  | BA    | 78   | A    | C8-N9-C4    | 5.16  | 107.86      | 105.80   |
| 35  | BB    | 518  | G    | N3-C2-N2    | 5.16  | 123.51      | 119.90   |
| 35  | BB    | 1026 | G    | C4'-C3'-C2' | -5.16 | 97.44       | 102.60   |
| 35  | BB    | 1076 | C    | C5-C6-N1    | -5.16 | 118.42      | 121.00   |
| 35  | BB    | 1325 | U    | C2-N1-C1'   | 5.16  | 123.89      | 117.70   |
| 35  | BB    | 1416 | G    | C5'-C4'-O4' | 5.16  | 115.30      | 109.10   |
| 35  | BB    | 2430 | A    | C5-N7-C8    | 5.16  | 106.48      | 103.90   |
| 35  | BB    | 2481 | G    | C2-N3-C4    | 5.16  | 114.48      | 111.90   |
| 1   | AA    | 646  | G    | P-O3'-C3'   | -5.16 | 113.51      | 119.70   |
| 34  | BA    | 8    | C    | C2-N1-C1'   | 5.16  | 124.48      | 118.80   |
| 34  | BA    | 41   | G    | C8-N9-C4    | -5.16 | 104.34      | 106.40   |
| 35  | BB    | 181  | A    | C4-C5-C6    | 5.16  | 119.58      | 117.00   |
| 35  | BB    | 263  | G    | N3-C4-C5    | -5.16 | 126.02      | 128.60   |
| 35  | BB    | 684  | G    | C5-C6-O6    | -5.16 | 125.50      | 128.60   |
| 35  | BB    | 742  | A    | C4-C5-C6    | 5.16  | 119.58      | 117.00   |
| 35  | BB    | 1978 | A    | N7-C8-N9    | -5.16 | 111.22      | 113.80   |
| 35  | BB    | 2019 | A    | C8-N9-C4    | 5.16  | 107.86      | 105.80   |
| 35  | BB    | 2059 | A    | C4-C5-C6    | 5.16  | 119.58      | 117.00   |
| 35  | BB    | 2874 | C    | C6-N1-C2    | -5.16 | 118.23      | 120.30   |
| 1   | AA    | 119  | A    | C5'-C4'-O4' | 5.16  | 115.29      | 109.10   |
| 1   | AA    | 314  | C    | N3-C4-N4    | 5.16  | 121.61      | 118.00   |
| 1   | AA    | 461  | A    | P-O3'-C3'   | -5.16 | 113.51      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 711  | G    | C6-C5-N7    | -5.16 | 127.31      | 130.40   |
| 1   | AA    | 859  | G    | C2-N3-C4    | 5.16  | 114.48      | 111.90   |
| 1   | AA    | 986  | U    | N3-C2-O2    | -5.16 | 118.59      | 122.20   |
| 34  | BA    | 83   | G    | C8-N9-C4    | -5.16 | 104.34      | 106.40   |
| 35  | BB    | 274  | C    | C5-C4-N4    | -5.16 | 116.59      | 120.20   |
| 35  | BB    | 653  | U    | O4'-C1'-N1  | 5.16  | 112.33      | 108.20   |
| 35  | BB    | 1649 | G    | C5-C6-O6    | -5.16 | 125.50      | 128.60   |
| 35  | BB    | 1801 | A    | O4'-C1'-N9  | 5.16  | 112.33      | 108.20   |
| 35  | BB    | 1935 | G    | N3-C2-N2    | 5.16  | 123.51      | 119.90   |
| 35  | BB    | 2026 | U    | C6-N1-C2    | -5.16 | 117.91      | 121.00   |
| 35  | BB    | 2524 | G    | C5'-C4'-O4' | -5.16 | 102.91      | 109.10   |
| 35  | BB    | 2578 | G    | P-O3'-C3'   | -5.16 | 113.51      | 119.70   |
| 35  | BB    | 2644 | G    | N3-C4-C5    | -5.16 | 126.02      | 128.60   |
| 1   | AA    | 224  | U    | C5-C6-N1    | 5.16  | 125.28      | 122.70   |
| 1   | AA    | 255  | G    | N3-C2-N2    | 5.16  | 123.51      | 119.90   |
| 1   | AA    | 573  | A    | O4'-C1'-N9  | 5.16  | 112.33      | 108.20   |
| 1   | AA    | 979  | C    | C3'-C2'-C1' | -5.16 | 97.38       | 101.50   |
| 1   | AA    | 1003 | G    | C5'-C4'-C3' | -5.16 | 107.75      | 116.00   |
| 1   | AA    | 1064 | G    | C2-N3-C4    | 5.16  | 114.48      | 111.90   |
| 6   | AF    | 24   | ARG  | NE-CZ-NH1   | 5.16  | 122.88      | 120.30   |
| 34  | BA    | 25   | U    | C6-N1-C1'   | 5.16  | 128.42      | 121.20   |
| 34  | BA    | 44   | G    | C8-N9-C4    | -5.16 | 104.34      | 106.40   |
| 35  | BB    | 206  | U    | C6-N1-C2    | 5.16  | 124.09      | 121.00   |
| 35  | BB    | 503  | A    | O4'-C1'-N9  | 5.16  | 112.33      | 108.20   |
| 35  | BB    | 856  | G    | N9-C1'-C2'  | -5.16 | 106.33      | 112.00   |
| 35  | BB    | 1051 | G    | N3-C2-N2    | 5.16  | 123.51      | 119.90   |
| 35  | BB    | 1088 | A    | N3-C4-N9    | 5.16  | 131.53      | 127.40   |
| 35  | BB    | 1256 | G    | OP2-P-O3'   | 5.16  | 116.55      | 105.20   |
| 35  | BB    | 2269 | G    | N3-C2-N2    | -5.16 | 116.29      | 119.90   |
| 35  | BB    | 2734 | A    | N9-C4-C5    | 5.16  | 107.86      | 105.80   |
| 1   | AA    | 63   | C    | C6-N1-C2    | -5.16 | 118.24      | 120.30   |
| 1   | AA    | 357  | G    | C8-N9-C4    | 5.16  | 108.46      | 106.40   |
| 1   | AA    | 624  | C    | N3-C4-C5    | -5.16 | 119.84      | 121.90   |
| 1   | AA    | 1387 | G    | C5-C6-O6    | -5.16 | 125.51      | 128.60   |
| 11  | AK    | 17   | ASP  | CB-CA-C     | 5.16  | 120.71      | 110.40   |
| 35  | BB    | 17   | G    | C6-C5-N7    | -5.16 | 127.31      | 130.40   |
| 35  | BB    | 52   | A    | N1-C2-N3    | 5.16  | 131.88      | 129.30   |
| 35  | BB    | 175  | G    | N3-C4-C5    | 5.16  | 131.18      | 128.60   |
| 35  | BB    | 239  | C    | N3-C4-N4    | 5.16  | 121.61      | 118.00   |
| 35  | BB    | 1505 | A    | N7-C8-N9    | 5.16  | 116.38      | 113.80   |
| 35  | BB    | 1524 | G    | C5-C6-N1    | -5.16 | 108.92      | 111.50   |
| 35  | BB    | 1805 | A    | C5-C6-N1    | -5.16 | 115.12      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2130 | U    | O4'-C4'-C3' | -5.16 | 98.84       | 104.00   |
| 35  | BB    | 2346 | A    | N9-C4-C5    | 5.16  | 107.86      | 105.80   |
| 38  | BE    | 147  | LEU  | CB-CA-C     | -5.16 | 100.41      | 110.20   |
| 1   | AA    | 188  | C    | N3-C4-N4    | 5.15  | 121.61      | 118.00   |
| 1   | AA    | 1287 | A    | C5'-C4'-O4' | 5.15  | 115.28      | 109.10   |
| 35  | BB    | 956  | G    | O4'-C1'-N9  | 5.15  | 112.32      | 108.20   |
| 35  | BB    | 2052 | A    | P-O3'-C3'   | -5.15 | 113.52      | 119.70   |
| 1   | AA    | 119  | A    | O4'-C1'-C2' | 5.15  | 112.24      | 107.60   |
| 1   | AA    | 371  | A    | C8-N9-C4    | 5.15  | 107.86      | 105.80   |
| 1   | AA    | 382  | A    | N9-C4-C5    | 5.15  | 107.86      | 105.80   |
| 1   | AA    | 519  | C    | OP1-P-OP2   | -5.15 | 111.87      | 119.60   |
| 1   | AA    | 553  | A    | C5-N7-C8    | 5.15  | 106.48      | 103.90   |
| 1   | AA    | 633  | G    | N1-C6-O6    | 5.15  | 122.99      | 119.90   |
| 1   | AA    | 705  | G    | OP1-P-OP2   | -5.15 | 111.87      | 119.60   |
| 16  | AP    | 39   | PHE  | CB-CG-CD1   | 5.15  | 124.41      | 120.80   |
| 35  | BB    | 58   | G    | C5-C6-N1    | -5.15 | 108.92      | 111.50   |
| 35  | BB    | 278  | A    | C4-N9-C1'   | 5.15  | 135.57      | 126.30   |
| 35  | BB    | 920  | A    | C8-N9-C4    | -5.15 | 103.74      | 105.80   |
| 35  | BB    | 1168 | G    | N7-C8-N9    | 5.15  | 115.68      | 113.10   |
| 35  | BB    | 1431 | A    | N1-C2-N3    | 5.15  | 131.88      | 129.30   |
| 35  | BB    | 1510 | G    | O4'-C4'-C3' | -5.15 | 98.85       | 104.00   |
| 35  | BB    | 1562 | U    | O4'-C1'-N1  | 5.15  | 112.32      | 108.20   |
| 35  | BB    | 1641 | A    | C5-N7-C8    | 5.15  | 106.48      | 103.90   |
| 35  | BB    | 1729 | U    | C2-N1-C1'   | 5.15  | 123.88      | 117.70   |
| 35  | BB    | 1900 | A    | C8-N9-C4    | -5.15 | 103.74      | 105.80   |
| 35  | BB    | 2183 | A    | O4'-C4'-C3' | -5.15 | 98.85       | 104.00   |
| 35  | BB    | 2491 | U    | C5'-C4'-C3' | -5.15 | 107.75      | 116.00   |
| 35  | BB    | 2537 | U    | O5'-P-OP2   | 5.15  | 116.88      | 110.70   |
| 35  | BB    | 2543 | G    | C5'-C4'-C3' | -5.15 | 107.76      | 116.00   |
| 35  | BB    | 2581 | G    | C2-N3-C4    | 5.15  | 114.48      | 111.90   |
| 35  | BB    | 2728 | U    | C5-C4-O4    | -5.15 | 122.81      | 125.90   |
| 49  | BP    | 34   | GLY  | C-N-CA      | 5.15  | 134.58      | 121.70   |
| 1   | AA    | 295  | C    | C2-N1-C1'   | 5.15  | 124.47      | 118.80   |
| 1   | AA    | 305  | G    | O4'-C1'-C2' | -5.15 | 100.65      | 105.80   |
| 1   | AA    | 328  | C    | C6-N1-C1'   | -5.15 | 114.62      | 120.80   |
| 1   | AA    | 652  | U    | O4'-C1'-N1  | 5.15  | 112.32      | 108.20   |
| 1   | AA    | 801  | U    | O4'-C4'-C3' | -5.15 | 98.85       | 104.00   |
| 1   | AA    | 900  | A    | C6-C5-N7    | -5.15 | 128.69      | 132.30   |
| 1   | AA    | 1112 | C    | C4-C5-C6    | 5.15  | 119.97      | 117.40   |
| 1   | AA    | 1482 | G    | N7-C8-N9    | 5.15  | 115.68      | 113.10   |
| 12  | AL    | 118  | VAL  | N-CA-CB     | 5.15  | 122.83      | 111.50   |
| 25  | B0    | 68   | ALA  | N-CA-CB     | 5.15  | 117.31      | 110.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 30  | B5    | 195  | ALA  | O-C-N       | -5.15 | 114.46      | 122.70   |
| 35  | BB    | 27   | G    | N1-C6-O6    | 5.15  | 122.99      | 119.90   |
| 35  | BB    | 73   | A    | C4-C5-N7    | -5.15 | 108.12      | 110.70   |
| 35  | BB    | 217  | A    | C6-N1-C2    | 5.15  | 121.69      | 118.60   |
| 35  | BB    | 535  | G    | N9-C4-C5    | 5.15  | 107.46      | 105.40   |
| 35  | BB    | 612  | G    | C6-C5-N7    | -5.15 | 127.31      | 130.40   |
| 35  | BB    | 713  | G    | C8-N9-C1'   | -5.15 | 120.30      | 127.00   |
| 35  | BB    | 931  | U    | C2-N1-C1'   | 5.15  | 123.88      | 117.70   |
| 35  | BB    | 936  | A    | C5-C6-N1    | -5.15 | 115.12      | 117.70   |
| 35  | BB    | 1595 | C    | C2-N1-C1'   | -5.15 | 113.13      | 118.80   |
| 35  | BB    | 1750 | G    | O4'-C4'-C3' | -5.15 | 98.85       | 104.00   |
| 35  | BB    | 2876 | G    | C8-N9-C1'   | 5.15  | 133.70      | 127.00   |
| 1   | AA    | 702  | A    | C6-C5-N7    | -5.15 | 128.70      | 132.30   |
| 35  | BB    | 414  | C    | C4-C5-C6    | 5.15  | 119.97      | 117.40   |
| 35  | BB    | 632  | A    | C5-N7-C8    | 5.15  | 106.47      | 103.90   |
| 35  | BB    | 974  | G    | C8-N9-C1'   | -5.15 | 120.31      | 127.00   |
| 35  | BB    | 1436 | G    | N3-C4-C5    | 5.15  | 131.18      | 128.60   |
| 35  | BB    | 1486 | U    | C3'-C2'-C1' | -5.15 | 97.38       | 101.50   |
| 35  | BB    | 2742 | G    | N1-C2-N3    | -5.15 | 120.81      | 123.90   |
| 55  | BW    | 63   | ILE  | N-CA-CB     | 5.15  | 122.64      | 110.80   |
| 1   | AA    | 143  | A    | N7-C8-N9    | -5.15 | 111.23      | 113.80   |
| 1   | AA    | 442  | G    | N9-C4-C5    | 5.15  | 107.46      | 105.40   |
| 1   | AA    | 466  | A    | N1-C2-N3    | -5.15 | 126.73      | 129.30   |
| 1   | AA    | 500  | G    | C5'-C4'-O4' | -5.15 | 102.92      | 109.10   |
| 1   | AA    | 846  | G    | N9-C4-C5    | -5.15 | 103.34      | 105.40   |
| 25  | B0    | 40   | GLU  | N-CA-CB     | 5.15  | 119.87      | 110.60   |
| 35  | BB    | 188  | G    | C1'-O4'-C4' | -5.15 | 105.78      | 109.90   |
| 35  | BB    | 1689 | A    | P-O5'-C5'   | 5.15  | 129.14      | 120.90   |
| 35  | BB    | 1763 | G    | C5-C6-O6    | -5.15 | 125.51      | 128.60   |
| 35  | BB    | 2252 | G    | C8-N9-C4    | -5.15 | 104.34      | 106.40   |
| 36  | BC    | 246  | PRO  | N-CD-CG     | 5.15  | 110.92      | 103.20   |
| 1   | AA    | 7    | A    | N1-C2-N3    | 5.15  | 131.87      | 129.30   |
| 1   | AA    | 1279 | G    | C6-C5-N7    | -5.15 | 127.31      | 130.40   |
| 1   | AA    | 1347 | G    | C4-C5-C6    | 5.15  | 121.89      | 118.80   |
| 34  | BA    | 108  | A    | P-O3'-C3'   | 5.15  | 125.88      | 119.70   |
| 35  | BB    | 46   | G    | C8-N9-C4    | -5.15 | 104.34      | 106.40   |
| 35  | BB    | 174  | U    | C5-C4-O4    | -5.15 | 122.81      | 125.90   |
| 35  | BB    | 622  | G    | C6-C5-N7    | -5.15 | 127.31      | 130.40   |
| 35  | BB    | 792  | A    | N9-C1'-C2'  | -5.15 | 106.34      | 112.00   |
| 35  | BB    | 1893 | C    | O4'-C1'-N1  | 5.15  | 112.32      | 108.20   |
| 35  | BB    | 2385 | C    | N1-C2-N3    | -5.15 | 115.60      | 119.20   |
| 1   | AA    | 22   | G    | N1-C2-N3    | -5.14 | 120.81      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 422  | C    | N1-C2-O2    | 5.14  | 121.99      | 118.90   |
| 1   | AA    | 639  | G    | C4-C5-N7    | 5.14  | 112.86      | 110.80   |
| 1   | AA    | 870  | U    | C5-C4-O4    | -5.14 | 122.81      | 125.90   |
| 1   | AA    | 1021 | A    | P-O5'-C5'   | 5.14  | 129.13      | 120.90   |
| 1   | AA    | 1147 | C    | N1-C2-N3    | -5.14 | 115.60      | 119.20   |
| 1   | AA    | 1440 | U    | O4'-C1'-N1  | 5.14  | 112.32      | 108.20   |
| 1   | AA    | 1462 | C    | O4'-C4'-C3' | -5.14 | 98.86       | 104.00   |
| 35  | BB    | 463  | G    | N1-C2-N3    | -5.14 | 120.81      | 123.90   |
| 35  | BB    | 634  | C    | N3-C2-O2    | 5.14  | 125.50      | 121.90   |
| 35  | BB    | 864  | G    | C5-C6-N1    | -5.14 | 108.93      | 111.50   |
| 35  | BB    | 951  | C    | C4-C5-C6    | 5.14  | 119.97      | 117.40   |
| 35  | BB    | 1202 | G    | N3-C4-N9    | -5.14 | 122.91      | 126.00   |
| 35  | BB    | 1626 | A    | C5-N7-C8    | 5.14  | 106.47      | 103.90   |
| 1   | AA    | 125  | U    | P-O3'-C3'   | -5.14 | 113.53      | 119.70   |
| 1   | AA    | 155  | A    | C8-N9-C4    | -5.14 | 103.74      | 105.80   |
| 1   | AA    | 168  | G    | C5-C6-N1    | -5.14 | 108.93      | 111.50   |
| 1   | AA    | 759  | A    | OP1-P-OP2   | -5.14 | 111.89      | 119.60   |
| 3   | AC    | 202  | PHE  | CB-CG-CD2   | -5.14 | 117.20      | 120.80   |
| 35  | BB    | 82   | U    | C6-N1-C2    | -5.14 | 117.92      | 121.00   |
| 35  | BB    | 381  | G    | N1-C6-O6    | 5.14  | 122.98      | 119.90   |
| 35  | BB    | 653  | U    | N3-C2-O2    | -5.14 | 118.60      | 122.20   |
| 35  | BB    | 1007 | C    | C2-N3-C4    | 5.14  | 122.47      | 119.90   |
| 35  | BB    | 1288 | G    | C5-N7-C8    | 5.14  | 106.87      | 104.30   |
| 35  | BB    | 1723 | G    | N3-C4-N9    | -5.14 | 122.92      | 126.00   |
| 35  | BB    | 2286 | G    | OP1-P-OP2   | -5.14 | 111.89      | 119.60   |
| 35  | BB    | 2306 | C    | P-O3'-C3'   | 5.14  | 125.87      | 119.70   |
| 35  | BB    | 2404 | U    | C2-N1-C1'   | -5.14 | 111.53      | 117.70   |
| 35  | BB    | 2599 | G    | C8-N9-C1'   | 5.14  | 133.69      | 127.00   |
| 35  | BB    | 2638 | G    | C5'-C4'-O4' | 5.14  | 115.27      | 109.10   |
| 35  | BB    | 2686 | G    | C4-N9-C1'   | 5.14  | 133.18      | 126.50   |
| 35  | BB    | 2755 | C    | C2-N1-C1'   | 5.14  | 124.46      | 118.80   |
| 35  | BB    | 2764 | A    | C2-N3-C4    | 5.14  | 113.17      | 110.60   |
| 1   | AA    | 117  | G    | P-O5'-C5'   | 5.14  | 129.12      | 120.90   |
| 34  | BA    | 4    | C    | C4-C5-C6    | 5.14  | 119.97      | 117.40   |
| 34  | BA    | 50   | A    | C5-N7-C8    | 5.14  | 106.47      | 103.90   |
| 34  | BA    | 57   | A    | C4-C5-C6    | 5.14  | 119.57      | 117.00   |
| 35  | BB    | 662  | G    | C2-N3-C4    | -5.14 | 109.33      | 111.90   |
| 35  | BB    | 1177 | G    | C1'-O4'-C4' | 5.14  | 114.01      | 109.90   |
| 35  | BB    | 1732 | C    | OP1-P-OP2   | -5.14 | 111.89      | 119.60   |
| 35  | BB    | 1920 | C    | N1-C1'-C2'  | -5.14 | 106.34      | 112.00   |
| 35  | BB    | 2045 | C    | C1'-O4'-C4' | -5.14 | 105.79      | 109.90   |
| 35  | BB    | 2250 | G    | OP2-P-O3'   | 5.14  | 116.51      | 105.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2498 | C    | C5-C4-N4    | 5.14  | 123.80      | 120.20   |
| 35  | BB    | 2737 | G    | P-O5'-C5'   | 5.14  | 129.12      | 120.90   |
| 1   | AA    | 195  | A    | O4'-C4'-C3' | -5.14 | 98.86       | 104.00   |
| 1   | AA    | 430  | A    | O4'-C1'-N9  | 5.14  | 112.31      | 108.20   |
| 1   | AA    | 431  | A    | O4'-C1'-N9  | 5.14  | 112.31      | 108.20   |
| 1   | AA    | 691  | G    | C5'-C4'-O4' | 5.14  | 115.27      | 109.10   |
| 1   | AA    | 826  | C    | C5-C4-N4    | -5.14 | 116.60      | 120.20   |
| 1   | AA    | 1109 | C    | C4-C5-C6    | 5.14  | 119.97      | 117.40   |
| 1   | AA    | 1137 | C    | C2-N1-C1'   | 5.14  | 124.45      | 118.80   |
| 34  | BA    | 118  | C    | N3-C2-O2    | 5.14  | 125.50      | 121.90   |
| 35  | BB    | 219  | A    | C5-C6-N1    | -5.14 | 115.13      | 117.70   |
| 35  | BB    | 451  | U    | C1'-O4'-C4' | -5.14 | 105.79      | 109.90   |
| 35  | BB    | 619  | G    | C5-C6-O6    | -5.14 | 125.52      | 128.60   |
| 35  | BB    | 1104 | C    | N3-C4-N4    | 5.14  | 121.60      | 118.00   |
| 35  | BB    | 1298 | C    | N1-C2-N3    | -5.14 | 115.60      | 119.20   |
| 35  | BB    | 2253 | G    | C6-N1-C2    | -5.14 | 122.02      | 125.10   |
| 35  | BB    | 2471 | A    | N7-C8-N9    | -5.14 | 111.23      | 113.80   |
| 35  | BB    | 2525 | G    | C4-N9-C1'   | -5.14 | 119.82      | 126.50   |
| 1   | AA    | 868  | C    | N3-C4-C5    | 5.14  | 123.95      | 121.90   |
| 1   | AA    | 1222 | G    | N1-C2-N2    | 5.14  | 120.82      | 116.20   |
| 1   | AA    | 1356 | G    | O4'-C1'-N9  | 5.14  | 112.31      | 108.20   |
| 1   | AA    | 1455 | G    | O4'-C1'-N9  | 5.14  | 112.31      | 108.20   |
| 1   | AA    | 1479 | C    | P-O3'-C3'   | -5.14 | 113.53      | 119.70   |
| 3   | AC    | 129  | PHE  | CB-CG-CD1   | 5.14  | 124.40      | 120.80   |
| 35  | BB    | 2566 | A    | N7-C8-N9    | -5.14 | 111.23      | 113.80   |
| 1   | AA    | 42   | G    | C8-N9-C4    | 5.14  | 108.45      | 106.40   |
| 1   | AA    | 85   | U    | C2-N1-C1'   | 5.14  | 123.86      | 117.70   |
| 1   | AA    | 183  | C    | N1-C2-O2    | -5.14 | 115.82      | 118.90   |
| 1   | AA    | 482  | A    | C3'-C2'-C1' | -5.14 | 97.39       | 101.50   |
| 1   | AA    | 1238 | A    | N1-C6-N6    | 5.14  | 121.68      | 118.60   |
| 1   | AA    | 1289 | A    | N1-C2-N3    | -5.14 | 126.73      | 129.30   |
| 1   | AA    | 1334 | G    | C2-N3-C4    | -5.14 | 109.33      | 111.90   |
| 34  | BA    | 21   | G    | C4-C5-N7    | 5.14  | 112.86      | 110.80   |
| 35  | BB    | 242  | G    | C6-N1-C2    | 5.14  | 128.18      | 125.10   |
| 35  | BB    | 283  | G    | C5'-C4'-C3' | 5.14  | 124.22      | 116.00   |
| 35  | BB    | 825  | A    | N7-C8-N9    | -5.14 | 111.23      | 113.80   |
| 35  | BB    | 979  | A    | C8-N9-C4    | 5.14  | 107.86      | 105.80   |
| 35  | BB    | 1200 | C    | O4'-C1'-N1  | 5.14  | 112.31      | 108.20   |
| 35  | BB    | 1228 | G    | C8-N9-C1'   | 5.14  | 133.68      | 127.00   |
| 35  | BB    | 1930 | G    | P-O3'-C3'   | 5.14  | 125.86      | 119.70   |
| 35  | BB    | 2114 | A    | C5-N7-C8    | 5.14  | 106.47      | 103.90   |
| 35  | BB    | 2530 | A    | C5-C6-N1    | -5.14 | 115.13      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2676 | C    | N3-C4-N4    | 5.14  | 121.59      | 118.00   |
| 35  | BB    | 2722 | G    | O5'-C5'-C4' | -5.14 | 101.94      | 111.70   |
| 1   | AA    | 47   | C    | N1-C2-O2    | -5.13 | 115.82      | 118.90   |
| 1   | AA    | 126  | G    | O4'-C1'-N9  | 5.13  | 112.31      | 108.20   |
| 1   | AA    | 266  | G    | C4-C5-N7    | -5.13 | 108.75      | 110.80   |
| 1   | AA    | 645  | G    | N1-C2-N2    | 5.13  | 120.82      | 116.20   |
| 1   | AA    | 1127 | G    | O4'-C1'-N9  | -5.13 | 104.09      | 108.20   |
| 1   | AA    | 1185 | G    | N3-C4-C5    | -5.13 | 126.03      | 128.60   |
| 1   | AA    | 1190 | G    | C6-N1-C2    | 5.13  | 128.18      | 125.10   |
| 1   | AA    | 1305 | G    | N3-C4-N9    | -5.13 | 122.92      | 126.00   |
| 8   | AH    | 14   | ARG  | C-N-CA      | 5.13  | 134.54      | 121.70   |
| 34  | BA    | 9    | G    | O4'-C1'-N9  | 5.13  | 112.31      | 108.20   |
| 35  | BB    | 102  | U    | C4-C5-C6    | -5.13 | 116.62      | 119.70   |
| 35  | BB    | 386  | G    | N1-C2-N3    | -5.13 | 120.82      | 123.90   |
| 35  | BB    | 632  | A    | C4-C5-C6    | 5.13  | 119.57      | 117.00   |
| 35  | BB    | 845  | A    | C8-N9-C4    | -5.13 | 103.75      | 105.80   |
| 35  | BB    | 1051 | G    | C5'-C4'-C3' | 5.13  | 124.21      | 116.00   |
| 35  | BB    | 1208 | C    | N3-C4-N4    | 5.13  | 121.59      | 118.00   |
| 35  | BB    | 1268 | A    | C2-N3-C4    | -5.13 | 108.03      | 110.60   |
| 35  | BB    | 1448 | G    | N3-C4-C5    | 5.13  | 131.17      | 128.60   |
| 35  | BB    | 1476 | U    | C4'-C3'-C2' | -5.13 | 97.47       | 102.60   |
| 35  | BB    | 1568 | G    | OP2-P-O3'   | 5.13  | 116.50      | 105.20   |
| 35  | BB    | 1599 | U    | OP1-P-OP2   | -5.13 | 111.90      | 119.60   |
| 35  | BB    | 1699 | G    | C4-N9-C1'   | 5.13  | 133.17      | 126.50   |
| 35  | BB    | 1745 | A    | C6-N1-C2    | -5.13 | 115.52      | 118.60   |
| 35  | BB    | 2055 | C    | N1-C1'-C2'  | -5.13 | 106.35      | 112.00   |
| 35  | BB    | 2239 | G    | C5-C6-N1    | -5.13 | 108.93      | 111.50   |
| 35  | BB    | 2379 | G    | N7-C8-N9    | 5.13  | 115.67      | 113.10   |
| 35  | BB    | 2398 | U    | C2-N3-C4    | 5.13  | 130.08      | 127.00   |
| 35  | BB    | 2788 | C    | N3-C4-N4    | 5.13  | 121.59      | 118.00   |
| 1   | AA    | 105  | G    | C5-C6-N1    | -5.13 | 108.93      | 111.50   |
| 12  | AL    | 94   | TYR  | N-CA-CB     | 5.13  | 119.84      | 110.60   |
| 35  | BB    | 216  | A    | N3-C4-C5    | -5.13 | 123.21      | 126.80   |
| 35  | BB    | 1119 | U    | O4'-C1'-N1  | 5.13  | 112.31      | 108.20   |
| 35  | BB    | 1567 | G    | C2-N3-C4    | 5.13  | 114.47      | 111.90   |
| 35  | BB    | 1796 | U    | N3-C4-O4    | 5.13  | 122.99      | 119.40   |
| 35  | BB    | 1933 | G    | C2-N3-C4    | 5.13  | 114.47      | 111.90   |
| 1   | AA    | 438  | U    | C1'-O4'-C4' | 5.13  | 114.00      | 109.90   |
| 1   | AA    | 1013 | G    | N1-C2-N3    | -5.13 | 120.82      | 123.90   |
| 1   | AA    | 1142 | G    | C4-C5-C6    | 5.13  | 121.88      | 118.80   |
| 1   | AA    | 1362 | A    | N1-C2-N3    | 5.13  | 131.87      | 129.30   |
| 1   | AA    | 1447 | A    | P-O3'-C3'   | 5.13  | 125.86      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1490 | U    | C5'-C4'-C3' | -5.13 | 107.79      | 116.00   |
| 35  | BB    | 87   | U    | C5-C6-N1    | -5.13 | 120.13      | 122.70   |
| 35  | BB    | 531  | C    | C4-C5-C6    | 5.13  | 119.97      | 117.40   |
| 35  | BB    | 784  | G    | P-O3'-C3'   | -5.13 | 113.54      | 119.70   |
| 35  | BB    | 907  | G    | N9-C4-C5    | -5.13 | 103.35      | 105.40   |
| 35  | BB    | 1241 | A    | C8-N9-C4    | -5.13 | 103.75      | 105.80   |
| 35  | BB    | 1360 | G    | N1-C6-O6    | 5.13  | 122.98      | 119.90   |
| 35  | BB    | 1366 | A    | C6-N1-C2    | 5.13  | 121.68      | 118.60   |
| 35  | BB    | 1427 | A    | C1'-O4'-C4' | 5.13  | 114.01      | 109.90   |
| 35  | BB    | 2614 | A    | C5-C6-N6    | -5.13 | 119.59      | 123.70   |
| 35  | BB    | 2736 | A    | C5'-C4'-O4' | 5.13  | 115.26      | 109.10   |
| 1   | AA    | 711  | G    | C5-C6-N1    | -5.13 | 108.94      | 111.50   |
| 1   | AA    | 1018 | G    | C5-C6-O6    | -5.13 | 125.52      | 128.60   |
| 1   | AA    | 1211 | U    | C5-C6-N1    | -5.13 | 120.14      | 122.70   |
| 1   | AA    | 1267 | C    | N1-C2-N3    | -5.13 | 115.61      | 119.20   |
| 1   | AA    | 1350 | A    | O4'-C1'-N9  | 5.13  | 112.30      | 108.20   |
| 35  | BB    | 521  | U    | C5-C6-N1    | 5.13  | 125.27      | 122.70   |
| 35  | BB    | 643  | A    | C4-C5-N7    | -5.13 | 108.14      | 110.70   |
| 35  | BB    | 985  | C    | N3-C2-O2    | 5.13  | 125.49      | 121.90   |
| 35  | BB    | 1157 | G    | C8-N9-C4    | -5.13 | 104.35      | 106.40   |
| 35  | BB    | 1159 | U    | C1'-O4'-C4' | 5.13  | 114.00      | 109.90   |
| 35  | BB    | 1726 | C    | N3-C4-N4    | 5.13  | 121.59      | 118.00   |
| 35  | BB    | 2519 | U    | N1-C2-O2    | -5.13 | 119.21      | 122.80   |
| 35  | BB    | 2692 | G    | P-O5'-C5'   | -5.13 | 112.69      | 120.90   |
| 1   | AA    | 363  | A    | N1-C2-N3    | -5.13 | 126.74      | 129.30   |
| 1   | AA    | 596  | A    | C5-C6-N1    | -5.13 | 115.14      | 117.70   |
| 1   | AA    | 842  | U    | O5'-P-OP1   | -5.13 | 101.08      | 105.70   |
| 1   | AA    | 853  | C    | C2-N1-C1'   | -5.13 | 113.16      | 118.80   |
| 1   | AA    | 1081 | A    | C5-C6-N1    | -5.13 | 115.14      | 117.70   |
| 1   | AA    | 1480 | A    | C5-C6-N1    | -5.13 | 115.14      | 117.70   |
| 2   | AB    | 126  | ASP  | CB-CG-OD1   | -5.13 | 113.69      | 118.30   |
| 34  | BA    | 53   | A    | OP1-P-OP2   | -5.13 | 111.91      | 119.60   |
| 35  | BB    | 345  | A    | C8-N9-C4    | -5.13 | 103.75      | 105.80   |
| 35  | BB    | 780  | G    | C4-C5-C6    | 5.13  | 121.88      | 118.80   |
| 35  | BB    | 1087 | G    | C3'-C2'-C1' | -5.13 | 97.40       | 101.50   |
| 35  | BB    | 1129 | A    | C6-C5-N7    | -5.13 | 128.71      | 132.30   |
| 35  | BB    | 1743 | G    | C6-C5-N7    | -5.13 | 127.32      | 130.40   |
| 35  | BB    | 2248 | C    | C3'-C2'-C1' | -5.13 | 97.40       | 101.50   |
| 35  | BB    | 2441 | U    | N3-C2-O2    | 5.13  | 125.79      | 122.20   |
| 35  | BB    | 2452 | C    | N1-C2-O2    | 5.13  | 121.98      | 118.90   |
| 35  | BB    | 2746 | U    | N3-C2-O2    | 5.13  | 125.79      | 122.20   |
| 1   | AA    | 50   | A    | O4'-C1'-N9  | 5.13  | 112.30      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 315  | A    | C2-N3-C4    | -5.13 | 108.04      | 110.60   |
| 1   | AA    | 459  | A    | C2-N3-C4    | -5.13 | 108.04      | 110.60   |
| 1   | AA    | 802  | A    | C5-C6-N6    | -5.13 | 119.60      | 123.70   |
| 1   | AA    | 1075 | U    | C1'-O4'-C4' | 5.13  | 114.00      | 109.90   |
| 1   | AA    | 1126 | U    | N3-C4-C5    | -5.13 | 111.52      | 114.60   |
| 1   | AA    | 1336 | C    | N3-C4-C5    | -5.13 | 119.85      | 121.90   |
| 1   | AA    | 1449 | C    | C5-C6-N1    | 5.13  | 123.56      | 121.00   |
| 34  | BA    | 57   | A    | C5-C6-N1    | -5.13 | 115.14      | 117.70   |
| 35  | BB    | 343  | C    | O3'-P-O5'   | -5.13 | 94.26       | 104.00   |
| 35  | BB    | 850  | U    | N3-C4-O4    | 5.13  | 122.99      | 119.40   |
| 35  | BB    | 1277 | G    | C8-N9-C4    | -5.13 | 104.35      | 106.40   |
| 35  | BB    | 2047 | C    | N1-C2-N3    | 5.13  | 122.79      | 119.20   |
| 35  | BB    | 2182 | U    | C2-N3-C4    | -5.13 | 123.92      | 127.00   |
| 35  | BB    | 2318 | G    | C8-N9-C4    | 5.13  | 108.45      | 106.40   |
| 35  | BB    | 2336 | A    | C6-N1-C2    | 5.13  | 121.68      | 118.60   |
| 35  | BB    | 2560 | A    | N7-C8-N9    | 5.13  | 116.36      | 113.80   |
| 35  | BB    | 2579 | C    | C2-N3-C4    | 5.13  | 122.46      | 119.90   |
| 1   | AA    | 81   | A    | C8-N9-C4    | -5.12 | 103.75      | 105.80   |
| 34  | BA    | 7    | G    | N9-C4-C5    | -5.12 | 103.35      | 105.40   |
| 35  | BB    | 138  | U    | C6-N1-C1'   | -5.12 | 114.03      | 121.20   |
| 35  | BB    | 191  | A    | C2-N3-C4    | -5.12 | 108.04      | 110.60   |
| 35  | BB    | 930  | G    | C5-N7-C8    | -5.12 | 101.74      | 104.30   |
| 35  | BB    | 1033 | U    | C6-N1-C2    | 5.12  | 124.08      | 121.00   |
| 35  | BB    | 2537 | U    | N1-C2-N3    | -5.12 | 111.83      | 114.90   |
| 35  | BB    | 2751 | G    | C5-C6-N1    | -5.12 | 108.94      | 111.50   |
| 1   | AA    | 33   | A    | O4'-C1'-N9  | 5.12  | 112.30      | 108.20   |
| 1   | AA    | 460  | A    | N1-C6-N6    | 5.12  | 121.67      | 118.60   |
| 1   | AA    | 761  | G    | O4'-C1'-N9  | 5.12  | 112.30      | 108.20   |
| 1   | AA    | 775  | G    | C5-N7-C8    | -5.12 | 101.74      | 104.30   |
| 1   | AA    | 1030 | U    | C5-C6-N1    | 5.12  | 125.26      | 122.70   |
| 1   | AA    | 1228 | C    | C4-C5-C6    | -5.12 | 114.84      | 117.40   |
| 35  | BB    | 290  | U    | P-O5'-C5'   | 5.12  | 129.10      | 120.90   |
| 35  | BB    | 610  | C    | C1'-O4'-C4' | 5.12  | 114.00      | 109.90   |
| 35  | BB    | 878  | A    | N1-C2-N3    | 5.12  | 131.86      | 129.30   |
| 35  | BB    | 904  | G    | C2-N3-C4    | 5.12  | 114.46      | 111.90   |
| 35  | BB    | 1445 | G    | C6-N1-C2    | -5.12 | 122.03      | 125.10   |
| 35  | BB    | 1891 | G    | N1-C2-N3    | -5.12 | 120.83      | 123.90   |
| 35  | BB    | 2168 | G    | N3-C2-N2    | 5.12  | 123.49      | 119.90   |
| 35  | BB    | 2210 | U    | O4'-C1'-N1  | 5.12  | 112.30      | 108.20   |
| 35  | BB    | 2795 | C    | C5-C4-N4    | -5.12 | 116.61      | 120.20   |
| 35  | BB    | 2890 | G    | C5-C6-O6    | -5.12 | 125.53      | 128.60   |
| 35  | BB    | 2892 | G    | N9-C4-C5    | -5.12 | 103.35      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 306  | A    | C6-C5-N7    | -5.12 | 128.71      | 132.30   |
| 1   | AA    | 509  | A    | O4'-C1'-N9  | 5.12  | 112.30      | 108.20   |
| 1   | AA    | 727  | G    | C5-C6-O6    | -5.12 | 125.53      | 128.60   |
| 1   | AA    | 976  | G    | C4'-C3'-C2' | 5.12  | 107.72      | 102.60   |
| 1   | AA    | 1025 | U    | C6-N1-C1'   | -5.12 | 114.03      | 121.20   |
| 1   | AA    | 1301 | U    | O4'-C1'-N1  | 5.12  | 112.30      | 108.20   |
| 29  | B4    | 8    | ILE  | CB-CA-C     | 5.12  | 121.84      | 111.60   |
| 35  | BB    | 38   | A    | P-O5'-C5'   | -5.12 | 112.71      | 120.90   |
| 35  | BB    | 213  | A    | C4-C5-C6    | 5.12  | 119.56      | 117.00   |
| 35  | BB    | 508  | A    | C6-N1-C2    | -5.12 | 115.53      | 118.60   |
| 35  | BB    | 1287 | A    | N3-C4-C5    | -5.12 | 123.22      | 126.80   |
| 35  | BB    | 1331 | G    | OP2-P-O3'   | 5.12  | 116.47      | 105.20   |
| 35  | BB    | 1581 | G    | N7-C8-N9    | 5.12  | 115.66      | 113.10   |
| 35  | BB    | 1740 | G    | O5'-P-OP1   | -5.12 | 101.09      | 105.70   |
| 35  | BB    | 2001 | C    | C2-N3-C4    | 5.12  | 122.46      | 119.90   |
| 35  | BB    | 2037 | A    | N1-C2-N3    | 5.12  | 131.86      | 129.30   |
| 35  | BB    | 2491 | U    | C5-C4-O4    | -5.12 | 122.83      | 125.90   |
| 35  | BB    | 2493 | U    | N1-C2-O2    | -5.12 | 119.22      | 122.80   |
| 35  | BB    | 2603 | G    | N7-C8-N9    | -5.12 | 110.54      | 113.10   |
| 35  | BB    | 2632 | A    | C5'-C4'-O4' | 5.12  | 115.25      | 109.10   |
| 35  | BB    | 2709 | G    | C4-C5-N7    | -5.12 | 108.75      | 110.80   |
| 44  | BK    | 82   | ASN  | CB-CA-C     | -5.12 | 100.16      | 110.40   |
| 1   | AA    | 966  | G    | C4-N9-C1'   | -5.12 | 119.84      | 126.50   |
| 1   | AA    | 1407 | C    | C5-C6-N1    | -5.12 | 118.44      | 121.00   |
| 7   | AG    | 101  | ARG  | NE-CZ-NH2   | 5.12  | 122.86      | 120.30   |
| 35  | BB    | 940  | G    | C3'-C2'-C1' | -5.12 | 97.40       | 101.50   |
| 35  | BB    | 1573 | G    | C4-N9-C1'   | -5.12 | 119.84      | 126.50   |
| 35  | BB    | 1583 | A    | N7-C8-N9    | 5.12  | 116.36      | 113.80   |
| 35  | BB    | 2076 | U    | C5'-C4'-C3' | 5.12  | 124.19      | 116.00   |
| 36  | BC    | 68   | ARG  | NE-CZ-NH1   | -5.12 | 117.74      | 120.30   |
| 39  | BF    | 111  | ARG  | NE-CZ-NH1   | 5.12  | 122.86      | 120.30   |
| 1   | AA    | 277  | C    | O4'-C1'-N1  | 5.12  | 112.30      | 108.20   |
| 1   | AA    | 475  | C    | N3-C4-N4    | 5.12  | 121.58      | 118.00   |
| 1   | AA    | 530  | G    | C4'-C3'-C2' | -5.12 | 97.48       | 102.60   |
| 1   | AA    | 1329 | A    | N9-C4-C5    | 5.12  | 107.85      | 105.80   |
| 34  | BA    | 99   | A    | N3-C4-C5    | -5.12 | 123.22      | 126.80   |
| 35  | BB    | 239  | C    | OP1-P-O3'   | 5.12  | 116.46      | 105.20   |
| 35  | BB    | 674  | G    | N1-C2-N3    | -5.12 | 120.83      | 123.90   |
| 35  | BB    | 1027 | A    | C5-C6-N1    | -5.12 | 115.14      | 117.70   |
| 35  | BB    | 1272 | A    | C1'-O4'-C4' | -5.12 | 105.81      | 109.90   |
| 35  | BB    | 2294 | G    | N3-C4-C5    | -5.12 | 126.04      | 128.60   |
| 35  | BB    | 2361 | G    | C6-C5-N7    | 5.12  | 133.47      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2643 | G    | C5-C6-O6    | -5.12 | 125.53      | 128.60   |
| 35  | BB    | 2759 | G    | N1-C2-N3    | -5.12 | 120.83      | 123.90   |
| 1   | AA    | 667  | G    | P-O5'-C5'   | -5.12 | 112.71      | 120.90   |
| 35  | BB    | 608  | A    | C3'-C2'-C1' | 5.12  | 105.59      | 101.50   |
| 35  | BB    | 2375 | G    | N1-C2-N3    | 5.12  | 126.97      | 123.90   |
| 35  | BB    | 2411 | A    | N3-C4-C5    | -5.12 | 123.22      | 126.80   |
| 41  | BH    | 93   | SER  | CB-CA-C     | 5.12  | 119.82      | 110.10   |
| 1   | AA    | 256  | U    | C5'-C4'-C3' | -5.12 | 107.81      | 116.00   |
| 1   | AA    | 375  | U    | C1'-O4'-C4' | -5.12 | 105.81      | 109.90   |
| 1   | AA    | 773  | G    | C4-N9-C1'   | -5.12 | 119.85      | 126.50   |
| 1   | AA    | 815  | A    | C6-N1-C2    | 5.12  | 121.67      | 118.60   |
| 1   | AA    | 908  | A    | C8-N9-C4    | -5.12 | 103.75      | 105.80   |
| 1   | AA    | 1275 | A    | C5-C6-N6    | -5.12 | 119.61      | 123.70   |
| 24  | AZ    | 23   | ALA  | CA-C-N      | 5.12  | 128.45      | 117.20   |
| 35  | BB    | 197  | A    | C5'-C4'-O4' | 5.12  | 115.24      | 109.10   |
| 35  | BB    | 256  | A    | C3'-C2'-C1' | 5.12  | 105.59      | 101.50   |
| 35  | BB    | 409  | G    | OP2-P-O3'   | 5.12  | 116.45      | 105.20   |
| 35  | BB    | 1372 | U    | C4-C5-C6    | 5.12  | 122.77      | 119.70   |
| 35  | BB    | 1829 | A    | C2-N3-C4    | -5.12 | 108.04      | 110.60   |
| 35  | BB    | 1839 | G    | C5-N7-C8    | -5.12 | 101.74      | 104.30   |
| 35  | BB    | 1931 | U    | C4-C5-C6    | -5.12 | 116.63      | 119.70   |
| 35  | BB    | 2012 | G    | C5-C6-O6    | -5.12 | 125.53      | 128.60   |
| 35  | BB    | 2071 | A    | C2-N3-C4    | -5.12 | 108.04      | 110.60   |
| 35  | BB    | 2125 | G    | C5-N7-C8    | 5.12  | 106.86      | 104.30   |
| 35  | BB    | 2209 | G    | C5-N7-C8    | -5.12 | 101.74      | 104.30   |
| 1   | AA    | 216  | U    | O5'-P-OP1   | 5.11  | 116.84      | 110.70   |
| 1   | AA    | 371  | A    | N3-C4-N9    | 5.11  | 131.49      | 127.40   |
| 1   | AA    | 651  | C    | C4-C5-C6    | 5.11  | 119.96      | 117.40   |
| 1   | AA    | 791  | G    | C5'-C4'-O4' | 5.11  | 115.24      | 109.10   |
| 1   | AA    | 1517 | G    | C1'-O4'-C4' | 5.11  | 113.99      | 109.90   |
| 35  | BB    | 22   | C    | P-O3'-C3'   | 5.11  | 125.83      | 119.70   |
| 35  | BB    | 362  | A    | O4'-C1'-N9  | 5.11  | 112.29      | 108.20   |
| 35  | BB    | 575  | A    | C6-N1-C2    | -5.11 | 115.53      | 118.60   |
| 35  | BB    | 661  | A    | C1'-O4'-C4' | -5.11 | 105.81      | 109.90   |
| 35  | BB    | 718  | A    | N1-C2-N3    | 5.11  | 131.86      | 129.30   |
| 35  | BB    | 1454 | C    | N3-C2-O2    | 5.11  | 125.48      | 121.90   |
| 35  | BB    | 1962 | C    | C2-N3-C4    | 5.11  | 122.46      | 119.90   |
| 35  | BB    | 1986 | C    | O4'-C1'-N1  | 5.11  | 112.29      | 108.20   |
| 35  | BB    | 2068 | U    | P-O3'-C3'   | 5.11  | 125.84      | 119.70   |
| 35  | BB    | 2234 | G    | O4'-C1'-N9  | 5.11  | 112.29      | 108.20   |
| 35  | BB    | 2381 | A    | C5-N7-C8    | 5.11  | 106.46      | 103.90   |
| 35  | BB    | 2729 | G    | C5-C6-N1    | -5.11 | 108.94      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2777 | G    | N3-C4-N9    | 5.11  | 129.07      | 126.00   |
| 44  | BK    | 17   | ARG  | NE-CZ-NH2   | -5.11 | 117.74      | 120.30   |
| 52  | BS    | 4    | ILE  | CA-CB-CG1   | 5.11  | 120.71      | 111.00   |
| 1   | AA    | 88   | U    | N1-C2-O2    | 5.11  | 126.38      | 122.80   |
| 1   | AA    | 297  | G    | C6-C5-N7    | -5.11 | 127.33      | 130.40   |
| 1   | AA    | 871  | U    | N3-C4-C5    | -5.11 | 111.53      | 114.60   |
| 1   | AA    | 1237 | C    | N1-C2-O2    | 5.11  | 121.97      | 118.90   |
| 1   | AA    | 1343 | G    | P-O3'-C3'   | -5.11 | 113.57      | 119.70   |
| 35  | BB    | 794  | A    | C4-C5-N7    | -5.11 | 108.14      | 110.70   |
| 35  | BB    | 1777 | U    | C4-C5-C6    | 5.11  | 122.77      | 119.70   |
| 35  | BB    | 1809 | A    | N1-C2-N3    | -5.11 | 126.74      | 129.30   |
| 35  | BB    | 2558 | C    | N3-C2-O2    | 5.11  | 125.48      | 121.90   |
| 56  | BY    | 18   | LYS  | N-CA-CB     | 5.11  | 119.80      | 110.60   |
| 1   | AA    | 100  | G    | P-O3'-C3'   | -5.11 | 113.57      | 119.70   |
| 1   | AA    | 172  | A    | N1-C6-N6    | 5.11  | 121.67      | 118.60   |
| 14  | AN    | 53   | ASP  | CB-CG-OD2   | -5.11 | 113.70      | 118.30   |
| 35  | BB    | 34   | U    | C4'-C3'-C2' | -5.11 | 97.49       | 102.60   |
| 35  | BB    | 81   | G    | C8-N9-C4    | -5.11 | 104.36      | 106.40   |
| 35  | BB    | 183  | C    | OP1-P-O3'   | 5.11  | 116.44      | 105.20   |
| 35  | BB    | 392  | U    | C1'-O4'-C4' | 5.11  | 113.99      | 109.90   |
| 35  | BB    | 700  | G    | C6-N1-C2    | -5.11 | 122.03      | 125.10   |
| 35  | BB    | 706  | A    | N9-C1'-C2'  | -5.11 | 106.38      | 112.00   |
| 35  | BB    | 753  | A    | C4-C5-C6    | 5.11  | 119.56      | 117.00   |
| 35  | BB    | 756  | A    | C2-N3-C4    | 5.11  | 113.16      | 110.60   |
| 35  | BB    | 913  | U    | C5'-C4'-C3' | 5.11  | 124.18      | 116.00   |
| 35  | BB    | 1080 | A    | N3-C4-C5    | -5.11 | 123.22      | 126.80   |
| 35  | BB    | 1108 | U    | C5-C4-O4    | 5.11  | 128.97      | 125.90   |
| 35  | BB    | 1346 | G    | N7-C8-N9    | 5.11  | 115.66      | 113.10   |
| 35  | BB    | 1346 | G    | P-O5'-C5'   | -5.11 | 112.72      | 120.90   |
| 35  | BB    | 1383 | A    | N3-C4-C5    | -5.11 | 123.22      | 126.80   |
| 35  | BB    | 1413 | A    | N3-C4-C5    | -5.11 | 123.22      | 126.80   |
| 35  | BB    | 1814 | G    | C3'-C2'-C1' | 5.11  | 105.59      | 101.50   |
| 35  | BB    | 1884 | G    | N1-C2-N3    | -5.11 | 120.83      | 123.90   |
| 35  | BB    | 2676 | C    | C1'-O4'-C4' | -5.11 | 105.81      | 109.90   |
| 41  | BH    | 3    | VAL  | N-CA-C      | -5.11 | 97.20       | 111.00   |
| 50  | BQ    | 75   | TYR  | CD1-CE1-CZ  | 5.11  | 124.40      | 119.80   |
| 55  | BW    | 30   | ILE  | N-CA-C      | -5.11 | 97.20       | 111.00   |
| 1   | AA    | 20   | U    | C2-N3-C4    | 5.11  | 130.06      | 127.00   |
| 1   | AA    | 1087 | G    | C5-C6-N1    | -5.11 | 108.94      | 111.50   |
| 1   | AA    | 1143 | G    | C5-C6-O6    | -5.11 | 125.53      | 128.60   |
| 1   | AA    | 1401 | G    | C2-N3-C4    | -5.11 | 109.35      | 111.90   |
| 35  | BB    | 235  | U    | N3-C4-C5    | 5.11  | 117.67      | 114.60   |

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| Mol | Chain | Res   | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-------------|-------|-------------|----------|
| 35  | BB    | 486   | C    | C5-C6-N1    | -5.11 | 118.44      | 121.00   |
| 35  | BB    | 526   | A    | C5-N7-C8    | 5.11  | 106.45      | 103.90   |
| 35  | BB    | 879   | G    | P-O5'-C5'   | -5.11 | 112.73      | 120.90   |
| 35  | BB    | 1613  | G    | P-O3'-C3'   | -5.11 | 113.57      | 119.70   |
| 43  | BJ    | 74    | TYR  | N-CA-C      | -5.11 | 97.20       | 111.00   |
| 1   | AA    | 487   | A    | P-O5'-C5'   | -5.11 | 112.73      | 120.90   |
| 1   | AA    | 659   | U    | C5-C4-O4    | -5.11 | 122.84      | 125.90   |
| 1   | AA    | 901   | A    | C4-C5-C6    | 5.11  | 119.55      | 117.00   |
| 1   | AA    | 1088  | G    | P-O3'-C3'   | -5.11 | 113.57      | 119.70   |
| 1   | AA    | 1195  | C    | N1-C1'-C2'  | -5.11 | 106.38      | 112.00   |
| 1   | AA    | 1204  | A    | C5-C6-N1    | -5.11 | 115.15      | 117.70   |
| 1   | AA    | 1232  | U    | N3-C4-O4    | 5.11  | 122.98      | 119.40   |
| 7   | AG    | 99    | ALA  | CB-CA-C     | -5.11 | 102.44      | 110.10   |
| 34  | BA    | 86    | G    | O4'-C1'-N9  | 5.11  | 112.29      | 108.20   |
| 35  | BB    | 131   | A    | N7-C8-N9    | -5.11 | 111.25      | 113.80   |
| 35  | BB    | 173   | A    | O4'-C4'-C3' | -5.11 | 98.89       | 104.00   |
| 35  | BB    | 269   | C    | C5-C4-N4    | -5.11 | 116.62      | 120.20   |
| 35  | BB    | 674   | G    | C5-C6-N1    | -5.11 | 108.95      | 111.50   |
| 35  | BB    | 1829  | A    | N1-C6-N6    | 5.11  | 121.66      | 118.60   |
| 35  | BB    | 1830  | C    | C5'-C4'-O4' | 5.11  | 115.23      | 109.10   |
| 35  | BB    | 2634  | A    | OP2-P-O3'   | 5.11  | 116.44      | 105.20   |
| 35  | BB    | 2660  | A    | C5-N7-C8    | 5.11  | 106.45      | 103.90   |
| 35  | BB    | 2702  | G    | C6-N1-C2    | 5.11  | 128.16      | 125.10   |
| 35  | BB    | 2883  | A    | N9-C4-C5    | 5.11  | 107.84      | 105.80   |
| 40  | BG    | 89    | VAL  | C-N-CA      | 5.11  | 133.03      | 122.30   |
| 54  | BU    | 13    | LEU  | CA-CB-CG    | 5.11  | 127.05      | 115.30   |
| 1   | AA    | 675   | A    | O5'-C5'-C4' | -5.11 | 102.00      | 111.70   |
| 1   | AA    | 1339  | A    | C6-C5-N7    | -5.11 | 128.73      | 132.30   |
| 1   | AA    | 1368  | A    | C3'-C2'-C1' | 5.11  | 105.58      | 101.50   |
| 22  | AV    | 17(A) | U    | O4'-C1'-N1  | 5.11  | 112.28      | 108.20   |
| 32  | B7    | 13    | PHE  | CD1-CE1-CZ  | 5.11  | 126.23      | 120.10   |
| 35  | BB    | 446   | G    | N3-C4-N9    | 5.11  | 129.06      | 126.00   |
| 35  | BB    | 497   | A    | N3-C4-N9    | -5.11 | 123.32      | 127.40   |
| 35  | BB    | 1199  | U    | C2-N1-C1'   | -5.11 | 111.57      | 117.70   |
| 35  | BB    | 2146  | C    | C4'-C3'-C2' | -5.11 | 97.50       | 102.60   |
| 35  | BB    | 2502  | G    | O4'-C1'-C2' | 5.11  | 112.20      | 107.60   |
| 35  | BB    | 2521  | C    | O4'-C1'-N1  | 5.11  | 112.28      | 108.20   |
| 35  | BB    | 2546  | U    | P-O3'-C3'   | 5.11  | 125.83      | 119.70   |
| 35  | BB    | 2590  | A    | C5-N7-C8    | 5.11  | 106.45      | 103.90   |
| 35  | BB    | 2605  | U    | C6-N1-C2    | -5.11 | 117.94      | 121.00   |
| 35  | BB    | 2809  | A    | C5'-C4'-C3' | 5.11  | 124.17      | 116.00   |
| 35  | BB    | 2844  | G    | N1-C6-O6    | 5.11  | 122.96      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 965  | U    | N3-C4-O4    | 5.10  | 122.97      | 119.40   |
| 35  | BB    | 72   | U    | N1-C2-N3    | -5.10 | 111.84      | 114.90   |
| 35  | BB    | 143  | C    | P-O5'-C5'   | 5.10  | 129.07      | 120.90   |
| 35  | BB    | 550  | C    | C5-C6-N1    | 5.10  | 123.55      | 121.00   |
| 35  | BB    | 860  | U    | C1'-O4'-C4' | 5.10  | 113.98      | 109.90   |
| 35  | BB    | 890  | C    | C5-C6-N1    | 5.10  | 123.55      | 121.00   |
| 35  | BB    | 1176 | U    | O4'-C1'-N1  | 5.10  | 112.28      | 108.20   |
| 35  | BB    | 1893 | C    | C5'-C4'-O4' | -5.10 | 102.97      | 109.10   |
| 35  | BB    | 2023 | C    | C2-N3-C4    | -5.10 | 117.35      | 119.90   |
| 35  | BB    | 2262 | U    | N3-C4-O4    | 5.10  | 122.97      | 119.40   |
| 35  | BB    | 2785 | C    | N1-C2-N3    | -5.10 | 115.63      | 119.20   |
| 47  | BN    | 80   | PHE  | CZ-CE2-CD2  | -5.10 | 113.97      | 120.10   |
| 1   | AA    | 50   | A    | C5'-C4'-C3' | -5.10 | 107.84      | 116.00   |
| 1   | AA    | 446  | G    | C4'-C3'-C2' | -5.10 | 97.50       | 102.60   |
| 1   | AA    | 489  | C    | N3-C2-O2    | 5.10  | 125.47      | 121.90   |
| 1   | AA    | 1069 | C    | O4'-C1'-N1  | 5.10  | 112.28      | 108.20   |
| 35  | BB    | 600  | G    | O4'-C1'-N9  | 5.10  | 112.28      | 108.20   |
| 35  | BB    | 663  | G    | N1-C6-O6    | 5.10  | 122.96      | 119.90   |
| 35  | BB    | 717  | C    | C2-N3-C4    | 5.10  | 122.45      | 119.90   |
| 35  | BB    | 1674 | G    | C4-C5-C6    | 5.10  | 121.86      | 118.80   |
| 35  | BB    | 1723 | G    | N3-C4-C5    | 5.10  | 131.15      | 128.60   |
| 35  | BB    | 1959 | G    | N3-C4-N9    | -5.10 | 122.94      | 126.00   |
| 35  | BB    | 2352 | A    | C6-N1-C2    | 5.10  | 121.66      | 118.60   |
| 35  | BB    | 2486 | C    | N3-C4-N4    | 5.10  | 121.57      | 118.00   |
| 1   | AA    | 98   | A    | N9-C1'-C2'  | -5.10 | 106.39      | 112.00   |
| 1   | AA    | 677  | U    | C5'-C4'-C3' | -5.10 | 107.84      | 116.00   |
| 1   | AA    | 802  | A    | N7-C8-N9    | -5.10 | 111.25      | 113.80   |
| 1   | AA    | 922  | G    | C8-N9-C1'   | 5.10  | 133.63      | 127.00   |
| 1   | AA    | 1034 | G    | N3-C4-N9    | -5.10 | 122.94      | 126.00   |
| 1   | AA    | 1159 | U    | C2-N3-C4    | 5.10  | 130.06      | 127.00   |
| 35  | BB    | 123  | G    | C4-N9-C1'   | -5.10 | 119.87      | 126.50   |
| 35  | BB    | 529  | A    | C8-N9-C4    | -5.10 | 103.76      | 105.80   |
| 1   | AA    | 82   | G    | C3'-C2'-C1' | -5.10 | 97.42       | 101.50   |
| 1   | AA    | 827  | U    | N1-C2-O2    | -5.10 | 119.23      | 122.80   |
| 1   | AA    | 1058 | G    | C6-C5-N7    | -5.10 | 127.34      | 130.40   |
| 35  | BB    | 54   | G    | C3'-C2'-C1' | 5.10  | 105.58      | 101.50   |
| 35  | BB    | 72   | U    | N3-C2-O2    | -5.10 | 118.63      | 122.20   |
| 35  | BB    | 386  | G    | P-O3'-C3'   | -5.10 | 113.58      | 119.70   |
| 35  | BB    | 567  | U    | N1-C2-N3    | -5.10 | 111.84      | 114.90   |
| 35  | BB    | 761  | A    | O4'-C1'-N9  | 5.10  | 112.28      | 108.20   |
| 35  | BB    | 1105 | U    | C5-C6-N1    | 5.10  | 125.25      | 122.70   |
| 35  | BB    | 1254 | A    | C5-C6-N6    | 5.10  | 127.78      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1728 | C    | N3-C4-N4    | 5.10  | 121.57      | 118.00   |
| 35  | BB    | 2134 | A    | N3-C4-C5    | -5.10 | 123.23      | 126.80   |
| 35  | BB    | 2140 | G    | O4'-C1'-N9  | 5.10  | 112.28      | 108.20   |
| 35  | BB    | 2367 | G    | C5-N7-C8    | -5.10 | 101.75      | 104.30   |
| 35  | BB    | 2704 | C    | C4-C5-C6    | 5.10  | 119.95      | 117.40   |
| 49  | BP    | 35   | SER  | N-CA-CB     | 5.10  | 118.15      | 110.50   |
| 1   | AA    | 431  | A    | P-O3'-C3'   | 5.10  | 125.82      | 119.70   |
| 1   | AA    | 558  | G    | N3-C4-N9    | 5.10  | 129.06      | 126.00   |
| 1   | AA    | 906  | A    | O4'-C4'-C3' | -5.10 | 98.90       | 104.00   |
| 1   | AA    | 1005 | A    | C5'-C4'-C3' | -5.10 | 107.84      | 116.00   |
| 1   | AA    | 1064 | G    | C8-N9-C1'   | 5.10  | 133.63      | 127.00   |
| 1   | AA    | 1419 | G    | O5'-C5'-C4' | -5.10 | 102.01      | 111.70   |
| 9   | AI    | 112  | ARG  | NE-CZ-NH1   | -5.10 | 117.75      | 120.30   |
| 14  | AN    | 41   | TRP  | CB-CG-CD2   | -5.10 | 119.97      | 126.60   |
| 20  | AT    | 58   | ASP  | N-CA-CB     | 5.10  | 119.77      | 110.60   |
| 22  | AV    | 71   | C    | C2-N3-C4    | 5.10  | 122.45      | 119.90   |
| 35  | BB    | 27   | G    | C4'-C3'-C2' | -5.10 | 97.50       | 102.60   |
| 35  | BB    | 238  | C    | OP1-P-OP2   | -5.10 | 111.95      | 119.60   |
| 35  | BB    | 327  | G    | C4'-C3'-C2' | -5.10 | 97.50       | 102.60   |
| 35  | BB    | 534  | U    | O4'-C1'-N1  | 5.10  | 112.28      | 108.20   |
| 35  | BB    | 1145 | C    | C2-N3-C4    | 5.10  | 122.45      | 119.90   |
| 35  | BB    | 1954 | G    | C5-C6-N1    | 5.10  | 114.05      | 111.50   |
| 35  | BB    | 2038 | G    | N3-C4-N9    | -5.10 | 122.94      | 126.00   |
| 35  | BB    | 2276 | G    | N3-C4-C5    | 5.10  | 131.15      | 128.60   |
| 35  | BB    | 2553 | G    | P-O3'-C3'   | 5.10  | 125.82      | 119.70   |
| 35  | BB    | 2554 | U    | P-O5'-C5'   | 5.10  | 129.06      | 120.90   |
| 35  | BB    | 2894 | G    | C4-N9-C1'   | 5.10  | 133.13      | 126.50   |
| 39  | BF    | 96   | TRP  | CE3-CZ3-CH2 | 5.10  | 126.81      | 121.20   |
| 1   | AA    | 281  | G    | C8-N9-C1'   | -5.10 | 120.38      | 127.00   |
| 1   | AA    | 772  | U    | C5-C6-N1    | 5.10  | 125.25      | 122.70   |
| 22  | AV    | 5    | A    | C5-C6-N6    | -5.10 | 119.62      | 123.70   |
| 35  | BB    | 581  | C    | C6-N1-C2    | -5.10 | 118.26      | 120.30   |
| 35  | BB    | 804  | A    | C6-C5-N7    | -5.10 | 128.73      | 132.30   |
| 35  | BB    | 1954 | G    | N3-C4-C5    | -5.10 | 126.05      | 128.60   |
| 49  | BP    | 98   | TYR  | CD1-CE1-CZ  | -5.10 | 115.21      | 119.80   |
| 1   | AA    | 209  | U    | C5-C4-O4    | -5.09 | 122.84      | 125.90   |
| 1   | AA    | 344  | A    | C2-N3-C4    | 5.09  | 113.15      | 110.60   |
| 1   | AA    | 1001 | C    | C2-N1-C1'   | 5.09  | 124.41      | 118.80   |
| 1   | AA    | 1015 | G    | N3-C4-C5    | -5.09 | 126.05      | 128.60   |
| 1   | AA    | 1111 | A    | C4-C5-C6    | 5.09  | 119.55      | 117.00   |
| 1   | AA    | 1139 | G    | C5-C6-N1    | -5.09 | 108.95      | 111.50   |
| 1   | AA    | 1173 | U    | N1-C2-N3    | -5.09 | 111.84      | 114.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 51   | G    | N9-C1'-C2'  | -5.09 | 106.40      | 112.00   |
| 35  | BB    | 279  | A    | N1-C2-N3    | 5.09  | 131.85      | 129.30   |
| 35  | BB    | 321  | U    | C1'-O4'-C4' | -5.09 | 105.83      | 109.90   |
| 35  | BB    | 328  | U    | C5-C6-N1    | 5.09  | 125.25      | 122.70   |
| 35  | BB    | 453  | A    | N3-C4-C5    | 5.09  | 130.37      | 126.80   |
| 35  | BB    | 726  | G    | P-O5'-C5'   | 5.09  | 129.05      | 120.90   |
| 35  | BB    | 1244 | A    | C5-N7-C8    | 5.09  | 106.45      | 103.90   |
| 35  | BB    | 1610 | A    | C5'-C4'-C3' | -5.09 | 107.85      | 116.00   |
| 35  | BB    | 1744 | A    | C5-C6-N1    | -5.09 | 115.15      | 117.70   |
| 35  | BB    | 2426 | A    | N9-C4-C5    | 5.09  | 107.84      | 105.80   |
| 35  | BB    | 2824 | C    | N3-C4-N4    | 5.09  | 121.57      | 118.00   |
| 1   | AA    | 78   | A    | OP2-P-O3'   | 5.09  | 116.40      | 105.20   |
| 1   | AA    | 165  | G    | C2-N3-C4    | 5.09  | 114.45      | 111.90   |
| 1   | AA    | 217  | C    | C6-N1-C1'   | -5.09 | 114.69      | 120.80   |
| 13  | AM    | 22   | TYR  | CG-CD1-CE1  | -5.09 | 117.22      | 121.30   |
| 35  | BB    | 1973 | G    | N1-C6-O6    | 5.09  | 122.96      | 119.90   |
| 35  | BB    | 2132 | U    | O4'-C1'-N1  | 5.09  | 112.27      | 108.20   |
| 35  | BB    | 2539 | C    | N1-C2-N3    | -5.09 | 115.64      | 119.20   |
| 44  | BK    | 121  | GLU  | OE1-CD-OE2  | 5.09  | 129.41      | 123.30   |
| 1   | AA    | 112  | G    | C4-C5-C6    | 5.09  | 121.86      | 118.80   |
| 1   | AA    | 196  | A    | C2-N3-C4    | -5.09 | 108.06      | 110.60   |
| 1   | AA    | 445  | G    | C5-C6-N1    | -5.09 | 108.95      | 111.50   |
| 1   | AA    | 445  | G    | N3-C4-N9    | -5.09 | 122.94      | 126.00   |
| 1   | AA    | 634  | C    | C3'-C2'-C1' | -5.09 | 97.43       | 101.50   |
| 1   | AA    | 868  | C    | P-O5'-C5'   | -5.09 | 112.75      | 120.90   |
| 1   | AA    | 918  | A    | N9-C4-C5    | 5.09  | 107.84      | 105.80   |
| 1   | AA    | 1272 | G    | C4-C5-C6    | 5.09  | 121.86      | 118.80   |
| 1   | AA    | 1327 | C    | N1-C2-O2    | -5.09 | 115.84      | 118.90   |
| 35  | BB    | 218  | A    | O4'-C4'-C3' | 5.09  | 110.17      | 106.10   |
| 35  | BB    | 250  | G    | C5-C6-O6    | 5.09  | 131.66      | 128.60   |
| 35  | BB    | 577  | G    | N3-C2-N2    | 5.09  | 123.46      | 119.90   |
| 35  | BB    | 911  | A    | C1'-O4'-C4' | 5.09  | 113.97      | 109.90   |
| 35  | BB    | 913  | U    | C2-N3-C4    | 5.09  | 130.05      | 127.00   |
| 35  | BB    | 1120 | G    | N3-C4-N9    | -5.09 | 122.95      | 126.00   |
| 35  | BB    | 1733 | G    | C4-C5-N7    | -5.09 | 108.76      | 110.80   |
| 35  | BB    | 1829 | A    | O4'-C1'-N9  | 5.09  | 112.27      | 108.20   |
| 35  | BB    | 2031 | A    | C4-C5-N7    | -5.09 | 108.16      | 110.70   |
| 35  | BB    | 2209 | G    | C8-N9-C4    | -5.09 | 104.36      | 106.40   |
| 35  | BB    | 2780 | G    | C6-C5-N7    | -5.09 | 127.34      | 130.40   |
| 35  | BB    | 2799 | A    | N9-C4-C5    | 5.09  | 107.84      | 105.80   |
| 1   | AA    | 96   | U    | C3'-C2'-C1' | 5.09  | 105.57      | 101.50   |
| 1   | AA    | 574  | A    | C5-C6-N6    | -5.09 | 119.63      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 686  | U    | C1'-O4'-C4' | -5.09 | 105.83      | 109.90   |
| 1   | AA    | 726  | C    | C4'-C3'-C2' | -5.09 | 97.51       | 102.60   |
| 1   | AA    | 784  | A    | C5-N7-C8    | 5.09  | 106.44      | 103.90   |
| 1   | AA    | 1094 | G    | O3'-P-O5'   | -5.09 | 94.33       | 104.00   |
| 1   | AA    | 1104 | G    | C6-N1-C2    | -5.09 | 122.05      | 125.10   |
| 1   | AA    | 1340 | A    | C1'-O4'-C4' | 5.09  | 113.97      | 109.90   |
| 22  | AV    | 7    | G    | N1-C2-N2    | -5.09 | 111.62      | 116.20   |
| 29  | B4    | 38   | PHE  | CB-CG-CD2   | -5.09 | 117.24      | 120.80   |
| 35  | BB    | 207  | A    | N9-C4-C5    | -5.09 | 103.76      | 105.80   |
| 35  | BB    | 401  | A    | C5-C6-N6    | -5.09 | 119.63      | 123.70   |
| 35  | BB    | 617  | G    | N7-C8-N9    | -5.09 | 110.56      | 113.10   |
| 35  | BB    | 705  | A    | P-O3'-C3'   | 5.09  | 125.81      | 119.70   |
| 35  | BB    | 815  | C    | C2-N3-C4    | 5.09  | 122.44      | 119.90   |
| 35  | BB    | 903  | C    | O4'-C1'-N1  | 5.09  | 112.27      | 108.20   |
| 35  | BB    | 953  | G    | N9-C4-C5    | -5.09 | 103.36      | 105.40   |
| 35  | BB    | 1168 | G    | N1-C2-N3    | -5.09 | 120.85      | 123.90   |
| 35  | BB    | 1482 | G    | N3-C2-N2    | 5.09  | 123.46      | 119.90   |
| 35  | BB    | 1504 | A    | N7-C8-N9    | 5.09  | 116.34      | 113.80   |
| 35  | BB    | 1957 | C    | C4'-C3'-C2' | -5.09 | 97.51       | 102.60   |
| 35  | BB    | 2490 | G    | C5-C6-N1    | -5.09 | 108.95      | 111.50   |
| 35  | BB    | 2880 | C    | C5-C6-N1    | -5.09 | 118.45      | 121.00   |
| 40  | BG    | 136  | ASP  | N-CA-CB     | 5.09  | 119.76      | 110.60   |
| 1   | AA    | 391  | G    | C4'-C3'-C2' | -5.09 | 97.51       | 102.60   |
| 1   | AA    | 585  | G    | N3-C4-N9    | 5.09  | 129.05      | 126.00   |
| 35  | BB    | 1023 | U    | N3-C2-O2    | 5.09  | 125.76      | 122.20   |
| 35  | BB    | 1964 | G    | C4-C5-C6    | 5.09  | 121.85      | 118.80   |
| 1   | AA    | 831  | A    | C4-C5-C6    | 5.09  | 119.54      | 117.00   |
| 1   | AA    | 919  | A    | C4-C5-N7    | 5.09  | 113.24      | 110.70   |
| 1   | AA    | 971  | G    | N1-C6-O6    | 5.09  | 122.95      | 119.90   |
| 1   | AA    | 1373 | G    | O4'-C4'-C3' | -5.09 | 98.91       | 104.00   |
| 1   | AA    | 1498 | U    | C5-C6-N1    | -5.09 | 120.16      | 122.70   |
| 1   | AA    | 1534 | A    | O4'-C1'-N9  | 5.09  | 112.27      | 108.20   |
| 2   | AB    | 183  | PHE  | CB-CG-CD1   | 5.09  | 124.36      | 120.80   |
| 30  | B5    | 179  | ASP  | O-C-N       | -5.09 | 114.56      | 122.70   |
| 35  | BB    | 301  | G    | C4-C5-N7    | -5.09 | 108.77      | 110.80   |
| 35  | BB    | 404  | A    | N9-C4-C5    | -5.09 | 103.77      | 105.80   |
| 35  | BB    | 435  | C    | C5-C4-N4    | -5.09 | 116.64      | 120.20   |
| 35  | BB    | 599  | A    | C4-C5-C6    | 5.09  | 119.54      | 117.00   |
| 35  | BB    | 671  | C    | C5-C4-N4    | -5.09 | 116.64      | 120.20   |
| 35  | BB    | 863  | A    | C5-C6-N1    | -5.09 | 115.16      | 117.70   |
| 35  | BB    | 986  | C    | N3-C2-O2    | 5.09  | 125.46      | 121.90   |
| 35  | BB    | 1037 | G    | C4-C5-C6    | 5.09  | 121.85      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1120 | G    | OP1-P-OP2   | -5.09 | 111.97      | 119.60   |
| 35  | BB    | 1173 | U    | N3-C4-O4    | 5.09  | 122.96      | 119.40   |
| 35  | BB    | 1174 | U    | C4-C5-C6    | -5.09 | 116.65      | 119.70   |
| 35  | BB    | 1318 | U    | C6-N1-C2    | -5.09 | 117.95      | 121.00   |
| 35  | BB    | 1412 | U    | N1-C2-O2    | 5.09  | 126.36      | 122.80   |
| 35  | BB    | 1488 | C    | OP1-P-O3'   | 5.09  | 116.39      | 105.20   |
| 35  | BB    | 1664 | A    | C4-C5-N7    | -5.09 | 108.16      | 110.70   |
| 35  | BB    | 2197 | U    | N1-C2-N3    | -5.09 | 111.85      | 114.90   |
| 35  | BB    | 2288 | A    | N7-C8-N9    | -5.09 | 111.26      | 113.80   |
| 35  | BB    | 2566 | A    | N1-C2-N3    | -5.09 | 126.76      | 129.30   |
| 35  | BB    | 2855 | C    | N1-C1'-C2'  | -5.09 | 106.41      | 112.00   |
| 35  | BB    | 2884 | U    | C4-C5-C6    | 5.09  | 122.75      | 119.70   |
| 1   | AA    | 378  | G    | N3-C2-N2    | 5.08  | 123.46      | 119.90   |
| 1   | AA    | 660  | C    | C5-C4-N4    | -5.08 | 116.64      | 120.20   |
| 1   | AA    | 1359 | C    | C5'-C4'-O4' | 5.08  | 115.20      | 109.10   |
| 1   | AA    | 1368 | A    | OP1-P-OP2   | -5.08 | 111.97      | 119.60   |
| 35  | BB    | 189  | G    | C4-C5-C6    | 5.08  | 121.85      | 118.80   |
| 35  | BB    | 396  | G    | N9-C1'-C2'  | -5.08 | 106.41      | 112.00   |
| 35  | BB    | 1071 | G    | C5-C6-O6    | -5.08 | 125.55      | 128.60   |
| 35  | BB    | 1868 | C    | C2-N1-C1'   | -5.08 | 113.21      | 118.80   |
| 35  | BB    | 1880 | U    | C6-N1-C2    | -5.08 | 117.95      | 121.00   |
| 35  | BB    | 1981 | A    | N1-C2-N3    | 5.08  | 131.84      | 129.30   |
| 35  | BB    | 2622 | U    | N1-C2-O2    | 5.08  | 126.36      | 122.80   |
| 35  | BB    | 2741 | A    | OP1-P-OP2   | -5.08 | 111.97      | 119.60   |
| 1   | AA    | 520  | A    | C4-C5-N7    | -5.08 | 108.16      | 110.70   |
| 1   | AA    | 644  | U    | C2-N3-C4    | -5.08 | 123.95      | 127.00   |
| 1   | AA    | 664  | G    | C6-C5-N7    | -5.08 | 127.35      | 130.40   |
| 1   | AA    | 947  | G    | C6-C5-N7    | -5.08 | 127.35      | 130.40   |
| 1   | AA    | 1513 | A    | OP1-P-OP2   | -5.08 | 111.97      | 119.60   |
| 35  | BB    | 115  | C    | C5'-C4'-O4' | -5.08 | 103.00      | 109.10   |
| 35  | BB    | 265  | A    | C4'-C3'-C2' | -5.08 | 97.52       | 102.60   |
| 35  | BB    | 1284 | A    | O4'-C1'-N9  | 5.08  | 112.27      | 108.20   |
| 35  | BB    | 1346 | G    | C8-N9-C4    | -5.08 | 104.37      | 106.40   |
| 35  | BB    | 1399 | C    | C4-C5-C6    | 5.08  | 119.94      | 117.40   |
| 35  | BB    | 1776 | G    | C3'-C2'-C1' | 5.08  | 105.57      | 101.50   |
| 35  | BB    | 1984 | G    | C3'-C2'-C1' | 5.08  | 105.57      | 101.50   |
| 35  | BB    | 2068 | U    | C4'-C3'-C2' | -5.08 | 97.52       | 102.60   |
| 35  | BB    | 2619 | C    | N1-C2-O2    | 5.08  | 121.95      | 118.90   |
| 35  | BB    | 2623 | G    | N1-C2-N2    | 5.08  | 120.78      | 116.20   |
| 35  | BB    | 2708 | G    | C2-N3-C4    | 5.08  | 114.44      | 111.90   |
| 35  | BB    | 2708 | G    | C5-C6-N1    | -5.08 | 108.96      | 111.50   |
| 35  | BB    | 2840 | C    | C6-N1-C2    | -5.08 | 118.27      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 113  | G    | N3-C4-N9    | -5.08 | 122.95      | 126.00   |
| 1   | AA    | 146  | G    | C3'-C2'-C1' | 5.08  | 105.57      | 101.50   |
| 1   | AA    | 501  | C    | C3'-C2'-C1' | -5.08 | 97.44       | 101.50   |
| 1   | AA    | 529  | G    | C5-C6-N1    | 5.08  | 114.04      | 111.50   |
| 1   | AA    | 669  | G    | C3'-C2'-C1' | -5.08 | 97.44       | 101.50   |
| 1   | AA    | 883  | C    | N1-C2-O2    | -5.08 | 115.85      | 118.90   |
| 1   | AA    | 1079 | G    | C6-C5-N7    | -5.08 | 127.35      | 130.40   |
| 1   | AA    | 1186 | G    | N1-C6-O6    | 5.08  | 122.95      | 119.90   |
| 1   | AA    | 1304 | G    | N9-C4-C5    | -5.08 | 103.37      | 105.40   |
| 1   | AA    | 1388 | C    | C3'-C2'-C1' | -5.08 | 97.44       | 101.50   |
| 1   | AA    | 1522 | U    | N3-C2-O2    | -5.08 | 118.64      | 122.20   |
| 5   | AE    | 24   | VAL  | CA-CB-CG1   | 5.08  | 118.52      | 110.90   |
| 12  | AL    | 120  | ARG  | NE-CZ-NH2   | -5.08 | 117.76      | 120.30   |
| 34  | BA    | 117  | G    | C8-N9-C4    | -5.08 | 104.37      | 106.40   |
| 35  | BB    | 205  | G    | C5-C6-O6    | -5.08 | 125.55      | 128.60   |
| 35  | BB    | 377  | G    | P-O3'-C3'   | -5.08 | 113.60      | 119.70   |
| 35  | BB    | 1001 | A    | C4-C5-N7    | 5.08  | 113.24      | 110.70   |
| 35  | BB    | 1679 | A    | OP2-P-O3'   | 5.08  | 116.38      | 105.20   |
| 35  | BB    | 1818 | U    | N3-C2-O2    | 5.08  | 125.76      | 122.20   |
| 35  | BB    | 1920 | C    | C6-N1-C2    | -5.08 | 118.27      | 120.30   |
| 35  | BB    | 1921 | G    | C6-N1-C2    | 5.08  | 128.15      | 125.10   |
| 35  | BB    | 2844 | G    | C5'-C4'-C3' | -5.08 | 107.87      | 116.00   |
| 1   | AA    | 1380 | U    | OP1-P-OP2   | -5.08 | 111.98      | 119.60   |
| 35  | BB    | 1234 | U    | N1-C2-N3    | -5.08 | 111.85      | 114.90   |
| 35  | BB    | 1237 | A    | C4'-C3'-C2' | -5.08 | 97.52       | 102.60   |
| 35  | BB    | 1674 | G    | N3-C4-N9    | -5.08 | 122.95      | 126.00   |
| 35  | BB    | 2396 | G    | C5'-C4'-C3' | -5.08 | 107.87      | 116.00   |
| 53  | BT    | 84   | TYR  | N-CA-CB     | 5.08  | 119.74      | 110.60   |
| 1   | AA    | 195  | A    | N9-C1'-C2'  | -5.08 | 106.41      | 112.00   |
| 1   | AA    | 283  | U    | O4'-C1'-N1  | 5.08  | 112.26      | 108.20   |
| 1   | AA    | 306  | A    | C6-N1-C2    | 5.08  | 121.65      | 118.60   |
| 1   | AA    | 664  | G    | C5-C6-N1    | -5.08 | 108.96      | 111.50   |
| 1   | AA    | 1313 | U    | C5-C6-N1    | 5.08  | 125.24      | 122.70   |
| 1   | AA    | 1350 | A    | C2-N3-C4    | -5.08 | 108.06      | 110.60   |
| 1   | AA    | 1499 | A    | N3-C4-C5    | -5.08 | 123.25      | 126.80   |
| 4   | AD    | 162  | GLU  | OE1-CD-OE2  | 5.08  | 129.40      | 123.30   |
| 22  | AV    | 32   | A    | N1-C6-N6    | 5.08  | 121.65      | 118.60   |
| 27  | B2    | 54   | VAL  | CA-CB-CG1   | -5.08 | 103.28      | 110.90   |
| 34  | BA    | 79   | G    | C5'-C4'-C3' | -5.08 | 107.88      | 116.00   |
| 35  | BB    | 35   | G    | O4'-C4'-C3' | -5.08 | 98.92       | 104.00   |
| 35  | BB    | 153  | U    | C3'-C2'-C1' | 5.08  | 105.56      | 101.50   |
| 35  | BB    | 179  | C    | N3-C4-N4    | 5.08  | 121.56      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 192  | C    | O4'-C1'-N1  | 5.08  | 112.26      | 108.20   |
| 35  | BB    | 1633 | G    | N7-C8-N9    | -5.08 | 110.56      | 113.10   |
| 35  | BB    | 1669 | A    | N9-C4-C5    | 5.08  | 107.83      | 105.80   |
| 35  | BB    | 2137 | U    | P-O3'-C3'   | 5.08  | 125.80      | 119.70   |
| 35  | BB    | 2184 | A    | C1'-O4'-C4' | 5.08  | 113.96      | 109.90   |
| 35  | BB    | 2383 | G    | O4'-C1'-N9  | 5.08  | 112.26      | 108.20   |
| 51  | BR    | 55   | ASP  | N-CA-CB     | 5.08  | 119.74      | 110.60   |
| 1   | AA    | 138  | G    | C4-N9-C1'   | -5.08 | 119.90      | 126.50   |
| 1   | AA    | 670  | G    | N3-C4-C5    | 5.08  | 131.14      | 128.60   |
| 10  | AJ    | 70   | HIS  | CA-CB-CG    | -5.08 | 104.97      | 113.60   |
| 34  | BA    | 72   | G    | C6-C5-N7    | -5.08 | 127.35      | 130.40   |
| 35  | BB    | 1941 | C    | C4-C5-C6    | -5.08 | 114.86      | 117.40   |
| 35  | BB    | 2214 | C    | C6-N1-C2    | -5.08 | 118.27      | 120.30   |
| 35  | BB    | 2588 | G    | C8-N9-C1'   | -5.08 | 120.40      | 127.00   |
| 35  | BB    | 2598 | A    | C8-N9-C4    | 5.08  | 107.83      | 105.80   |
| 1   | AA    | 45   | G    | C5'-C4'-O4' | -5.08 | 103.01      | 109.10   |
| 1   | AA    | 241  | G    | C4-C5-C6    | 5.08  | 121.84      | 118.80   |
| 1   | AA    | 354  | G    | O4'-C1'-N9  | 5.08  | 112.26      | 108.20   |
| 1   | AA    | 623  | C    | OP2-P-O3'   | 5.08  | 116.36      | 105.20   |
| 1   | AA    | 723  | U    | N3-C2-O2    | 5.08  | 125.75      | 122.20   |
| 1   | AA    | 738  | C    | C4-C5-C6    | -5.08 | 114.86      | 117.40   |
| 1   | AA    | 833  | G    | C4-C5-C6    | 5.08  | 121.85      | 118.80   |
| 1   | AA    | 997  | U    | N1-C2-N3    | -5.08 | 111.85      | 114.90   |
| 1   | AA    | 1400 | C    | C1'-O4'-C4' | -5.08 | 105.84      | 109.90   |
| 4   | AD    | 174  | ALA  | CA-C-N      | 5.08  | 126.35      | 116.20   |
| 6   | AF    | 92   | THR  | CA-CB-CG2   | -5.08 | 105.29      | 112.40   |
| 35  | BB    | 56   | A    | N1-C6-N6    | 5.08  | 121.65      | 118.60   |
| 35  | BB    | 78   | U    | C6-N1-C2    | -5.08 | 117.95      | 121.00   |
| 35  | BB    | 181  | A    | N3-C4-C5    | -5.08 | 123.25      | 126.80   |
| 35  | BB    | 437  | U    | N3-C4-O4    | 5.08  | 122.95      | 119.40   |
| 35  | BB    | 553  | G    | N7-C8-N9    | -5.08 | 110.56      | 113.10   |
| 35  | BB    | 670  | A    | C4-N9-C1'   | 5.08  | 135.44      | 126.30   |
| 35  | BB    | 679  | C    | P-O5'-C5'   | -5.08 | 112.78      | 120.90   |
| 35  | BB    | 1400 | U    | P-O3'-C3'   | -5.08 | 113.61      | 119.70   |
| 35  | BB    | 1478 | G    | O4'-C1'-N9  | 5.08  | 112.26      | 108.20   |
| 35  | BB    | 1501 | G    | N9-C4-C5    | -5.08 | 103.37      | 105.40   |
| 35  | BB    | 1623 | G    | C8-N9-C4    | 5.08  | 108.43      | 106.40   |
| 35  | BB    | 1667 | G    | C6-N1-C2    | 5.08  | 128.15      | 125.10   |
| 35  | BB    | 2110 | G    | C1'-O4'-C4' | 5.08  | 113.96      | 109.90   |
| 35  | BB    | 2257 | U    | O4'-C1'-N1  | 5.08  | 112.26      | 108.20   |
| 35  | BB    | 2610 | C    | C3'-C2'-C1' | -5.08 | 97.44       | 101.50   |
| 35  | BB    | 2627 | G    | P-O3'-C3'   | 5.08  | 125.79      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 50  | BQ    | 18   | LYS  | N-CA-CB     | 5.08  | 119.74      | 110.60   |
| 1   | AA    | 32   | A    | N3-C4-C5    | -5.07 | 123.25      | 126.80   |
| 1   | AA    | 190  | A    | C3'-C2'-C1' | -5.07 | 97.44       | 101.50   |
| 1   | AA    | 645  | G    | C5-N7-C8    | 5.07  | 106.84      | 104.30   |
| 1   | AA    | 1019 | A    | N1-C2-N3    | -5.07 | 126.76      | 129.30   |
| 1   | AA    | 1275 | A    | C1'-O4'-C4' | -5.07 | 105.84      | 109.90   |
| 1   | AA    | 1410 | A    | O4'-C1'-N9  | 5.07  | 112.26      | 108.20   |
| 2   | AB    | 158  | ASP  | O-C-N       | -5.07 | 114.58      | 122.70   |
| 13  | AM    | 75   | SER  | CB-CA-C     | -5.07 | 100.46      | 110.10   |
| 35  | BB    | 249  | C    | O4'-C4'-C3' | 5.07  | 110.16      | 106.10   |
| 35  | BB    | 268  | C    | N3-C2-O2    | -5.07 | 118.35      | 121.90   |
| 35  | BB    | 857  | G    | P-O3'-C3'   | -5.07 | 113.61      | 119.70   |
| 35  | BB    | 916  | G    | C1'-O4'-C4' | -5.07 | 105.84      | 109.90   |
| 35  | BB    | 1454 | C    | C5-C6-N1    | 5.07  | 123.54      | 121.00   |
| 35  | BB    | 1496 | A    | C4-C5-C6    | 5.07  | 119.54      | 117.00   |
| 35  | BB    | 2149 | U    | P-O3'-C3'   | 5.07  | 125.79      | 119.70   |
| 35  | BB    | 2220 | U    | C5-C4-O4    | 5.07  | 128.94      | 125.90   |
| 35  | BB    | 2402 | U    | C4-C5-C6    | -5.07 | 116.66      | 119.70   |
| 1   | AA    | 133  | U    | N1-C2-O2    | -5.07 | 119.25      | 122.80   |
| 1   | AA    | 432  | A    | C3'-C2'-C1' | -5.07 | 97.44       | 101.50   |
| 1   | AA    | 722  | G    | N9-C4-C5    | 5.07  | 107.43      | 105.40   |
| 35  | BB    | 32   | C    | C6-N1-C2    | -5.07 | 118.27      | 120.30   |
| 35  | BB    | 877  | A    | C5-N7-C8    | 5.07  | 106.44      | 103.90   |
| 35  | BB    | 1235 | G    | C5-C6-N1    | -5.07 | 108.96      | 111.50   |
| 35  | BB    | 2810 | A    | C5-C6-N6    | -5.07 | 119.64      | 123.70   |
| 47  | BN    | 45   | ARG  | NE-CZ-NH1   | -5.07 | 117.76      | 120.30   |
| 1   | AA    | 6    | G    | C4-C5-N7    | 5.07  | 112.83      | 110.80   |
| 1   | AA    | 84   | U    | N3-C4-O4    | 5.07  | 122.95      | 119.40   |
| 1   | AA    | 141  | G    | P-O5'-C5'   | -5.07 | 112.79      | 120.90   |
| 1   | AA    | 303  | A    | C5-N7-C8    | -5.07 | 101.36      | 103.90   |
| 1   | AA    | 585  | G    | N1-C6-O6    | 5.07  | 122.94      | 119.90   |
| 1   | AA    | 633  | G    | N1-C2-N2    | -5.07 | 111.64      | 116.20   |
| 1   | AA    | 689  | C    | C2-N1-C1'   | 5.07  | 124.38      | 118.80   |
| 2   | AB    | 77   | GLU  | N-CA-CB     | 5.07  | 119.73      | 110.60   |
| 35  | BB    | 44   | A    | N7-C8-N9    | -5.07 | 111.27      | 113.80   |
| 35  | BB    | 127  | A    | O4'-C1'-N9  | 5.07  | 112.26      | 108.20   |
| 35  | BB    | 656  | G    | C6-N1-C2    | 5.07  | 128.14      | 125.10   |
| 35  | BB    | 956  | G    | P-O3'-C3'   | -5.07 | 113.61      | 119.70   |
| 35  | BB    | 1203 | U    | C3'-C2'-C1' | 5.07  | 105.56      | 101.50   |
| 35  | BB    | 1309 | G    | N3-C4-C5    | -5.07 | 126.06      | 128.60   |
| 35  | BB    | 1683 | U    | P-O5'-C5'   | 5.07  | 129.01      | 120.90   |
| 35  | BB    | 1938 | A    | C5-C6-N1    | -5.07 | 115.17      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2093 | G    | N3-C4-C5    | 5.07  | 131.14      | 128.60   |
| 35  | BB    | 2238 | G    | C8-N9-C4    | 5.07  | 108.43      | 106.40   |
| 35  | BB    | 2751 | G    | C4-C5-C6    | 5.07  | 121.84      | 118.80   |
| 45  | BL    | 48   | ARG  | NE-CZ-NH2   | 5.07  | 122.83      | 120.30   |
| 48  | BO    | 97   | PHE  | O-C-N       | 5.07  | 130.81      | 122.70   |
| 1   | AA    | 773  | G    | N3-C4-N9    | 5.07  | 129.04      | 126.00   |
| 1   | AA    | 868  | C    | N3-C2-O2    | -5.07 | 118.35      | 121.90   |
| 35  | BB    | 378  | C    | P-O3'-C3'   | -5.07 | 113.62      | 119.70   |
| 35  | BB    | 1473 | G    | N3-C4-N9    | -5.07 | 122.96      | 126.00   |
| 35  | BB    | 1643 | G    | N1-C2-N3    | -5.07 | 120.86      | 123.90   |
| 35  | BB    | 2117 | A    | N9-C1'-C2'  | -5.07 | 106.42      | 112.00   |
| 35  | BB    | 2396 | G    | C5-C6-N1    | 5.07  | 114.03      | 111.50   |
| 35  | BB    | 2471 | A    | C4'-C3'-C2' | -5.07 | 97.53       | 102.60   |
| 1   | AA    | 400  | C    | C1'-O4'-C4' | 5.07  | 113.95      | 109.90   |
| 1   | AA    | 567  | G    | C4-C5-N7    | 5.07  | 112.83      | 110.80   |
| 1   | AA    | 1372 | U    | N1-C2-N3    | 5.07  | 117.94      | 114.90   |
| 2   | AB    | 31   | PHE  | CB-CG-CD2   | -5.07 | 117.25      | 120.80   |
| 35  | BB    | 679  | C    | OP1-P-O3'   | 5.07  | 116.35      | 105.20   |
| 35  | BB    | 680  | C    | N3-C2-O2    | 5.07  | 125.45      | 121.90   |
| 35  | BB    | 1354 | A    | C4-N9-C1'   | -5.07 | 117.18      | 126.30   |
| 35  | BB    | 1357 | C    | C2-N3-C4    | 5.07  | 122.43      | 119.90   |
| 35  | BB    | 1444 | G    | O4'-C1'-C2' | -5.07 | 100.73      | 105.80   |
| 35  | BB    | 1536 | C    | OP1-P-O3'   | 5.07  | 116.35      | 105.20   |
| 35  | BB    | 1810 | A    | C8-N9-C4    | -5.07 | 103.77      | 105.80   |
| 35  | BB    | 2002 | G    | N3-C2-N2    | 5.07  | 123.45      | 119.90   |
| 35  | BB    | 2257 | U    | C5-C6-N1    | -5.07 | 120.17      | 122.70   |
| 35  | BB    | 2261 | C    | C6-N1-C1'   | -5.07 | 114.72      | 120.80   |
| 35  | BB    | 2669 | G    | P-O3'-C3'   | -5.07 | 113.62      | 119.70   |
| 1   | AA    | 354  | G    | C5-C6-O6    | -5.07 | 125.56      | 128.60   |
| 1   | AA    | 548  | G    | N1-C6-O6    | 5.07  | 122.94      | 119.90   |
| 1   | AA    | 615  | G    | N3-C2-N2    | 5.07  | 123.45      | 119.90   |
| 1   | AA    | 1293 | C    | N3-C4-N4    | 5.07  | 121.55      | 118.00   |
| 1   | AA    | 1295 | U    | C2-N3-C4    | -5.07 | 123.96      | 127.00   |
| 1   | AA    | 1297 | G    | N3-C2-N2    | 5.07  | 123.45      | 119.90   |
| 35  | BB    | 187  | G    | N3-C4-C5    | 5.07  | 131.13      | 128.60   |
| 35  | BB    | 264  | C    | N3-C2-O2    | 5.07  | 125.45      | 121.90   |
| 35  | BB    | 420  | C    | P-O5'-C5'   | -5.07 | 112.79      | 120.90   |
| 35  | BB    | 682  | G    | O4'-C1'-N9  | 5.07  | 112.25      | 108.20   |
| 35  | BB    | 735  | A    | O4'-C1'-N9  | 5.07  | 112.25      | 108.20   |
| 35  | BB    | 760  | G    | O4'-C1'-N9  | 5.07  | 112.25      | 108.20   |
| 35  | BB    | 1145 | C    | C4-C5-C6    | -5.07 | 114.87      | 117.40   |
| 35  | BB    | 1771 | C    | C1'-O4'-C4' | -5.07 | 105.85      | 109.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2280 | G    | N1-C2-N3    | -5.07 | 120.86      | 123.90   |
| 35  | BB    | 2334 | U    | C2'-C3'-O3' | 5.07  | 121.81      | 113.70   |
| 35  | BB    | 2718 | G    | C6-N1-C2    | 5.07  | 128.14      | 125.10   |
| 1   | AA    | 130  | A    | C5-C6-N1    | -5.06 | 115.17      | 117.70   |
| 1   | AA    | 273  | U    | O4'-C1'-N1  | 5.06  | 112.25      | 108.20   |
| 1   | AA    | 463  | U    | N3-C2-O2    | 5.06  | 125.75      | 122.20   |
| 1   | AA    | 541  | G    | C8-N9-C4    | 5.06  | 108.43      | 106.40   |
| 1   | AA    | 1093 | A    | C6-C5-N7    | -5.06 | 128.75      | 132.30   |
| 35  | BB    | 595  | C    | N3-C4-N4    | 5.06  | 121.55      | 118.00   |
| 35  | BB    | 845  | A    | O4'-C1'-N9  | 5.06  | 112.25      | 108.20   |
| 35  | BB    | 1017 | G    | N3-C4-N9    | 5.06  | 129.04      | 126.00   |
| 35  | BB    | 1056 | G    | C5'-C4'-C3' | 5.06  | 124.10      | 116.00   |
| 35  | BB    | 1667 | G    | OP2-P-O3'   | 5.06  | 116.34      | 105.20   |
| 35  | BB    | 2042 | A    | N7-C8-N9    | -5.06 | 111.27      | 113.80   |
| 35  | BB    | 2152 | G    | C5'-C4'-O4' | 5.06  | 115.18      | 109.10   |
| 35  | BB    | 2251 | G    | N1-C2-N2    | -5.06 | 111.64      | 116.20   |
| 1   | AA    | 164  | G    | OP1-P-OP2   | -5.06 | 112.01      | 119.60   |
| 1   | AA    | 580  | C    | C2-N3-C4    | -5.06 | 117.37      | 119.90   |
| 1   | AA    | 587  | G    | P-O3'-C3'   | 5.06  | 125.78      | 119.70   |
| 1   | AA    | 650  | G    | N3-C2-N2    | 5.06  | 123.44      | 119.90   |
| 1   | AA    | 891  | U    | N3-C4-O4    | 5.06  | 122.94      | 119.40   |
| 1   | AA    | 1017 | U    | P-O3'-C3'   | -5.06 | 113.62      | 119.70   |
| 1   | AA    | 1064 | G    | C6-N1-C2    | 5.06  | 128.14      | 125.10   |
| 1   | AA    | 1397 | C    | OP1-P-OP2   | -5.06 | 112.01      | 119.60   |
| 34  | BA    | 54   | G    | C3'-C2'-C1' | -5.06 | 97.45       | 101.50   |
| 34  | BA    | 61   | G    | O4'-C1'-N9  | 5.06  | 112.25      | 108.20   |
| 34  | BA    | 84   | G    | O4'-C1'-N9  | 5.06  | 112.25      | 108.20   |
| 35  | BB    | 339  | U    | P-O3'-C3'   | -5.06 | 113.62      | 119.70   |
| 35  | BB    | 715  | A    | C6-N1-C2    | -5.06 | 115.56      | 118.60   |
| 35  | BB    | 738  | G    | C3'-C2'-C1' | 5.06  | 105.55      | 101.50   |
| 35  | BB    | 1696 | G    | N7-C8-N9    | -5.06 | 110.57      | 113.10   |
| 35  | BB    | 1949 | G    | O4'-C1'-N9  | 5.06  | 112.25      | 108.20   |
| 35  | BB    | 2076 | U    | C6-N1-C2    | -5.06 | 117.96      | 121.00   |
| 35  | BB    | 2103 | C    | N1-C2-N3    | -5.06 | 115.66      | 119.20   |
| 35  | BB    | 2284 | A    | C5-N7-C8    | 5.06  | 106.43      | 103.90   |
| 35  | BB    | 2338 | C    | C5'-C4'-C3' | 5.06  | 124.10      | 116.00   |
| 40  | BG    | 150  | TYR  | CB-CG-CD2   | 5.06  | 124.04      | 121.00   |
| 1   | AA    | 349  | A    | O4'-C1'-N9  | 5.06  | 112.25      | 108.20   |
| 1   | AA    | 396  | C    | O4'-C1'-N1  | 5.06  | 112.25      | 108.20   |
| 35  | BB    | 1413 | A    | C5-N7-C8    | 5.06  | 106.43      | 103.90   |
| 35  | BB    | 2016 | U    | C3'-C2'-C1' | 5.06  | 105.55      | 101.50   |
| 52  | BS    | 77   | ASP  | N-CA-CB     | 5.06  | 119.71      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 166  | U    | C2-N3-C4    | 5.06  | 130.04      | 127.00   |
| 1   | AA    | 255  | G    | C6-C5-N7    | -5.06 | 127.36      | 130.40   |
| 1   | AA    | 262  | A    | C4'-C3'-C2' | -5.06 | 97.54       | 102.60   |
| 1   | AA    | 1443 | C    | C2-N1-C1'   | 5.06  | 124.37      | 118.80   |
| 4   | AD    | 159  | GLU  | OE1-CD-OE2  | 5.06  | 129.37      | 123.30   |
| 13  | AM    | 55   | LEU  | CB-CG-CD2   | 5.06  | 119.60      | 111.00   |
| 22  | AV    | 21   | A    | O4'-C1'-N9  | 5.06  | 112.25      | 108.20   |
| 35  | BB    | 295  | G    | C4'-C3'-C2' | -5.06 | 97.54       | 102.60   |
| 35  | BB    | 311  | A    | C8-N9-C4    | -5.06 | 103.78      | 105.80   |
| 35  | BB    | 715  | A    | OP1-P-OP2   | -5.06 | 112.01      | 119.60   |
| 35  | BB    | 965  | C    | N3-C4-C5    | -5.06 | 119.88      | 121.90   |
| 35  | BB    | 1006 | C    | C4-C5-C6    | 5.06  | 119.93      | 117.40   |
| 35  | BB    | 1440 | U    | C3'-C2'-C1' | 5.06  | 105.55      | 101.50   |
| 35  | BB    | 2171 | A    | O4'-C1'-C2' | -5.06 | 100.74      | 105.80   |
| 35  | BB    | 2311 | A    | C4-C5-C6    | 5.06  | 119.53      | 117.00   |
| 35  | BB    | 2366 | A    | N3-C4-N9    | 5.06  | 131.45      | 127.40   |
| 1   | AA    | 423  | G    | N1-C2-N3    | -5.06 | 120.87      | 123.90   |
| 1   | AA    | 501  | C    | N1-C2-O2    | 5.06  | 121.93      | 118.90   |
| 1   | AA    | 682  | G    | C8-N9-C1'   | 5.06  | 133.57      | 127.00   |
| 4   | AD    | 24   | VAL  | O-C-N       | -5.06 | 114.61      | 122.70   |
| 7   | AG    | 64   | ALA  | CB-CA-C     | -5.06 | 102.51      | 110.10   |
| 35  | BB    | 255  | A    | C6-C5-N7    | -5.06 | 128.76      | 132.30   |
| 35  | BB    | 309  | A    | O4'-C1'-N9  | 5.06  | 112.25      | 108.20   |
| 35  | BB    | 752  | A    | O4'-C1'-N9  | 5.06  | 112.25      | 108.20   |
| 35  | BB    | 874  | G    | N1-C6-O6    | 5.06  | 122.93      | 119.90   |
| 35  | BB    | 927  | A    | C2-N3-C4    | -5.06 | 108.07      | 110.60   |
| 35  | BB    | 1329 | U    | OP1-P-OP2   | -5.06 | 112.01      | 119.60   |
| 35  | BB    | 1651 | G    | C4-C5-C6    | 5.06  | 121.83      | 118.80   |
| 35  | BB    | 1845 | G    | N3-C4-N9    | 5.06  | 129.03      | 126.00   |
| 35  | BB    | 1888 | G    | C5-C6-O6    | -5.06 | 125.57      | 128.60   |
| 35  | BB    | 2017 | U    | O4'-C1'-C2' | 5.06  | 112.15      | 107.60   |
| 41  | BH    | 81   | ALA  | N-CA-CB     | 5.06  | 117.18      | 110.10   |
| 1   | AA    | 143  | A    | O4'-C4'-C3' | 5.06  | 110.14      | 106.10   |
| 1   | AA    | 202  | G    | C4'-C3'-C2' | -5.06 | 97.54       | 102.60   |
| 1   | AA    | 497  | G    | N7-C8-N9    | -5.06 | 110.57      | 113.10   |
| 34  | BA    | 108  | A    | C4-C5-N7    | -5.06 | 108.17      | 110.70   |
| 35  | BB    | 248  | G    | C5-N7-C8    | 5.06  | 106.83      | 104.30   |
| 35  | BB    | 483  | A    | C4-C5-C6    | 5.06  | 119.53      | 117.00   |
| 35  | BB    | 720  | U    | P-O3'-C3'   | -5.06 | 113.63      | 119.70   |
| 35  | BB    | 1055 | G    | C8-N9-C1'   | 5.06  | 133.57      | 127.00   |
| 35  | BB    | 1383 | A    | C2'-C3'-O3' | 5.06  | 121.79      | 113.70   |
| 35  | BB    | 1419 | A    | C4-C5-C6    | 5.06  | 119.53      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 448  | A    | C8-N9-C4    | 5.05  | 107.82      | 105.80   |
| 1   | AA    | 766  | A    | C4'-C3'-C2' | -5.05 | 97.55       | 102.60   |
| 1   | AA    | 1029 | U    | C5'-C4'-O4' | -5.05 | 103.04      | 109.10   |
| 1   | AA    | 1421 | G    | C4'-C3'-C2' | -5.05 | 97.55       | 102.60   |
| 10  | AJ    | 28   | THR  | CA-CB-CG2   | -5.05 | 105.32      | 112.40   |
| 17  | AQ    | 33   | TYR  | CG-CD2-CE2  | 5.05  | 125.34      | 121.30   |
| 34  | BA    | 101  | A    | C6-N1-C2    | -5.05 | 115.57      | 118.60   |
| 35  | BB    | 3    | U    | O4'-C1'-C2' | -5.05 | 100.75      | 105.80   |
| 35  | BB    | 68   | G    | C5-N7-C8    | 5.05  | 106.83      | 104.30   |
| 35  | BB    | 277  | G    | C6-N1-C2    | 5.05  | 128.13      | 125.10   |
| 35  | BB    | 1558 | C    | C4-C5-C6    | -5.05 | 114.87      | 117.40   |
| 35  | BB    | 1837 | C    | C5-C4-N4    | 5.05  | 123.74      | 120.20   |
| 35  | BB    | 2417 | C    | N1-C2-O2    | 5.05  | 121.93      | 118.90   |
| 35  | BB    | 2448 | A    | P-O3'-C3'   | 5.05  | 125.77      | 119.70   |
| 35  | BB    | 2478 | A    | C4-C5-N7    | -5.05 | 108.17      | 110.70   |
| 35  | BB    | 2489 | U    | O4'-C1'-C2' | 5.05  | 112.15      | 107.60   |
| 35  | BB    | 2684 | U    | N3-C2-O2    | 5.05  | 125.74      | 122.20   |
| 35  | BB    | 2698 | U    | N3-C4-C5    | -5.05 | 111.57      | 114.60   |
| 35  | BB    | 2863 | C    | N1-C2-O2    | 5.05  | 121.93      | 118.90   |
| 1   | AA    | 799  | G    | C4-C5-C6    | 5.05  | 121.83      | 118.80   |
| 1   | AA    | 1466 | C    | O4'-C4'-C3' | -5.05 | 98.95       | 104.00   |
| 35  | BB    | 1072 | C    | N3-C4-N4    | 5.05  | 121.54      | 118.00   |
| 35  | BB    | 1695 | G    | O5'-P-OP2   | 5.05  | 116.76      | 110.70   |
| 35  | BB    | 1808 | A    | C5-C6-N1    | -5.05 | 115.17      | 117.70   |
| 35  | BB    | 1977 | A    | N3-C4-C5    | -5.05 | 123.26      | 126.80   |
| 35  | BB    | 2531 | A    | O4'-C1'-C2' | -5.05 | 100.75      | 105.80   |
| 35  | BB    | 2902 | C    | C4'-C3'-C2' | -5.05 | 97.55       | 102.60   |
| 1   | AA    | 20   | U    | C5-C4-O4    | -5.05 | 122.87      | 125.90   |
| 1   | AA    | 109  | A    | C5-N7-C8    | -5.05 | 101.37      | 103.90   |
| 1   | AA    | 755  | G    | C2-N3-C4    | 5.05  | 114.43      | 111.90   |
| 1   | AA    | 1246 | A    | C5-N7-C8    | 5.05  | 106.43      | 103.90   |
| 1   | AA    | 1285 | A    | C5-C6-N1    | -5.05 | 115.17      | 117.70   |
| 34  | BA    | 98   | G    | N3-C4-C5    | 5.05  | 131.13      | 128.60   |
| 35  | BB    | 224  | U    | O4'-C1'-N1  | 5.05  | 112.24      | 108.20   |
| 35  | BB    | 259  | G    | C5'-C4'-O4' | 5.05  | 115.16      | 109.10   |
| 35  | BB    | 317  | G    | N7-C8-N9    | -5.05 | 110.57      | 113.10   |
| 35  | BB    | 343  | C    | C6-N1-C2    | -5.05 | 118.28      | 120.30   |
| 35  | BB    | 675  | A    | C6-N1-C2    | -5.05 | 115.57      | 118.60   |
| 35  | BB    | 792  | A    | C5-N7-C8    | 5.05  | 106.43      | 103.90   |
| 35  | BB    | 1328 | A    | N9-C4-C5    | 5.05  | 107.82      | 105.80   |
| 35  | BB    | 1591 | A    | C2-N3-C4    | -5.05 | 108.07      | 110.60   |
| 35  | BB    | 1805 | A    | N7-C8-N9    | 5.05  | 116.33      | 113.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1887 | C    | C4'-C3'-C2' | -5.05 | 97.55       | 102.60   |
| 35  | BB    | 1982 | U    | N3-C4-O4    | 5.05  | 122.94      | 119.40   |
| 35  | BB    | 2070 | A    | N3-C4-C5    | 5.05  | 130.34      | 126.80   |
| 35  | BB    | 2146 | C    | C4-C5-C6    | 5.05  | 119.93      | 117.40   |
| 35  | BB    | 2206 | C    | N1-C2-O2    | -5.05 | 115.87      | 118.90   |
| 35  | BB    | 2721 | A    | C6-C5-N7    | -5.05 | 128.76      | 132.30   |
| 35  | BB    | 2732 | G    | O4'-C1'-C2' | 5.05  | 112.15      | 107.60   |
| 35  | BB    | 2759 | G    | C4-C5-C6    | 5.05  | 121.83      | 118.80   |
| 35  | BB    | 2813 | A    | N7-C8-N9    | 5.05  | 116.33      | 113.80   |
| 38  | BE    | 77   | ILE  | CB-CA-C     | -5.05 | 101.50      | 111.60   |
| 41  | BH    | 11   | ASN  | CB-CA-C     | 5.05  | 120.50      | 110.40   |
| 45  | BL    | 30   | THR  | N-CA-CB     | 5.05  | 119.90      | 110.30   |
| 1   | AA    | 151  | A    | C5-C6-N6    | -5.05 | 119.66      | 123.70   |
| 1   | AA    | 1089 | G    | OP1-P-OP2   | -5.05 | 112.03      | 119.60   |
| 1   | AA    | 1183 | U    | N3-C2-O2    | 5.05  | 125.73      | 122.20   |
| 1   | AA    | 1336 | C    | C5'-C4'-O4' | 5.05  | 115.16      | 109.10   |
| 1   | AA    | 1355 | G    | C4'-C3'-C2' | -5.05 | 97.55       | 102.60   |
| 1   | AA    | 1404 | C    | C5-C6-N1    | 5.05  | 123.53      | 121.00   |
| 34  | BA    | 18   | G    | C4-C5-C6    | 5.05  | 121.83      | 118.80   |
| 35  | BB    | 86   | G    | N3-C4-N9    | -5.05 | 122.97      | 126.00   |
| 35  | BB    | 115  | C    | N1-C2-O2    | 5.05  | 121.93      | 118.90   |
| 35  | BB    | 257  | C    | C4'-C3'-C2' | -5.05 | 97.55       | 102.60   |
| 35  | BB    | 350  | G    | N1-C2-N2    | -5.05 | 111.66      | 116.20   |
| 35  | BB    | 455  | C    | C6-N1-C1'   | -5.05 | 114.74      | 120.80   |
| 35  | BB    | 497  | A    | C6-N1-C2    | -5.05 | 115.57      | 118.60   |
| 35  | BB    | 610  | C    | N3-C4-C5    | -5.05 | 119.88      | 121.90   |
| 35  | BB    | 927  | A    | N1-C2-N3    | 5.05  | 131.82      | 129.30   |
| 35  | BB    | 1105 | U    | P-O3'-C3'   | -5.05 | 113.64      | 119.70   |
| 35  | BB    | 1260 | A    | N1-C2-N3    | 5.05  | 131.82      | 129.30   |
| 35  | BB    | 1468 | U    | N1-C2-N3    | 5.05  | 117.93      | 114.90   |
| 35  | BB    | 1807 | G    | C6-N1-C2    | -5.05 | 122.07      | 125.10   |
| 35  | BB    | 2083 | G    | N3-C4-N9    | -5.05 | 122.97      | 126.00   |
| 35  | BB    | 2239 | G    | C4-C5-C6    | 5.05  | 121.83      | 118.80   |
| 35  | BB    | 2838 | G    | C5-N7-C8    | -5.05 | 101.78      | 104.30   |
| 1   | AA    | 1310 | G    | C4'-C3'-C2' | -5.05 | 97.55       | 102.60   |
| 35  | BB    | 1974 | C    | C3'-C2'-C1' | 5.05  | 105.54      | 101.50   |
| 35  | BB    | 1989 | G    | N9-C4-C5    | 5.05  | 107.42      | 105.40   |
| 39  | BF    | 134  | GLN  | N-CA-CB     | 5.05  | 119.69      | 110.60   |
| 1   | AA    | 203  | G    | C5-C6-N1    | -5.05 | 108.98      | 111.50   |
| 1   | AA    | 576  | C    | C5-C6-N1    | 5.05  | 123.52      | 121.00   |
| 1   | AA    | 583  | A    | C5-C6-N6    | -5.05 | 119.66      | 123.70   |
| 1   | AA    | 606  | G    | C5-C6-N1    | -5.05 | 108.98      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 823  | C    | OP2-P-O3'   | 5.05  | 116.30      | 105.20   |
| 1   | AA    | 997  | U    | C5-C6-N1    | 5.05  | 125.22      | 122.70   |
| 1   | AA    | 1257 | A    | N7-C8-N9    | -5.05 | 111.28      | 113.80   |
| 5   | AE    | 115  | GLU  | N-CA-C      | -5.05 | 97.38       | 111.00   |
| 14  | AN    | 99   | SER  | N-CA-C      | -5.05 | 97.37       | 111.00   |
| 22  | AV    | 4    | C    | C4'-C3'-C2' | -5.05 | 97.55       | 102.60   |
| 35  | BB    | 204  | A    | P-O3'-C3'   | 5.05  | 125.76      | 119.70   |
| 35  | BB    | 283  | G    | P-O5'-C5'   | 5.05  | 128.97      | 120.90   |
| 35  | BB    | 284  | U    | N3-C4-O4    | 5.05  | 122.93      | 119.40   |
| 35  | BB    | 570  | G    | N3-C2-N2    | 5.05  | 123.43      | 119.90   |
| 35  | BB    | 902  | C    | C5'-C4'-O4' | -5.05 | 103.04      | 109.10   |
| 35  | BB    | 1097 | U    | O4'-C1'-N1  | 5.05  | 112.24      | 108.20   |
| 35  | BB    | 1312 | U    | C6-N1-C2    | 5.05  | 124.03      | 121.00   |
| 35  | BB    | 1574 | C    | N3-C2-O2    | 5.05  | 125.43      | 121.90   |
| 35  | BB    | 1944 | U    | C1'-O4'-C4' | 5.05  | 113.94      | 109.90   |
| 35  | BB    | 2150 | C    | N3-C2-O2    | 5.05  | 125.43      | 121.90   |
| 35  | BB    | 2846 | G    | N7-C8-N9    | -5.05 | 110.58      | 113.10   |
| 1   | AA    | 660  | C    | P-O5'-C5'   | 5.04  | 128.97      | 120.90   |
| 1   | AA    | 773  | G    | P-O5'-C5'   | -5.04 | 112.83      | 120.90   |
| 7   | AG    | 116  | ALA  | C-N-CA      | 5.04  | 134.31      | 121.70   |
| 35  | BB    | 143  | C    | C6-N1-C2    | -5.04 | 118.28      | 120.30   |
| 35  | BB    | 751  | A    | N1-C2-N3    | -5.04 | 126.78      | 129.30   |
| 35  | BB    | 1992 | G    | N3-C4-N9    | -5.04 | 122.97      | 126.00   |
| 35  | BB    | 2572 | A    | C6-N1-C2    | 5.04  | 121.63      | 118.60   |
| 35  | BB    | 2574 | G    | C2-N3-C4    | -5.04 | 109.38      | 111.90   |
| 35  | BB    | 2761 | A    | O5'-C5'-C4' | -5.04 | 102.11      | 111.70   |
| 1   | AA    | 103  | U    | C5-C4-O4    | -5.04 | 122.87      | 125.90   |
| 1   | AA    | 237  | G    | C8-N9-C1'   | 5.04  | 133.56      | 127.00   |
| 1   | AA    | 282  | A    | C5'-C4'-O4' | 5.04  | 115.15      | 109.10   |
| 1   | AA    | 393  | A    | N3-C4-C5    | -5.04 | 123.27      | 126.80   |
| 1   | AA    | 716  | A    | C1'-O4'-C4' | 5.04  | 113.93      | 109.90   |
| 1   | AA    | 779  | C    | N1-C2-N3    | 5.04  | 122.73      | 119.20   |
| 1   | AA    | 1506 | U    | C4'-C3'-C2' | -5.04 | 97.56       | 102.60   |
| 35  | BB    | 119  | A    | C4-C5-C6    | 5.04  | 119.52      | 117.00   |
| 35  | BB    | 338  | G    | C8-N9-C4    | -5.04 | 104.38      | 106.40   |
| 35  | BB    | 438  | G    | C3'-C2'-C1' | -5.04 | 97.47       | 101.50   |
| 35  | BB    | 585  | G    | N3-C2-N2    | 5.04  | 123.43      | 119.90   |
| 35  | BB    | 653  | U    | N3-C4-O4    | 5.04  | 122.93      | 119.40   |
| 35  | BB    | 696  | G    | N3-C2-N2    | 5.04  | 123.43      | 119.90   |
| 35  | BB    | 748  | G    | C5'-C4'-O4' | 5.04  | 115.15      | 109.10   |
| 35  | BB    | 787  | C    | C5'-C4'-C3' | -5.04 | 107.93      | 116.00   |
| 35  | BB    | 801  | G    | O4'-C1'-N9  | 5.04  | 112.23      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1130 | U    | C1'-O4'-C4' | 5.04  | 113.93      | 109.90   |
| 35  | BB    | 1968 | G    | N1-C2-N3    | -5.04 | 120.87      | 123.90   |
| 35  | BB    | 2320 | U    | N3-C4-O4    | 5.04  | 122.93      | 119.40   |
| 35  | BB    | 2588 | G    | C4-N9-C1'   | 5.04  | 133.06      | 126.50   |
| 35  | BB    | 2603 | G    | C5'-C4'-O4' | 5.04  | 115.15      | 109.10   |
| 35  | BB    | 2766 | A    | C5'-C4'-O4' | 5.04  | 115.15      | 109.10   |
| 35  | BB    | 2798 | U    | P-O3'-C3'   | -5.04 | 113.65      | 119.70   |
| 39  | BF    | 134  | GLN  | O-C-N       | 5.04  | 130.77      | 122.70   |
| 1   | AA    | 76   | G    | N3-C2-N2    | 5.04  | 123.43      | 119.90   |
| 1   | AA    | 100  | G    | P-O5'-C5'   | -5.04 | 112.83      | 120.90   |
| 1   | AA    | 616  | G    | C5-C6-O6    | -5.04 | 125.58      | 128.60   |
| 1   | AA    | 1264 | U    | C1'-O4'-C4' | 5.04  | 113.93      | 109.90   |
| 1   | AA    | 1304 | G    | C8-N9-C4    | -5.04 | 104.38      | 106.40   |
| 1   | AA    | 1374 | A    | N7-C8-N9    | -5.04 | 111.28      | 113.80   |
| 5   | AE    | 51   | LYS  | O-C-N       | 5.04  | 130.77      | 122.70   |
| 9   | AI    | 7    | GLY  | N-CA-C      | -5.04 | 100.50      | 113.10   |
| 18  | AR    | 71   | ASP  | CB-CG-OD1   | -5.04 | 113.76      | 118.30   |
| 35  | BB    | 26   | G    | N3-C2-N2    | 5.04  | 123.43      | 119.90   |
| 35  | BB    | 1135 | C    | O4'-C4'-C3' | -5.04 | 98.96       | 104.00   |
| 35  | BB    | 1914 | C    | P-O3'-C3'   | 5.04  | 125.75      | 119.70   |
| 35  | BB    | 2014 | A    | C8-N9-C4    | -5.04 | 103.78      | 105.80   |
| 35  | BB    | 2293 | G    | N1-C2-N2    | 5.04  | 120.74      | 116.20   |
| 35  | BB    | 2296 | U    | C6-N1-C2    | -5.04 | 117.97      | 121.00   |
| 35  | BB    | 2491 | U    | O4'-C1'-C2' | -5.04 | 100.76      | 105.80   |
| 35  | BB    | 2558 | C    | C2-N3-C4    | 5.04  | 122.42      | 119.90   |
| 1   | AA    | 34   | C    | C1'-O4'-C4' | 5.04  | 113.93      | 109.90   |
| 1   | AA    | 922  | G    | N3-C2-N2    | 5.04  | 123.43      | 119.90   |
| 1   | AA    | 1020 | G    | C5'-C4'-O4' | 5.04  | 115.15      | 109.10   |
| 22  | AV    | 27   | C    | N3-C4-C5    | -5.04 | 119.88      | 121.90   |
| 35  | BB    | 188  | G    | P-O5'-C5'   | -5.04 | 112.84      | 120.90   |
| 35  | BB    | 244  | A    | C5-N7-C8    | 5.04  | 106.42      | 103.90   |
| 35  | BB    | 402  | A    | C6-C5-N7    | -5.04 | 128.77      | 132.30   |
| 35  | BB    | 516  | C    | C2-N3-C4    | 5.04  | 122.42      | 119.90   |
| 35  | BB    | 687  | C    | C5'-C4'-C3' | -5.04 | 107.94      | 116.00   |
| 35  | BB    | 1331 | G    | N7-C8-N9    | 5.04  | 115.62      | 113.10   |
| 35  | BB    | 1356 | G    | O4'-C1'-N9  | 5.04  | 112.23      | 108.20   |
| 35  | BB    | 1795 | C    | P-O5'-C5'   | 5.04  | 128.96      | 120.90   |
| 35  | BB    | 1804 | C    | C2-N1-C1'   | 5.04  | 124.34      | 118.80   |
| 35  | BB    | 1935 | G    | N3-C4-C5    | -5.04 | 126.08      | 128.60   |
| 35  | BB    | 2117 | A    | N1-C6-N6    | 5.04  | 121.62      | 118.60   |
| 35  | BB    | 2385 | C    | O5'-C5'-C4' | -5.04 | 102.12      | 111.70   |
| 1   | AA    | 45   | G    | P-O3'-C3'   | 5.04  | 125.75      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 323  | U    | C3'-C2'-C1' | -5.04 | 97.47       | 101.50   |
| 1   | AA    | 620  | C    | C5-C4-N4    | -5.04 | 116.67      | 120.20   |
| 1   | AA    | 1260 | G    | C5-C6-N1    | 5.04  | 114.02      | 111.50   |
| 1   | AA    | 1266 | G    | P-O5'-C5'   | -5.04 | 112.84      | 120.90   |
| 1   | AA    | 1437 | A    | C1'-O4'-C4' | 5.04  | 113.93      | 109.90   |
| 1   | AA    | 1519 | A    | N7-C8-N9    | 5.04  | 116.32      | 113.80   |
| 4   | AD    | 169  | TRP  | N-CA-CB     | 5.04  | 119.67      | 110.60   |
| 22  | AV    | 11   | C    | N3-C4-N4    | 5.04  | 121.53      | 118.00   |
| 35  | BB    | 1    | G    | N3-C2-N2    | 5.04  | 123.43      | 119.90   |
| 35  | BB    | 232  | G    | C5-C6-O6    | -5.04 | 125.58      | 128.60   |
| 35  | BB    | 414  | C    | N1-C2-N3    | 5.04  | 122.73      | 119.20   |
| 35  | BB    | 516  | C    | P-O3'-C3'   | -5.04 | 113.65      | 119.70   |
| 35  | BB    | 677  | A    | C6-C5-N7    | -5.04 | 128.77      | 132.30   |
| 35  | BB    | 694  | U    | C2-N1-C1'   | 5.04  | 123.75      | 117.70   |
| 35  | BB    | 1381 | G    | O5'-C5'-C4' | -5.04 | 102.13      | 111.70   |
| 35  | BB    | 1426 | G    | N3-C4-N9    | 5.04  | 129.02      | 126.00   |
| 35  | BB    | 1640 | A    | C4-C5-C6    | 5.04  | 119.52      | 117.00   |
| 35  | BB    | 1712 | U    | C6-N1-C2    | -5.04 | 117.98      | 121.00   |
| 35  | BB    | 1924 | C    | C4'-C3'-C2' | -5.04 | 97.56       | 102.60   |
| 35  | BB    | 2033 | A    | C5'-C4'-O4' | 5.04  | 115.15      | 109.10   |
| 35  | BB    | 2359 | C    | N1-C2-O2    | -5.04 | 115.88      | 118.90   |
| 35  | BB    | 2397 | G    | O4'-C4'-C3' | -5.04 | 98.96       | 104.00   |
| 35  | BB    | 2727 | A    | C4-C5-C6    | 5.04  | 119.52      | 117.00   |
| 55  | BW    | 47   | VAL  | CA-CB-CG2   | -5.04 | 103.34      | 110.90   |
| 1   | AA    | 685  | G    | C5-C6-O6    | -5.04 | 125.58      | 128.60   |
| 35  | BB    | 770  | G    | C5-C6-O6    | -5.04 | 125.58      | 128.60   |
| 35  | BB    | 773  | U    | C4-C5-C6    | -5.04 | 116.68      | 119.70   |
| 35  | BB    | 877  | A    | N3-C4-N9    | -5.04 | 123.37      | 127.40   |
| 35  | BB    | 1248 | G    | N3-C2-N2    | 5.04  | 123.43      | 119.90   |
| 35  | BB    | 1475 | G    | O4'-C1'-N9  | 5.04  | 112.23      | 108.20   |
| 35  | BB    | 1579 | A    | C4-C5-C6    | 5.04  | 119.52      | 117.00   |
| 35  | BB    | 1677 | A    | C4-C5-N7    | -5.04 | 108.18      | 110.70   |
| 35  | BB    | 1888 | G    | C6-N1-C2    | 5.04  | 128.12      | 125.10   |
| 39  | BF    | 8    | LYS  | CA-CB-CG    | 5.04  | 124.48      | 113.40   |
| 1   | AA    | 176  | C    | C6-N1-C1'   | -5.04 | 114.76      | 120.80   |
| 1   | AA    | 334  | C    | N1-C2-N3    | 5.04  | 122.72      | 119.20   |
| 1   | AA    | 478  | A    | C2-N3-C4    | -5.04 | 108.08      | 110.60   |
| 1   | AA    | 845  | A    | C4-C5-C6    | 5.04  | 119.52      | 117.00   |
| 1   | AA    | 902  | G    | C5-C6-N1    | -5.04 | 108.98      | 111.50   |
| 1   | AA    | 1132 | C    | OP1-P-OP2   | -5.04 | 112.05      | 119.60   |
| 1   | AA    | 1320 | C    | C4-C5-C6    | 5.04  | 119.92      | 117.40   |
| 16  | AP    | 40   | ASN  | N-CA-C      | -5.04 | 97.41       | 111.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 19  | AS    | 9    | PHE  | CD1-CE1-CZ  | -5.04 | 114.06      | 120.10   |
| 27  | B2    | 29   | ARG  | NE-CZ-NH2   | 5.04  | 122.82      | 120.30   |
| 34  | BA    | 27   | C    | C2-N1-C1'   | 5.04  | 124.34      | 118.80   |
| 35  | BB    | 118  | A    | N7-C8-N9    | -5.04 | 111.28      | 113.80   |
| 35  | BB    | 266  | G    | C4'-C3'-C2' | -5.04 | 97.56       | 102.60   |
| 35  | BB    | 586  | A    | C4-C5-C6    | 5.04  | 119.52      | 117.00   |
| 35  | BB    | 1016 | G    | C4'-C3'-C2' | -5.04 | 97.56       | 102.60   |
| 35  | BB    | 1059 | G    | N3-C2-N2    | 5.04  | 123.42      | 119.90   |
| 35  | BB    | 1578 | U    | P-O3'-C3'   | 5.04  | 125.74      | 119.70   |
| 35  | BB    | 2113 | U    | C5-C4-O4    | -5.04 | 122.88      | 125.90   |
| 35  | BB    | 2126 | A    | C4-C5-C6    | 5.04  | 119.52      | 117.00   |
| 35  | BB    | 2232 | C    | O4'-C1'-N1  | 5.04  | 112.23      | 108.20   |
| 35  | BB    | 2289 | G    | C4-N9-C1'   | 5.04  | 133.05      | 126.50   |
| 35  | BB    | 2392 | A    | C8-N9-C4    | -5.04 | 103.78      | 105.80   |
| 35  | BB    | 2555 | U    | C4'-C3'-C2' | -5.04 | 97.56       | 102.60   |
| 35  | BB    | 2732 | G    | C4-C5-C6    | 5.04  | 121.82      | 118.80   |
| 40  | BG    | 129  | GLU  | N-CA-CB     | 5.04  | 119.66      | 110.60   |
| 1   | AA    | 231  | U    | N1-C2-N3    | -5.03 | 111.88      | 114.90   |
| 1   | AA    | 295  | C    | N1-C2-N3    | -5.03 | 115.68      | 119.20   |
| 1   | AA    | 858  | G    | C5-C6-O6    | -5.03 | 125.58      | 128.60   |
| 1   | AA    | 1032 | G    | C1'-O4'-C4' | -5.03 | 105.87      | 109.90   |
| 1   | AA    | 1046 | A    | C2-N3-C4    | -5.03 | 108.08      | 110.60   |
| 1   | AA    | 1076 | U    | N3-C2-O2    | 5.03  | 125.72      | 122.20   |
| 11  | AK    | 121  | ARG  | NE-CZ-NH2   | -5.03 | 117.78      | 120.30   |
| 35  | BB    | 60   | G    | N3-C4-C5    | -5.03 | 126.08      | 128.60   |
| 35  | BB    | 69   | C    | N3-C4-N4    | 5.03  | 121.52      | 118.00   |
| 35  | BB    | 321  | U    | O4'-C1'-N1  | 5.03  | 112.23      | 108.20   |
| 35  | BB    | 577  | G    | C4-C5-N7    | 5.03  | 112.81      | 110.80   |
| 35  | BB    | 699  | A    | P-O3'-C3'   | 5.03  | 125.74      | 119.70   |
| 35  | BB    | 839  | U    | C6-N1-C2    | 5.03  | 124.02      | 121.00   |
| 35  | BB    | 844  | A    | C5-C6-N6    | -5.03 | 119.67      | 123.70   |
| 35  | BB    | 942  | G    | C8-N9-C1'   | 5.03  | 133.54      | 127.00   |
| 35  | BB    | 966  | G    | N9-C4-C5    | 5.03  | 107.41      | 105.40   |
| 35  | BB    | 1023 | U    | N3-C4-O4    | 5.03  | 122.92      | 119.40   |
| 35  | BB    | 1286 | A    | C8-N9-C4    | 5.03  | 107.81      | 105.80   |
| 35  | BB    | 1382 | G    | C4'-C3'-C2' | -5.03 | 97.57       | 102.60   |
| 35  | BB    | 1509 | A    | P-O5'-C5'   | -5.03 | 112.85      | 120.90   |
| 35  | BB    | 1916 | A    | C4-C5-N7    | -5.03 | 108.18      | 110.70   |
| 35  | BB    | 2116 | G    | C8-N9-C4    | -5.03 | 104.39      | 106.40   |
| 1   | AA    | 561  | U    | C2-N1-C1'   | 5.03  | 123.74      | 117.70   |
| 1   | AA    | 867  | G    | OP1-P-OP2   | -5.03 | 112.05      | 119.60   |
| 1   | AA    | 970  | C    | C1'-O4'-C4' | -5.03 | 105.87      | 109.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 1441 | G    | C5-C6-N1    | -5.03 | 108.98      | 111.50   |
| 35  | BB    | 2526 | G    | O4'-C1'-N9  | 5.03  | 112.22      | 108.20   |
| 35  | BB    | 2693 | G    | C5-C6-N1    | -5.03 | 108.98      | 111.50   |
| 1   | AA    | 305  | G    | C5-N7-C8    | 5.03  | 106.81      | 104.30   |
| 1   | AA    | 357  | G    | N1-C2-N2    | 5.03  | 120.73      | 116.20   |
| 1   | AA    | 387  | U    | P-O5'-C5'   | -5.03 | 112.85      | 120.90   |
| 1   | AA    | 854  | U    | P-O3'-C3'   | -5.03 | 113.66      | 119.70   |
| 1   | AA    | 1393 | U    | OP2-P-O3'   | 5.03  | 116.27      | 105.20   |
| 1   | AA    | 1457 | G    | P-O3'-C3'   | -5.03 | 113.67      | 119.70   |
| 5   | AE    | 28   | ARG  | N-CA-CB     | 5.03  | 119.66      | 110.60   |
| 35  | BB    | 252  | G    | C3'-C2'-C1' | 5.03  | 105.52      | 101.50   |
| 35  | BB    | 631  | A    | N1-C2-N3    | 5.03  | 131.81      | 129.30   |
| 35  | BB    | 771  | G    | C4-C5-C6    | 5.03  | 121.82      | 118.80   |
| 35  | BB    | 1039 | A    | C6-N1-C2    | 5.03  | 121.62      | 118.60   |
| 35  | BB    | 1143 | A    | N3-C4-N9    | 5.03  | 131.42      | 127.40   |
| 35  | BB    | 1179 | G    | C5'-C4'-O4' | 5.03  | 115.14      | 109.10   |
| 35  | BB    | 1916 | A    | C5-C6-N1    | -5.03 | 115.19      | 117.70   |
| 35  | BB    | 2052 | A    | C4'-C3'-C2' | -5.03 | 97.57       | 102.60   |
| 35  | BB    | 2078 | C    | C6-N1-C2    | -5.03 | 118.29      | 120.30   |
| 35  | BB    | 2502 | G    | C4-C5-C6    | 5.03  | 121.82      | 118.80   |
| 35  | BB    | 2513 | A    | C5-N7-C8    | 5.03  | 106.42      | 103.90   |
| 35  | BB    | 2541 | A    | C5-N7-C8    | 5.03  | 106.42      | 103.90   |
| 1   | AA    | 18   | C    | O4'-C4'-C3' | -5.03 | 98.97       | 104.00   |
| 1   | AA    | 431  | A    | N7-C8-N9    | -5.03 | 111.28      | 113.80   |
| 1   | AA    | 1170 | A    | N3-C4-C5    | -5.03 | 123.28      | 126.80   |
| 35  | BB    | 717  | C    | P-O3'-C3'   | -5.03 | 113.67      | 119.70   |
| 35  | BB    | 988  | A    | C5-C6-N6    | -5.03 | 119.68      | 123.70   |
| 35  | BB    | 2232 | C    | C1'-O4'-C4' | 5.03  | 113.92      | 109.90   |
| 35  | BB    | 2320 | U    | O4'-C1'-N1  | 5.03  | 112.22      | 108.20   |
| 35  | BB    | 2579 | C    | C6-N1-C2    | -5.03 | 118.29      | 120.30   |
| 1   | AA    | 370  | C    | N3-C4-C5    | -5.03 | 119.89      | 121.90   |
| 1   | AA    | 575  | G    | N7-C8-N9    | -5.03 | 110.59      | 113.10   |
| 1   | AA    | 808  | C    | C5-C6-N1    | 5.03  | 123.51      | 121.00   |
| 34  | BA    | 114  | C    | N1-C2-O2    | 5.03  | 121.92      | 118.90   |
| 35  | BB    | 7    | G    | N9-C4-C5    | -5.03 | 103.39      | 105.40   |
| 35  | BB    | 237  | C    | C2-N1-C1'   | 5.03  | 124.33      | 118.80   |
| 35  | BB    | 250  | G    | C4-N9-C1'   | -5.03 | 119.96      | 126.50   |
| 35  | BB    | 1196 | C    | P-O3'-C3'   | -5.03 | 113.67      | 119.70   |
| 35  | BB    | 1286 | A    | P-O5'-C5'   | -5.03 | 112.86      | 120.90   |
| 35  | BB    | 1570 | A    | C5-C6-N1    | 5.03  | 120.21      | 117.70   |
| 35  | BB    | 2137 | U    | P-O5'-C5'   | 5.03  | 128.94      | 120.90   |
| 35  | BB    | 2496 | C    | O4'-C1'-N1  | 5.03  | 112.22      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 2685 | G    | N1-C6-O6    | 5.03  | 122.92      | 119.90   |
| 35  | BB    | 2764 | A    | C4-C5-N7    | -5.03 | 108.19      | 110.70   |
| 35  | BB    | 2780 | G    | N3-C4-N9    | 5.03  | 129.02      | 126.00   |
| 35  | BB    | 2887 | A    | C5-N7-C8    | 5.03  | 106.41      | 103.90   |
| 1   | AA    | 151  | A    | O4'-C1'-N9  | 5.03  | 112.22      | 108.20   |
| 1   | AA    | 666  | G    | C6-N1-C2    | 5.03  | 128.12      | 125.10   |
| 1   | AA    | 937  | A    | C6-C5-N7    | -5.03 | 128.78      | 132.30   |
| 22  | AV    | 69   | G    | N7-C8-N9    | -5.03 | 110.59      | 113.10   |
| 34  | BA    | 23   | G    | C4-C5-C6    | 5.03  | 121.81      | 118.80   |
| 35  | BB    | 12   | U    | C2-N3-C4    | -5.03 | 123.98      | 127.00   |
| 35  | BB    | 42   | A    | C5-C6-N6    | -5.03 | 119.68      | 123.70   |
| 35  | BB    | 142  | A    | C5-N7-C8    | 5.03  | 106.41      | 103.90   |
| 35  | BB    | 417  | C    | P-O3'-C3'   | -5.03 | 113.67      | 119.70   |
| 35  | BB    | 463  | G    | P-O3'-C3'   | -5.03 | 113.67      | 119.70   |
| 35  | BB    | 621  | A    | C4-C5-C6    | 5.03  | 119.51      | 117.00   |
| 35  | BB    | 833  | A    | C4-C5-N7    | -5.03 | 108.19      | 110.70   |
| 35  | BB    | 1060 | U    | C6-N1-C2    | -5.03 | 117.98      | 121.00   |
| 35  | BB    | 1193 | G    | C8-N9-C4    | -5.03 | 104.39      | 106.40   |
| 35  | BB    | 1259 | G    | C4-C5-C6    | 5.03  | 121.81      | 118.80   |
| 35  | BB    | 1336 | A    | C5-C6-N6    | -5.03 | 119.68      | 123.70   |
| 35  | BB    | 1345 | C    | C5-C4-N4    | -5.03 | 116.68      | 120.20   |
| 35  | BB    | 1792 | G    | C4-N9-C1'   | -5.03 | 119.97      | 126.50   |
| 35  | BB    | 2289 | G    | P-O3'-C3'   | -5.03 | 113.67      | 119.70   |
| 35  | BB    | 2482 | A    | C5'-C4'-O4' | 5.03  | 115.13      | 109.10   |
| 35  | BB    | 2510 | C    | P-O3'-C3'   | 5.03  | 125.73      | 119.70   |
| 35  | BB    | 2823 | A    | O4'-C1'-N9  | 5.03  | 112.22      | 108.20   |
| 1   | AA    | 375  | U    | OP1-P-OP2   | -5.02 | 112.06      | 119.60   |
| 1   | AA    | 555  | U    | OP2-P-O3'   | 5.02  | 116.25      | 105.20   |
| 1   | AA    | 1453 | G    | C6-C5-N7    | -5.02 | 127.39      | 130.40   |
| 35  | BB    | 5    | A    | C8-N9-C4    | -5.02 | 103.79      | 105.80   |
| 35  | BB    | 500  | G    | C8-N9-C4    | 5.02  | 108.41      | 106.40   |
| 35  | BB    | 517  | C    | O4'-C4'-C3' | -5.02 | 98.98       | 104.00   |
| 35  | BB    | 880  | G    | P-O5'-C5'   | -5.02 | 112.86      | 120.90   |
| 35  | BB    | 1322 | A    | C6-C5-N7    | -5.02 | 128.78      | 132.30   |
| 35  | BB    | 1394 | U    | P-O3'-C3'   | -5.02 | 113.67      | 119.70   |
| 35  | BB    | 1430 | G    | C5-C6-O6    | -5.02 | 125.58      | 128.60   |
| 35  | BB    | 2420 | C    | C5-C4-N4    | -5.02 | 116.68      | 120.20   |
| 1   | AA    | 373  | A    | N3-C4-N9    | 5.02  | 131.42      | 127.40   |
| 1   | AA    | 659  | U    | O5'-P-OP1   | -5.02 | 101.18      | 105.70   |
| 1   | AA    | 670  | G    | N7-C8-N9    | -5.02 | 110.59      | 113.10   |
| 1   | AA    | 682  | G    | N1-C2-N2    | -5.02 | 111.68      | 116.20   |
| 1   | AA    | 785  | G    | N3-C2-N2    | 5.02  | 123.42      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1074 | G    | C4-C5-C6    | 5.02  | 121.81      | 118.80   |
| 1   | AA    | 1352 | C    | OP1-P-OP2   | -5.02 | 112.07      | 119.60   |
| 14  | AN    | 23   | ARG  | NE-CZ-NH1   | 5.02  | 122.81      | 120.30   |
| 22  | AV    | 5    | A    | C5-C6-N1    | -5.02 | 115.19      | 117.70   |
| 35  | BB    | 137  | U    | N1-C2-O2    | -5.02 | 119.28      | 122.80   |
| 35  | BB    | 141  | G    | C4'-C3'-C2' | -5.02 | 97.58       | 102.60   |
| 35  | BB    | 152  | A    | C4-C5-N7    | -5.02 | 108.19      | 110.70   |
| 35  | BB    | 484  | C    | C6-N1-C1'   | 5.02  | 126.83      | 120.80   |
| 35  | BB    | 578  | G    | C6-N1-C2    | 5.02  | 128.11      | 125.10   |
| 35  | BB    | 969  | G    | C4-C5-N7    | 5.02  | 112.81      | 110.80   |
| 35  | BB    | 1233 | C    | N1-C2-O2    | -5.02 | 115.89      | 118.90   |
| 35  | BB    | 1938 | A    | C5-C6-N6    | -5.02 | 119.68      | 123.70   |
| 1   | AA    | 183  | C    | P-O3'-C3'   | 5.02  | 125.72      | 119.70   |
| 1   | AA    | 206  | C    | C2-N3-C4    | 5.02  | 122.41      | 119.90   |
| 1   | AA    | 681  | A    | N7-C8-N9    | -5.02 | 111.29      | 113.80   |
| 35  | BB    | 449  | A    | O4'-C1'-N9  | 5.02  | 112.22      | 108.20   |
| 35  | BB    | 724  | U    | OP1-P-OP2   | -5.02 | 112.07      | 119.60   |
| 35  | BB    | 930  | G    | C5'-C4'-O4' | 5.02  | 115.12      | 109.10   |
| 35  | BB    | 1102 | C    | N1-C2-N3    | -5.02 | 115.69      | 119.20   |
| 35  | BB    | 1141 | U    | C5-C6-N1    | -5.02 | 120.19      | 122.70   |
| 35  | BB    | 1385 | A    | C6-N1-C2    | 5.02  | 121.61      | 118.60   |
| 35  | BB    | 2120 | G    | N3-C4-C5    | 5.02  | 131.11      | 128.60   |
| 35  | BB    | 2698 | U    | C6-N1-C2    | -5.02 | 117.99      | 121.00   |
| 1   | AA    | 335  | C    | C6-N1-C2    | -5.02 | 118.29      | 120.30   |
| 1   | AA    | 475  | C    | C2-N1-C1'   | 5.02  | 124.32      | 118.80   |
| 1   | AA    | 877  | G    | O3'-P-O5'   | -5.02 | 94.46       | 104.00   |
| 1   | AA    | 1527 | U    | O4'-C1'-N1  | 5.02  | 112.22      | 108.20   |
| 35  | BB    | 153  | U    | C1'-O4'-C4' | 5.02  | 113.92      | 109.90   |
| 35  | BB    | 233  | A    | C4-C5-N7    | -5.02 | 108.19      | 110.70   |
| 35  | BB    | 332  | A    | N9-C4-C5    | 5.02  | 107.81      | 105.80   |
| 35  | BB    | 701  | G    | N1-C2-N2    | -5.02 | 111.68      | 116.20   |
| 35  | BB    | 885  | C    | C2-N3-C4    | 5.02  | 122.41      | 119.90   |
| 35  | BB    | 1085 | A    | N1-C2-N3    | -5.02 | 126.79      | 129.30   |
| 35  | BB    | 1138 | G    | N1-C2-N3    | -5.02 | 120.89      | 123.90   |
| 35  | BB    | 1701 | A    | O4'-C1'-N9  | 5.02  | 112.22      | 108.20   |
| 35  | BB    | 2064 | C    | C5-C6-N1    | 5.02  | 123.51      | 121.00   |
| 35  | BB    | 2728 | U    | C3'-C2'-C1' | 5.02  | 105.52      | 101.50   |
| 52  | BS    | 57   | ASN  | N-CA-CB     | 5.02  | 119.64      | 110.60   |
| 1   | AA    | 49   | U    | C6-N1-C2    | -5.02 | 117.99      | 121.00   |
| 1   | AA    | 363  | A    | N3-C4-C5    | -5.02 | 123.29      | 126.80   |
| 1   | AA    | 378  | G    | C6-C5-N7    | -5.02 | 127.39      | 130.40   |
| 1   | AA    | 483  | C    | C5-C6-N1    | 5.02  | 123.51      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 536  | C    | C5-C4-N4    | -5.02 | 116.69      | 120.20   |
| 1   | AA    | 677  | U    | N1-C2-O2    | -5.02 | 119.29      | 122.80   |
| 1   | AA    | 678  | U    | N3-C2-O2    | -5.02 | 118.69      | 122.20   |
| 1   | AA    | 1015 | G    | O5'-P-OP1   | 5.02  | 116.72      | 110.70   |
| 35  | BB    | 35   | G    | C4-N9-C1'   | 5.02  | 133.02      | 126.50   |
| 35  | BB    | 607  | U    | C4'-C3'-C2' | -5.02 | 97.58       | 102.60   |
| 35  | BB    | 704  | G    | C3'-C2'-C1' | 5.02  | 105.51      | 101.50   |
| 35  | BB    | 829  | A    | N3-C4-N9    | 5.02  | 131.41      | 127.40   |
| 35  | BB    | 882  | G    | C6-C5-N7    | -5.02 | 127.39      | 130.40   |
| 35  | BB    | 1695 | G    | N3-C4-C5    | -5.02 | 126.09      | 128.60   |
| 35  | BB    | 2230 | G    | N3-C4-C5    | 5.02  | 131.11      | 128.60   |
| 35  | BB    | 2245 | U    | N3-C4-C5    | 5.02  | 117.61      | 114.60   |
| 1   | AA    | 191  | G    | N1-C2-N3    | -5.02 | 120.89      | 123.90   |
| 1   | AA    | 246  | A    | O4'-C1'-N9  | 5.02  | 112.21      | 108.20   |
| 1   | AA    | 1170 | A    | OP1-P-OP2   | -5.02 | 112.08      | 119.60   |
| 1   | AA    | 1417 | G    | P-O3'-C3'   | -5.02 | 113.68      | 119.70   |
| 34  | BA    | 77   | U    | C3'-C2'-C1' | -5.02 | 97.49       | 101.50   |
| 34  | BA    | 112  | G    | N9-C4-C5    | 5.02  | 107.41      | 105.40   |
| 35  | BB    | 589  | U    | N3-C2-O2    | 5.02  | 125.71      | 122.20   |
| 35  | BB    | 650  | C    | C6-N1-C2    | -5.02 | 118.29      | 120.30   |
| 35  | BB    | 816  | C    | C2-N3-C4    | 5.02  | 122.41      | 119.90   |
| 35  | BB    | 854  | C    | N1-C1'-C2'  | -5.02 | 106.48      | 112.00   |
| 35  | BB    | 945  | A    | C6-N1-C2    | -5.02 | 115.59      | 118.60   |
| 35  | BB    | 1620 | G    | O4'-C1'-N9  | 5.02  | 112.21      | 108.20   |
| 35  | BB    | 2038 | G    | C6-C5-N7    | -5.02 | 127.39      | 130.40   |
| 1   | AA    | 34   | C    | N3-C4-C5    | -5.01 | 119.89      | 121.90   |
| 1   | AA    | 189  | A    | N3-C4-C5    | -5.01 | 123.29      | 126.80   |
| 1   | AA    | 482  | A    | C5-C6-N1    | -5.01 | 115.19      | 117.70   |
| 1   | AA    | 551  | U    | N3-C2-O2    | 5.01  | 125.71      | 122.20   |
| 2   | AB    | 15   | PHE  | N-CA-CB     | 5.01  | 119.63      | 110.60   |
| 34  | BA    | 106  | G    | C4-C5-N7    | 5.01  | 112.81      | 110.80   |
| 35  | BB    | 926  | G    | P-O5'-C5'   | 5.01  | 128.92      | 120.90   |
| 35  | BB    | 989  | G    | C5'-C4'-C3' | -5.01 | 107.98      | 116.00   |
| 35  | BB    | 1133 | A    | N7-C8-N9    | -5.01 | 111.29      | 113.80   |
| 35  | BB    | 1298 | C    | N3-C4-N4    | 5.01  | 121.51      | 118.00   |
| 35  | BB    | 1515 | A    | C6-N1-C2    | 5.01  | 121.61      | 118.60   |
| 35  | BB    | 1844 | C    | C6-N1-C1'   | -5.01 | 114.78      | 120.80   |
| 35  | BB    | 1922 | G    | N1-C2-N3    | -5.01 | 120.89      | 123.90   |
| 35  | BB    | 2067 | G    | C5-N7-C8    | -5.01 | 101.79      | 104.30   |
| 35  | BB    | 2148 | G    | N1-C2-N2    | 5.01  | 120.71      | 116.20   |
| 35  | BB    | 2795 | C    | C2-N3-C4    | 5.01  | 122.41      | 119.90   |
| 41  | BH    | 82   | SER  | C-N-CA      | 5.01  | 134.24      | 121.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 83   | C    | O4'-C1'-N1  | 5.01  | 112.21      | 108.20   |
| 35  | BB    | 206  | U    | N1-C2-N3    | -5.01 | 111.89      | 114.90   |
| 35  | BB    | 612  | G    | N3-C4-C5    | -5.01 | 126.09      | 128.60   |
| 35  | BB    | 1254 | A    | C2'-C3'-O3' | 5.01  | 121.72      | 113.70   |
| 35  | BB    | 1472 | C    | N1-C2-O2    | 5.01  | 121.91      | 118.90   |
| 35  | BB    | 1587 | G    | N9-C1'-C2'  | 5.01  | 120.52      | 114.00   |
| 35  | BB    | 1624 | U    | C5-C6-N1    | 5.01  | 125.21      | 122.70   |
| 35  | BB    | 1979 | U    | C5-C6-N1    | 5.01  | 125.21      | 122.70   |
| 35  | BB    | 2328 | A    | N3-C4-N9    | 5.01  | 131.41      | 127.40   |
| 35  | BB    | 2719 | G    | C8-N9-C4    | -5.01 | 104.39      | 106.40   |
| 1   | AA    | 41   | G    | C1'-O4'-C4' | -5.01 | 105.89      | 109.90   |
| 1   | AA    | 211  | G    | C5-N7-C8    | 5.01  | 106.81      | 104.30   |
| 1   | AA    | 659  | U    | N3-C4-O4    | 5.01  | 122.91      | 119.40   |
| 1   | AA    | 1241 | G    | N3-C4-C5    | -5.01 | 126.09      | 128.60   |
| 1   | AA    | 1300 | G    | C2-N3-C4    | -5.01 | 109.39      | 111.90   |
| 1   | AA    | 1521 | C    | C2-N3-C4    | 5.01  | 122.41      | 119.90   |
| 12  | AL    | 82   | ARG  | CD-NE-CZ    | 5.01  | 130.62      | 123.60   |
| 34  | BA    | 14   | U    | C2-N1-C1'   | 5.01  | 123.71      | 117.70   |
| 34  | BA    | 23   | G    | N1-C2-N3    | -5.01 | 120.89      | 123.90   |
| 35  | BB    | 60   | G    | N3-C2-N2    | 5.01  | 123.41      | 119.90   |
| 35  | BB    | 242  | G    | N9-C4-C5    | -5.01 | 103.39      | 105.40   |
| 35  | BB    | 683  | U    | N3-C4-C5    | -5.01 | 111.59      | 114.60   |
| 35  | BB    | 879  | G    | C5-N7-C8    | -5.01 | 101.79      | 104.30   |
| 35  | BB    | 1035 | U    | C4'-C3'-C2' | -5.01 | 97.59       | 102.60   |
| 35  | BB    | 1060 | U    | N3-C2-O2    | -5.01 | 118.69      | 122.20   |
| 35  | BB    | 1191 | G    | C4-C5-C6    | 5.01  | 121.81      | 118.80   |
| 35  | BB    | 1236 | G    | N1-C2-N3    | -5.01 | 120.89      | 123.90   |
| 35  | BB    | 1279 | G    | N1-C2-N3    | -5.01 | 120.89      | 123.90   |
| 35  | BB    | 1353 | A    | C6-C5-N7    | -5.01 | 128.79      | 132.30   |
| 35  | BB    | 1639 | C    | N3-C4-N4    | 5.01  | 121.51      | 118.00   |
| 35  | BB    | 1697 | G    | C4-C5-C6    | 5.01  | 121.81      | 118.80   |
| 35  | BB    | 1719 | G    | N1-C2-N3    | -5.01 | 120.89      | 123.90   |
| 35  | BB    | 2147 | A    | O4'-C1'-C2' | 5.01  | 112.11      | 107.60   |
| 35  | BB    | 2548 | U    | N1-C2-O2    | -5.01 | 119.29      | 122.80   |
| 41  | BH    | 31   | VAL  | CA-CB-CG2   | -5.01 | 103.38      | 110.90   |
| 41  | BH    | 76   | GLU  | C-N-CA      | 5.01  | 134.23      | 121.70   |
| 1   | AA    | 207  | C    | C4'-C3'-C2' | -5.01 | 97.59       | 102.60   |
| 1   | AA    | 873  | A    | N9-C4-C5    | 5.01  | 107.80      | 105.80   |
| 1   | AA    | 1363 | A    | O4'-C1'-N9  | 5.01  | 112.21      | 108.20   |
| 28  | B3    | 16   | ARG  | NE-CZ-NH2   | -5.01 | 117.80      | 120.30   |
| 35  | BB    | 2    | G    | C2-N3-C4    | -5.01 | 109.39      | 111.90   |
| 35  | BB    | 325  | G    | C5-C6-O6    | -5.01 | 125.59      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 543  | G    | P-O5'-C5'   | -5.01 | 112.89      | 120.90   |
| 35  | BB    | 841  | G    | C4'-C3'-C2' | -5.01 | 97.59       | 102.60   |
| 35  | BB    | 941  | A    | C4-C5-N7    | -5.01 | 108.19      | 110.70   |
| 35  | BB    | 974  | G    | C4-N9-C1'   | 5.01  | 133.01      | 126.50   |
| 35  | BB    | 1450 | G    | N3-C4-C5    | 5.01  | 131.10      | 128.60   |
| 35  | BB    | 2780 | G    | C8-N9-C4    | 5.01  | 108.40      | 106.40   |
| 41  | BH    | 47   | PHE  | CB-CG-CD1   | -5.01 | 117.29      | 120.80   |
| 45  | BL    | 61   | LEU  | CB-CG-CD2   | 5.01  | 119.52      | 111.00   |
| 1   | AA    | 462  | G    | P-O3'-C3'   | 5.01  | 125.71      | 119.70   |
| 1   | AA    | 719  | C    | O4'-C1'-N1  | 5.01  | 112.21      | 108.20   |
| 1   | AA    | 741  | G    | N1-C2-N3    | -5.01 | 120.89      | 123.90   |
| 1   | AA    | 770  | C    | N1-C2-N3    | -5.01 | 115.69      | 119.20   |
| 20  | AT    | 24   | ARG  | NH1-CZ-NH2  | 5.01  | 124.91      | 119.40   |
| 35  | BB    | 1148 | U    | P-O3'-C3'   | -5.01 | 113.69      | 119.70   |
| 35  | BB    | 1648 | U    | C6-N1-C2    | 5.01  | 124.00      | 121.00   |
| 35  | BB    | 1987 | A    | C5-C6-N6    | -5.01 | 119.69      | 123.70   |
| 35  | BB    | 2799 | A    | C4-C5-C6    | 5.01  | 119.50      | 117.00   |
| 1   | AA    | 182  | A    | C3'-C2'-C1' | 5.01  | 105.51      | 101.50   |
| 1   | AA    | 449  | G    | N3-C2-N2    | 5.01  | 123.41      | 119.90   |
| 1   | AA    | 888  | G    | C5-N7-C8    | 5.01  | 106.80      | 104.30   |
| 1   | AA    | 924  | C    | N3-C4-N4    | 5.01  | 121.50      | 118.00   |
| 1   | AA    | 1229 | A    | O4'-C1'-N9  | 5.01  | 112.20      | 108.20   |
| 1   | AA    | 1471 | U    | OP1-P-OP2   | -5.01 | 112.09      | 119.60   |
| 10  | AJ    | 59   | LYS  | CA-CB-CG    | 5.01  | 124.42      | 113.40   |
| 35  | BB    | 91   | A    | C5'-C4'-O4' | 5.01  | 115.11      | 109.10   |
| 35  | BB    | 143  | C    | O3'-P-O5'   | -5.01 | 94.49       | 104.00   |
| 35  | BB    | 275  | C    | N3-C4-N4    | 5.01  | 121.50      | 118.00   |
| 35  | BB    | 818  | G    | C8-N9-C1'   | -5.01 | 120.49      | 127.00   |
| 35  | BB    | 1221 | C    | C6-N1-C2    | 5.01  | 122.30      | 120.30   |
| 35  | BB    | 1299 | G    | C8-N9-C4    | -5.01 | 104.40      | 106.40   |
| 35  | BB    | 1486 | U    | P-O5'-C5'   | 5.01  | 128.91      | 120.90   |
| 35  | BB    | 1687 | G    | C4-C5-N7    | 5.01  | 112.80      | 110.80   |
| 35  | BB    | 1744 | A    | C8-N9-C4    | -5.01 | 103.80      | 105.80   |
| 35  | BB    | 1797 | G    | N1-C2-N2    | 5.01  | 120.71      | 116.20   |
| 35  | BB    | 1938 | A    | C4-C5-C6    | 5.01  | 119.50      | 117.00   |
| 35  | BB    | 1956 | U    | C2-N3-C4    | 5.01  | 130.00      | 127.00   |
| 35  | BB    | 2186 | G    | N7-C8-N9    | 5.01  | 115.60      | 113.10   |
| 35  | BB    | 2610 | C    | C5-C6-N1    | 5.01  | 123.50      | 121.00   |
| 35  | BB    | 2825 | G    | C8-N9-C4    | 5.01  | 108.40      | 106.40   |
| 43  | BJ    | 129  | GLU  | O-C-N       | -5.01 | 114.69      | 122.70   |
| 1   | AA    | 575  | G    | C2-N3-C4    | 5.00  | 114.40      | 111.90   |
| 1   | AA    | 745  | G    | C5'-C4'-C3' | -5.00 | 107.99      | 116.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 35  | BB    | 144  | A    | N1-C2-N3    | -5.00 | 126.80      | 129.30   |
| 35  | BB    | 305  | C    | N3-C2-O2    | -5.00 | 118.40      | 121.90   |
| 35  | BB    | 569  | U    | C6-N1-C2    | -5.00 | 118.00      | 121.00   |
| 35  | BB    | 1444 | G    | C4-C5-C6    | 5.00  | 121.80      | 118.80   |
| 35  | BB    | 1752 | C    | P-O5'-C5'   | 5.00  | 128.91      | 120.90   |
| 35  | BB    | 2392 | A    | C6-N1-C2    | 5.00  | 121.60      | 118.60   |
| 35  | BB    | 2455 | G    | O5'-P-OP1   | -5.00 | 101.20      | 105.70   |
| 35  | BB    | 2589 | A    | C5-C6-N6    | -5.00 | 119.70      | 123.70   |
| 54  | BU    | 81   | ARG  | NE-CZ-NH1   | -5.00 | 117.80      | 120.30   |
| 1   | AA    | 21   | G    | OP1-P-OP2   | -5.00 | 112.10      | 119.60   |
| 1   | AA    | 38   | G    | N9-C4-C5    | -5.00 | 103.40      | 105.40   |
| 1   | AA    | 113  | G    | C4-C5-N7    | 5.00  | 112.80      | 110.80   |
| 1   | AA    | 208  | U    | N1-C2-O2    | -5.00 | 119.30      | 122.80   |
| 1   | AA    | 633  | G    | N1-C2-N3    | -5.00 | 120.90      | 123.90   |
| 1   | AA    | 699  | C    | O4'-C1'-C2' | -5.00 | 100.80      | 105.80   |
| 1   | AA    | 740  | U    | C5-C6-N1    | 5.00  | 125.20      | 122.70   |
| 1   | AA    | 1000 | A    | C5-N7-C8    | 5.00  | 106.40      | 103.90   |
| 20  | AT    | 65   | LEU  | CB-CG-CD1   | 5.00  | 119.50      | 111.00   |
| 29  | B4    | 43   | ARG  | NE-CZ-NH1   | 5.00  | 122.80      | 120.30   |
| 30  | B5    | 65   | LEU  | CB-CG-CD2   | -5.00 | 102.50      | 111.00   |
| 34  | BA    | 98   | G    | C6-N1-C2    | 5.00  | 128.10      | 125.10   |
| 35  | BB    | 28   | A    | N1-C6-N6    | 5.00  | 121.60      | 118.60   |
| 35  | BB    | 122  | G    | P-O5'-C5'   | 5.00  | 128.91      | 120.90   |
| 35  | BB    | 213  | A    | O4'-C4'-C3' | -5.00 | 99.00       | 104.00   |
| 35  | BB    | 461  | C    | C5-C4-N4    | -5.00 | 116.70      | 120.20   |
| 35  | BB    | 523  | C    | C2-N3-C4    | 5.00  | 122.40      | 119.90   |
| 35  | BB    | 536  | G    | C4-N9-C1'   | -5.00 | 120.00      | 126.50   |
| 35  | BB    | 897  | C    | C3'-C2'-C1' | 5.00  | 105.50      | 101.50   |
| 35  | BB    | 1114 | C    | O5'-C5'-C4' | -5.00 | 102.19      | 111.70   |
| 35  | BB    | 1248 | G    | OP1-P-OP2   | -5.00 | 112.09      | 119.60   |
| 35  | BB    | 1512 | C    | N1-C2-O2    | -5.00 | 115.90      | 118.90   |
| 35  | BB    | 1516 | G    | C5-C6-O6    | -5.00 | 125.60      | 128.60   |
| 35  | BB    | 1732 | C    | O4'-C4'-C3' | -5.00 | 99.00       | 104.00   |
| 35  | BB    | 1732 | C    | C5-C6-N1    | 5.00  | 123.50      | 121.00   |
| 35  | BB    | 1953 | A    | C5-C6-N6    | -5.00 | 119.70      | 123.70   |
| 35  | BB    | 2419 | U    | C3'-C2'-C1' | 5.00  | 105.50      | 101.50   |
| 35  | BB    | 2526 | G    | N7-C8-N9    | -5.00 | 110.60      | 113.10   |
| 38  | BE    | 187  | VAL  | CG1-CB-CG2  | 5.00  | 118.91      | 110.90   |
| 41  | BH    | 49   | ALA  | CB-CA-C     | -5.00 | 102.59      | 110.10   |
| 1   | AA    | 651  | C    | C2-N3-C4    | -5.00 | 117.40      | 119.90   |
| 1   | AA    | 1004 | A    | C5'-C4'-C3' | 5.00  | 124.00      | 116.00   |
| 1   | AA    | 1061 | G    | C4-C5-C6    | 5.00  | 121.80      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1304 | G    | C4-C5-C6    | -5.00 | 115.80      | 118.80   |
| 1   | AA    | 1308 | U    | C1'-O4'-C4' | 5.00  | 113.90      | 109.90   |
| 13  | AM    | 11   | HIS  | N-CA-CB     | 5.00  | 119.60      | 110.60   |
| 21  | AU    | 16   | ARG  | NE-CZ-NH2   | -5.00 | 117.80      | 120.30   |
| 23  | AX    | 17   | C    | O4'-C1'-N1  | 5.00  | 112.20      | 108.20   |
| 25  | B0    | 68   | ALA  | O-C-N       | 5.00  | 130.70      | 122.70   |
| 35  | BB    | 223  | A    | N9-C4-C5    | -5.00 | 103.80      | 105.80   |
| 35  | BB    | 581  | C    | C1'-O4'-C4' | 5.00  | 113.90      | 109.90   |
| 35  | BB    | 1000 | A    | C4-C5-C6    | 5.00  | 119.50      | 117.00   |
| 35  | BB    | 1132 | U    | C2-N3-C4    | 5.00  | 130.00      | 127.00   |
| 35  | BB    | 1248 | G    | N3-C4-N9    | 5.00  | 129.00      | 126.00   |
| 35  | BB    | 1371 | G    | N7-C8-N9    | 5.00  | 115.60      | 113.10   |
| 35  | BB    | 2124 | G    | C5'-C4'-C3' | 5.00  | 124.00      | 116.00   |
| 35  | BB    | 2609 | U    | C1'-O4'-C4' | -5.00 | 105.90      | 109.90   |

There are no chirality outliers.

All (2342) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 100  | G    | Sidechain |
| 1   | AA    | 1001 | C    | Sidechain |
| 1   | AA    | 1003 | G    | Sidechain |
| 1   | AA    | 1005 | A    | Sidechain |
| 1   | AA    | 1006 | G    | Sidechain |
| 1   | AA    | 1007 | U    | Sidechain |
| 1   | AA    | 1008 | U    | Sidechain |
| 1   | AA    | 101  | A    | Sidechain |
| 1   | AA    | 1010 | U    | Sidechain |
| 1   | AA    | 1011 | C    | Sidechain |
| 1   | AA    | 1012 | A    | Sidechain |
| 1   | AA    | 1013 | G    | Sidechain |
| 1   | AA    | 1014 | A    | Sidechain |
| 1   | AA    | 1015 | G    | Sidechain |
| 1   | AA    | 1016 | A    | Sidechain |
| 1   | AA    | 1018 | G    | Sidechain |
| 1   | AA    | 1019 | A    | Sidechain |
| 1   | AA    | 1024 | G    | Sidechain |
| 1   | AA    | 1025 | U    | Sidechain |
| 1   | AA    | 1026 | G    | Sidechain |
| 1   | AA    | 1029 | U    | Sidechain |
| 1   | AA    | 103  | U    | Sidechain |
| 1   | AA    | 1031 | C    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 1035 | A    | Sidechain |
| 1   | AA    | 1039 | G    | Sidechain |
| 1   | AA    | 1042 | A    | Sidechain |
| 1   | AA    | 1044 | A    | Sidechain |
| 1   | AA    | 1046 | A    | Sidechain |
| 1   | AA    | 1047 | G    | Sidechain |
| 1   | AA    | 1048 | G    | Sidechain |
| 1   | AA    | 1049 | U    | Sidechain |
| 1   | AA    | 1050 | G    | Sidechain |
| 1   | AA    | 1053 | G    | Sidechain |
| 1   | AA    | 1055 | A    | Sidechain |
| 1   | AA    | 1056 | U    | Sidechain |
| 1   | AA    | 1058 | G    | Sidechain |
| 1   | AA    | 1059 | C    | Sidechain |
| 1   | AA    | 106  | C    | Sidechain |
| 1   | AA    | 1060 | U    | Sidechain |
| 1   | AA    | 1061 | G    | Sidechain |
| 1   | AA    | 1062 | U    | Sidechain |
| 1   | AA    | 1065 | U    | Sidechain |
| 1   | AA    | 1069 | C    | Sidechain |
| 1   | AA    | 107  | G    | Sidechain |
| 1   | AA    | 1070 | U    | Sidechain |
| 1   | AA    | 1071 | C    | Sidechain |
| 1   | AA    | 1073 | U    | Sidechain |
| 1   | AA    | 1075 | U    | Sidechain |
| 1   | AA    | 1076 | U    | Sidechain |
| 1   | AA    | 1077 | G    | Sidechain |
| 1   | AA    | 1080 | A    | Sidechain |
| 1   | AA    | 1082 | A    | Sidechain |
| 1   | AA    | 1084 | G    | Sidechain |
| 1   | AA    | 1085 | U    | Sidechain |
| 1   | AA    | 1086 | U    | Sidechain |
| 1   | AA    | 1087 | G    | Sidechain |
| 1   | AA    | 1089 | G    | Sidechain |
| 1   | AA    | 109  | A    | Sidechain |
| 1   | AA    | 1091 | U    | Sidechain |
| 1   | AA    | 1092 | A    | Sidechain |
| 1   | AA    | 1094 | G    | Sidechain |
| 1   | AA    | 1097 | C    | Sidechain |
| 1   | AA    | 1099 | G    | Sidechain |
| 1   | AA    | 11   | G    | Sidechain |
| 1   | AA    | 1101 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 1104 | G    | Sidechain |
| 1   | AA    | 1106 | G    | Sidechain |
| 1   | AA    | 1108 | G    | Sidechain |
| 1   | AA    | 111  | G    | Sidechain |
| 1   | AA    | 1114 | C    | Sidechain |
| 1   | AA    | 1117 | A    | Sidechain |
| 1   | AA    | 1118 | U    | Sidechain |
| 1   | AA    | 1119 | C    | Sidechain |
| 1   | AA    | 112  | G    | Sidechain |
| 1   | AA    | 1122 | U    | Sidechain |
| 1   | AA    | 1124 | G    | Sidechain |
| 1   | AA    | 1125 | U    | Sidechain |
| 1   | AA    | 1128 | C    | Sidechain |
| 1   | AA    | 1129 | C    | Sidechain |
| 1   | AA    | 1130 | A    | Sidechain |
| 1   | AA    | 1131 | G    | Sidechain |
| 1   | AA    | 1132 | C    | Sidechain |
| 1   | AA    | 1135 | U    | Sidechain |
| 1   | AA    | 1136 | C    | Sidechain |
| 1   | AA    | 1139 | G    | Sidechain |
| 1   | AA    | 114  | U    | Sidechain |
| 1   | AA    | 1143 | G    | Sidechain |
| 1   | AA    | 1144 | G    | Sidechain |
| 1   | AA    | 1147 | C    | Sidechain |
| 1   | AA    | 115  | G    | Sidechain |
| 1   | AA    | 1150 | A    | Sidechain |
| 1   | AA    | 1151 | A    | Sidechain |
| 1   | AA    | 1152 | A    | Sidechain |
| 1   | AA    | 1153 | G    | Sidechain |
| 1   | AA    | 1156 | G    | Sidechain |
| 1   | AA    | 1158 | C    | Sidechain |
| 1   | AA    | 1161 | C    | Sidechain |
| 1   | AA    | 1165 | U    | Sidechain |
| 1   | AA    | 1166 | G    | Sidechain |
| 1   | AA    | 117  | G    | Sidechain |
| 1   | AA    | 1171 | A    | Sidechain |
| 1   | AA    | 1172 | C    | Sidechain |
| 1   | AA    | 1173 | U    | Sidechain |
| 1   | AA    | 1177 | G    | Sidechain |
| 1   | AA    | 1178 | G    | Sidechain |
| 1   | AA    | 118  | U    | Sidechain |
| 1   | AA    | 1180 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 1181 | G    | Sidechain |
| 1   | AA    | 1185 | G    | Sidechain |
| 1   | AA    | 1187 | G    | Sidechain |
| 1   | AA    | 119  | A    | Sidechain |
| 1   | AA    | 1190 | G    | Sidechain |
| 1   | AA    | 1192 | C    | Sidechain |
| 1   | AA    | 1193 | G    | Sidechain |
| 1   | AA    | 1195 | C    | Sidechain |
| 1   | AA    | 12   | U    | Sidechain |
| 1   | AA    | 1200 | C    | Sidechain |
| 1   | AA    | 1203 | C    | Sidechain |
| 1   | AA    | 1205 | U    | Sidechain |
| 1   | AA    | 1206 | G    | Sidechain |
| 1   | AA    | 1207 | G    | Sidechain |
| 1   | AA    | 1208 | C    | Sidechain |
| 1   | AA    | 1211 | U    | Sidechain |
| 1   | AA    | 1216 | A    | Sidechain |
| 1   | AA    | 1218 | C    | Sidechain |
| 1   | AA    | 1219 | A    | Sidechain |
| 1   | AA    | 122  | G    | Sidechain |
| 1   | AA    | 1221 | G    | Sidechain |
| 1   | AA    | 1222 | G    | Sidechain |
| 1   | AA    | 1224 | U    | Sidechain |
| 1   | AA    | 1225 | A    | Sidechain |
| 1   | AA    | 1226 | C    | Sidechain |
| 1   | AA    | 1227 | A    | Sidechain |
| 1   | AA    | 123  | U    | Sidechain |
| 1   | AA    | 1231 | G    | Sidechain |
| 1   | AA    | 1236 | A    | Sidechain |
| 1   | AA    | 1237 | C    | Sidechain |
| 1   | AA    | 1240 | U    | Sidechain |
| 1   | AA    | 1244 | G    | Sidechain |
| 1   | AA    | 1246 | A    | Sidechain |
| 1   | AA    | 1248 | A    | Sidechain |
| 1   | AA    | 1250 | A    | Sidechain |
| 1   | AA    | 1252 | A    | Sidechain |
| 1   | AA    | 1258 | G    | Sidechain |
| 1   | AA    | 1259 | C    | Sidechain |
| 1   | AA    | 1260 | G    | Sidechain |
| 1   | AA    | 1261 | A    | Sidechain |
| 1   | AA    | 1267 | C    | Sidechain |
| 1   | AA    | 1269 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 1272 | G    | Sidechain |
| 1   | AA    | 1274 | A    | Sidechain |
| 1   | AA    | 1276 | G    | Sidechain |
| 1   | AA    | 1277 | C    | Sidechain |
| 1   | AA    | 1278 | G    | Sidechain |
| 1   | AA    | 1279 | G    | Sidechain |
| 1   | AA    | 128  | G    | Sidechain |
| 1   | AA    | 1280 | A    | Sidechain |
| 1   | AA    | 1282 | C    | Sidechain |
| 1   | AA    | 1283 | U    | Sidechain |
| 1   | AA    | 1284 | C    | Sidechain |
| 1   | AA    | 1287 | A    | Sidechain |
| 1   | AA    | 1289 | A    | Sidechain |
| 1   | AA    | 1291 | U    | Sidechain |
| 1   | AA    | 1292 | G    | Sidechain |
| 1   | AA    | 1293 | C    | Sidechain |
| 1   | AA    | 1294 | G    | Sidechain |
| 1   | AA    | 1295 | U    | Sidechain |
| 1   | AA    | 1299 | A    | Sidechain |
| 1   | AA    | 13   | U    | Sidechain |
| 1   | AA    | 130  | A    | Sidechain |
| 1   | AA    | 1300 | G    | Sidechain |
| 1   | AA    | 1302 | C    | Sidechain |
| 1   | AA    | 1304 | G    | Sidechain |
| 1   | AA    | 1305 | G    | Sidechain |
| 1   | AA    | 1307 | U    | Sidechain |
| 1   | AA    | 1311 | A    | Sidechain |
| 1   | AA    | 1312 | G    | Sidechain |
| 1   | AA    | 1319 | A    | Sidechain |
| 1   | AA    | 1320 | C    | Sidechain |
| 1   | AA    | 1323 | G    | Sidechain |
| 1   | AA    | 1325 | C    | Sidechain |
| 1   | AA    | 1327 | C    | Sidechain |
| 1   | AA    | 133  | U    | Sidechain |
| 1   | AA    | 1330 | U    | Sidechain |
| 1   | AA    | 1331 | G    | Sidechain |
| 1   | AA    | 1334 | G    | Sidechain |
| 1   | AA    | 1335 | U    | Sidechain |
| 1   | AA    | 1337 | G    | Sidechain |
| 1   | AA    | 1339 | A    | Sidechain |
| 1   | AA    | 134  | G    | Sidechain |
| 1   | AA    | 1340 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 1344 | C    | Sidechain |
| 1   | AA    | 1345 | U    | Sidechain |
| 1   | AA    | 1346 | A    | Sidechain |
| 1   | AA    | 1347 | G    | Sidechain |
| 1   | AA    | 1348 | U    | Sidechain |
| 1   | AA    | 1349 | A    | Sidechain |
| 1   | AA    | 1353 | G    | Sidechain |
| 1   | AA    | 1354 | U    | Sidechain |
| 1   | AA    | 1355 | G    | Sidechain |
| 1   | AA    | 136  | C    | Sidechain |
| 1   | AA    | 1360 | A    | Sidechain |
| 1   | AA    | 1363 | A    | Sidechain |
| 1   | AA    | 1365 | G    | Sidechain |
| 1   | AA    | 137  | U    | Sidechain |
| 1   | AA    | 1370 | G    | Sidechain |
| 1   | AA    | 1371 | G    | Sidechain |
| 1   | AA    | 1373 | G    | Sidechain |
| 1   | AA    | 1374 | A    | Sidechain |
| 1   | AA    | 1375 | A    | Sidechain |
| 1   | AA    | 1376 | U    | Sidechain |
| 1   | AA    | 1378 | C    | Sidechain |
| 1   | AA    | 1379 | G    | Sidechain |
| 1   | AA    | 1383 | C    | Sidechain |
| 1   | AA    | 1385 | G    | Sidechain |
| 1   | AA    | 1386 | G    | Sidechain |
| 1   | AA    | 1387 | G    | Sidechain |
| 1   | AA    | 1388 | C    | Sidechain |
| 1   | AA    | 1394 | A    | Sidechain |
| 1   | AA    | 1399 | C    | Sidechain |
| 1   | AA    | 14   | U    | Sidechain |
| 1   | AA    | 1401 | G    | Sidechain |
| 1   | AA    | 1403 | C    | Sidechain |
| 1   | AA    | 1404 | C    | Sidechain |
| 1   | AA    | 1413 | A    | Sidechain |
| 1   | AA    | 1415 | G    | Sidechain |
| 1   | AA    | 1418 | A    | Sidechain |
| 1   | AA    | 142  | G    | Sidechain |
| 1   | AA    | 1422 | G    | Sidechain |
| 1   | AA    | 1423 | G    | Sidechain |
| 1   | AA    | 1425 | U    | Sidechain |
| 1   | AA    | 1432 | G    | Sidechain |
| 1   | AA    | 1433 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 1437 | A    | Sidechain |
| 1   | AA    | 1439 | G    | Sidechain |
| 1   | AA    | 1441 | A    | Sidechain |
| 1   | AA    | 1442 | G    | Sidechain |
| 1   | AA    | 1444 | U    | Sidechain |
| 1   | AA    | 1445 | U    | Sidechain |
| 1   | AA    | 1446 | A    | Sidechain |
| 1   | AA    | 1447 | A    | Sidechain |
| 1   | AA    | 1455 | G    | Sidechain |
| 1   | AA    | 1456 | A    | Sidechain |
| 1   | AA    | 1457 | G    | Sidechain |
| 1   | AA    | 1458 | G    | Sidechain |
| 1   | AA    | 1459 | G    | Sidechain |
| 1   | AA    | 146  | G    | Sidechain |
| 1   | AA    | 1465 | A    | Sidechain |
| 1   | AA    | 1468 | A    | Sidechain |
| 1   | AA    | 1469 | C    | Sidechain |
| 1   | AA    | 147  | G    | Sidechain |
| 1   | AA    | 1470 | U    | Sidechain |
| 1   | AA    | 1472 | U    | Sidechain |
| 1   | AA    | 1473 | G    | Sidechain |
| 1   | AA    | 1475 | G    | Sidechain |
| 1   | AA    | 1476 | A    | Sidechain |
| 1   | AA    | 1478 | U    | Sidechain |
| 1   | AA    | 1479 | C    | Sidechain |
| 1   | AA    | 1480 | A    | Sidechain |
| 1   | AA    | 1482 | G    | Sidechain |
| 1   | AA    | 1483 | A    | Sidechain |
| 1   | AA    | 1484 | C    | Sidechain |
| 1   | AA    | 1486 | G    | Sidechain |
| 1   | AA    | 1488 | G    | Sidechain |
| 1   | AA    | 1490 | U    | Sidechain |
| 1   | AA    | 1492 | A    | Sidechain |
| 1   | AA    | 1493 | A    | Sidechain |
| 1   | AA    | 1499 | A    | Sidechain |
| 1   | AA    | 1500 | A    | Sidechain |
| 1   | AA    | 1501 | C    | Sidechain |
| 1   | AA    | 1502 | A    | Sidechain |
| 1   | AA    | 1503 | A    | Sidechain |
| 1   | AA    | 1504 | G    | Sidechain |
| 1   | AA    | 1505 | G    | Sidechain |
| 1   | AA    | 1507 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 1508 | A    | Sidechain |
| 1   | AA    | 151  | A    | Sidechain |
| 1   | AA    | 1512 | U    | Sidechain |
| 1   | AA    | 1513 | A    | Sidechain |
| 1   | AA    | 1516 | G    | Sidechain |
| 1   | AA    | 1517 | G    | Sidechain |
| 1   | AA    | 1518 | A    | Sidechain |
| 1   | AA    | 1519 | A    | Sidechain |
| 1   | AA    | 1520 | C    | Sidechain |
| 1   | AA    | 1521 | C    | Sidechain |
| 1   | AA    | 1522 | U    | Sidechain |
| 1   | AA    | 1524 | C    | Sidechain |
| 1   | AA    | 1525 | G    | Sidechain |
| 1   | AA    | 1526 | G    | Sidechain |
| 1   | AA    | 1528 | U    | Sidechain |
| 1   | AA    | 1529 | G    | Sidechain |
| 1   | AA    | 153  | C    | Sidechain |
| 1   | AA    | 1531 | A    | Sidechain |
| 1   | AA    | 156  | C    | Sidechain |
| 1   | AA    | 157  | U    | Sidechain |
| 1   | AA    | 158  | G    | Sidechain |
| 1   | AA    | 161  | A    | Sidechain |
| 1   | AA    | 162  | A    | Sidechain |
| 1   | AA    | 163  | C    | Sidechain |
| 1   | AA    | 166  | U    | Sidechain |
| 1   | AA    | 173  | U    | Sidechain |
| 1   | AA    | 177  | G    | Sidechain |
| 1   | AA    | 18   | C    | Sidechain |
| 1   | AA    | 180  | U    | Sidechain |
| 1   | AA    | 181  | A    | Sidechain |
| 1   | AA    | 183  | C    | Sidechain |
| 1   | AA    | 185  | U    | Sidechain |
| 1   | AA    | 187  | G    | Sidechain |
| 1   | AA    | 188  | C    | Sidechain |
| 1   | AA    | 189  | A    | Sidechain |
| 1   | AA    | 19   | A    | Sidechain |
| 1   | AA    | 191  | G    | Sidechain |
| 1   | AA    | 193  | C    | Sidechain |
| 1   | AA    | 194  | C    | Sidechain |
| 1   | AA    | 195  | A    | Sidechain |
| 1   | AA    | 196  | A    | Sidechain |
| 1   | AA    | 197  | A    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AA    | 200 | G    | Sidechain |
| 1   | AA    | 201 | G    | Sidechain |
| 1   | AA    | 202 | G    | Sidechain |
| 1   | AA    | 203 | G    | Sidechain |
| 1   | AA    | 205 | A    | Sidechain |
| 1   | AA    | 208 | U    | Sidechain |
| 1   | AA    | 210 | C    | Sidechain |
| 1   | AA    | 211 | G    | Sidechain |
| 1   | AA    | 212 | G    | Sidechain |
| 1   | AA    | 216 | U    | Sidechain |
| 1   | AA    | 217 | C    | Sidechain |
| 1   | AA    | 219 | U    | Sidechain |
| 1   | AA    | 22  | G    | Sidechain |
| 1   | AA    | 221 | C    | Sidechain |
| 1   | AA    | 223 | A    | Sidechain |
| 1   | AA    | 227 | G    | Sidechain |
| 1   | AA    | 229 | U    | Sidechain |
| 1   | AA    | 230 | G    | Sidechain |
| 1   | AA    | 233 | C    | Sidechain |
| 1   | AA    | 238 | A    | Sidechain |
| 1   | AA    | 239 | U    | Sidechain |
| 1   | AA    | 240 | G    | Sidechain |
| 1   | AA    | 242 | G    | Sidechain |
| 1   | AA    | 244 | U    | Sidechain |
| 1   | AA    | 245 | U    | Sidechain |
| 1   | AA    | 249 | U    | Sidechain |
| 1   | AA    | 25  | C    | Sidechain |
| 1   | AA    | 250 | A    | Sidechain |
| 1   | AA    | 251 | G    | Sidechain |
| 1   | AA    | 252 | U    | Sidechain |
| 1   | AA    | 253 | A    | Sidechain |
| 1   | AA    | 255 | G    | Sidechain |
| 1   | AA    | 259 | G    | Sidechain |
| 1   | AA    | 262 | A    | Sidechain |
| 1   | AA    | 264 | C    | Sidechain |
| 1   | AA    | 266 | G    | Sidechain |
| 1   | AA    | 27  | G    | Sidechain |
| 1   | AA    | 275 | G    | Sidechain |
| 1   | AA    | 276 | G    | Sidechain |
| 1   | AA    | 277 | C    | Sidechain |
| 1   | AA    | 278 | G    | Sidechain |
| 1   | AA    | 281 | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AA    | 282 | A    | Sidechain |
| 1   | AA    | 283 | U    | Sidechain |
| 1   | AA    | 291 | U    | Sidechain |
| 1   | AA    | 292 | G    | Sidechain |
| 1   | AA    | 293 | G    | Sidechain |
| 1   | AA    | 295 | C    | Sidechain |
| 1   | AA    | 297 | G    | Sidechain |
| 1   | AA    | 298 | A    | Sidechain |
| 1   | AA    | 299 | G    | Sidechain |
| 1   | AA    | 30  | U    | Sidechain |
| 1   | AA    | 302 | G    | Sidechain |
| 1   | AA    | 303 | A    | Sidechain |
| 1   | AA    | 305 | G    | Sidechain |
| 1   | AA    | 306 | A    | Sidechain |
| 1   | AA    | 309 | A    | Sidechain |
| 1   | AA    | 31  | G    | Sidechain |
| 1   | AA    | 318 | G    | Sidechain |
| 1   | AA    | 323 | U    | Sidechain |
| 1   | AA    | 326 | G    | Sidechain |
| 1   | AA    | 327 | A    | Sidechain |
| 1   | AA    | 328 | C    | Sidechain |
| 1   | AA    | 331 | G    | Sidechain |
| 1   | AA    | 332 | G    | Sidechain |
| 1   | AA    | 333 | U    | Sidechain |
| 1   | AA    | 336 | A    | Sidechain |
| 1   | AA    | 339 | C    | Sidechain |
| 1   | AA    | 340 | U    | Sidechain |
| 1   | AA    | 342 | C    | Sidechain |
| 1   | AA    | 343 | U    | Sidechain |
| 1   | AA    | 345 | C    | Sidechain |
| 1   | AA    | 348 | G    | Sidechain |
| 1   | AA    | 349 | A    | Sidechain |
| 1   | AA    | 35  | G    | Sidechain |
| 1   | AA    | 350 | G    | Sidechain |
| 1   | AA    | 352 | C    | Sidechain |
| 1   | AA    | 354 | G    | Sidechain |
| 1   | AA    | 356 | A    | Sidechain |
| 1   | AA    | 36  | C    | Sidechain |
| 1   | AA    | 360 | G    | Sidechain |
| 1   | AA    | 361 | G    | Sidechain |
| 1   | AA    | 363 | A    | Sidechain |
| 1   | AA    | 365 | U    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AA    | 366 | A    | Sidechain |
| 1   | AA    | 369 | G    | Sidechain |
| 1   | AA    | 37  | U    | Sidechain |
| 1   | AA    | 370 | C    | Sidechain |
| 1   | AA    | 372 | C    | Sidechain |
| 1   | AA    | 375 | U    | Sidechain |
| 1   | AA    | 377 | G    | Sidechain |
| 1   | AA    | 378 | G    | Sidechain |
| 1   | AA    | 380 | G    | Sidechain |
| 1   | AA    | 381 | C    | Sidechain |
| 1   | AA    | 383 | A    | Sidechain |
| 1   | AA    | 387 | U    | Sidechain |
| 1   | AA    | 388 | G    | Sidechain |
| 1   | AA    | 395 | C    | Sidechain |
| 1   | AA    | 396 | C    | Sidechain |
| 1   | AA    | 397 | A    | Sidechain |
| 1   | AA    | 399 | G    | Sidechain |
| 1   | AA    | 40  | C    | Sidechain |
| 1   | AA    | 400 | C    | Sidechain |
| 1   | AA    | 401 | C    | Sidechain |
| 1   | AA    | 402 | G    | Sidechain |
| 1   | AA    | 405 | U    | Sidechain |
| 1   | AA    | 406 | G    | Sidechain |
| 1   | AA    | 407 | U    | Sidechain |
| 1   | AA    | 408 | A    | Sidechain |
| 1   | AA    | 409 | U    | Sidechain |
| 1   | AA    | 410 | G    | Sidechain |
| 1   | AA    | 411 | A    | Sidechain |
| 1   | AA    | 412 | A    | Sidechain |
| 1   | AA    | 418 | C    | Sidechain |
| 1   | AA    | 420 | U    | Sidechain |
| 1   | AA    | 422 | C    | Sidechain |
| 1   | AA    | 423 | G    | Sidechain |
| 1   | AA    | 424 | G    | Sidechain |
| 1   | AA    | 425 | G    | Sidechain |
| 1   | AA    | 426 | U    | Sidechain |
| 1   | AA    | 428 | G    | Sidechain |
| 1   | AA    | 429 | U    | Sidechain |
| 1   | AA    | 43  | C    | Sidechain |
| 1   | AA    | 430 | A    | Sidechain |
| 1   | AA    | 431 | A    | Sidechain |
| 1   | AA    | 438 | U    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AA    | 439 | U    | Sidechain |
| 1   | AA    | 44  | A    | Sidechain |
| 1   | AA    | 441 | A    | Sidechain |
| 1   | AA    | 442 | G    | Sidechain |
| 1   | AA    | 443 | C    | Sidechain |
| 1   | AA    | 444 | G    | Sidechain |
| 1   | AA    | 445 | G    | Sidechain |
| 1   | AA    | 446 | G    | Sidechain |
| 1   | AA    | 449 | G    | Sidechain |
| 1   | AA    | 450 | G    | Sidechain |
| 1   | AA    | 452 | A    | Sidechain |
| 1   | AA    | 455 | G    | Sidechain |
| 1   | AA    | 46  | G    | Sidechain |
| 1   | AA    | 460 | A    | Sidechain |
| 1   | AA    | 461 | A    | Sidechain |
| 1   | AA    | 462 | G    | Sidechain |
| 1   | AA    | 464 | U    | Sidechain |
| 1   | AA    | 468 | A    | Sidechain |
| 1   | AA    | 47  | C    | Sidechain |
| 1   | AA    | 471 | U    | Sidechain |
| 1   | AA    | 473 | U    | Sidechain |
| 1   | AA    | 474 | G    | Sidechain |
| 1   | AA    | 477 | C    | Sidechain |
| 1   | AA    | 478 | A    | Sidechain |
| 1   | AA    | 48  | C    | Sidechain |
| 1   | AA    | 482 | A    | Sidechain |
| 1   | AA    | 484 | G    | Sidechain |
| 1   | AA    | 486 | U    | Sidechain |
| 1   | AA    | 487 | A    | Sidechain |
| 1   | AA    | 489 | C    | Sidechain |
| 1   | AA    | 49  | U    | Sidechain |
| 1   | AA    | 490 | C    | Sidechain |
| 1   | AA    | 491 | G    | Sidechain |
| 1   | AA    | 493 | A    | Sidechain |
| 1   | AA    | 495 | A    | Sidechain |
| 1   | AA    | 496 | A    | Sidechain |
| 1   | AA    | 499 | A    | Sidechain |
| 1   | AA    | 5   | U    | Sidechain |
| 1   | AA    | 50  | A    | Sidechain |
| 1   | AA    | 504 | C    | Sidechain |
| 1   | AA    | 505 | G    | Sidechain |
| 1   | AA    | 509 | A    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AA    | 512 | U    | Sidechain |
| 1   | AA    | 513 | C    | Sidechain |
| 1   | AA    | 517 | G    | Sidechain |
| 1   | AA    | 518 | C    | Sidechain |
| 1   | AA    | 519 | C    | Sidechain |
| 1   | AA    | 52  | C    | Sidechain |
| 1   | AA    | 524 | G    | Sidechain |
| 1   | AA    | 525 | C    | Sidechain |
| 1   | AA    | 526 | C    | Sidechain |
| 1   | AA    | 527 | G    | Sidechain |
| 1   | AA    | 532 | A    | Sidechain |
| 1   | AA    | 540 | G    | Sidechain |
| 1   | AA    | 542 | G    | Sidechain |
| 1   | AA    | 548 | G    | Sidechain |
| 1   | AA    | 551 | U    | Sidechain |
| 1   | AA    | 553 | A    | Sidechain |
| 1   | AA    | 558 | G    | Sidechain |
| 1   | AA    | 561 | U    | Sidechain |
| 1   | AA    | 565 | U    | Sidechain |
| 1   | AA    | 566 | G    | Sidechain |
| 1   | AA    | 567 | G    | Sidechain |
| 1   | AA    | 569 | C    | Sidechain |
| 1   | AA    | 571 | U    | Sidechain |
| 1   | AA    | 572 | A    | Sidechain |
| 1   | AA    | 573 | A    | Sidechain |
| 1   | AA    | 574 | A    | Sidechain |
| 1   | AA    | 578 | C    | Sidechain |
| 1   | AA    | 58  | C    | Sidechain |
| 1   | AA    | 581 | G    | Sidechain |
| 1   | AA    | 584 | G    | Sidechain |
| 1   | AA    | 587 | G    | Sidechain |
| 1   | AA    | 59  | A    | Sidechain |
| 1   | AA    | 590 | U    | Sidechain |
| 1   | AA    | 594 | U    | Sidechain |
| 1   | AA    | 595 | A    | Sidechain |
| 1   | AA    | 597 | G    | Sidechain |
| 1   | AA    | 598 | U    | Sidechain |
| 1   | AA    | 599 | C    | Sidechain |
| 1   | AA    | 6   | G    | Sidechain |
| 1   | AA    | 600 | A    | Sidechain |
| 1   | AA    | 608 | A    | Sidechain |
| 1   | AA    | 61  | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AA    | 610 | U    | Sidechain |
| 1   | AA    | 612 | C    | Sidechain |
| 1   | AA    | 614 | C    | Sidechain |
| 1   | AA    | 615 | G    | Sidechain |
| 1   | AA    | 616 | G    | Sidechain |
| 1   | AA    | 619 | U    | Sidechain |
| 1   | AA    | 620 | C    | Sidechain |
| 1   | AA    | 622 | A    | Sidechain |
| 1   | AA    | 623 | C    | Sidechain |
| 1   | AA    | 624 | C    | Sidechain |
| 1   | AA    | 625 | U    | Sidechain |
| 1   | AA    | 626 | G    | Sidechain |
| 1   | AA    | 628 | G    | Sidechain |
| 1   | AA    | 63  | C    | Sidechain |
| 1   | AA    | 632 | U    | Sidechain |
| 1   | AA    | 633 | G    | Sidechain |
| 1   | AA    | 636 | U    | Sidechain |
| 1   | AA    | 638 | U    | Sidechain |
| 1   | AA    | 639 | G    | Sidechain |
| 1   | AA    | 64  | G    | Sidechain |
| 1   | AA    | 642 | A    | Sidechain |
| 1   | AA    | 644 | U    | Sidechain |
| 1   | AA    | 646 | G    | Sidechain |
| 1   | AA    | 648 | A    | Sidechain |
| 1   | AA    | 649 | A    | Sidechain |
| 1   | AA    | 650 | G    | Sidechain |
| 1   | AA    | 651 | C    | Sidechain |
| 1   | AA    | 652 | U    | Sidechain |
| 1   | AA    | 654 | G    | Sidechain |
| 1   | AA    | 657 | U    | Sidechain |
| 1   | AA    | 661 | G    | Sidechain |
| 1   | AA    | 664 | G    | Sidechain |
| 1   | AA    | 665 | A    | Sidechain |
| 1   | AA    | 667 | G    | Sidechain |
| 1   | AA    | 668 | G    | Sidechain |
| 1   | AA    | 669 | G    | Sidechain |
| 1   | AA    | 673 | A    | Sidechain |
| 1   | AA    | 674 | G    | Sidechain |
| 1   | AA    | 676 | A    | Sidechain |
| 1   | AA    | 681 | A    | Sidechain |
| 1   | AA    | 683 | G    | Sidechain |
| 1   | AA    | 684 | U    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AA    | 69  | G    | Sidechain |
| 1   | AA    | 690 | G    | Sidechain |
| 1   | AA    | 696 | A    | Sidechain |
| 1   | AA    | 697 | U    | Sidechain |
| 1   | AA    | 7   | A    | Sidechain |
| 1   | AA    | 700 | G    | Sidechain |
| 1   | AA    | 701 | U    | Sidechain |
| 1   | AA    | 708 | C    | Sidechain |
| 1   | AA    | 709 | U    | Sidechain |
| 1   | AA    | 71  | A    | Sidechain |
| 1   | AA    | 711 | G    | Sidechain |
| 1   | AA    | 714 | G    | Sidechain |
| 1   | AA    | 718 | A    | Sidechain |
| 1   | AA    | 720 | C    | Sidechain |
| 1   | AA    | 722 | G    | Sidechain |
| 1   | AA    | 726 | C    | Sidechain |
| 1   | AA    | 728 | A    | Sidechain |
| 1   | AA    | 729 | A    | Sidechain |
| 1   | AA    | 73  | C    | Sidechain |
| 1   | AA    | 730 | G    | Sidechain |
| 1   | AA    | 732 | C    | Sidechain |
| 1   | AA    | 733 | G    | Sidechain |
| 1   | AA    | 734 | G    | Sidechain |
| 1   | AA    | 737 | C    | Sidechain |
| 1   | AA    | 738 | C    | Sidechain |
| 1   | AA    | 739 | C    | Sidechain |
| 1   | AA    | 740 | U    | Sidechain |
| 1   | AA    | 742 | G    | Sidechain |
| 1   | AA    | 747 | A    | Sidechain |
| 1   | AA    | 748 | G    | Sidechain |
| 1   | AA    | 75  | G    | Sidechain |
| 1   | AA    | 751 | U    | Sidechain |
| 1   | AA    | 752 | G    | Sidechain |
| 1   | AA    | 754 | C    | Sidechain |
| 1   | AA    | 755 | G    | Sidechain |
| 1   | AA    | 757 | U    | Sidechain |
| 1   | AA    | 758 | C    | Sidechain |
| 1   | AA    | 761 | G    | Sidechain |
| 1   | AA    | 762 | U    | Sidechain |
| 1   | AA    | 763 | G    | Sidechain |
| 1   | AA    | 764 | C    | Sidechain |
| 1   | AA    | 77  | A    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AA    | 771 | G    | Sidechain |
| 1   | AA    | 772 | U    | Sidechain |
| 1   | AA    | 774 | G    | Sidechain |
| 1   | AA    | 776 | G    | Sidechain |
| 1   | AA    | 778 | G    | Sidechain |
| 1   | AA    | 779 | C    | Sidechain |
| 1   | AA    | 784 | A    | Sidechain |
| 1   | AA    | 785 | G    | Sidechain |
| 1   | AA    | 786 | G    | Sidechain |
| 1   | AA    | 787 | A    | Sidechain |
| 1   | AA    | 788 | U    | Sidechain |
| 1   | AA    | 789 | U    | Sidechain |
| 1   | AA    | 790 | A    | Sidechain |
| 1   | AA    | 791 | G    | Sidechain |
| 1   | AA    | 799 | G    | Sidechain |
| 1   | AA    | 80  | A    | Sidechain |
| 1   | AA    | 800 | G    | Sidechain |
| 1   | AA    | 801 | U    | Sidechain |
| 1   | AA    | 805 | C    | Sidechain |
| 1   | AA    | 809 | G    | Sidechain |
| 1   | AA    | 810 | C    | Sidechain |
| 1   | AA    | 814 | A    | Sidechain |
| 1   | AA    | 817 | C    | Sidechain |
| 1   | AA    | 818 | G    | Sidechain |
| 1   | AA    | 819 | A    | Sidechain |
| 1   | AA    | 820 | U    | Sidechain |
| 1   | AA    | 821 | G    | Sidechain |
| 1   | AA    | 822 | U    | Sidechain |
| 1   | AA    | 824 | G    | Sidechain |
| 1   | AA    | 827 | U    | Sidechain |
| 1   | AA    | 828 | U    | Sidechain |
| 1   | AA    | 829 | G    | Sidechain |
| 1   | AA    | 830 | G    | Sidechain |
| 1   | AA    | 836 | G    | Sidechain |
| 1   | AA    | 838 | G    | Sidechain |
| 1   | AA    | 839 | C    | Sidechain |
| 1   | AA    | 84  | U    | Sidechain |
| 1   | AA    | 841 | C    | Sidechain |
| 1   | AA    | 843 | U    | Sidechain |
| 1   | AA    | 844 | G    | Sidechain |
| 1   | AA    | 846 | G    | Sidechain |
| 1   | AA    | 847 | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AA    | 849 | G    | Sidechain |
| 1   | AA    | 850 | U    | Sidechain |
| 1   | AA    | 852 | G    | Sidechain |
| 1   | AA    | 853 | C    | Sidechain |
| 1   | AA    | 855 | U    | Sidechain |
| 1   | AA    | 856 | C    | Sidechain |
| 1   | AA    | 858 | G    | Sidechain |
| 1   | AA    | 86  | G    | Sidechain |
| 1   | AA    | 860 | A    | Sidechain |
| 1   | AA    | 861 | G    | Sidechain |
| 1   | AA    | 863 | U    | Sidechain |
| 1   | AA    | 864 | A    | Sidechain |
| 1   | AA    | 865 | A    | Sidechain |
| 1   | AA    | 867 | G    | Sidechain |
| 1   | AA    | 869 | G    | Sidechain |
| 1   | AA    | 87  | C    | Sidechain |
| 1   | AA    | 870 | U    | Sidechain |
| 1   | AA    | 871 | U    | Sidechain |
| 1   | AA    | 872 | A    | Sidechain |
| 1   | AA    | 874 | G    | Sidechain |
| 1   | AA    | 875 | U    | Sidechain |
| 1   | AA    | 876 | C    | Sidechain |
| 1   | AA    | 879 | C    | Sidechain |
| 1   | AA    | 88  | U    | Sidechain |
| 1   | AA    | 883 | C    | Sidechain |
| 1   | AA    | 884 | U    | Sidechain |
| 1   | AA    | 886 | G    | Sidechain |
| 1   | AA    | 888 | G    | Sidechain |
| 1   | AA    | 890 | G    | Sidechain |
| 1   | AA    | 894 | G    | Sidechain |
| 1   | AA    | 895 | G    | Sidechain |
| 1   | AA    | 897 | C    | Sidechain |
| 1   | AA    | 898 | G    | Sidechain |
| 1   | AA    | 900 | A    | Sidechain |
| 1   | AA    | 903 | G    | Sidechain |
| 1   | AA    | 906 | A    | Sidechain |
| 1   | AA    | 909 | A    | Sidechain |
| 1   | AA    | 91  | U    | Sidechain |
| 1   | AA    | 915 | A    | Sidechain |
| 1   | AA    | 917 | G    | Sidechain |
| 1   | AA    | 918 | A    | Sidechain |
| 1   | AA    | 921 | U    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AA    | 923 | A    | Sidechain |
| 1   | AA    | 925 | G    | Sidechain |
| 1   | AA    | 927 | G    | Sidechain |
| 1   | AA    | 929 | G    | Sidechain |
| 1   | AA    | 93  | U    | Sidechain |
| 1   | AA    | 931 | C    | Sidechain |
| 1   | AA    | 933 | G    | Sidechain |
| 1   | AA    | 937 | A    | Sidechain |
| 1   | AA    | 938 | A    | Sidechain |
| 1   | AA    | 94  | G    | Sidechain |
| 1   | AA    | 942 | G    | Sidechain |
| 1   | AA    | 943 | U    | Sidechain |
| 1   | AA    | 944 | G    | Sidechain |
| 1   | AA    | 945 | G    | Sidechain |
| 1   | AA    | 947 | G    | Sidechain |
| 1   | AA    | 948 | C    | Sidechain |
| 1   | AA    | 949 | A    | Sidechain |
| 1   | AA    | 95  | C    | Sidechain |
| 1   | AA    | 951 | G    | Sidechain |
| 1   | AA    | 952 | U    | Sidechain |
| 1   | AA    | 954 | G    | Sidechain |
| 1   | AA    | 955 | U    | Sidechain |
| 1   | AA    | 959 | A    | Sidechain |
| 1   | AA    | 962 | C    | Sidechain |
| 1   | AA    | 963 | G    | Sidechain |
| 1   | AA    | 964 | A    | Sidechain |
| 1   | AA    | 966 | G    | Sidechain |
| 1   | AA    | 969 | A    | Sidechain |
| 1   | AA    | 970 | C    | Sidechain |
| 1   | AA    | 971 | G    | Sidechain |
| 1   | AA    | 973 | G    | Sidechain |
| 1   | AA    | 974 | A    | Sidechain |
| 1   | AA    | 976 | G    | Sidechain |
| 1   | AA    | 978 | A    | Sidechain |
| 1   | AA    | 979 | C    | Sidechain |
| 1   | AA    | 98  | A    | Sidechain |
| 1   | AA    | 985 | C    | Sidechain |
| 1   | AA    | 988 | G    | Sidechain |
| 1   | AA    | 989 | U    | Sidechain |
| 1   | AA    | 99  | C    | Sidechain |
| 1   | AA    | 990 | C    | Sidechain |
| 1   | AA    | 992 | U    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AA    | 994 | A    | Sidechain |
| 1   | AA    | 997 | U    | Sidechain |
| 1   | AA    | 999 | C    | Sidechain |
| 2   | AB    | 112 | ARG  | Sidechain |
| 2   | AB    | 136 | ARG  | Sidechain |
| 2   | AB    | 212 | TYR  | Sidechain |
| 2   | AB    | 89  | PHE  | Sidechain |
| 2   | AB    | 94  | ARG  | Sidechain |
| 3   | AC    | 126 | ARG  | Sidechain |
| 3   | AC    | 142 | ARG  | Sidechain |
| 3   | AC    | 155 | ARG  | Sidechain |
| 3   | AC    | 163 | ARG  | Sidechain |
| 3   | AC    | 39  | ARG  | Sidechain |
| 3   | AC    | 41  | TYR  | Sidechain |
| 3   | AC    | 53  | ARG  | Sidechain |
| 4   | AD    | 110 | ARG  | Sidechain |
| 4   | AD    | 114 | ARG  | Sidechain |
| 4   | AD    | 127 | ARG  | Sidechain |
| 4   | AD    | 134 | TYR  | Sidechain |
| 4   | AD    | 164 | ARG  | Sidechain |
| 4   | AD    | 181 | PHE  | Peptide   |
| 4   | AD    | 187 | ARG  | Sidechain |
| 4   | AD    | 203 | TYR  | Sidechain |
| 4   | AD    | 3   | TYR  | Sidechain |
| 4   | AD    | 62  | ARG  | Sidechain |
| 4   | AD    | 64  | TYR  | Sidechain |
| 5   | AE    | 111 | ARG  | Peptide   |
| 5   | AE    | 127 | TYR  | Sidechain |
| 5   | AE    | 19  | ARG  | Sidechain |
| 5   | AE    | 33  | THR  | Peptide   |
| 5   | AE    | 94  | PHE  | Sidechain |
| 6   | AF    | 2   | ARG  | Sidechain |
| 6   | AF    | 44  | ARG  | Sidechain |
| 6   | AF    | 49  | TYR  | Sidechain |
| 7   | AG    | 118 | ARG  | Sidechain |
| 7   | AG    | 52  | ARG  | Sidechain |
| 7   | AG    | 77  | ARG  | Sidechain |
| 8   | AH    | 113 | ARG  | Sidechain |
| 8   | AH    | 12  | ARG  | Sidechain |
| 8   | AH    | 127 | TYR  | Sidechain |
| 9   | AI    | 121 | ARG  | Sidechain |
| 9   | AI    | 129 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 9   | AI    | 20  | ILE  | Peptide   |
| 9   | AI    | 32  | ARG  | Sidechain |
| 9   | AI    | 48  | ARG  | Sidechain |
| 9   | AI    | 6   | TYR  | Sidechain |
| 9   | AI    | 89  | TYR  | Sidechain |
| 10  | AJ    | 48  | ARG  | Sidechain |
| 10  | AJ    | 49  | PHE  | Sidechain |
| 10  | AJ    | 62  | ARG  | Sidechain |
| 10  | AJ    | 68  | ARG  | Sidechain |
| 10  | AJ    | 7   | ARG  | Sidechain |
| 10  | AJ    | 72  | ARG  | Sidechain |
| 11  | AK    | 104 | PHE  | Sidechain |
| 11  | AK    | 51  | PHE  | Sidechain |
| 11  | AK    | 52  | ARG  | Sidechain |
| 12  | AL    | 109 | ARG  | Sidechain |
| 12  | AL    | 37  | TYR  | Sidechain |
| 12  | AL    | 65  | TYR  | Sidechain |
| 12  | AL    | 93  | ARG  | Sidechain |
| 12  | AL    | 94  | TYR  | Sidechain |
| 13  | AM    | 112 | ARG  | Sidechain |
| 13  | AM    | 2   | ARG  | Sidechain |
| 13  | AM    | 22  | TYR  | Sidechain |
| 13  | AM    | 25  | GLY  | Peptide   |
| 13  | AM    | 69  | ARG  | Sidechain |
| 13  | AM    | 86  | ARG  | Sidechain |
| 13  | AM    | 89  | ARG  | Sidechain |
| 13  | AM    | 91  | ARG  | Sidechain |
| 13  | AM    | 92  | ARG  | Sidechain |
| 14  | AN    | 74  | ARG  | Sidechain |
| 14  | AN    | 8   | ARG  | Sidechain |
| 14  | AN    | 89  | ARG  | Sidechain |
| 15  | AO    | 37  | HIS  | Sidechain |
| 15  | AO    | 68  | TYR  | Sidechain |
| 15  | AO    | 71  | ARG  | Sidechain |
| 15  | AO    | 76  | ARG  | Sidechain |
| 15  | AO    | 79  | ARG  | Sidechain |
| 15  | AO    | 87  | ARG  | Sidechain |
| 16  | AP    | 17  | TYR  | Sidechain |
| 16  | AP    | 28  | ARG  | Sidechain |
| 16  | AP    | 5   | ARG  | Sidechain |
| 16  | AP    | 51  | ARG  | Sidechain |
| 17  | AQ    | 33  | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 18  | AR    | 22  | TYR  | Sidechain |
| 18  | AR    | 42  | ARG  | Sidechain |
| 18  | AR    | 50  | TYR  | Sidechain |
| 18  | AR    | 56  | ARG  | Sidechain |
| 18  | AR    | 69  | TYR  | Sidechain |
| 19  | AS    | 54  | ARG  | Sidechain |
| 19  | AS    | 74  | ALA  | Peptide   |
| 19  | AS    | 77  | ARG  | Sidechain |
| 19  | AS    | 79  | TYR  | Sidechain |
| 20  | AT    | 17  | ARG  | Sidechain |
| 20  | AT    | 28  | ARG  | Sidechain |
| 20  | AT    | 74  | HIS  | Sidechain |
| 22  | AV    | 13  | C    | Sidechain |
| 22  | AV    | 3   | G    | Sidechain |
| 22  | AV    | 33  | U    | Sidechain |
| 22  | AV    | 37  | G    | Sidechain |
| 22  | AV    | 39  | G    | Sidechain |
| 22  | AV    | 4   | C    | Sidechain |
| 22  | AV    | 5   | A    | Sidechain |
| 22  | AV    | 66  | C    | Sidechain |
| 22  | AV    | 67  | G    | Sidechain |
| 22  | AV    | 69  | G    | Sidechain |
| 22  | AV    | 70  | C    | Sidechain |
| 22  | AV    | 71  | C    | Sidechain |
| 22  | AV    | 75  | C    | Sidechain |
| 23  | AX    | 13  | A    | Sidechain |
| 23  | AX    | 14  | A    | Sidechain |
| 23  | AX    | 15  | A    | Sidechain |
| 23  | AX    | 20  | G    | Sidechain |
| 25  | B0    | 36  | ARG  | Sidechain |
| 25  | B0    | 49  | ARG  | Sidechain |
| 25  | B0    | 52  | ALA  | Peptide   |
| 25  | B0    | 73  | ARG  | Sidechain |
| 26  | B1    | 26  | PHE  | Sidechain |
| 28  | B3    | 12  | ARG  | Sidechain |
| 28  | B3    | 51  | ARG  | Sidechain |
| 29  | B4    | 13  | SER  | Peptide   |
| 29  | B4    | 37  | LYS  | Peptide   |
| 29  | B4    | 48  | TYR  | Sidechain |
| 30  | B5    | 144 | THR  | Peptide   |
| 30  | B5    | 164 | ARG  | Sidechain |
| 30  | B5    | 208 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 30  | B5    | 60  | ARG  | Sidechain |
| 30  | B5    | 71  | ARG  | Sidechain |
| 30  | B5    | 9   | ARG  | Sidechain |
| 31  | B6    | 12  | ARG  | Sidechain |
| 31  | B6    | 28  | ARG  | Sidechain |
| 31  | B6    | 39  | ARG  | Peptide   |
| 32  | B7    | 25  | HIS  | Sidechain |
| 34  | BA    | 10  | G    | Sidechain |
| 34  | BA    | 100 | G    | Sidechain |
| 34  | BA    | 105 | G    | Sidechain |
| 34  | BA    | 107 | G    | Sidechain |
| 34  | BA    | 108 | A    | Sidechain |
| 34  | BA    | 112 | G    | Sidechain |
| 34  | BA    | 113 | C    | Sidechain |
| 34  | BA    | 114 | C    | Sidechain |
| 34  | BA    | 115 | A    | Sidechain |
| 34  | BA    | 116 | G    | Sidechain |
| 34  | BA    | 117 | G    | Sidechain |
| 34  | BA    | 12  | C    | Sidechain |
| 34  | BA    | 16  | G    | Sidechain |
| 34  | BA    | 17  | C    | Sidechain |
| 34  | BA    | 18  | G    | Sidechain |
| 34  | BA    | 2   | G    | Sidechain |
| 34  | BA    | 21  | G    | Sidechain |
| 34  | BA    | 24  | G    | Sidechain |
| 34  | BA    | 26  | C    | Sidechain |
| 34  | BA    | 27  | C    | Sidechain |
| 34  | BA    | 31  | C    | Sidechain |
| 34  | BA    | 37  | C    | Sidechain |
| 34  | BA    | 4   | C    | Sidechain |
| 34  | BA    | 40  | U    | Sidechain |
| 34  | BA    | 41  | G    | Sidechain |
| 34  | BA    | 44  | G    | Sidechain |
| 34  | BA    | 45  | A    | Sidechain |
| 34  | BA    | 47  | C    | Sidechain |
| 34  | BA    | 49  | C    | Sidechain |
| 34  | BA    | 5   | U    | Sidechain |
| 34  | BA    | 51  | G    | Sidechain |
| 34  | BA    | 54  | G    | Sidechain |
| 34  | BA    | 58  | A    | Sidechain |
| 34  | BA    | 59  | A    | Sidechain |
| 34  | BA    | 61  | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 34  | BA    | 64   | G    | Sidechain |
| 34  | BA    | 66   | A    | Sidechain |
| 34  | BA    | 68   | C    | Sidechain |
| 34  | BA    | 7    | G    | Sidechain |
| 34  | BA    | 70   | C    | Sidechain |
| 34  | BA    | 71   | C    | Sidechain |
| 34  | BA    | 72   | G    | Sidechain |
| 34  | BA    | 75   | G    | Sidechain |
| 34  | BA    | 78   | A    | Sidechain |
| 34  | BA    | 79   | G    | Sidechain |
| 34  | BA    | 83   | G    | Sidechain |
| 34  | BA    | 87   | U    | Sidechain |
| 34  | BA    | 90   | C    | Sidechain |
| 34  | BA    | 92   | C    | Sidechain |
| 34  | BA    | 96   | G    | Sidechain |
| 35  | BB    | 1    | G    | Sidechain |
| 35  | BB    | 1002 | G    | Sidechain |
| 35  | BB    | 1005 | C    | Sidechain |
| 35  | BB    | 1008 | A    | Sidechain |
| 35  | BB    | 1010 | A    | Sidechain |
| 35  | BB    | 1011 | G    | Sidechain |
| 35  | BB    | 1015 | U    | Sidechain |
| 35  | BB    | 102  | U    | Sidechain |
| 35  | BB    | 1021 | A    | Sidechain |
| 35  | BB    | 1023 | U    | Sidechain |
| 35  | BB    | 1025 | G    | Sidechain |
| 35  | BB    | 1026 | G    | Sidechain |
| 35  | BB    | 1027 | A    | Sidechain |
| 35  | BB    | 1031 | G    | Sidechain |
| 35  | BB    | 1035 | U    | Sidechain |
| 35  | BB    | 1037 | G    | Sidechain |
| 35  | BB    | 104  | A    | Sidechain |
| 35  | BB    | 1040 | A    | Sidechain |
| 35  | BB    | 1041 | G    | Sidechain |
| 35  | BB    | 1045 | C    | Sidechain |
| 35  | BB    | 1046 | A    | Sidechain |
| 35  | BB    | 1047 | G    | Sidechain |
| 35  | BB    | 1048 | A    | Sidechain |
| 35  | BB    | 1049 | C    | Sidechain |
| 35  | BB    | 1051 | G    | Sidechain |
| 35  | BB    | 1052 | C    | Sidechain |
| 35  | BB    | 1053 | C    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 1055 | G    | Sidechain |
| 35  | BB    | 1057 | A    | Sidechain |
| 35  | BB    | 1059 | G    | Sidechain |
| 35  | BB    | 1060 | U    | Sidechain |
| 35  | BB    | 1061 | U    | Sidechain |
| 35  | BB    | 1062 | G    | Sidechain |
| 35  | BB    | 1064 | C    | Sidechain |
| 35  | BB    | 1067 | A    | Sidechain |
| 35  | BB    | 1069 | A    | Sidechain |
| 35  | BB    | 1071 | G    | Sidechain |
| 35  | BB    | 1074 | G    | Sidechain |
| 35  | BB    | 1077 | A    | Sidechain |
| 35  | BB    | 1079 | C    | Sidechain |
| 35  | BB    | 108  | G    | Sidechain |
| 35  | BB    | 1081 | U    | Sidechain |
| 35  | BB    | 1085 | A    | Sidechain |
| 35  | BB    | 109  | C    | Sidechain |
| 35  | BB    | 1095 | A    | Sidechain |
| 35  | BB    | 1097 | U    | Sidechain |
| 35  | BB    | 1098 | A    | Sidechain |
| 35  | BB    | 1099 | G    | Sidechain |
| 35  | BB    | 11   | C    | Sidechain |
| 35  | BB    | 1103 | A    | Sidechain |
| 35  | BB    | 1107 | G    | Sidechain |
| 35  | BB    | 1108 | U    | Sidechain |
| 35  | BB    | 1109 | C    | Sidechain |
| 35  | BB    | 111  | A    | Sidechain |
| 35  | BB    | 1110 | G    | Sidechain |
| 35  | BB    | 1115 | G    | Sidechain |
| 35  | BB    | 112  | U    | Sidechain |
| 35  | BB    | 1120 | G    | Sidechain |
| 35  | BB    | 1123 | C    | Sidechain |
| 35  | BB    | 1124 | G    | Sidechain |
| 35  | BB    | 1125 | G    | Sidechain |
| 35  | BB    | 1126 | A    | Sidechain |
| 35  | BB    | 1129 | A    | Sidechain |
| 35  | BB    | 113  | U    | Sidechain |
| 35  | BB    | 1131 | G    | Sidechain |
| 35  | BB    | 1133 | A    | Sidechain |
| 35  | BB    | 1137 | G    | Sidechain |
| 35  | BB    | 1138 | G    | Sidechain |
| 35  | BB    | 1143 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 1148 | U    | Sidechain |
| 35  | BB    | 1149 | G    | Sidechain |
| 35  | BB    | 1151 | A    | Sidechain |
| 35  | BB    | 1153 | C    | Sidechain |
| 35  | BB    | 1154 | G    | Sidechain |
| 35  | BB    | 1159 | U    | Sidechain |
| 35  | BB    | 116  | C    | Sidechain |
| 35  | BB    | 1164 | C    | Sidechain |
| 35  | BB    | 1165 | A    | Sidechain |
| 35  | BB    | 1166 | G    | Sidechain |
| 35  | BB    | 1167 | C    | Sidechain |
| 35  | BB    | 1170 | C    | Sidechain |
| 35  | BB    | 1171 | G    | Sidechain |
| 35  | BB    | 1172 | C    | Sidechain |
| 35  | BB    | 1173 | U    | Sidechain |
| 35  | BB    | 1174 | U    | Sidechain |
| 35  | BB    | 1177 | G    | Sidechain |
| 35  | BB    | 1180 | U    | Sidechain |
| 35  | BB    | 1184 | U    | Sidechain |
| 35  | BB    | 1185 | G    | Sidechain |
| 35  | BB    | 1186 | G    | Sidechain |
| 35  | BB    | 1187 | G    | Sidechain |
| 35  | BB    | 1188 | U    | Sidechain |
| 35  | BB    | 1191 | G    | Sidechain |
| 35  | BB    | 1192 | G    | Sidechain |
| 35  | BB    | 1195 | G    | Sidechain |
| 35  | BB    | 1198 | U    | Sidechain |
| 35  | BB    | 12   | U    | Sidechain |
| 35  | BB    | 1204 | A    | Sidechain |
| 35  | BB    | 1206 | G    | Sidechain |
| 35  | BB    | 1207 | C    | Sidechain |
| 35  | BB    | 1209 | U    | Sidechain |
| 35  | BB    | 1211 | C    | Sidechain |
| 35  | BB    | 1212 | G    | Sidechain |
| 35  | BB    | 1216 | G    | Sidechain |
| 35  | BB    | 122  | G    | Sidechain |
| 35  | BB    | 1220 | G    | Sidechain |
| 35  | BB    | 1221 | C    | Sidechain |
| 35  | BB    | 1222 | U    | Sidechain |
| 35  | BB    | 1223 | G    | Sidechain |
| 35  | BB    | 1224 | U    | Sidechain |
| 35  | BB    | 123  | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 1231 | U    | Sidechain |
| 35  | BB    | 1234 | U    | Sidechain |
| 35  | BB    | 1235 | G    | Sidechain |
| 35  | BB    | 1237 | A    | Sidechain |
| 35  | BB    | 1238 | G    | Sidechain |
| 35  | BB    | 1242 | U    | Sidechain |
| 35  | BB    | 1244 | A    | Sidechain |
| 35  | BB    | 1245 | G    | Sidechain |
| 35  | BB    | 1249 | U    | Sidechain |
| 35  | BB    | 1250 | G    | Sidechain |
| 35  | BB    | 1252 | G    | Sidechain |
| 35  | BB    | 1253 | A    | Sidechain |
| 35  | BB    | 1254 | A    | Sidechain |
| 35  | BB    | 1255 | U    | Sidechain |
| 35  | BB    | 1260 | A    | Sidechain |
| 35  | BB    | 1264 | A    | Sidechain |
| 35  | BB    | 1267 | U    | Sidechain |
| 35  | BB    | 1269 | A    | Sidechain |
| 35  | BB    | 127  | A    | Sidechain |
| 35  | BB    | 1270 | C    | Sidechain |
| 35  | BB    | 1273 | U    | Sidechain |
| 35  | BB    | 1274 | A    | Sidechain |
| 35  | BB    | 1275 | A    | Sidechain |
| 35  | BB    | 1276 | A    | Sidechain |
| 35  | BB    | 1277 | G    | Sidechain |
| 35  | BB    | 1281 | G    | Sidechain |
| 35  | BB    | 1282 | U    | Sidechain |
| 35  | BB    | 1283 | G    | Sidechain |
| 35  | BB    | 1286 | A    | Sidechain |
| 35  | BB    | 1288 | G    | Sidechain |
| 35  | BB    | 1290 | C    | Sidechain |
| 35  | BB    | 1292 | G    | Sidechain |
| 35  | BB    | 1298 | C    | Sidechain |
| 35  | BB    | 1300 | G    | Sidechain |
| 35  | BB    | 1302 | A    | Sidechain |
| 35  | BB    | 1303 | G    | Sidechain |
| 35  | BB    | 1306 | C    | Sidechain |
| 35  | BB    | 1310 | G    | Sidechain |
| 35  | BB    | 1311 | G    | Sidechain |
| 35  | BB    | 1312 | U    | Sidechain |
| 35  | BB    | 1316 | U    | Sidechain |
| 35  | BB    | 1319 | C    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 132  | G    | Sidechain |
| 35  | BB    | 1320 | C    | Sidechain |
| 35  | BB    | 1321 | A    | Sidechain |
| 35  | BB    | 1322 | A    | Sidechain |
| 35  | BB    | 1325 | U    | Sidechain |
| 35  | BB    | 1327 | A    | Sidechain |
| 35  | BB    | 1332 | G    | Sidechain |
| 35  | BB    | 1334 | G    | Sidechain |
| 35  | BB    | 1336 | A    | Sidechain |
| 35  | BB    | 1338 | G    | Sidechain |
| 35  | BB    | 134  | G    | Sidechain |
| 35  | BB    | 1343 | G    | Sidechain |
| 35  | BB    | 1346 | G    | Sidechain |
| 35  | BB    | 1347 | A    | Sidechain |
| 35  | BB    | 1349 | C    | Sidechain |
| 35  | BB    | 135  | U    | Sidechain |
| 35  | BB    | 1350 | C    | Sidechain |
| 35  | BB    | 1351 | C    | Sidechain |
| 35  | BB    | 1359 | A    | Sidechain |
| 35  | BB    | 136  | G    | Sidechain |
| 35  | BB    | 1360 | G    | Sidechain |
| 35  | BB    | 1361 | G    | Sidechain |
| 35  | BB    | 1363 | C    | Sidechain |
| 35  | BB    | 1367 | A    | Sidechain |
| 35  | BB    | 1368 | G    | Sidechain |
| 35  | BB    | 1369 | G    | Sidechain |
| 35  | BB    | 1371 | G    | Sidechain |
| 35  | BB    | 1372 | U    | Sidechain |
| 35  | BB    | 1373 | A    | Sidechain |
| 35  | BB    | 1374 | G    | Sidechain |
| 35  | BB    | 1376 | C    | Sidechain |
| 35  | BB    | 1377 | G    | Sidechain |
| 35  | BB    | 1381 | G    | Sidechain |
| 35  | BB    | 1382 | G    | Sidechain |
| 35  | BB    | 1384 | A    | Sidechain |
| 35  | BB    | 1387 | A    | Sidechain |
| 35  | BB    | 1388 | G    | Sidechain |
| 35  | BB    | 1389 | G    | Sidechain |
| 35  | BB    | 139  | U    | Sidechain |
| 35  | BB    | 1390 | U    | Sidechain |
| 35  | BB    | 1394 | U    | Sidechain |
| 35  | BB    | 1396 | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 1399 | C    | Sidechain |
| 35  | BB    | 140  | C    | Sidechain |
| 35  | BB    | 1401 | G    | Sidechain |
| 35  | BB    | 1404 | C    | Sidechain |
| 35  | BB    | 1406 | U    | Sidechain |
| 35  | BB    | 1408 | G    | Sidechain |
| 35  | BB    | 141  | G    | Sidechain |
| 35  | BB    | 1413 | A    | Sidechain |
| 35  | BB    | 1415 | U    | Sidechain |
| 35  | BB    | 1416 | G    | Sidechain |
| 35  | BB    | 1418 | G    | Sidechain |
| 35  | BB    | 1419 | A    | Sidechain |
| 35  | BB    | 1421 | G    | Sidechain |
| 35  | BB    | 1423 | G    | Sidechain |
| 35  | BB    | 1424 | G    | Sidechain |
| 35  | BB    | 1427 | A    | Sidechain |
| 35  | BB    | 1428 | C    | Sidechain |
| 35  | BB    | 1429 | G    | Sidechain |
| 35  | BB    | 1433 | A    | Sidechain |
| 35  | BB    | 1435 | G    | Sidechain |
| 35  | BB    | 1438 | U    | Sidechain |
| 35  | BB    | 1441 | G    | Sidechain |
| 35  | BB    | 1442 | U    | Sidechain |
| 35  | BB    | 1445 | G    | Sidechain |
| 35  | BB    | 1447 | C    | Sidechain |
| 35  | BB    | 1449 | G    | Sidechain |
| 35  | BB    | 1451 | C    | Sidechain |
| 35  | BB    | 1453 | A    | Sidechain |
| 35  | BB    | 1459 | G    | Sidechain |
| 35  | BB    | 1461 | C    | Sidechain |
| 35  | BB    | 1463 | C    | Sidechain |
| 35  | BB    | 1465 | G    | Sidechain |
| 35  | BB    | 1467 | U    | Sidechain |
| 35  | BB    | 1468 | U    | Sidechain |
| 35  | BB    | 1469 | A    | Sidechain |
| 35  | BB    | 1470 | A    | Sidechain |
| 35  | BB    | 1471 | G    | Sidechain |
| 35  | BB    | 1473 | G    | Sidechain |
| 35  | BB    | 1474 | U    | Sidechain |
| 35  | BB    | 1475 | G    | Sidechain |
| 35  | BB    | 1477 | A    | Sidechain |
| 35  | BB    | 1479 | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 148  | U    | Sidechain |
| 35  | BB    | 1480 | C    | Sidechain |
| 35  | BB    | 1482 | G    | Sidechain |
| 35  | BB    | 1487 | U    | Sidechain |
| 35  | BB    | 1488 | C    | Sidechain |
| 35  | BB    | 1490 | A    | Sidechain |
| 35  | BB    | 1491 | G    | Sidechain |
| 35  | BB    | 1493 | C    | Sidechain |
| 35  | BB    | 1494 | A    | Sidechain |
| 35  | BB    | 1496 | A    | Sidechain |
| 35  | BB    | 1498 | C    | Sidechain |
| 35  | BB    | 15   | G    | Sidechain |
| 35  | BB    | 150  | U    | Sidechain |
| 35  | BB    | 1501 | G    | Sidechain |
| 35  | BB    | 1503 | A    | Sidechain |
| 35  | BB    | 1506 | U    | Sidechain |
| 35  | BB    | 1508 | A    | Sidechain |
| 35  | BB    | 1509 | A    | Sidechain |
| 35  | BB    | 1510 | G    | Sidechain |
| 35  | BB    | 1513 | U    | Sidechain |
| 35  | BB    | 1514 | G    | Sidechain |
| 35  | BB    | 1517 | G    | Sidechain |
| 35  | BB    | 1519 | G    | Sidechain |
| 35  | BB    | 152  | A    | Sidechain |
| 35  | BB    | 1520 | U    | Sidechain |
| 35  | BB    | 1521 | G    | Sidechain |
| 35  | BB    | 1522 | A    | Sidechain |
| 35  | BB    | 1524 | G    | Sidechain |
| 35  | BB    | 1525 | A    | Sidechain |
| 35  | BB    | 1528 | A    | Sidechain |
| 35  | BB    | 1532 | A    | Sidechain |
| 35  | BB    | 1533 | C    | Sidechain |
| 35  | BB    | 1535 | A    | Sidechain |
| 35  | BB    | 1537 | G    | Sidechain |
| 35  | BB    | 1538 | G    | Sidechain |
| 35  | BB    | 1539 | U    | Sidechain |
| 35  | BB    | 1540 | G    | Sidechain |
| 35  | BB    | 1545 | A    | Sidechain |
| 35  | BB    | 1547 | C    | Sidechain |
| 35  | BB    | 1548 | A    | Sidechain |
| 35  | BB    | 1552 | A    | Sidechain |
| 35  | BB    | 1553 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 1555 | G    | Sidechain |
| 35  | BB    | 1558 | C    | Sidechain |
| 35  | BB    | 1559 | U    | Sidechain |
| 35  | BB    | 1560 | G    | Sidechain |
| 35  | BB    | 1561 | C    | Sidechain |
| 35  | BB    | 1562 | U    | Sidechain |
| 35  | BB    | 1564 | C    | Sidechain |
| 35  | BB    | 1569 | A    | Sidechain |
| 35  | BB    | 1573 | G    | Sidechain |
| 35  | BB    | 1574 | C    | Sidechain |
| 35  | BB    | 1578 | U    | Sidechain |
| 35  | BB    | 158  | U    | Sidechain |
| 35  | BB    | 1582 | C    | Sidechain |
| 35  | BB    | 1583 | A    | Sidechain |
| 35  | BB    | 1587 | G    | Sidechain |
| 35  | BB    | 1588 | G    | Sidechain |
| 35  | BB    | 159  | G    | Sidechain |
| 35  | BB    | 1590 | A    | Sidechain |
| 35  | BB    | 1591 | A    | Sidechain |
| 35  | BB    | 1596 | A    | Sidechain |
| 35  | BB    | 1597 | A    | Sidechain |
| 35  | BB    | 16   | C    | Sidechain |
| 35  | BB    | 160  | A    | Sidechain |
| 35  | BB    | 1602 | U    | Sidechain |
| 35  | BB    | 1605 | C    | Sidechain |
| 35  | BB    | 1607 | C    | Sidechain |
| 35  | BB    | 1608 | A    | Sidechain |
| 35  | BB    | 161  | A    | Sidechain |
| 35  | BB    | 1610 | A    | Sidechain |
| 35  | BB    | 1613 | G    | Sidechain |
| 35  | BB    | 1614 | A    | Sidechain |
| 35  | BB    | 1616 | A    | Sidechain |
| 35  | BB    | 1617 | C    | Sidechain |
| 35  | BB    | 1618 | A    | Sidechain |
| 35  | BB    | 1619 | G    | Sidechain |
| 35  | BB    | 1620 | G    | Sidechain |
| 35  | BB    | 1621 | U    | Sidechain |
| 35  | BB    | 1622 | G    | Sidechain |
| 35  | BB    | 1628 | G    | Sidechain |
| 35  | BB    | 163  | C    | Sidechain |
| 35  | BB    | 1631 | G    | Sidechain |
| 35  | BB    | 1635 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 1636 | U    | Sidechain |
| 35  | BB    | 1638 | C    | Sidechain |
| 35  | BB    | 164  | C    | Sidechain |
| 35  | BB    | 1646 | C    | Sidechain |
| 35  | BB    | 1651 | G    | Sidechain |
| 35  | BB    | 1652 | A    | Sidechain |
| 35  | BB    | 1653 | G    | Sidechain |
| 35  | BB    | 1657 | U    | Sidechain |
| 35  | BB    | 1659 | G    | Sidechain |
| 35  | BB    | 1660 | G    | Sidechain |
| 35  | BB    | 1661 | G    | Sidechain |
| 35  | BB    | 1662 | U    | Sidechain |
| 35  | BB    | 1668 | A    | Sidechain |
| 35  | BB    | 1671 | U    | Sidechain |
| 35  | BB    | 1672 | A    | Sidechain |
| 35  | BB    | 1674 | G    | Sidechain |
| 35  | BB    | 1676 | A    | Sidechain |
| 35  | BB    | 1678 | A    | Sidechain |
| 35  | BB    | 168  | G    | Sidechain |
| 35  | BB    | 1680 | U    | Sidechain |
| 35  | BB    | 1681 | G    | Sidechain |
| 35  | BB    | 1682 | G    | Sidechain |
| 35  | BB    | 1686 | C    | Sidechain |
| 35  | BB    | 1688 | U    | Sidechain |
| 35  | BB    | 169  | G    | Sidechain |
| 35  | BB    | 1692 | U    | Sidechain |
| 35  | BB    | 1693 | U    | Sidechain |
| 35  | BB    | 1695 | G    | Sidechain |
| 35  | BB    | 1696 | G    | Sidechain |
| 35  | BB    | 1697 | G    | Sidechain |
| 35  | BB    | 1698 | A    | Sidechain |
| 35  | BB    | 1699 | G    | Sidechain |
| 35  | BB    | 1700 | A    | Sidechain |
| 35  | BB    | 1702 | G    | Sidechain |
| 35  | BB    | 1707 | G    | Sidechain |
| 35  | BB    | 171  | U    | Sidechain |
| 35  | BB    | 1710 | G    | Sidechain |
| 35  | BB    | 1714 | U    | Sidechain |
| 35  | BB    | 1715 | G    | Sidechain |
| 35  | BB    | 1716 | U    | Sidechain |
| 35  | BB    | 1718 | G    | Sidechain |
| 35  | BB    | 172  | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 1720 | U    | Sidechain |
| 35  | BB    | 1721 | G    | Sidechain |
| 35  | BB    | 1724 | G    | Sidechain |
| 35  | BB    | 1725 | U    | Sidechain |
| 35  | BB    | 173  | A    | Sidechain |
| 35  | BB    | 1730 | C    | Sidechain |
| 35  | BB    | 1731 | G    | Sidechain |
| 35  | BB    | 1734 | G    | Sidechain |
| 35  | BB    | 1736 | U    | Sidechain |
| 35  | BB    | 1740 | G    | Sidechain |
| 35  | BB    | 1741 | C    | Sidechain |
| 35  | BB    | 1747 | U    | Sidechain |
| 35  | BB    | 1754 | A    | Sidechain |
| 35  | BB    | 1756 | G    | Sidechain |
| 35  | BB    | 1759 | A    | Sidechain |
| 35  | BB    | 1760 | C    | Sidechain |
| 35  | BB    | 1761 | C    | Sidechain |
| 35  | BB    | 1763 | G    | Sidechain |
| 35  | BB    | 1765 | U    | Sidechain |
| 35  | BB    | 1767 | G    | Sidechain |
| 35  | BB    | 1768 | C    | Sidechain |
| 35  | BB    | 1769 | U    | Sidechain |
| 35  | BB    | 177  | G    | Sidechain |
| 35  | BB    | 1777 | U    | Sidechain |
| 35  | BB    | 1778 | U    | Sidechain |
| 35  | BB    | 1779 | U    | Sidechain |
| 35  | BB    | 1780 | A    | Sidechain |
| 35  | BB    | 1781 | U    | Sidechain |
| 35  | BB    | 1783 | A    | Sidechain |
| 35  | BB    | 1784 | A    | Sidechain |
| 35  | BB    | 1785 | A    | Sidechain |
| 35  | BB    | 1786 | A    | Sidechain |
| 35  | BB    | 1787 | A    | Sidechain |
| 35  | BB    | 1788 | C    | Sidechain |
| 35  | BB    | 1791 | A    | Sidechain |
| 35  | BB    | 1794 | A    | Sidechain |
| 35  | BB    | 1797 | G    | Sidechain |
| 35  | BB    | 180  | G    | Sidechain |
| 35  | BB    | 1800 | C    | Sidechain |
| 35  | BB    | 1801 | A    | Sidechain |
| 35  | BB    | 1802 | A    | Sidechain |
| 35  | BB    | 1803 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 1807 | G    | Sidechain |
| 35  | BB    | 1809 | A    | Sidechain |
| 35  | BB    | 1813 | G    | Sidechain |
| 35  | BB    | 1814 | G    | Sidechain |
| 35  | BB    | 1815 | A    | Sidechain |
| 35  | BB    | 1816 | C    | Sidechain |
| 35  | BB    | 1818 | U    | Sidechain |
| 35  | BB    | 1820 | U    | Sidechain |
| 35  | BB    | 1821 | A    | Sidechain |
| 35  | BB    | 1823 | G    | Sidechain |
| 35  | BB    | 1825 | U    | Sidechain |
| 35  | BB    | 1826 | G    | Sidechain |
| 35  | BB    | 1829 | A    | Sidechain |
| 35  | BB    | 1839 | G    | Sidechain |
| 35  | BB    | 1841 | U    | Sidechain |
| 35  | BB    | 1842 | G    | Sidechain |
| 35  | BB    | 1844 | C    | Sidechain |
| 35  | BB    | 1845 | G    | Sidechain |
| 35  | BB    | 1846 | G    | Sidechain |
| 35  | BB    | 1854 | A    | Sidechain |
| 35  | BB    | 1855 | U    | Sidechain |
| 35  | BB    | 1856 | U    | Sidechain |
| 35  | BB    | 1857 | G    | Sidechain |
| 35  | BB    | 1858 | A    | Sidechain |
| 35  | BB    | 1859 | U    | Sidechain |
| 35  | BB    | 1860 | G    | Sidechain |
| 35  | BB    | 1863 | G    | Sidechain |
| 35  | BB    | 1866 | A    | Sidechain |
| 35  | BB    | 1868 | C    | Sidechain |
| 35  | BB    | 1869 | G    | Sidechain |
| 35  | BB    | 187  | G    | Sidechain |
| 35  | BB    | 1872 | A    | Sidechain |
| 35  | BB    | 1875 | G    | Sidechain |
| 35  | BB    | 1876 | A    | Sidechain |
| 35  | BB    | 1878 | G    | Sidechain |
| 35  | BB    | 188  | G    | Sidechain |
| 35  | BB    | 1880 | U    | Sidechain |
| 35  | BB    | 1885 | A    | Sidechain |
| 35  | BB    | 1888 | G    | Sidechain |
| 35  | BB    | 1891 | G    | Sidechain |
| 35  | BB    | 1896 | G    | Sidechain |
| 35  | BB    | 1898 | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 1899 | A    | Sidechain |
| 35  | BB    | 190  | A    | Sidechain |
| 35  | BB    | 1901 | A    | Sidechain |
| 35  | BB    | 1903 | G    | Sidechain |
| 35  | BB    | 1904 | G    | Sidechain |
| 35  | BB    | 1905 | C    | Sidechain |
| 35  | BB    | 1907 | G    | Sidechain |
| 35  | BB    | 191  | A    | Sidechain |
| 35  | BB    | 1911 | U    | Sidechain |
| 35  | BB    | 1913 | A    | Sidechain |
| 35  | BB    | 1914 | C    | Sidechain |
| 35  | BB    | 1917 | U    | Sidechain |
| 35  | BB    | 1918 | A    | Sidechain |
| 35  | BB    | 192  | C    | Sidechain |
| 35  | BB    | 1920 | C    | Sidechain |
| 35  | BB    | 1921 | G    | Sidechain |
| 35  | BB    | 1923 | U    | Sidechain |
| 35  | BB    | 1927 | A    | Sidechain |
| 35  | BB    | 1929 | G    | Sidechain |
| 35  | BB    | 1930 | G    | Sidechain |
| 35  | BB    | 1931 | U    | Sidechain |
| 35  | BB    | 1933 | G    | Sidechain |
| 35  | BB    | 1937 | A    | Sidechain |
| 35  | BB    | 194  | G    | Sidechain |
| 35  | BB    | 1940 | U    | Sidechain |
| 35  | BB    | 1941 | C    | Sidechain |
| 35  | BB    | 1942 | C    | Sidechain |
| 35  | BB    | 1943 | U    | Sidechain |
| 35  | BB    | 1945 | G    | Sidechain |
| 35  | BB    | 1949 | G    | Sidechain |
| 35  | BB    | 195  | A    | Sidechain |
| 35  | BB    | 1952 | A    | Sidechain |
| 35  | BB    | 1953 | A    | Sidechain |
| 35  | BB    | 1957 | C    | Sidechain |
| 35  | BB    | 196  | A    | Sidechain |
| 35  | BB    | 1960 | A    | Sidechain |
| 35  | BB    | 1961 | C    | Sidechain |
| 35  | BB    | 1963 | U    | Sidechain |
| 35  | BB    | 1964 | G    | Sidechain |
| 35  | BB    | 1966 | A    | Sidechain |
| 35  | BB    | 197  | A    | Sidechain |
| 35  | BB    | 1971 | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 1974 | C    | Sidechain |
| 35  | BB    | 1975 | G    | Sidechain |
| 35  | BB    | 1976 | U    | Sidechain |
| 35  | BB    | 1978 | A    | Sidechain |
| 35  | BB    | 1979 | U    | Sidechain |
| 35  | BB    | 198  | C    | Sidechain |
| 35  | BB    | 1980 | G    | Sidechain |
| 35  | BB    | 1981 | A    | Sidechain |
| 35  | BB    | 1982 | U    | Sidechain |
| 35  | BB    | 1983 | G    | Sidechain |
| 35  | BB    | 1986 | C    | Sidechain |
| 35  | BB    | 1989 | G    | Sidechain |
| 35  | BB    | 1993 | U    | Sidechain |
| 35  | BB    | 1996 | C    | Sidechain |
| 35  | BB    | 1998 | A    | Sidechain |
| 35  | BB    | 1999 | C    | Sidechain |
| 35  | BB    | 20   | C    | Sidechain |
| 35  | BB    | 2002 | G    | Sidechain |
| 35  | BB    | 2003 | A    | Sidechain |
| 35  | BB    | 2005 | A    | Sidechain |
| 35  | BB    | 2009 | A    | Sidechain |
| 35  | BB    | 2010 | G    | Sidechain |
| 35  | BB    | 2011 | U    | Sidechain |
| 35  | BB    | 2012 | G    | Sidechain |
| 35  | BB    | 2019 | A    | Sidechain |
| 35  | BB    | 2021 | C    | Sidechain |
| 35  | BB    | 2023 | C    | Sidechain |
| 35  | BB    | 2025 | C    | Sidechain |
| 35  | BB    | 2026 | U    | Sidechain |
| 35  | BB    | 2029 | G    | Sidechain |
| 35  | BB    | 2034 | U    | Sidechain |
| 35  | BB    | 2035 | G    | Sidechain |
| 35  | BB    | 2037 | A    | Sidechain |
| 35  | BB    | 2043 | C    | Sidechain |
| 35  | BB    | 2044 | C    | Sidechain |
| 35  | BB    | 2046 | G    | Sidechain |
| 35  | BB    | 2047 | C    | Sidechain |
| 35  | BB    | 2048 | G    | Sidechain |
| 35  | BB    | 205  | G    | Sidechain |
| 35  | BB    | 2053 | G    | Sidechain |
| 35  | BB    | 2054 | A    | Sidechain |
| 35  | BB    | 2057 | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 2058 | A    | Sidechain |
| 35  | BB    | 2059 | A    | Sidechain |
| 35  | BB    | 206  | U    | Sidechain |
| 35  | BB    | 2062 | A    | Sidechain |
| 35  | BB    | 2065 | C    | Sidechain |
| 35  | BB    | 2066 | C    | Sidechain |
| 35  | BB    | 2068 | U    | Sidechain |
| 35  | BB    | 2069 | G    | Sidechain |
| 35  | BB    | 207  | A    | Sidechain |
| 35  | BB    | 2070 | A    | Sidechain |
| 35  | BB    | 2071 | A    | Sidechain |
| 35  | BB    | 2072 | C    | Sidechain |
| 35  | BB    | 2073 | C    | Sidechain |
| 35  | BB    | 2074 | U    | Sidechain |
| 35  | BB    | 2075 | U    | Sidechain |
| 35  | BB    | 2076 | U    | Sidechain |
| 35  | BB    | 2081 | U    | Sidechain |
| 35  | BB    | 2085 | U    | Sidechain |
| 35  | BB    | 2086 | U    | Sidechain |
| 35  | BB    | 2088 | A    | Sidechain |
| 35  | BB    | 2093 | G    | Sidechain |
| 35  | BB    | 210  | C    | Sidechain |
| 35  | BB    | 2100 | G    | Sidechain |
| 35  | BB    | 2102 | G    | Sidechain |
| 35  | BB    | 2104 | C    | Sidechain |
| 35  | BB    | 2106 | U    | Sidechain |
| 35  | BB    | 2109 | U    | Sidechain |
| 35  | BB    | 2115 | G    | Sidechain |
| 35  | BB    | 2117 | A    | Sidechain |
| 35  | BB    | 2119 | A    | Sidechain |
| 35  | BB    | 2122 | U    | Sidechain |
| 35  | BB    | 2124 | G    | Sidechain |
| 35  | BB    | 2125 | G    | Sidechain |
| 35  | BB    | 2126 | A    | Sidechain |
| 35  | BB    | 2128 | G    | Sidechain |
| 35  | BB    | 213  | A    | Sidechain |
| 35  | BB    | 2130 | U    | Sidechain |
| 35  | BB    | 2133 | G    | Sidechain |
| 35  | BB    | 2135 | A    | Sidechain |
| 35  | BB    | 2137 | U    | Sidechain |
| 35  | BB    | 2138 | G    | Sidechain |
| 35  | BB    | 2139 | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 2142 | A    | Sidechain |
| 35  | BB    | 2144 | G    | Sidechain |
| 35  | BB    | 2146 | C    | Sidechain |
| 35  | BB    | 2147 | A    | Sidechain |
| 35  | BB    | 2148 | G    | Sidechain |
| 35  | BB    | 2149 | U    | Sidechain |
| 35  | BB    | 215  | G    | Sidechain |
| 35  | BB    | 2150 | C    | Sidechain |
| 35  | BB    | 2151 | U    | Sidechain |
| 35  | BB    | 2152 | G    | Sidechain |
| 35  | BB    | 2156 | G    | Sidechain |
| 35  | BB    | 2157 | G    | Sidechain |
| 35  | BB    | 2158 | A    | Sidechain |
| 35  | BB    | 2159 | G    | Sidechain |
| 35  | BB    | 2166 | U    | Sidechain |
| 35  | BB    | 2167 | U    | Sidechain |
| 35  | BB    | 2168 | G    | Sidechain |
| 35  | BB    | 217  | A    | Sidechain |
| 35  | BB    | 2170 | A    | Sidechain |
| 35  | BB    | 2172 | U    | Sidechain |
| 35  | BB    | 2173 | A    | Sidechain |
| 35  | BB    | 2176 | A    | Sidechain |
| 35  | BB    | 2178 | C    | Sidechain |
| 35  | BB    | 218  | A    | Sidechain |
| 35  | BB    | 2180 | U    | Sidechain |
| 35  | BB    | 2181 | U    | Sidechain |
| 35  | BB    | 2182 | U    | Sidechain |
| 35  | BB    | 2183 | A    | Sidechain |
| 35  | BB    | 2186 | G    | Sidechain |
| 35  | BB    | 2187 | U    | Sidechain |
| 35  | BB    | 2189 | U    | Sidechain |
| 35  | BB    | 219  | A    | Sidechain |
| 35  | BB    | 2190 | G    | Sidechain |
| 35  | BB    | 2192 | U    | Sidechain |
| 35  | BB    | 2197 | U    | Sidechain |
| 35  | BB    | 220  | G    | Sidechain |
| 35  | BB    | 2201 | G    | Sidechain |
| 35  | BB    | 2203 | U    | Sidechain |
| 35  | BB    | 2204 | G    | Sidechain |
| 35  | BB    | 2205 | A    | Sidechain |
| 35  | BB    | 2206 | C    | Sidechain |
| 35  | BB    | 2209 | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 221  | A    | Sidechain |
| 35  | BB    | 2213 | U    | Sidechain |
| 35  | BB    | 2219 | U    | Sidechain |
| 35  | BB    | 2222 | C    | Sidechain |
| 35  | BB    | 2224 | G    | Sidechain |
| 35  | BB    | 2226 | C    | Sidechain |
| 35  | BB    | 2227 | A    | Sidechain |
| 35  | BB    | 2228 | G    | Sidechain |
| 35  | BB    | 223  | A    | Sidechain |
| 35  | BB    | 2230 | G    | Sidechain |
| 35  | BB    | 2231 | U    | Sidechain |
| 35  | BB    | 2234 | G    | Sidechain |
| 35  | BB    | 2238 | G    | Sidechain |
| 35  | BB    | 2239 | G    | Sidechain |
| 35  | BB    | 2240 | U    | Sidechain |
| 35  | BB    | 2242 | G    | Sidechain |
| 35  | BB    | 2243 | U    | Sidechain |
| 35  | BB    | 2247 | A    | Sidechain |
| 35  | BB    | 2249 | U    | Sidechain |
| 35  | BB    | 2251 | G    | Sidechain |
| 35  | BB    | 2252 | G    | Sidechain |
| 35  | BB    | 2253 | G    | Sidechain |
| 35  | BB    | 2256 | G    | Sidechain |
| 35  | BB    | 2258 | C    | Sidechain |
| 35  | BB    | 2261 | C    | Sidechain |
| 35  | BB    | 2262 | U    | Sidechain |
| 35  | BB    | 2267 | A    | Sidechain |
| 35  | BB    | 2268 | A    | Sidechain |
| 35  | BB    | 2269 | G    | Sidechain |
| 35  | BB    | 2271 | G    | Sidechain |
| 35  | BB    | 2272 | U    | Sidechain |
| 35  | BB    | 2279 | G    | Sidechain |
| 35  | BB    | 2281 | A    | Sidechain |
| 35  | BB    | 2282 | G    | Sidechain |
| 35  | BB    | 2285 | C    | Sidechain |
| 35  | BB    | 2287 | A    | Sidechain |
| 35  | BB    | 2288 | A    | Sidechain |
| 35  | BB    | 2289 | G    | Sidechain |
| 35  | BB    | 229  | C    | Sidechain |
| 35  | BB    | 2290 | G    | Sidechain |
| 35  | BB    | 2292 | U    | Sidechain |
| 35  | BB    | 2294 | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 2296 | U    | Sidechain |
| 35  | BB    | 2297 | A    | Sidechain |
| 35  | BB    | 2299 | U    | Sidechain |
| 35  | BB    | 23   | G    | Sidechain |
| 35  | BB    | 230  | G    | Sidechain |
| 35  | BB    | 2300 | C    | Sidechain |
| 35  | BB    | 2301 | C    | Sidechain |
| 35  | BB    | 2302 | U    | Sidechain |
| 35  | BB    | 2303 | G    | Sidechain |
| 35  | BB    | 2305 | U    | Sidechain |
| 35  | BB    | 2307 | G    | Sidechain |
| 35  | BB    | 2308 | G    | Sidechain |
| 35  | BB    | 231  | A    | Sidechain |
| 35  | BB    | 2310 | C    | Sidechain |
| 35  | BB    | 2312 | U    | Sidechain |
| 35  | BB    | 2313 | C    | Sidechain |
| 35  | BB    | 2316 | G    | Sidechain |
| 35  | BB    | 2317 | A    | Sidechain |
| 35  | BB    | 2318 | G    | Sidechain |
| 35  | BB    | 232  | G    | Sidechain |
| 35  | BB    | 2320 | U    | Sidechain |
| 35  | BB    | 2322 | A    | Sidechain |
| 35  | BB    | 2327 | A    | Sidechain |
| 35  | BB    | 2329 | U    | Sidechain |
| 35  | BB    | 2330 | G    | Sidechain |
| 35  | BB    | 2333 | A    | Sidechain |
| 35  | BB    | 2335 | A    | Sidechain |
| 35  | BB    | 2336 | A    | Sidechain |
| 35  | BB    | 234  | U    | Sidechain |
| 35  | BB    | 2340 | A    | Sidechain |
| 35  | BB    | 2343 | U    | Sidechain |
| 35  | BB    | 2345 | G    | Sidechain |
| 35  | BB    | 2348 | U    | Sidechain |
| 35  | BB    | 235  | U    | Sidechain |
| 35  | BB    | 2350 | C    | Sidechain |
| 35  | BB    | 2352 | A    | Sidechain |
| 35  | BB    | 2355 | G    | Sidechain |
| 35  | BB    | 2356 | U    | Sidechain |
| 35  | BB    | 2357 | G    | Sidechain |
| 35  | BB    | 236  | C    | Sidechain |
| 35  | BB    | 2360 | G    | Sidechain |
| 35  | BB    | 2362 | C    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 2363 | G    | Sidechain |
| 35  | BB    | 2368 | C    | Sidechain |
| 35  | BB    | 2369 | A    | Sidechain |
| 35  | BB    | 237  | C    | Sidechain |
| 35  | BB    | 2372 | U    | Sidechain |
| 35  | BB    | 2375 | G    | Sidechain |
| 35  | BB    | 2379 | G    | Sidechain |
| 35  | BB    | 2381 | A    | Sidechain |
| 35  | BB    | 2382 | G    | Sidechain |
| 35  | BB    | 2383 | G    | Sidechain |
| 35  | BB    | 2385 | C    | Sidechain |
| 35  | BB    | 2388 | A    | Sidechain |
| 35  | BB    | 2389 | G    | Sidechain |
| 35  | BB    | 2390 | U    | Sidechain |
| 35  | BB    | 2392 | A    | Sidechain |
| 35  | BB    | 2393 | U    | Sidechain |
| 35  | BB    | 24   | G    | Sidechain |
| 35  | BB    | 2400 | G    | Sidechain |
| 35  | BB    | 2401 | U    | Sidechain |
| 35  | BB    | 2402 | U    | Sidechain |
| 35  | BB    | 2403 | C    | Sidechain |
| 35  | BB    | 2404 | U    | Sidechain |
| 35  | BB    | 2405 | G    | Sidechain |
| 35  | BB    | 2406 | A    | Sidechain |
| 35  | BB    | 2407 | A    | Sidechain |
| 35  | BB    | 2408 | U    | Sidechain |
| 35  | BB    | 2410 | G    | Sidechain |
| 35  | BB    | 2412 | A    | Sidechain |
| 35  | BB    | 2414 | G    | Sidechain |
| 35  | BB    | 2415 | G    | Sidechain |
| 35  | BB    | 242  | G    | Sidechain |
| 35  | BB    | 2428 | G    | Sidechain |
| 35  | BB    | 2429 | G    | Sidechain |
| 35  | BB    | 243  | U    | Sidechain |
| 35  | BB    | 2432 | A    | Sidechain |
| 35  | BB    | 2437 | G    | Sidechain |
| 35  | BB    | 2440 | C    | Sidechain |
| 35  | BB    | 2441 | U    | Sidechain |
| 35  | BB    | 2442 | C    | Sidechain |
| 35  | BB    | 2444 | G    | Sidechain |
| 35  | BB    | 2447 | G    | Sidechain |
| 35  | BB    | 2448 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 2449 | U    | Sidechain |
| 35  | BB    | 245  | G    | Sidechain |
| 35  | BB    | 2454 | G    | Sidechain |
| 35  | BB    | 2455 | G    | Sidechain |
| 35  | BB    | 2456 | C    | Sidechain |
| 35  | BB    | 2457 | U    | Sidechain |
| 35  | BB    | 2458 | G    | Sidechain |
| 35  | BB    | 2459 | A    | Sidechain |
| 35  | BB    | 246  | C    | Sidechain |
| 35  | BB    | 2461 | A    | Sidechain |
| 35  | BB    | 2462 | C    | Sidechain |
| 35  | BB    | 2467 | C    | Sidechain |
| 35  | BB    | 2469 | A    | Sidechain |
| 35  | BB    | 2471 | A    | Sidechain |
| 35  | BB    | 2472 | G    | Sidechain |
| 35  | BB    | 2475 | C    | Sidechain |
| 35  | BB    | 2476 | A    | Sidechain |
| 35  | BB    | 2477 | U    | Sidechain |
| 35  | BB    | 2479 | U    | Sidechain |
| 35  | BB    | 248  | G    | Sidechain |
| 35  | BB    | 2483 | C    | Sidechain |
| 35  | BB    | 2486 | C    | Sidechain |
| 35  | BB    | 2488 | G    | Sidechain |
| 35  | BB    | 249  | C    | Sidechain |
| 35  | BB    | 2491 | U    | Sidechain |
| 35  | BB    | 2492 | U    | Sidechain |
| 35  | BB    | 2494 | G    | Sidechain |
| 35  | BB    | 2495 | G    | Sidechain |
| 35  | BB    | 25   | U    | Sidechain |
| 35  | BB    | 2500 | U    | Sidechain |
| 35  | BB    | 2503 | A    | Sidechain |
| 35  | BB    | 2504 | U    | Sidechain |
| 35  | BB    | 2505 | G    | Sidechain |
| 35  | BB    | 2507 | C    | Sidechain |
| 35  | BB    | 251  | A    | Sidechain |
| 35  | BB    | 2515 | C    | Sidechain |
| 35  | BB    | 2516 | A    | Sidechain |
| 35  | BB    | 2517 | C    | Sidechain |
| 35  | BB    | 2523 | G    | Sidechain |
| 35  | BB    | 2525 | G    | Sidechain |
| 35  | BB    | 2528 | U    | Sidechain |
| 35  | BB    | 253  | C    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 2530 | A    | Sidechain |
| 35  | BB    | 2532 | G    | Sidechain |
| 35  | BB    | 2534 | A    | Sidechain |
| 35  | BB    | 2535 | G    | Sidechain |
| 35  | BB    | 2536 | G    | Sidechain |
| 35  | BB    | 2538 | C    | Sidechain |
| 35  | BB    | 2540 | C    | Sidechain |
| 35  | BB    | 2541 | A    | Sidechain |
| 35  | BB    | 2542 | A    | Sidechain |
| 35  | BB    | 2546 | U    | Sidechain |
| 35  | BB    | 255  | A    | Sidechain |
| 35  | BB    | 2550 | G    | Sidechain |
| 35  | BB    | 2551 | C    | Sidechain |
| 35  | BB    | 2553 | G    | Sidechain |
| 35  | BB    | 2556 | C    | Sidechain |
| 35  | BB    | 2557 | G    | Sidechain |
| 35  | BB    | 2560 | A    | Sidechain |
| 35  | BB    | 2561 | U    | Sidechain |
| 35  | BB    | 2565 | A    | Sidechain |
| 35  | BB    | 2568 | U    | Sidechain |
| 35  | BB    | 257  | C    | Sidechain |
| 35  | BB    | 2570 | G    | Sidechain |
| 35  | BB    | 2572 | A    | Sidechain |
| 35  | BB    | 2574 | G    | Sidechain |
| 35  | BB    | 2576 | G    | Sidechain |
| 35  | BB    | 2578 | G    | Sidechain |
| 35  | BB    | 2580 | U    | Sidechain |
| 35  | BB    | 2581 | G    | Sidechain |
| 35  | BB    | 2582 | G    | Sidechain |
| 35  | BB    | 2583 | G    | Sidechain |
| 35  | BB    | 2584 | U    | Sidechain |
| 35  | BB    | 2585 | U    | Sidechain |
| 35  | BB    | 2587 | A    | Sidechain |
| 35  | BB    | 2588 | G    | Sidechain |
| 35  | BB    | 2593 | U    | Sidechain |
| 35  | BB    | 2596 | U    | Sidechain |
| 35  | BB    | 2598 | A    | Sidechain |
| 35  | BB    | 26   | G    | Sidechain |
| 35  | BB    | 260  | G    | Sidechain |
| 35  | BB    | 2601 | C    | Sidechain |
| 35  | BB    | 2602 | A    | Sidechain |
| 35  | BB    | 2604 | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 261  | G    | Sidechain |
| 35  | BB    | 2610 | C    | Sidechain |
| 35  | BB    | 2612 | C    | Sidechain |
| 35  | BB    | 2613 | U    | Sidechain |
| 35  | BB    | 2614 | A    | Sidechain |
| 35  | BB    | 2616 | C    | Sidechain |
| 35  | BB    | 2618 | G    | Sidechain |
| 35  | BB    | 2619 | C    | Sidechain |
| 35  | BB    | 262  | A    | Sidechain |
| 35  | BB    | 2620 | C    | Sidechain |
| 35  | BB    | 2622 | U    | Sidechain |
| 35  | BB    | 2624 | G    | Sidechain |
| 35  | BB    | 2627 | G    | Sidechain |
| 35  | BB    | 263  | G    | Sidechain |
| 35  | BB    | 2631 | G    | Sidechain |
| 35  | BB    | 2637 | U    | Sidechain |
| 35  | BB    | 264  | C    | Sidechain |
| 35  | BB    | 2641 | G    | Sidechain |
| 35  | BB    | 2643 | G    | Sidechain |
| 35  | BB    | 2645 | G    | Sidechain |
| 35  | BB    | 2648 | G    | Sidechain |
| 35  | BB    | 265  | A    | Sidechain |
| 35  | BB    | 2650 | U    | Sidechain |
| 35  | BB    | 2652 | C    | Sidechain |
| 35  | BB    | 2654 | A    | Sidechain |
| 35  | BB    | 2656 | U    | Sidechain |
| 35  | BB    | 2659 | G    | Sidechain |
| 35  | BB    | 2661 | G    | Sidechain |
| 35  | BB    | 2662 | A    | Sidechain |
| 35  | BB    | 2663 | G    | Sidechain |
| 35  | BB    | 2664 | G    | Sidechain |
| 35  | BB    | 2666 | C    | Sidechain |
| 35  | BB    | 2669 | G    | Sidechain |
| 35  | BB    | 2670 | A    | Sidechain |
| 35  | BB    | 2674 | G    | Sidechain |
| 35  | BB    | 2679 | A    | Sidechain |
| 35  | BB    | 268  | C    | Sidechain |
| 35  | BB    | 2680 | U    | Sidechain |
| 35  | BB    | 2683 | C    | Sidechain |
| 35  | BB    | 2685 | G    | Sidechain |
| 35  | BB    | 2688 | G    | Sidechain |
| 35  | BB    | 2689 | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 2690 | U    | Sidechain |
| 35  | BB    | 2692 | G    | Sidechain |
| 35  | BB    | 2694 | G    | Sidechain |
| 35  | BB    | 2695 | U    | Sidechain |
| 35  | BB    | 2699 | C    | Sidechain |
| 35  | BB    | 2700 | A    | Sidechain |
| 35  | BB    | 2702 | G    | Sidechain |
| 35  | BB    | 2703 | C    | Sidechain |
| 35  | BB    | 2706 | A    | Sidechain |
| 35  | BB    | 2708 | G    | Sidechain |
| 35  | BB    | 271  | G    | Sidechain |
| 35  | BB    | 2711 | A    | Sidechain |
| 35  | BB    | 2713 | U    | Sidechain |
| 35  | BB    | 2715 | C    | Sidechain |
| 35  | BB    | 2716 | C    | Sidechain |
| 35  | BB    | 2717 | C    | Sidechain |
| 35  | BB    | 2720 | U    | Sidechain |
| 35  | BB    | 2722 | G    | Sidechain |
| 35  | BB    | 2724 | U    | Sidechain |
| 35  | BB    | 2727 | A    | Sidechain |
| 35  | BB    | 273  | G    | Sidechain |
| 35  | BB    | 2731 | G    | Sidechain |
| 35  | BB    | 2732 | G    | Sidechain |
| 35  | BB    | 2735 | G    | Sidechain |
| 35  | BB    | 2737 | G    | Sidechain |
| 35  | BB    | 2738 | A    | Sidechain |
| 35  | BB    | 2739 | U    | Sidechain |
| 35  | BB    | 274  | C    | Sidechain |
| 35  | BB    | 2741 | A    | Sidechain |
| 35  | BB    | 2742 | G    | Sidechain |
| 35  | BB    | 2744 | G    | Sidechain |
| 35  | BB    | 2746 | U    | Sidechain |
| 35  | BB    | 2751 | G    | Sidechain |
| 35  | BB    | 2756 | U    | Sidechain |
| 35  | BB    | 2759 | G    | Sidechain |
| 35  | BB    | 2765 | A    | Sidechain |
| 35  | BB    | 2766 | A    | Sidechain |
| 35  | BB    | 277  | G    | Sidechain |
| 35  | BB    | 2770 | G    | Sidechain |
| 35  | BB    | 2771 | C    | Sidechain |
| 35  | BB    | 2773 | C    | Sidechain |
| 35  | BB    | 2774 | C    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 2775 | G    | Sidechain |
| 35  | BB    | 2776 | A    | Sidechain |
| 35  | BB    | 2778 | A    | Sidechain |
| 35  | BB    | 2779 | U    | Sidechain |
| 35  | BB    | 278  | A    | Sidechain |
| 35  | BB    | 2782 | G    | Sidechain |
| 35  | BB    | 2784 | U    | Sidechain |
| 35  | BB    | 2785 | C    | Sidechain |
| 35  | BB    | 2786 | U    | Sidechain |
| 35  | BB    | 2787 | C    | Sidechain |
| 35  | BB    | 2788 | C    | Sidechain |
| 35  | BB    | 279  | A    | Sidechain |
| 35  | BB    | 2790 | U    | Sidechain |
| 35  | BB    | 2791 | G    | Sidechain |
| 35  | BB    | 2792 | A    | Sidechain |
| 35  | BB    | 2794 | C    | Sidechain |
| 35  | BB    | 2798 | U    | Sidechain |
| 35  | BB    | 28   | A    | Sidechain |
| 35  | BB    | 280  | U    | Sidechain |
| 35  | BB    | 2802 | G    | Sidechain |
| 35  | BB    | 2804 | U    | Sidechain |
| 35  | BB    | 2806 | C    | Sidechain |
| 35  | BB    | 2809 | A    | Sidechain |
| 35  | BB    | 2810 | A    | Sidechain |
| 35  | BB    | 2813 | A    | Sidechain |
| 35  | BB    | 2816 | G    | Sidechain |
| 35  | BB    | 2818 | U    | Sidechain |
| 35  | BB    | 282  | A    | Sidechain |
| 35  | BB    | 2828 | G    | Sidechain |
| 35  | BB    | 2829 | A    | Sidechain |
| 35  | BB    | 2831 | G    | Sidechain |
| 35  | BB    | 2832 | U    | Sidechain |
| 35  | BB    | 2838 | G    | Sidechain |
| 35  | BB    | 2847 | U    | Sidechain |
| 35  | BB    | 2848 | G    | Sidechain |
| 35  | BB    | 2849 | U    | Sidechain |
| 35  | BB    | 285  | G    | Sidechain |
| 35  | BB    | 2850 | A    | Sidechain |
| 35  | BB    | 2851 | A    | Sidechain |
| 35  | BB    | 2854 | G    | Sidechain |
| 35  | BB    | 2856 | A    | Sidechain |
| 35  | BB    | 2858 | C    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 35  | BB    | 286  | U    | Sidechain |
| 35  | BB    | 2866 | U    | Sidechain |
| 35  | BB    | 2867 | G    | Sidechain |
| 35  | BB    | 287  | G    | Sidechain |
| 35  | BB    | 2872 | A    | Sidechain |
| 35  | BB    | 2874 | C    | Sidechain |
| 35  | BB    | 2876 | G    | Sidechain |
| 35  | BB    | 2877 | G    | Sidechain |
| 35  | BB    | 2879 | A    | Sidechain |
| 35  | BB    | 2881 | U    | Sidechain |
| 35  | BB    | 2884 | U    | Sidechain |
| 35  | BB    | 2885 | G    | Sidechain |
| 35  | BB    | 2886 | A    | Sidechain |
| 35  | BB    | 2888 | C    | Sidechain |
| 35  | BB    | 289  | G    | Sidechain |
| 35  | BB    | 2890 | G    | Sidechain |
| 35  | BB    | 2891 | U    | Sidechain |
| 35  | BB    | 2892 | G    | Sidechain |
| 35  | BB    | 2895 | G    | Sidechain |
| 35  | BB    | 2897 | U    | Sidechain |
| 35  | BB    | 2900 | A    | Sidechain |
| 35  | BB    | 2901 | C    | Sidechain |
| 35  | BB    | 2902 | C    | Sidechain |
| 35  | BB    | 2903 | U    | Sidechain |
| 35  | BB    | 292  | U    | Sidechain |
| 35  | BB    | 293  | U    | Sidechain |
| 35  | BB    | 294  | A    | Sidechain |
| 35  | BB    | 295  | G    | Sidechain |
| 35  | BB    | 300  | A    | Sidechain |
| 35  | BB    | 303  | G    | Sidechain |
| 35  | BB    | 304  | U    | Sidechain |
| 35  | BB    | 309  | A    | Sidechain |
| 35  | BB    | 310  | A    | Sidechain |
| 35  | BB    | 313  | G    | Sidechain |
| 35  | BB    | 316  | C    | Sidechain |
| 35  | BB    | 321  | U    | Sidechain |
| 35  | BB    | 324  | A    | Sidechain |
| 35  | BB    | 325  | G    | Sidechain |
| 35  | BB    | 327  | G    | Sidechain |
| 35  | BB    | 333  | G    | Sidechain |
| 35  | BB    | 336  | C    | Sidechain |
| 35  | BB    | 338  | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 35  | BB    | 339 | U    | Sidechain |
| 35  | BB    | 340 | A    | Sidechain |
| 35  | BB    | 344 | A    | Sidechain |
| 35  | BB    | 345 | A    | Sidechain |
| 35  | BB    | 346 | A    | Sidechain |
| 35  | BB    | 347 | A    | Sidechain |
| 35  | BB    | 35  | G    | Sidechain |
| 35  | BB    | 350 | G    | Sidechain |
| 35  | BB    | 352 | A    | Sidechain |
| 35  | BB    | 353 | C    | Sidechain |
| 35  | BB    | 354 | A    | Sidechain |
| 35  | BB    | 356 | G    | Sidechain |
| 35  | BB    | 358 | U    | Sidechain |
| 35  | BB    | 359 | G    | Sidechain |
| 35  | BB    | 36  | G    | Sidechain |
| 35  | BB    | 361 | G    | Sidechain |
| 35  | BB    | 363 | G    | Sidechain |
| 35  | BB    | 364 | C    | Sidechain |
| 35  | BB    | 366 | C    | Sidechain |
| 35  | BB    | 367 | G    | Sidechain |
| 35  | BB    | 37  | C    | Sidechain |
| 35  | BB    | 370 | G    | Sidechain |
| 35  | BB    | 372 | G    | Sidechain |
| 35  | BB    | 373 | U    | Sidechain |
| 35  | BB    | 376 | G    | Sidechain |
| 35  | BB    | 377 | G    | Sidechain |
| 35  | BB    | 379 | G    | Sidechain |
| 35  | BB    | 381 | G    | Sidechain |
| 35  | BB    | 385 | C    | Sidechain |
| 35  | BB    | 387 | U    | Sidechain |
| 35  | BB    | 388 | G    | Sidechain |
| 35  | BB    | 39  | G    | Sidechain |
| 35  | BB    | 390 | U    | Sidechain |
| 35  | BB    | 392 | U    | Sidechain |
| 35  | BB    | 395 | U    | Sidechain |
| 35  | BB    | 40  | U    | Sidechain |
| 35  | BB    | 400 | G    | Sidechain |
| 35  | BB    | 401 | A    | Sidechain |
| 35  | BB    | 402 | A    | Sidechain |
| 35  | BB    | 404 | A    | Sidechain |
| 35  | BB    | 405 | U    | Sidechain |
| 35  | BB    | 407 | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 35  | BB    | 410 | G    | Sidechain |
| 35  | BB    | 411 | G    | Sidechain |
| 35  | BB    | 414 | C    | Sidechain |
| 35  | BB    | 415 | A    | Sidechain |
| 35  | BB    | 417 | C    | Sidechain |
| 35  | BB    | 419 | U    | Sidechain |
| 35  | BB    | 420 | C    | Sidechain |
| 35  | BB    | 421 | C    | Sidechain |
| 35  | BB    | 422 | A    | Sidechain |
| 35  | BB    | 426 | C    | Sidechain |
| 35  | BB    | 428 | A    | Sidechain |
| 35  | BB    | 429 | A    | Sidechain |
| 35  | BB    | 43  | G    | Sidechain |
| 35  | BB    | 431 | U    | Sidechain |
| 35  | BB    | 434 | U    | Sidechain |
| 35  | BB    | 437 | U    | Sidechain |
| 35  | BB    | 438 | G    | Sidechain |
| 35  | BB    | 442 | G    | Sidechain |
| 35  | BB    | 443 | A    | Sidechain |
| 35  | BB    | 446 | G    | Sidechain |
| 35  | BB    | 449 | A    | Sidechain |
| 35  | BB    | 450 | G    | Sidechain |
| 35  | BB    | 452 | G    | Sidechain |
| 35  | BB    | 457 | A    | Sidechain |
| 35  | BB    | 458 | G    | Sidechain |
| 35  | BB    | 459 | U    | Sidechain |
| 35  | BB    | 46  | G    | Sidechain |
| 35  | BB    | 463 | G    | Sidechain |
| 35  | BB    | 464 | U    | Sidechain |
| 35  | BB    | 465 | G    | Sidechain |
| 35  | BB    | 466 | A    | Sidechain |
| 35  | BB    | 467 | G    | Sidechain |
| 35  | BB    | 468 | G    | Sidechain |
| 35  | BB    | 472 | A    | Sidechain |
| 35  | BB    | 473 | G    | Sidechain |
| 35  | BB    | 475 | C    | Sidechain |
| 35  | BB    | 479 | A    | Sidechain |
| 35  | BB    | 480 | A    | Sidechain |
| 35  | BB    | 484 | C    | Sidechain |
| 35  | BB    | 485 | C    | Sidechain |
| 35  | BB    | 488 | G    | Sidechain |
| 35  | BB    | 489 | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 35  | BB    | 491 | G    | Sidechain |
| 35  | BB    | 492 | A    | Sidechain |
| 35  | BB    | 494 | G    | Sidechain |
| 35  | BB    | 495 | G    | Sidechain |
| 35  | BB    | 497 | A    | Sidechain |
| 35  | BB    | 499 | U    | Sidechain |
| 35  | BB    | 5   | A    | Sidechain |
| 35  | BB    | 50  | U    | Sidechain |
| 35  | BB    | 500 | G    | Sidechain |
| 35  | BB    | 501 | A    | Sidechain |
| 35  | BB    | 505 | A    | Sidechain |
| 35  | BB    | 506 | G    | Sidechain |
| 35  | BB    | 507 | A    | Sidechain |
| 35  | BB    | 508 | A    | Sidechain |
| 35  | BB    | 51  | G    | Sidechain |
| 35  | BB    | 510 | C    | Sidechain |
| 35  | BB    | 511 | U    | Sidechain |
| 35  | BB    | 512 | G    | Sidechain |
| 35  | BB    | 513 | A    | Sidechain |
| 35  | BB    | 514 | A    | Sidechain |
| 35  | BB    | 52  | A    | Sidechain |
| 35  | BB    | 520 | G    | Sidechain |
| 35  | BB    | 521 | U    | Sidechain |
| 35  | BB    | 530 | G    | Sidechain |
| 35  | BB    | 532 | A    | Sidechain |
| 35  | BB    | 537 | G    | Sidechain |
| 35  | BB    | 539 | G    | Sidechain |
| 35  | BB    | 54  | G    | Sidechain |
| 35  | BB    | 542 | C    | Sidechain |
| 35  | BB    | 543 | G    | Sidechain |
| 35  | BB    | 544 | C    | Sidechain |
| 35  | BB    | 546 | U    | Sidechain |
| 35  | BB    | 548 | G    | Sidechain |
| 35  | BB    | 55  | G    | Sidechain |
| 35  | BB    | 551 | G    | Sidechain |
| 35  | BB    | 553 | G    | Sidechain |
| 35  | BB    | 555 | G    | Sidechain |
| 35  | BB    | 565 | C    | Sidechain |
| 35  | BB    | 567 | U    | Sidechain |
| 35  | BB    | 568 | U    | Sidechain |
| 35  | BB    | 569 | U    | Sidechain |
| 35  | BB    | 570 | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 35  | BB    | 574 | A    | Sidechain |
| 35  | BB    | 575 | A    | Sidechain |
| 35  | BB    | 577 | G    | Sidechain |
| 35  | BB    | 578 | G    | Sidechain |
| 35  | BB    | 580 | U    | Sidechain |
| 35  | BB    | 590 | A    | Sidechain |
| 35  | BB    | 594 | U    | Sidechain |
| 35  | BB    | 596 | U    | Sidechain |
| 35  | BB    | 597 | G    | Sidechain |
| 35  | BB    | 598 | U    | Sidechain |
| 35  | BB    | 599 | A    | Sidechain |
| 35  | BB    | 60  | G    | Sidechain |
| 35  | BB    | 600 | G    | Sidechain |
| 35  | BB    | 602 | A    | Sidechain |
| 35  | BB    | 610 | C    | Sidechain |
| 35  | BB    | 611 | C    | Sidechain |
| 35  | BB    | 612 | G    | Sidechain |
| 35  | BB    | 615 | U    | Sidechain |
| 35  | BB    | 616 | A    | Sidechain |
| 35  | BB    | 617 | G    | Sidechain |
| 35  | BB    | 619 | G    | Sidechain |
| 35  | BB    | 62  | U    | Sidechain |
| 35  | BB    | 622 | G    | Sidechain |
| 35  | BB    | 624 | C    | Sidechain |
| 35  | BB    | 625 | G    | Sidechain |
| 35  | BB    | 628 | G    | Sidechain |
| 35  | BB    | 629 | G    | Sidechain |
| 35  | BB    | 630 | G    | Sidechain |
| 35  | BB    | 631 | A    | Sidechain |
| 35  | BB    | 633 | A    | Sidechain |
| 35  | BB    | 634 | C    | Sidechain |
| 35  | BB    | 635 | C    | Sidechain |
| 35  | BB    | 636 | G    | Sidechain |
| 35  | BB    | 638 | G    | Sidechain |
| 35  | BB    | 64  | A    | Sidechain |
| 35  | BB    | 640 | C    | Sidechain |
| 35  | BB    | 642 | U    | Sidechain |
| 35  | BB    | 645 | C    | Sidechain |
| 35  | BB    | 646 | U    | Sidechain |
| 35  | BB    | 647 | G    | Sidechain |
| 35  | BB    | 648 | G    | Sidechain |
| 35  | BB    | 650 | C    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 35  | BB    | 651 | G    | Sidechain |
| 35  | BB    | 653 | U    | Sidechain |
| 35  | BB    | 658 | U    | Sidechain |
| 35  | BB    | 659 | G    | Sidechain |
| 35  | BB    | 66  | C    | Sidechain |
| 35  | BB    | 660 | C    | Sidechain |
| 35  | BB    | 661 | A    | Sidechain |
| 35  | BB    | 663 | G    | Sidechain |
| 35  | BB    | 664 | G    | Sidechain |
| 35  | BB    | 668 | A    | Sidechain |
| 35  | BB    | 669 | G    | Sidechain |
| 35  | BB    | 673 | C    | Sidechain |
| 35  | BB    | 674 | G    | Sidechain |
| 35  | BB    | 675 | A    | Sidechain |
| 35  | BB    | 676 | A    | Sidechain |
| 35  | BB    | 68  | G    | Sidechain |
| 35  | BB    | 680 | C    | Sidechain |
| 35  | BB    | 682 | G    | Sidechain |
| 35  | BB    | 685 | A    | Sidechain |
| 35  | BB    | 686 | U    | Sidechain |
| 35  | BB    | 687 | C    | Sidechain |
| 35  | BB    | 688 | U    | Sidechain |
| 35  | BB    | 689 | A    | Sidechain |
| 35  | BB    | 696 | G    | Sidechain |
| 35  | BB    | 698 | C    | Sidechain |
| 35  | BB    | 70  | G    | Sidechain |
| 35  | BB    | 700 | G    | Sidechain |
| 35  | BB    | 703 | U    | Sidechain |
| 35  | BB    | 704 | G    | Sidechain |
| 35  | BB    | 708 | G    | Sidechain |
| 35  | BB    | 710 | U    | Sidechain |
| 35  | BB    | 711 | G    | Sidechain |
| 35  | BB    | 712 | G    | Sidechain |
| 35  | BB    | 713 | G    | Sidechain |
| 35  | BB    | 714 | U    | Sidechain |
| 35  | BB    | 715 | A    | Sidechain |
| 35  | BB    | 720 | U    | Sidechain |
| 35  | BB    | 722 | A    | Sidechain |
| 35  | BB    | 723 | C    | Sidechain |
| 35  | BB    | 725 | G    | Sidechain |
| 35  | BB    | 726 | G    | Sidechain |
| 35  | BB    | 728 | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 35  | BB    | 730 | A    | Sidechain |
| 35  | BB    | 732 | C    | Sidechain |
| 35  | BB    | 733 | G    | Sidechain |
| 35  | BB    | 737 | C    | Sidechain |
| 35  | BB    | 738 | G    | Sidechain |
| 35  | BB    | 744 | U    | Sidechain |
| 35  | BB    | 748 | G    | Sidechain |
| 35  | BB    | 749 | A    | Sidechain |
| 35  | BB    | 75  | G    | Sidechain |
| 35  | BB    | 750 | A    | Sidechain |
| 35  | BB    | 752 | A    | Sidechain |
| 35  | BB    | 755 | U    | Sidechain |
| 35  | BB    | 758 | C    | Sidechain |
| 35  | BB    | 76  | C    | Sidechain |
| 35  | BB    | 760 | G    | Sidechain |
| 35  | BB    | 761 | A    | Sidechain |
| 35  | BB    | 763 | G    | Sidechain |
| 35  | BB    | 764 | A    | Sidechain |
| 35  | BB    | 767 | U    | Sidechain |
| 35  | BB    | 77  | G    | Sidechain |
| 35  | BB    | 771 | G    | Sidechain |
| 35  | BB    | 772 | C    | Sidechain |
| 35  | BB    | 773 | U    | Sidechain |
| 35  | BB    | 774 | G    | Sidechain |
| 35  | BB    | 775 | G    | Sidechain |
| 35  | BB    | 778 | G    | Sidechain |
| 35  | BB    | 78  | U    | Sidechain |
| 35  | BB    | 780 | G    | Sidechain |
| 35  | BB    | 784 | G    | Sidechain |
| 35  | BB    | 785 | G    | Sidechain |
| 35  | BB    | 787 | C    | Sidechain |
| 35  | BB    | 79  | C    | Sidechain |
| 35  | BB    | 791 | C    | Sidechain |
| 35  | BB    | 794 | A    | Sidechain |
| 35  | BB    | 795 | C    | Sidechain |
| 35  | BB    | 797 | G    | Sidechain |
| 35  | BB    | 798 | G    | Sidechain |
| 35  | BB    | 799 | G    | Sidechain |
| 35  | BB    | 800 | A    | Sidechain |
| 35  | BB    | 801 | G    | Sidechain |
| 35  | BB    | 805 | G    | Sidechain |
| 35  | BB    | 809 | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 35  | BB    | 81  | G    | Sidechain |
| 35  | BB    | 811 | U    | Sidechain |
| 35  | BB    | 814 | C    | Sidechain |
| 35  | BB    | 817 | C    | Sidechain |
| 35  | BB    | 82  | U    | Sidechain |
| 35  | BB    | 820 | A    | Sidechain |
| 35  | BB    | 821 | A    | Sidechain |
| 35  | BB    | 823 | C    | Sidechain |
| 35  | BB    | 824 | U    | Sidechain |
| 35  | BB    | 826 | U    | Sidechain |
| 35  | BB    | 830 | G    | Sidechain |
| 35  | BB    | 833 | A    | Sidechain |
| 35  | BB    | 838 | C    | Sidechain |
| 35  | BB    | 84  | A    | Sidechain |
| 35  | BB    | 842 | U    | Sidechain |
| 35  | BB    | 847 | U    | Sidechain |
| 35  | BB    | 849 | A    | Sidechain |
| 35  | BB    | 85  | G    | Sidechain |
| 35  | BB    | 852 | U    | Sidechain |
| 35  | BB    | 857 | G    | Sidechain |
| 35  | BB    | 858 | G    | Sidechain |
| 35  | BB    | 859 | G    | Sidechain |
| 35  | BB    | 86  | G    | Sidechain |
| 35  | BB    | 863 | A    | Sidechain |
| 35  | BB    | 864 | G    | Sidechain |
| 35  | BB    | 869 | G    | Sidechain |
| 35  | BB    | 871 | U    | Sidechain |
| 35  | BB    | 872 | U    | Sidechain |
| 35  | BB    | 877 | A    | Sidechain |
| 35  | BB    | 88  | G    | Sidechain |
| 35  | BB    | 880 | G    | Sidechain |
| 35  | BB    | 882 | G    | Sidechain |
| 35  | BB    | 883 | G    | Sidechain |
| 35  | BB    | 887 | U    | Sidechain |
| 35  | BB    | 89  | A    | Sidechain |
| 35  | BB    | 891 | G    | Sidechain |
| 35  | BB    | 892 | A    | Sidechain |
| 35  | BB    | 894 | U    | Sidechain |
| 35  | BB    | 896 | A    | Sidechain |
| 35  | BB    | 897 | C    | Sidechain |
| 35  | BB    | 898 | C    | Sidechain |
| 35  | BB    | 899 | A    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 35  | BB    | 9   | G    | Sidechain |
| 35  | BB    | 901 | C    | Sidechain |
| 35  | BB    | 903 | C    | Sidechain |
| 35  | BB    | 906 | U    | Sidechain |
| 35  | BB    | 907 | G    | Sidechain |
| 35  | BB    | 909 | A    | Sidechain |
| 35  | BB    | 91  | A    | Sidechain |
| 35  | BB    | 911 | A    | Sidechain |
| 35  | BB    | 912 | C    | Sidechain |
| 35  | BB    | 915 | C    | Sidechain |
| 35  | BB    | 917 | A    | Sidechain |
| 35  | BB    | 919 | U    | Sidechain |
| 35  | BB    | 921 | C    | Sidechain |
| 35  | BB    | 924 | G    | Sidechain |
| 35  | BB    | 926 | G    | Sidechain |
| 35  | BB    | 93  | G    | Sidechain |
| 35  | BB    | 933 | A    | Sidechain |
| 35  | BB    | 937 | C    | Sidechain |
| 35  | BB    | 938 | G    | Sidechain |
| 35  | BB    | 939 | G    | Sidechain |
| 35  | BB    | 943 | A    | Sidechain |
| 35  | BB    | 945 | A    | Sidechain |
| 35  | BB    | 946 | C    | Sidechain |
| 35  | BB    | 947 | A    | Sidechain |
| 35  | BB    | 949 | G    | Sidechain |
| 35  | BB    | 95  | A    | Sidechain |
| 35  | BB    | 950 | G    | Sidechain |
| 35  | BB    | 952 | G    | Sidechain |
| 35  | BB    | 953 | G    | Sidechain |
| 35  | BB    | 954 | G    | Sidechain |
| 35  | BB    | 955 | U    | Sidechain |
| 35  | BB    | 956 | G    | Sidechain |
| 35  | BB    | 957 | C    | Sidechain |
| 35  | BB    | 958 | U    | Sidechain |
| 35  | BB    | 959 | A    | Sidechain |
| 35  | BB    | 96  | C    | Sidechain |
| 35  | BB    | 962 | G    | Sidechain |
| 35  | BB    | 963 | U    | Sidechain |
| 35  | BB    | 966 | G    | Sidechain |
| 35  | BB    | 968 | C    | Sidechain |
| 35  | BB    | 969 | G    | Sidechain |
| 35  | BB    | 971 | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 35  | BB    | 972 | A    | Sidechain |
| 35  | BB    | 974 | G    | Sidechain |
| 35  | BB    | 976 | G    | Sidechain |
| 35  | BB    | 979 | A    | Sidechain |
| 35  | BB    | 98  | G    | Sidechain |
| 35  | BB    | 980 | A    | Sidechain |
| 35  | BB    | 981 | A    | Sidechain |
| 35  | BB    | 982 | C    | Sidechain |
| 35  | BB    | 984 | A    | Sidechain |
| 35  | BB    | 988 | A    | Sidechain |
| 35  | BB    | 989 | G    | Sidechain |
| 35  | BB    | 991 | C    | Sidechain |
| 35  | BB    | 995 | C    | Sidechain |
| 35  | BB    | 998 | C    | Sidechain |
| 36  | BC    | 132 | ARG  | Sidechain |
| 36  | BC    | 174 | ARG  | Sidechain |
| 36  | BC    | 188 | ARG  | Sidechain |
| 36  | BC    | 261 | ARG  | Sidechain |
| 36  | BC    | 269 | ARG  | Sidechain |
| 36  | BC    | 61  | TYR  | Sidechain |
| 36  | BC    | 82  | TYR  | Sidechain |
| 36  | BC    | 86  | ARG  | Sidechain |
| 37  | BD    | 124 | ARG  | Sidechain |
| 37  | BD    | 13  | ARG  | Sidechain |
| 37  | BD    | 151 | THR  | Peptide   |
| 37  | BD    | 156 | PHE  | Sidechain |
| 37  | BD    | 184 | ARG  | Sidechain |
| 37  | BD    | 89  | GLU  | Peptide   |
| 38  | BE    | 117 | ARG  | Sidechain |
| 38  | BE    | 170 | ARG  | Sidechain |
| 38  | BE    | 49  | ARG  | Sidechain |
| 38  | BE    | 57  | LYS  | Peptide   |
| 38  | BE    | 88  | ARG  | Peptide   |
| 39  | BF    | 111 | ARG  | Sidechain |
| 39  | BF    | 124 | ARG  | Sidechain |
| 39  | BF    | 127 | TYR  | Sidechain |
| 39  | BF    | 142 | TYR  | Sidechain |
| 39  | BF    | 147 | ARG  | Sidechain |
| 39  | BF    | 173 | ASP  | Peptide   |
| 39  | BF    | 18  | GLU  | Peptide   |
| 39  | BF    | 21  | TYR  | Sidechain |
| 39  | BF    | 6   | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 39  | BF    | 82  | TYR  | Sidechain |
| 40  | BG    | 150 | TYR  | Sidechain |
| 40  | BG    | 156 | TYR  | Sidechain |
| 40  | BG    | 83  | THR  | Peptide   |
| 41  | BH    | 31  | VAL  | Peptide   |
| 43  | BJ    | 112 | GLY  | Peptide   |
| 43  | BJ    | 13  | ARG  | Sidechain |
| 43  | BJ    | 16  | TYR  | Sidechain |
| 43  | BJ    | 35  | ARG  | Sidechain |
| 44  | BK    | 17  | ARG  | Sidechain |
| 44  | BK    | 30  | ARG  | Sidechain |
| 44  | BK    | 70  | ARG  | Peptide   |
| 44  | BK    | 71  | ARG  | Peptide   |
| 44  | BK    | 88  | ASN  | Peptide   |
| 45  | BL    | 41  | ARG  | Sidechain |
| 46  | BM    | 10  | ARG  | Sidechain |
| 46  | BM    | 37  | GLY  | Peptide   |
| 46  | BM    | 66  | ARG  | Sidechain |
| 47  | BN    | 112 | TYR  | Sidechain |
| 47  | BN    | 4   | ARG  | Sidechain |
| 47  | BN    | 80  | PHE  | Sidechain |
| 47  | BN    | 86  | ARG  | Sidechain |
| 47  | BN    | 95  | THR  | Peptide   |
| 48  | BO    | 102 | ARG  | Sidechain |
| 48  | BO    | 13  | ARG  | Sidechain |
| 49  | BP    | 108 | ARG  | Sidechain |
| 49  | BP    | 51  | ASN  | Peptide   |
| 49  | BP    | 60  | VAL  | Peptide   |
| 49  | BP    | 61  | ARG  | Sidechain |
| 49  | BP    | 97  | TYR  | Sidechain |
| 50  | BQ    | 10  | ARG  | Sidechain |
| 50  | BQ    | 23  | TYR  | Sidechain |
| 50  | BQ    | 24  | TYR  | Sidechain |
| 50  | BQ    | 57  | ARG  | Sidechain |
| 50  | BQ    | 6   | GLY  | Peptide   |
| 51  | BR    | 21  | ARG  | Sidechain |
| 51  | BR    | 89  | HIS  | Sidechain |
| 51  | BR    | 90  | ARG  | Sidechain |
| 52  | BS    | 25  | ARG  | Sidechain |
| 53  | BT    | 76  | ARG  | Sidechain |
| 54  | BU    | 6   | ARG  | Sidechain |
| 54  | BU    | 95  | PHE  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 55  | BW    | 18  | ARG  | Sidechain |
| 55  | BW    | 19  | ARG  | Sidechain |
| 55  | BW    | 57  | TYR  | Sidechain |
| 55  | BW    | 82  | TYR  | Sidechain |
| 56  | BY    | 19  | ARG  | Sidechain |
| 56  | BY    | 34  | SER  | Mainchain |
| 56  | BY    | 40  | ARG  | Sidechain |
| 56  | BY    | 54  | ARG  | Sidechain |
| 56  | BY    | 68  | PHE  | Peptide   |

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 32831 | 0        | 16502    | 183     | 0            |
| 2   | AB    | 1704  | 0        | 1732     | 3       | 0            |
| 3   | AC    | 1624  | 0        | 1699     | 12      | 0            |
| 4   | AD    | 1643  | 0        | 1710     | 5       | 0            |
| 5   | AE    | 1105  | 0        | 1148     | 6       | 0            |
| 6   | AF    | 817   | 0        | 808      | 7       | 0            |
| 7   | AG    | 1174  | 0        | 1230     | 5       | 0            |
| 8   | AH    | 979   | 0        | 1034     | 1       | 0            |
| 9   | AI    | 1022  | 0        | 1070     | 9       | 0            |
| 10  | AJ    | 786   | 0        | 828      | 3       | 0            |
| 11  | AK    | 877   | 0        | 887      | 9       | 0            |
| 12  | AL    | 955   | 0        | 1019     | 2       | 0            |
| 13  | AM    | 876   | 0        | 937      | 7       | 0            |
| 14  | AN    | 774   | 0        | 827      | 2       | 0            |
| 15  | AO    | 716   | 0        | 742      | 3       | 0            |
| 16  | AP    | 638   | 0        | 656      | 0       | 0            |
| 17  | AQ    | 648   | 0        | 691      | 4       | 0            |
| 18  | AR    | 455   | 0        | 478      | 1       | 0            |
| 19  | AS    | 637   | 0        | 665      | 5       | 0            |
| 20  | AT    | 665   | 0        | 714      | 4       | 0            |
| 21  | AU    | 425   | 0        | 449      | 2       | 0            |
| 22  | AV    | 1649  | 0        | 832      | 21      | 0            |
| 23  | AX    | 236   | 0        | 121      | 10      | 0            |
| 24  | AZ    | 100   | 0        | 99       | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 25  | B0    | 625    | 0        | 655      | 1       | 0            |
| 26  | B1    | 509    | 0        | 543      | 1       | 0            |
| 27  | B2    | 449    | 0        | 491      | 1       | 0            |
| 28  | B3    | 444    | 0        | 461      | 3       | 0            |
| 29  | B4    | 409    | 0        | 440      | 0       | 0            |
| 30  | B5    | 1733   | 0        | 1824     | 4       | 0            |
| 31  | B6    | 377    | 0        | 418      | 3       | 0            |
| 32  | B7    | 504    | 0        | 574      | 5       | 0            |
| 33  | B8    | 302    | 0        | 343      | 0       | 0            |
| 34  | BA    | 2464   | 0        | 1246     | 8       | 0            |
| 35  | BB    | 62321  | 0        | 31294    | 336     | 0            |
| 36  | BC    | 2082   | 0        | 2157     | 14      | 0            |
| 37  | BD    | 1565   | 0        | 1616     | 8       | 0            |
| 38  | BE    | 1552   | 0        | 1619     | 9       | 0            |
| 39  | BF    | 1420   | 0        | 1460     | 9       | 0            |
| 40  | BG    | 1316   | 0        | 1364     | 4       | 0            |
| 41  | BH    | 1111   | 0        | 1148     | 1       | 0            |
| 42  | BI    | 1032   | 0        | 1088     | 118     | 0            |
| 43  | BJ    | 1129   | 0        | 1162     | 8       | 0            |
| 44  | BK    | 930    | 0        | 1003     | 6       | 0            |
| 45  | BL    | 1045   | 0        | 1117     | 6       | 0            |
| 46  | BM    | 1074   | 0        | 1157     | 4       | 0            |
| 47  | BN    | 960    | 0        | 1000     | 2       | 0            |
| 48  | BO    | 892    | 0        | 923      | 2       | 0            |
| 49  | BP    | 917    | 0        | 965      | 4       | 0            |
| 50  | BQ    | 947    | 0        | 1022     | 8       | 0            |
| 51  | BR    | 816    | 0        | 839      | 8       | 0            |
| 52  | BS    | 857    | 0        | 922      | 3       | 0            |
| 53  | BT    | 738    | 0        | 807      | 5       | 0            |
| 54  | BU    | 755    | 0        | 807      | 10      | 0            |
| 55  | BW    | 753    | 0        | 780      | 5       | 0            |
| 56  | BY    | 596    | 0        | 610      | 1       | 0            |
| All | All   | 145960 | 0        | 98733    | 840     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (840) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1        | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|---------------|--------------------------|-------------------|
| 22:AV:35:G:N2 | 23:AX:18:C:C2 | 2.08                     | 1.22              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BI:11:GLN:HG2   | 42:BI:55:PRO:HB3   | 1.51                     | 0.91              |
| 42:BI:140:GLU:O    | 42:BI:141:ASP:OXT  | 1.91                     | 0.89              |
| 42:BI:27:LEU:H     | 42:BI:27:LEU:HD23  | 1.43                     | 0.82              |
| 42:BI:121:ILE:HD13 | 42:BI:121:ILE:H    | 1.44                     | 0.82              |
| 42:BI:21:PRO:HB2   | 42:BI:22:PRO:HD3   | 1.63                     | 0.80              |
| 42:BI:9:LYS:HG2    | 42:BI:57:VAL:HG13  | 1.63                     | 0.79              |
| 42:BI:45:THR:HA    | 42:BI:48:ILE:HG22  | 1.66                     | 0.78              |
| 42:BI:105:LEU:HD13 | 42:BI:129:GLU:HG2  | 1.67                     | 0.76              |
| 42:BI:102:ARG:HG3  | 42:BI:141:ASP:HA   | 1.66                     | 0.75              |
| 42:BI:72:THR:HG21  | 42:BI:112:LYS:HA   | 1.69                     | 0.75              |
| 42:BI:20:SER:HB3   | 42:BI:21:PRO:HD3   | 1.69                     | 0.74              |
| 42:BI:55:PRO:HD3   | 42:BI:74:PRO:HD3   | 1.70                     | 0.74              |
| 22:AV:35:G:N2      | 23:AX:18:C:N3      | 2.35                     | 0.74              |
| 22:AV:35:G:C2      | 23:AX:18:C:C2      | 2.79                     | 0.71              |
| 36:BC:257:ARG:HE   | 36:BC:260:LYS:H    | 1.39                     | 0.70              |
| 42:BI:105:LEU:HD11 | 42:BI:139:VAL:HG21 | 1.73                     | 0.70              |
| 42:BI:85:ILE:HD13  | 42:BI:137:LEU:HD21 | 1.73                     | 0.70              |
| 42:BI:73:PRO:HG2   | 42:BI:78:LEU:HD21  | 1.75                     | 0.69              |
| 54:BU:82:VAL:HG11  | 54:BU:93:ARG:HH11  | 1.56                     | 0.69              |
| 50:BQ:87:VAL:HG12  | 51:BR:39:LEU:HD22  | 1.76                     | 0.68              |
| 1:AA:827:U:H2'     | 1:AA:870:U:H3      | 1.59                     | 0.67              |
| 35:BB:2091:C:H3'   | 35:BB:2092:U:H5''  | 1.77                     | 0.67              |
| 1:AA:781:A:H2'     | 1:AA:782:A:H5'     | 1.75                     | 0.67              |
| 5:AE:137:ARG:HE    | 5:AE:137:ARG:HA    | 1.60                     | 0.67              |
| 35:BB:2132:U:H3'   | 35:BB:2132:U:H6    | 1.60                     | 0.66              |
| 42:BI:112:LYS:O    | 42:BI:116:MET:HG3  | 1.96                     | 0.66              |
| 35:BB:1082:U:C4    | 35:BB:1086:A:C2    | 2.84                     | 0.65              |
| 35:BB:962:G:H21    | 35:BB:2250:G:H1    | 1.43                     | 0.65              |
| 35:BB:877:A:C2     | 35:BB:901:C:C2     | 2.84                     | 0.65              |
| 42:BI:121:ILE:N    | 42:BI:121:ILE:HD13 | 2.12                     | 0.64              |
| 35:BB:900:A:H2'    | 35:BB:901:C:H5'    | 1.79                     | 0.64              |
| 42:BI:27:LEU:HD12  | 42:BI:32:VAL:HG11  | 1.78                     | 0.64              |
| 54:BU:35:VAL:H     | 54:BU:39:ASN:HD21  | 1.45                     | 0.64              |
| 42:BI:123:ALA:HA   | 42:BI:126:ARG:HH12 | 1.63                     | 0.64              |
| 1:AA:243:A:H4'     | 1:AA:244:U:H5'     | 1.78                     | 0.63              |
| 42:BI:41:PHE:O     | 42:BI:45:THR:HG23  | 1.98                     | 0.63              |
| 35:BB:1358:G:C2    | 35:BB:1372:U:C5    | 2.87                     | 0.63              |
| 1:AA:1305:G:H21    | 1:AA:1332:A:H8     | 1.46                     | 0.63              |
| 1:AA:764:C:H2'     | 1:AA:765:G:H5'     | 1.81                     | 0.62              |
| 53:BT:15:HIS:CE1   | 53:BT:17:SER:HB2   | 2.34                     | 0.62              |
| 42:BI:72:THR:HG22  | 42:BI:115:ASP:OD2  | 1.99                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 42:BI:42:ASN:HA    | 42:BI:45:THR:OG1  | 1.99                     | 0.62              |
| 42:BI:78:LEU:HA    | 42:BI:81:LYS:HE2  | 1.82                     | 0.62              |
| 22:AV:35:G:C2      | 23:AX:18:C:N3     | 2.68                     | 0.61              |
| 35:BB:28:A:C2      | 35:BB:513:A:C8    | 2.88                     | 0.61              |
| 35:BB:1082:U:C5    | 35:BB:1083:U:C5   | 2.88                     | 0.61              |
| 42:BI:27:LEU:H     | 42:BI:27:LEU:CD2  | 2.13                     | 0.61              |
| 35:BB:2132:U:H3'   | 35:BB:2132:U:C6   | 2.35                     | 0.61              |
| 42:BI:20:SER:O     | 42:BI:25:PRO:HD2  | 2.00                     | 0.61              |
| 35:BB:2091:C:H3'   | 35:BB:2092:U:C5'  | 2.31                     | 0.61              |
| 35:BB:940:G:H2'    | 35:BB:941:A:H4'   | 1.83                     | 0.61              |
| 1:AA:769:G:H4'     | 1:AA:1513:A:H4'   | 1.82                     | 0.61              |
| 42:BI:121:ILE:CD1  | 42:BI:121:ILE:H   | 2.14                     | 0.60              |
| 35:BB:1024:G:H3'   | 35:BB:1025:G:H5'' | 1.82                     | 0.60              |
| 45:BL:81:ASP:HA    | 45:BL:84:LYS:HD2  | 1.83                     | 0.60              |
| 9:AI:83:THR:HG22   | 9:AI:97:LEU:HD22  | 1.84                     | 0.60              |
| 35:BB:337:C:C5     | 35:BB:338:G:C8    | 2.89                     | 0.60              |
| 49:BP:77:SER:HB3   | 49:BP:80:VAL:HG23 | 1.84                     | 0.60              |
| 1:AA:920:U:H2'     | 1:AA:921:U:C6     | 2.37                     | 0.60              |
| 35:BB:571:U:C5     | 35:BB:575:A:C6    | 2.90                     | 0.59              |
| 46:BM:33:LEU:HD11  | 46:BM:117:PHE:HB3 | 1.84                     | 0.59              |
| 42:BI:32:VAL:HG22  | 42:BI:60:VAL:HG21 | 1.85                     | 0.59              |
| 1:AA:1526:G:OP1    | 21:AU:37:TYR:CG   | 2.55                     | 0.59              |
| 9:AI:10:ARG:H      | 9:AI:80:HIS:CD2   | 2.21                     | 0.59              |
| 35:BB:1216:G:H5''  | 50:BQ:10:ARG:HH12 | 1.65                     | 0.59              |
| 23:AX:17:C:H2'     | 23:AX:18:C:C5     | 2.38                     | 0.59              |
| 1:AA:979:C:H3'     | 1:AA:980:C:C6     | 2.38                     | 0.58              |
| 36:BC:141:HIS:CE1  | 36:BC:190:THR:HB  | 2.38                     | 0.58              |
| 42:BI:25:PRO:O     | 42:BI:29:GLN:HG3  | 2.03                     | 0.58              |
| 35:BB:1551:A:H3'   | 35:BB:1552:A:H5'' | 1.84                     | 0.58              |
| 1:AA:673:A:H4'     | 6:AF:86:ARG:HE    | 1.69                     | 0.58              |
| 1:AA:82:G:H3'      | 1:AA:83:C:H4'     | 1.85                     | 0.58              |
| 1:AA:1306:A:C2     | 1:AA:1332:A:H1'   | 2.39                     | 0.58              |
| 39:BF:4:HIS:HB2    | 39:BF:96:TRP:CE2  | 2.39                     | 0.57              |
| 51:BR:36:ALA:HB2   | 51:BR:58:VAL:HG12 | 1.86                     | 0.57              |
| 42:BI:99:LYS:H     | 42:BI:99:LYS:HD3  | 1.69                     | 0.57              |
| 1:AA:1526:G:C4     | 1:AA:1527:U:C5    | 2.93                     | 0.57              |
| 35:BB:1978:A:C5    | 35:BB:1979:U:C5   | 2.92                     | 0.57              |
| 42:BI:45:THR:CA    | 42:BI:48:ILE:HG22 | 2.35                     | 0.57              |
| 35:BB:2123:G:H22   | 35:BB:2176:A:H1'  | 1.70                     | 0.57              |
| 39:BF:134:GLN:HE21 | 39:BF:149:ARG:HD2 | 1.68                     | 0.57              |
| 1:AA:667:G:H4'     | 15:AO:50:HIS:CD2  | 2.39                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BB:1437:C:H2'   | 35:BB:1438:U:C6    | 2.39                     | 0.57              |
| 42:BI:37:PHE:CZ    | 42:BI:58:ILE:HD11  | 2.40                     | 0.57              |
| 35:BB:1803:A:C8    | 35:BB:1804:C:C6    | 2.93                     | 0.56              |
| 42:BI:108:ILE:HG22 | 42:BI:128:ILE:HD13 | 1.88                     | 0.56              |
| 51:BR:26:ASP:O     | 51:BR:27:ILE:HG22  | 2.05                     | 0.56              |
| 42:BI:125:THR:O    | 42:BI:129:GLU:HG3  | 2.05                     | 0.56              |
| 42:BI:17:ALA:O     | 42:BI:18:ASN:CB    | 2.54                     | 0.56              |
| 35:BB:1082:U:N3    | 35:BB:1086:A:C2    | 2.74                     | 0.56              |
| 30:B5:1:MET:HE1    | 35:BB:2175:C:H5    | 1.71                     | 0.56              |
| 35:BB:641:U:C5     | 35:BB:642:U:C4     | 2.94                     | 0.56              |
| 1:AA:350:G:H2'     | 1:AA:351:G:C8      | 2.41                     | 0.56              |
| 35:BB:250:G:C6     | 35:BB:251:A:C6     | 2.94                     | 0.56              |
| 1:AA:413:G:H21     | 1:AA:428:G:H1'     | 1.70                     | 0.56              |
| 7:AG:78:ARG:HE     | 23:AX:13:A:N6      | 2.04                     | 0.56              |
| 35:BB:851:C:H2'    | 35:BB:852:U:C6     | 2.41                     | 0.56              |
| 1:AA:516:U:C4      | 1:AA:517:G:C6      | 2.94                     | 0.56              |
| 32:B7:60:CYS:O     | 32:B7:61:LEU:HD23  | 2.06                     | 0.56              |
| 55:BW:44:HIS:CE1   | 55:BW:85:LYS:HA    | 2.41                     | 0.56              |
| 35:BB:1273:U:H5'   | 47:BN:12:ARG:HH12  | 1.71                     | 0.55              |
| 42:BI:129:GLU:HB3  | 42:BI:133:ARG:HH12 | 1.71                     | 0.55              |
| 35:BB:877:A:C6     | 35:BB:901:C:N3     | 2.75                     | 0.55              |
| 35:BB:98:G:H22     | 54:BU:6:ARG:HH22   | 1.54                     | 0.55              |
| 35:BB:418:C:C4     | 35:BB:419:U:C4     | 2.94                     | 0.55              |
| 56:BY:51:GLY:HA2   | 56:BY:59:PHE:H     | 1.72                     | 0.55              |
| 1:AA:973:G:H3'     | 1:AA:974:A:H5''    | 1.89                     | 0.55              |
| 30:B5:1:MET:SD     | 35:BB:2174:C:H3'   | 2.47                     | 0.55              |
| 1:AA:1111:A:H61    | 3:AC:175:HIS:HB3   | 1.72                     | 0.55              |
| 35:BB:819:A:C4     | 35:BB:1189:A:C2    | 2.95                     | 0.55              |
| 42:BI:54:ILE:HD13  | 42:BI:55:PRO:N     | 2.22                     | 0.55              |
| 1:AA:1110:A:H3'    | 1:AA:1111:A:H8     | 1.72                     | 0.55              |
| 6:AF:18:VAL:HG21   | 6:AF:58:HIS:CD2    | 2.42                     | 0.55              |
| 35:BB:1100:C:H2'   | 35:BB:1101:U:H6    | 1.71                     | 0.55              |
| 42:BI:49:GLU:CB    | 42:BI:52:LEU:HD12  | 2.37                     | 0.55              |
| 35:BB:704:G:H2'    | 35:BB:726:G:H22    | 1.72                     | 0.55              |
| 35:BB:1410:G:C6    | 35:BB:1411:U:C4    | 2.94                     | 0.54              |
| 35:BB:1805:A:H5''  | 36:BC:247:TRP:CD2  | 2.43                     | 0.54              |
| 1:AA:71:A:H61      | 1:AA:99:C:H1'      | 1.72                     | 0.54              |
| 5:AE:33:THR:HG22   | 5:AE:34:ALA:H      | 1.72                     | 0.54              |
| 11:AK:21:HIS:CE1   | 11:AK:23:HIS:HB2   | 2.42                     | 0.54              |
| 35:BB:1269:A:H2'   | 35:BB:1270:C:C6    | 2.42                     | 0.54              |
| 35:BB:2643:G:C6    | 35:BB:2644:G:C6    | 2.96                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BB:2308:G:H5'  | 35:BB:2308:G:C8   | 2.42                     | 0.54              |
| 42:BI:71:LYS:HB3  | 42:BI:115:ASP:OD2 | 2.07                     | 0.54              |
| 35:BB:2147:A:H3'  | 35:BB:2148:G:H5'  | 1.88                     | 0.54              |
| 35:BB:2229:U:H2'  | 35:BB:2230:G:H8   | 1.73                     | 0.54              |
| 35:BB:880:G:H2'   | 35:BB:881:G:C8    | 2.43                     | 0.54              |
| 1:AA:818:G:H3'    | 1:AA:819:A:H5''   | 1.89                     | 0.54              |
| 11:AK:20:ALA:HB2  | 11:AK:81:LEU:HD22 | 1.89                     | 0.54              |
| 42:BI:76:ALA:HA   | 42:BI:135:MET:SD  | 2.48                     | 0.54              |
| 35:BB:1057:A:C2   | 35:BB:1082:U:C2   | 2.95                     | 0.54              |
| 35:BB:1022:G:C6   | 35:BB:1141:U:C5   | 2.96                     | 0.54              |
| 35:BB:1483:G:C6   | 35:BB:1484:U:C4   | 2.96                     | 0.54              |
| 35:BB:1311:G:H21  | 35:BB:1603:A:H62  | 1.55                     | 0.54              |
| 35:BB:877:A:N1    | 35:BB:901:C:C2    | 2.76                     | 0.54              |
| 42:BI:140:GLU:C   | 42:BI:141:ASP:OXT | 2.38                     | 0.54              |
| 42:BI:63:ASP:O    | 42:BI:64:ARG:HB2  | 2.08                     | 0.53              |
| 35:BB:2128:G:C6   | 35:BB:2160:C:C5   | 2.96                     | 0.53              |
| 5:AE:57:ALA:HA    | 5:AE:60:GLN:HB3   | 1.90                     | 0.53              |
| 20:AT:24:ARG:HE   | 20:AT:28:ARG:HE   | 1.56                     | 0.53              |
| 35:BB:2723:C:C4   | 35:BB:2724:U:C4   | 2.97                     | 0.53              |
| 1:AA:1531:A:H2'   | 1:AA:1532:U:C6    | 2.43                     | 0.53              |
| 1:AA:668:G:H21    | 15:AO:45:HIS:HE1  | 1.57                     | 0.53              |
| 42:BI:52:LEU:HD22 | 42:BI:81:LYS:HD3  | 1.90                     | 0.53              |
| 42:BI:99:LYS:N    | 42:BI:99:LYS:HD3  | 2.24                     | 0.53              |
| 42:BI:57:VAL:HG23 | 42:BI:71:LYS:NZ   | 2.24                     | 0.53              |
| 35:BB:1858:A:C2   | 35:BB:1885:A:H1'  | 2.44                     | 0.53              |
| 35:BB:396:G:C6    | 35:BB:397:U:C4    | 2.97                     | 0.53              |
| 18:AR:38:ILE:HG22 | 18:AR:39:VAL:H    | 1.73                     | 0.52              |
| 44:BK:30:ARG:HH21 | 44:BK:33:ALA:HB1  | 1.74                     | 0.52              |
| 6:AF:38:ARG:HH12  | 6:AF:96:VAL:HG12  | 1.74                     | 0.52              |
| 42:BI:54:ILE:C    | 42:BI:54:ILE:HD13 | 2.30                     | 0.52              |
| 1:AA:1446:A:H3'   | 1:AA:1447:A:H5''  | 1.91                     | 0.52              |
| 35:BB:1065:U:H3   | 35:BB:1069:A:H2'  | 1.73                     | 0.52              |
| 35:BB:15:G:C4     | 35:BB:16:C:C6     | 2.98                     | 0.52              |
| 35:BB:962:G:N2    | 35:BB:2250:G:H1   | 2.08                     | 0.52              |
| 42:BI:32:VAL:HG22 | 42:BI:60:VAL:CG2  | 2.40                     | 0.52              |
| 36:BC:172:THR:HA  | 36:BC:182:LYS:HA  | 1.90                     | 0.52              |
| 35:BB:1995:U:H2'  | 35:BB:1996:C:C5   | 2.44                     | 0.52              |
| 42:BI:3:LYS:HG2   | 42:BI:4:VAL:H     | 1.75                     | 0.52              |
| 42:BI:57:VAL:HG23 | 42:BI:71:LYS:HZ1  | 1.73                     | 0.52              |
| 35:BB:2345:G:C4   | 35:BB:2347:C:C5   | 2.98                     | 0.52              |
| 35:BB:19:A:C2     | 35:BB:522:A:C2    | 2.98                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BB:1805:A:H4'   | 36:BC:247:TRP:CZ2  | 2.44                     | 0.52              |
| 42:BI:85:ILE:CD1   | 42:BI:137:LEU:HD21 | 2.39                     | 0.52              |
| 50:BQ:87:VAL:CG1   | 51:BR:39:LEU:HD22  | 2.40                     | 0.52              |
| 1:AA:664:G:H22     | 1:AA:741:G:H1      | 1.57                     | 0.51              |
| 35:BB:831:G:H22    | 45:BL:53:GLY:H     | 1.58                     | 0.51              |
| 35:BB:870:U:C2'    | 35:BB:871:U:H5''   | 2.40                     | 0.51              |
| 42:BI:79:LEU:HD11  | 42:BI:131:THR:OG1  | 2.09                     | 0.51              |
| 46:BM:19:GLY:CA    | 46:BM:38:ARG:HH12  | 2.23                     | 0.51              |
| 55:BW:4:ILE:HG21   | 55:BW:42:LEU:HD23  | 1.91                     | 0.51              |
| 35:BB:2014:A:C2    | 35:BB:2015:A:N1    | 2.78                     | 0.51              |
| 42:BI:21:PRO:CB    | 42:BI:22:PRO:HD3   | 2.38                     | 0.51              |
| 1:AA:184:G:C6      | 1:AA:185:U:C4      | 2.98                     | 0.51              |
| 1:AA:688:G:C6      | 1:AA:700:G:C5      | 2.98                     | 0.51              |
| 35:BB:424:G:C6     | 35:BB:425:G:C5     | 2.99                     | 0.51              |
| 43:BJ:77:HIS:CD2   | 43:BJ:79:GLY:H     | 2.29                     | 0.51              |
| 35:BB:589:U:H2'    | 35:BB:590:A:C8     | 2.45                     | 0.51              |
| 40:BG:96:ALA:HB2   | 40:BG:103:ASN:HD22 | 1.75                     | 0.51              |
| 35:BB:1844:C:H5'   | 36:BC:254:LYS:H    | 1.75                     | 0.51              |
| 35:BB:720:U:H2'    | 35:BB:721:A:C8     | 2.46                     | 0.51              |
| 1:AA:1390:U:H2'    | 1:AA:1391:U:C6     | 2.46                     | 0.51              |
| 1:AA:646:G:C5      | 1:AA:647:C:C5      | 2.99                     | 0.51              |
| 42:BI:45:THR:HA    | 42:BI:48:ILE:CG2   | 2.39                     | 0.51              |
| 22:AV:33:U:C4      | 22:AV:35:G:OP2     | 2.63                     | 0.51              |
| 35:BB:1506:U:H2'   | 35:BB:1507:C:C6    | 2.46                     | 0.51              |
| 1:AA:507:C:H3'     | 1:AA:508:U:H5''    | 1.92                     | 0.51              |
| 42:BI:126:ARG:HH11 | 42:BI:126:ARG:HB3  | 1.76                     | 0.51              |
| 1:AA:858:G:C5      | 1:AA:869:G:C5      | 2.98                     | 0.51              |
| 2:AB:103:TRP:CH2   | 2:AB:107:ARG:HD2   | 2.46                     | 0.51              |
| 7:AG:78:ARG:HE     | 23:AX:13:A:H61     | 1.59                     | 0.51              |
| 1:AA:895:G:C5      | 1:AA:896:C:C5      | 2.99                     | 0.51              |
| 35:BB:18:U:H2'     | 35:BB:19:A:C8      | 2.46                     | 0.51              |
| 39:BF:4:HIS:HB2    | 39:BF:96:TRP:CD2   | 2.46                     | 0.51              |
| 1:AA:699:C:H2'     | 1:AA:700:G:H5''    | 1.92                     | 0.50              |
| 26:B1:25:GLN:HB3   | 26:B1:29:ARG:HH11  | 1.76                     | 0.50              |
| 35:BB:15:G:C5      | 35:BB:16:C:C5      | 2.99                     | 0.50              |
| 35:BB:2267:A:C8    | 35:BB:2267:A:H3'   | 2.45                     | 0.50              |
| 30:B5:173:THR:HG21 | 30:B5:192:LEU:HG   | 1.93                     | 0.50              |
| 35:BB:2792:A:H3'   | 35:BB:2793:C:H5''  | 1.93                     | 0.50              |
| 35:BB:704:G:C2'    | 35:BB:726:G:H22    | 2.24                     | 0.50              |
| 42:BI:52:LEU:HD13  | 42:BI:81:LYS:HZ3   | 1.77                     | 0.50              |
| 35:BB:2591:C:H2'   | 35:BB:2592:G:C8    | 2.46                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BB:480:A:H3'   | 35:BB:481:G:H5''   | 1.93                     | 0.50              |
| 42:BI:92:PRO:O    | 42:BI:93:ASN:HB2   | 2.12                     | 0.50              |
| 42:BI:72:THR:HG23 | 42:BI:112:LYS:NZ   | 2.27                     | 0.50              |
| 35:BB:1000:A:H2'  | 35:BB:1001:A:C8    | 2.47                     | 0.50              |
| 35:BB:2233:U:H2'  | 35:BB:2234:G:C8    | 2.45                     | 0.50              |
| 35:BB:294:A:C5    | 35:BB:345:A:C5     | 2.99                     | 0.50              |
| 1:AA:1320:C:H42   | 19:AS:36:ARG:HH11  | 1.60                     | 0.50              |
| 35:BB:1206:G:C5   | 35:BB:1207:C:C5    | 3.00                     | 0.50              |
| 3:AC:174:LEU:HD23 | 3:AC:200:TRP:CZ3   | 2.47                     | 0.49              |
| 23:AX:16:C:C4     | 23:AX:17:C:C5      | 3.00                     | 0.49              |
| 35:BB:2851:A:C5   | 35:BB:2852:G:C5    | 3.00                     | 0.49              |
| 42:BI:78:LEU:HD13 | 42:BI:108:ILE:HG23 | 1.93                     | 0.49              |
| 1:AA:1012:A:C6    | 1:AA:1013:G:C6     | 3.00                     | 0.49              |
| 35:BB:2063:C:C5   | 35:BB:2064:C:C5    | 2.99                     | 0.49              |
| 35:BB:569:U:C4    | 35:BB:570:G:C6     | 3.00                     | 0.49              |
| 42:BI:10:LEU:HD12 | 42:BI:10:LEU:O     | 2.13                     | 0.49              |
| 42:BI:24:GLY:HA2  | 42:BI:34:ILE:HD12  | 1.93                     | 0.49              |
| 35:BB:584:C:H5''  | 50:BQ:2:ARG:HH12   | 1.77                     | 0.49              |
| 1:AA:914:A:C6     | 1:AA:915:A:C5      | 3.00                     | 0.49              |
| 35:BB:2360:G:N2   | 35:BB:2428:G:C4    | 2.80                     | 0.49              |
| 4:AD:145:ARG:HE   | 4:AD:148:ALA:HB2   | 1.77                     | 0.49              |
| 10:AJ:39:PRO:HA   | 10:AJ:74:VAL:HA    | 1.94                     | 0.49              |
| 35:BB:950:G:C5    | 35:BB:951:C:C5     | 3.00                     | 0.49              |
| 35:BB:870:U:H2'   | 35:BB:871:U:H5''   | 1.94                     | 0.49              |
| 1:AA:1492:A:H2'   | 35:BB:1913:A:C2    | 2.48                     | 0.49              |
| 35:BB:1100:C:H2'  | 35:BB:1101:U:C6    | 2.48                     | 0.49              |
| 43:BJ:47:HIS:CE1  | 43:BJ:48:VAL:HG22  | 2.48                     | 0.49              |
| 35:BB:2131:U:O3'  | 35:BB:2132:U:H4'   | 2.13                     | 0.49              |
| 35:BB:2557:G:H2'  | 35:BB:2558:C:C6    | 2.47                     | 0.49              |
| 35:BB:2709:G:C6   | 35:BB:2710:C:C4    | 3.01                     | 0.49              |
| 3:AC:48:LYS:HD2   | 3:AC:74:ILE:HG22   | 1.95                     | 0.49              |
| 4:AD:9:LYS:O      | 4:AD:12:ARG:HB2    | 2.13                     | 0.49              |
| 35:BB:204:A:O3'   | 35:BB:205:G:H4'    | 2.12                     | 0.49              |
| 35:BB:2540:C:C4   | 35:BB:2541:A:C5    | 3.01                     | 0.49              |
| 36:BC:70:LYS:H    | 36:BC:101:ARG:HH12 | 1.61                     | 0.49              |
| 55:BW:30:ILE:HG23 | 55:BW:72:VAL:HG11  | 1.94                     | 0.49              |
| 55:BW:80:HIS:CG   | 55:BW:81:PRO:HD2   | 2.48                     | 0.49              |
| 1:AA:527:G:C5     | 1:AA:528:C:C5      | 3.01                     | 0.49              |
| 3:AC:133:MET:HB2  | 3:AC:150:VAL:HG21  | 1.94                     | 0.49              |
| 35:BB:1584:U:H2'  | 35:BB:1585:C:H5'   | 1.95                     | 0.48              |
| 35:BB:2776:A:C5   | 35:BB:2782:G:C4    | 3.01                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BB:396:G:C5    | 35:BB:397:U:C5     | 3.00                     | 0.48              |
| 35:BB:974:G:C6    | 35:BB:1186:G:C6    | 3.01                     | 0.48              |
| 54:BU:41:VAL:HG22 | 54:BU:60:LYS:O     | 2.13                     | 0.48              |
| 1:AA:1391:U:H2'   | 1:AA:1392:G:C8     | 2.47                     | 0.48              |
| 35:BB:24:G:C5     | 35:BB:25:U:C4      | 3.01                     | 0.48              |
| 1:AA:795:C:C5     | 1:AA:796:C:C5      | 3.00                     | 0.48              |
| 1:AA:895:G:C6     | 1:AA:896:C:C4      | 3.02                     | 0.48              |
| 35:BB:1351:C:H2'  | 35:BB:1352:U:O4'   | 2.12                     | 0.48              |
| 1:AA:1239:A:H62   | 1:AA:1299:A:H62    | 1.61                     | 0.48              |
| 22:AV:35:G:N2     | 23:AX:18:C:N1      | 2.56                     | 0.48              |
| 35:BB:2234:G:C4   | 35:BB:2235:G:C8    | 3.02                     | 0.48              |
| 35:BB:711:G:C6    | 35:BB:712:G:C5     | 3.01                     | 0.48              |
| 35:BB:976:G:C6    | 35:BB:988:A:C2     | 3.00                     | 0.48              |
| 42:BI:100:ILE:O   | 42:BI:139:VAL:HA   | 2.14                     | 0.48              |
| 42:BI:17:ALA:O    | 42:BI:18:ASN:HB3   | 2.13                     | 0.48              |
| 42:BI:85:ILE:HD12 | 42:BI:87:SER:O     | 2.13                     | 0.48              |
| 1:AA:668:G:H21    | 15:AO:45:HIS:CE1   | 2.31                     | 0.48              |
| 35:BB:2235:G:C6   | 35:BB:2236:U:C4    | 3.01                     | 0.48              |
| 35:BB:82:U:H3     | 35:BB:104:A:H61    | 1.61                     | 0.48              |
| 42:BI:100:ILE:O   | 42:BI:139:VAL:HG13 | 2.13                     | 0.48              |
| 42:BI:79:LEU:HD12 | 42:BI:135:MET:SD   | 2.53                     | 0.48              |
| 44:BK:3:GLN:HA    | 44:BK:24:VAL:HG23  | 1.96                     | 0.48              |
| 1:AA:1118:U:O2    | 1:AA:1118:U:H2'    | 2.14                     | 0.48              |
| 1:AA:1446:A:C3'   | 1:AA:1447:A:H5''   | 2.44                     | 0.48              |
| 35:BB:2123:G:N2   | 35:BB:2176:A:H1'   | 2.29                     | 0.48              |
| 35:BB:2694:G:C6   | 35:BB:2695:U:C4    | 3.01                     | 0.48              |
| 35:BB:827:U:H4'   | 35:BB:828:U:OP2    | 2.14                     | 0.48              |
| 40:BG:53:PRO:HD3  | 40:BG:61:TRP:CH2   | 2.49                     | 0.48              |
| 42:BI:129:GLU:HB3 | 42:BI:133:ARG:NH1  | 2.28                     | 0.48              |
| 46:BM:114:ARG:HG3 | 46:BM:130:PHE:CE1  | 2.49                     | 0.48              |
| 35:BB:460:A:C2    | 35:BB:470:A:C5     | 3.01                     | 0.48              |
| 42:BI:11:GLN:HA   | 42:BI:55:PRO:HA    | 1.96                     | 0.48              |
| 51:BR:5:PHE:HB3   | 51:BR:38:VAL:HA    | 1.96                     | 0.48              |
| 1:AA:842:U:H3'    | 1:AA:843:U:H4'     | 1.94                     | 0.48              |
| 1:AA:967:C:C4     | 1:AA:968:A:C5      | 3.02                     | 0.48              |
| 22:AV:6:C:H2'     | 22:AV:7:G:H8       | 1.78                     | 0.48              |
| 35:BB:1025:G:C5   | 35:BB:1135:C:H1'   | 2.49                     | 0.48              |
| 35:BB:17:G:H2'    | 35:BB:18:U:C6      | 2.49                     | 0.48              |
| 42:BI:19:PRO:HB2  | 42:BI:22:PRO:HD2   | 1.95                     | 0.48              |
| 52:BS:30:SER:H    | 52:BS:33:LEU:HD13  | 1.78                     | 0.48              |
| 1:AA:836:G:C6     | 1:AA:851:G:C6      | 3.02                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:AV:34:G:C2     | 22:AV:35:G:C4      | 3.02                     | 0.48              |
| 44:BK:114:LYS:HD3 | 44:BK:114:LYS:H    | 1.79                     | 0.48              |
| 5:AE:29:ILE:HG21  | 5:AE:53:ARG:HH21   | 1.79                     | 0.47              |
| 42:BI:18:ASN:HB2  | 42:BI:38:CYS:SG    | 2.53                     | 0.47              |
| 53:BT:68:LYS:HG2  | 53:BT:69:ARG:H     | 1.79                     | 0.47              |
| 1:AA:879:C:H2'    | 1:AA:880:C:O4'     | 2.14                     | 0.47              |
| 1:AA:920:U:H2'    | 1:AA:921:U:H6      | 1.79                     | 0.47              |
| 20:AT:66:ILE:O    | 20:AT:67:HIS:CG    | 2.68                     | 0.47              |
| 35:BB:46:G:C6     | 35:BB:180:G:C6     | 3.02                     | 0.47              |
| 35:BB:1878:G:C5   | 35:BB:1879:C:C5    | 3.02                     | 0.47              |
| 35:BB:2132:U:C6   | 35:BB:2132:U:C3'   | 2.95                     | 0.47              |
| 35:BB:2898:U:H2'  | 35:BB:2899:A:C8    | 2.49                     | 0.47              |
| 35:BB:2073:C:H5'' | 36:BC:227:VAL:HG13 | 1.95                     | 0.47              |
| 54:BU:35:VAL:H    | 54:BU:39:ASN:ND2   | 2.10                     | 0.47              |
| 1:AA:691:G:H1     | 11:AK:52:ARG:HH21  | 1.61                     | 0.47              |
| 22:AV:6:C:H2'     | 22:AV:7:G:C8       | 2.49                     | 0.47              |
| 35:BB:273:G:C5    | 35:BB:274:C:C5     | 3.02                     | 0.47              |
| 39:BF:107:VAL:H   | 39:BF:108:PRO:CD   | 2.27                     | 0.47              |
| 42:BI:37:PHE:HB2  | 42:BI:66:PHE:CE2   | 2.49                     | 0.47              |
| 42:BI:75:ALA:O    | 42:BI:79:LEU:HG    | 2.13                     | 0.47              |
| 1:AA:1518:A:H2'   | 1:AA:1519:A:C8     | 2.49                     | 0.47              |
| 35:BB:1268:A:C2   | 35:BB:2013:A:C4    | 3.02                     | 0.47              |
| 35:BB:2684:U:C4   | 35:BB:2685:G:N7    | 2.82                     | 0.47              |
| 42:BI:129:GLU:CB  | 42:BI:133:ARG:HH12 | 2.27                     | 0.47              |
| 42:BI:69:VAL:O    | 42:BI:69:VAL:HG23  | 2.14                     | 0.47              |
| 50:BQ:5:ARG:O     | 50:BQ:8:ILE:HG22   | 2.14                     | 0.47              |
| 1:AA:199:A:H61    | 1:AA:218:U:H3      | 1.61                     | 0.47              |
| 3:AC:88:LYS:HE2   | 3:AC:88:LYS:HA     | 1.95                     | 0.47              |
| 35:BB:308:G:C8    | 35:BB:501:A:H1'    | 2.50                     | 0.47              |
| 42:BI:102:ARG:CG  | 42:BI:141:ASP:HA   | 2.40                     | 0.47              |
| 35:BB:695:G:N2    | 35:BB:696:G:H1'    | 2.30                     | 0.47              |
| 35:BB:890:C:H41   | 35:BB:891:G:H21    | 1.63                     | 0.47              |
| 4:AD:79:ALA:HA    | 4:AD:85:THR:HG21   | 1.96                     | 0.47              |
| 35:BB:1871:A:C8   | 35:BB:1872:A:C5    | 3.03                     | 0.47              |
| 35:BB:43:G:C2     | 35:BB:437:U:C2     | 3.03                     | 0.47              |
| 50:BQ:30:VAL:HG12 | 50:BQ:33:VAL:H     | 1.79                     | 0.47              |
| 6:AF:81:ASN:HD21  | 6:AF:83:ALA:HB3    | 1.80                     | 0.47              |
| 9:AI:10:ARG:H     | 9:AI:80:HIS:HD2    | 1.60                     | 0.47              |
| 35:BB:2064:C:H2'  | 35:BB:2065:C:C6    | 2.50                     | 0.47              |
| 51:BR:11:GLN:O    | 51:BR:12:HIS:CG    | 2.68                     | 0.47              |
| 1:AA:384:G:H2'    | 1:AA:385:C:C6      | 2.49                     | 0.47              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:AA:600:A:H2'   | 1:AA:601:G:C8      | 2.50                     | 0.47              |
| 1:AA:846:G:N3    | 1:AA:846:G:H2'     | 2.29                     | 0.47              |
| 28:B3:22:THR:O   | 28:B3:24:VAL:HG23  | 2.15                     | 0.47              |
| 35:BB:2214:C:C5  | 35:BB:2215:C:C5    | 3.03                     | 0.47              |
| 35:BB:2229:U:H2' | 35:BB:2230:G:C8    | 2.50                     | 0.47              |
| 35:BB:2371:G:C6  | 35:BB:2372:U:C5    | 3.03                     | 0.47              |
| 37:BD:56:LYS:HB2 | 37:BD:59:ARG:HG2   | 1.97                     | 0.47              |
| 42:BI:27:LEU:N   | 42:BI:27:LEU:HD23  | 2.21                     | 0.47              |
| 1:AA:98:A:H2'    | 1:AA:99:C:C6       | 2.49                     | 0.47              |
| 12:AL:67:GLY:HA3 | 12:AL:116:TYR:CE2  | 2.50                     | 0.47              |
| 35:BB:322:A:H3'  | 38:BE:163:ASN:HD21 | 1.80                     | 0.47              |
| 35:BB:338:G:C5   | 35:BB:339:U:C5     | 3.02                     | 0.47              |
| 42:BI:18:ASN:N   | 42:BI:19:PRO:CD    | 2.77                     | 0.47              |
| 1:AA:1004:A:H1'  | 1:AA:1026:G:C6     | 2.50                     | 0.47              |
| 19:AS:15:LEU:O   | 19:AS:18:VAL:HG12  | 2.16                     | 0.47              |
| 35:BB:1437:C:H2' | 35:BB:1438:U:H6    | 1.80                     | 0.47              |
| 42:BI:140:GLU:CD | 42:BI:140:GLU:H    | 2.19                     | 0.47              |
| 1:AA:1323:G:H2'  | 1:AA:1324:A:C8     | 2.50                     | 0.46              |
| 1:AA:171:A:C2    | 1:AA:172:A:C2      | 3.03                     | 0.46              |
| 1:AA:323:U:C5    | 1:AA:324:G:C5      | 3.03                     | 0.46              |
| 31:B6:30:VAL:HA  | 31:B6:33:ARG:HH11  | 1.80                     | 0.46              |
| 35:BB:570:G:C5   | 35:BB:2030:A:C6    | 3.02                     | 0.46              |
| 52:BS:75:PHE:CZ  | 52:BS:104:THR:HG21 | 2.50                     | 0.46              |
| 1:AA:1083:U:C5   | 1:AA:1084:G:C6     | 3.03                     | 0.46              |
| 1:AA:1112:C:C5   | 3:AC:177:LEU:HD12  | 2.50                     | 0.46              |
| 20:AT:46:ALA:HB1 | 20:AT:82:ILE:HG22  | 1.98                     | 0.46              |
| 35:BB:1560:G:C5  | 35:BB:1561:C:C4    | 3.03                     | 0.46              |
| 35:BB:1566:A:C6  | 36:BC:212:TRP:CZ3  | 3.03                     | 0.46              |
| 42:BI:96:LYS:HD3 | 42:BI:138:VAL:HG21 | 1.98                     | 0.46              |
| 35:BB:2292:U:H2' | 35:BB:2293:G:C8    | 2.50                     | 0.46              |
| 35:BB:367:G:C6   | 35:BB:368:A:C5     | 3.04                     | 0.46              |
| 44:BK:11:ALA:HB2 | 44:BK:83:ALA:HB1   | 1.96                     | 0.46              |
| 35:BB:1461:C:C4  | 35:BB:1462:C:C5    | 3.04                     | 0.46              |
| 32:B7:63:TYR:CE2 | 35:BB:242:G:H5''   | 2.51                     | 0.46              |
| 34:BA:75:G:H21   | 55:BW:88:HIS:CD2   | 2.33                     | 0.46              |
| 1:AA:1026:G:C5   | 1:AA:1027:C:C5     | 3.04                     | 0.46              |
| 35:BB:1059:G:H4' | 42:BI:116:MET:HE2  | 1.96                     | 0.46              |
| 50:BQ:56:PHE:HB3 | 50:BQ:60:TRP:CE2   | 2.51                     | 0.46              |
| 1:AA:1390:U:C4   | 1:AA:1391:U:C4     | 3.03                     | 0.46              |
| 1:AA:792:A:C2    | 1:AA:794:A:C4      | 3.03                     | 0.46              |
| 22:AV:26:A:H61   | 22:AV:44:G:H1      | 1.64                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BB:2175:C:C2   | 35:BB:2176:A:C8   | 3.04                     | 0.46              |
| 35:BB:2287:A:C2   | 35:BB:2289:G:C6   | 3.04                     | 0.46              |
| 1:AA:332:G:C5     | 1:AA:333:U:C5     | 3.03                     | 0.46              |
| 1:AA:665:A:C2     | 1:AA:733:G:C8     | 3.04                     | 0.46              |
| 1:AA:978:A:C2     | 1:AA:1319:A:C4    | 3.03                     | 0.46              |
| 35:BB:572:A:C2    | 35:BB:2033:A:C2   | 3.04                     | 0.46              |
| 35:BB:2724:U:H2'  | 35:BB:2725:A:C8   | 2.51                     | 0.46              |
| 35:BB:877:A:C2    | 35:BB:900:A:N6    | 2.84                     | 0.46              |
| 42:BI:23:VAL:HG12 | 42:BI:24:GLY:N    | 2.30                     | 0.46              |
| 53:BT:29:THR:HA   | 53:BT:87:LEU:HG   | 1.97                     | 0.46              |
| 1:AA:1360:A:OP1   | 1:AA:1360:A:C8    | 2.69                     | 0.46              |
| 1:AA:1347:G:C4    | 1:AA:1373:G:C6    | 3.04                     | 0.46              |
| 5:AE:148:SER:HB2  | 5:AE:151:MET:HB2  | 1.97                     | 0.46              |
| 13:AM:79:LEU:HA   | 13:AM:82:LEU:HD12 | 1.96                     | 0.46              |
| 35:BB:1833:C:H2'  | 35:BB:1834:U:H6   | 1.81                     | 0.46              |
| 35:BB:877:A:C5    | 35:BB:901:C:N3    | 2.84                     | 0.46              |
| 42:BI:17:ALA:C    | 42:BI:19:PRO:HD3  | 2.36                     | 0.46              |
| 1:AA:1295:U:H2'   | 1:AA:1296:C:C6    | 2.51                     | 0.46              |
| 35:BB:1803:A:C8   | 35:BB:1804:C:C5   | 3.04                     | 0.46              |
| 36:BC:12:ARG:HA   | 36:BC:15:VAL:HB   | 1.98                     | 0.46              |
| 45:BL:8:PRO:HB3   | 45:BL:13:LYS:H    | 1.79                     | 0.46              |
| 54:BU:45:GLN:HE22 | 54:BU:54:PRO:HD2  | 1.79                     | 0.46              |
| 22:AV:70:C:H2'    | 22:AV:71:C:H5'    | 1.98                     | 0.46              |
| 35:BB:1322:A:H2'  | 35:BB:1323:C:H5'  | 1.97                     | 0.46              |
| 38:BE:3:LEU:O     | 38:BE:4:VAL:HG22  | 2.15                     | 0.46              |
| 40:BG:44:HIS:CG   | 40:BG:45:ALA:N    | 2.84                     | 0.46              |
| 42:BI:23:VAL:HG12 | 42:BI:27:LEU:HD21 | 1.96                     | 0.46              |
| 1:AA:1223:C:H3'   | 1:AA:1224:U:C5'   | 2.46                     | 0.45              |
| 1:AA:1486:G:C6    | 1:AA:1487:G:C6    | 3.03                     | 0.45              |
| 1:AA:966:G:C2     | 22:AV:34:G:H5'    | 2.50                     | 0.45              |
| 22:AV:2:G:C6      | 22:AV:3:G:C5      | 3.04                     | 0.45              |
| 35:BB:2694:G:C5   | 35:BB:2695:U:C5   | 3.04                     | 0.45              |
| 48:BO:31:THR:HG22 | 48:BO:33:ARG:H    | 1.81                     | 0.45              |
| 1:AA:1421:G:C2    | 1:AA:1480:A:C2    | 3.04                     | 0.45              |
| 1:AA:1190:G:OP2   | 3:AC:4:VAL:HG22   | 2.16                     | 0.45              |
| 22:AV:36:G:H2'    | 22:AV:37:G:O4'    | 2.17                     | 0.45              |
| 35:BB:173:A:C5    | 35:BB:174:U:C5    | 3.04                     | 0.45              |
| 35:BB:940:G:H2'   | 35:BB:941:A:C4'   | 2.46                     | 0.45              |
| 43:BJ:93:ILE:HG23 | 43:BJ:97:PRO:HG3  | 1.97                     | 0.45              |
| 1:AA:1055:A:C2    | 1:AA:1056:U:H1'   | 2.52                     | 0.45              |
| 1:AA:519:C:C4     | 1:AA:520:A:C5     | 3.05                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:B7:18:LYS:HG3  | 32:B7:20:GLY:H     | 1.81                     | 0.45              |
| 35:BB:2684:U:C4   | 35:BB:2685:G:C8    | 3.04                     | 0.45              |
| 35:BB:504:A:H4'   | 35:BB:505:A:H5'    | 1.98                     | 0.45              |
| 46:BM:43:ALA:HA   | 46:BM:46:ILE:HG13  | 1.98                     | 0.45              |
| 47:BN:44:LEU:HD23 | 47:BN:113:ILE:HD13 | 1.99                     | 0.45              |
| 1:AA:1148:U:C5    | 1:AA:1149:C:C4     | 3.04                     | 0.45              |
| 1:AA:691:G:N2     | 1:AA:695:A:C8      | 2.85                     | 0.45              |
| 11:AK:79:LYS:HA   | 11:AK:104:PHE:HA   | 1.99                     | 0.45              |
| 35:BB:629:G:C6    | 35:BB:630:G:C5     | 3.04                     | 0.45              |
| 1:AA:1044:A:C5    | 1:AA:1045:C:H1'    | 2.51                     | 0.45              |
| 1:AA:1321:U:OP2   | 1:AA:1321:U:C6     | 2.69                     | 0.45              |
| 7:AG:31:VAL:HG11  | 7:AG:108:ARG:HH12  | 1.80                     | 0.45              |
| 35:BB:1302:A:H5'  | 35:BB:1608:A:OP1   | 2.17                     | 0.45              |
| 35:BB:45:G:H5'    | 35:BB:46:G:H5'     | 1.99                     | 0.45              |
| 1:AA:565:U:H5     | 1:AA:566:G:HO2'    | 1.62                     | 0.45              |
| 7:AG:49:LEU:HB3   | 7:AG:60:ALA:HB1    | 1.98                     | 0.45              |
| 34:BA:48:U:H2'    | 34:BA:49:C:C6      | 2.52                     | 0.45              |
| 35:BB:1054:A:C2   | 35:BB:1106:G:C6    | 3.05                     | 0.45              |
| 35:BB:2637:U:C5   | 35:BB:2638:G:C5    | 3.05                     | 0.45              |
| 42:BI:49:GLU:HB3  | 42:BI:52:LEU:HD12  | 1.97                     | 0.45              |
| 1:AA:1024:G:C5    | 1:AA:1025:U:C4     | 3.05                     | 0.45              |
| 1:AA:455:G:C2     | 1:AA:478:A:C2      | 3.04                     | 0.45              |
| 35:BB:370:G:C5    | 35:BB:424:G:C8     | 3.05                     | 0.45              |
| 37:BD:122:VAL:HA  | 37:BD:127:PHE:H    | 1.82                     | 0.45              |
| 42:BI:78:LEU:HD23 | 42:BI:81:LYS:HE2   | 1.98                     | 0.45              |
| 42:BI:52:LEU:HD13 | 42:BI:81:LYS:NZ    | 2.32                     | 0.45              |
| 35:BB:1021:A:C2   | 35:BB:1023:U:C2    | 3.05                     | 0.45              |
| 35:BB:2199:A:N3   | 35:BB:2199:A:H2'   | 2.31                     | 0.45              |
| 35:BB:541:A:C5    | 35:BB:542:C:C5     | 3.04                     | 0.45              |
| 35:BB:589:U:H2'   | 35:BB:590:A:H8     | 1.81                     | 0.45              |
| 37:BD:157:LYS:HB2 | 43:BJ:80:HIS:CD2   | 2.52                     | 0.45              |
| 42:BI:27:LEU:HB2  | 42:BI:32:VAL:HG21  | 1.98                     | 0.45              |
| 42:BI:46:ASP:HA   | 42:BI:50:LYS:HE2   | 1.99                     | 0.45              |
| 1:AA:257:G:C2     | 1:AA:258:G:C8      | 3.05                     | 0.45              |
| 17:AQ:58:VAL:HG12 | 17:AQ:77:VAL:HA    | 1.99                     | 0.45              |
| 1:AA:1526:G:OP1   | 21:AU:37:TYR:CD2   | 2.70                     | 0.45              |
| 35:BB:1025:G:C4   | 35:BB:1135:C:H1'   | 2.52                     | 0.45              |
| 35:BB:1651:G:C6   | 35:BB:1652:A:C6    | 3.05                     | 0.45              |
| 35:BB:196:A:C2    | 35:BB:805:G:C6     | 3.04                     | 0.45              |
| 35:BB:2809:A:C6   | 35:BB:2810:A:C6    | 3.05                     | 0.45              |
| 35:BB:327:G:C6    | 35:BB:328:U:C4     | 3.05                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BB:822:G:C6     | 35:BB:823:C:C4     | 3.05                     | 0.45              |
| 1:AA:38:G:N1       | 1:AA:397:A:C2      | 2.85                     | 0.45              |
| 13:AM:2:ARG:HA     | 13:AM:8:ILE:HG13   | 1.99                     | 0.45              |
| 35:BB:2116:G:H2'   | 35:BB:2116:G:N3    | 2.31                     | 0.45              |
| 42:BI:126:ARG:NH1  | 42:BI:126:ARG:HB3  | 2.32                     | 0.45              |
| 42:BI:90:GLY:C     | 42:BI:92:PRO:HD3   | 2.38                     | 0.45              |
| 1:AA:527:G:C6      | 1:AA:528:C:C5      | 3.06                     | 0.44              |
| 1:AA:764:C:C2'     | 1:AA:765:G:H5'     | 2.46                     | 0.44              |
| 9:AI:117:LEU:HD13  | 9:AI:121:ARG:HA    | 1.98                     | 0.44              |
| 28:B3:2:VAL:HG22   | 35:BB:2015:A:C2    | 2.51                     | 0.44              |
| 35:BB:748:G:C8     | 35:BB:750:A:C8     | 3.05                     | 0.44              |
| 35:BB:825:A:C6     | 35:BB:826:U:C4     | 3.05                     | 0.44              |
| 35:BB:1501:G:H4'   | 36:BC:94:LEU:HD21  | 1.99                     | 0.44              |
| 37:BD:111:GLY:HA2  | 37:BD:201:LEU:HA   | 1.98                     | 0.44              |
| 37:BD:78:GLY:HA3   | 37:BD:80:TRP:CH2   | 2.52                     | 0.44              |
| 45:BL:121:THR:HB   | 45:BL:123:ARG:HG2  | 1.99                     | 0.44              |
| 1:AA:224:U:H2'     | 1:AA:225:C:C6      | 2.52                     | 0.44              |
| 1:AA:296:U:C4      | 1:AA:297:G:C5      | 3.05                     | 0.44              |
| 35:BB:1659:G:C6    | 35:BB:1660:G:C5    | 3.05                     | 0.44              |
| 35:BB:2259:U:H2'   | 35:BB:2260:C:C6    | 2.52                     | 0.44              |
| 35:BB:1027:A:C2    | 35:BB:2488:G:H5'   | 2.52                     | 0.44              |
| 22:AV:34:G:H2'     | 22:AV:35:G:C8      | 2.52                     | 0.44              |
| 31:B6:19:ARG:NH1   | 35:BB:124:G:C5     | 2.85                     | 0.44              |
| 35:BB:2117:A:C5'   | 35:BB:2148:G:H21   | 2.30                     | 0.44              |
| 35:BB:730:A:C2     | 35:BB:731:C:C6     | 3.05                     | 0.44              |
| 1:AA:468:A:H3'     | 1:AA:469:C:C6      | 2.52                     | 0.44              |
| 1:AA:855:U:C2      | 1:AA:856:C:C5      | 3.06                     | 0.44              |
| 10:AJ:25:ILE:HG21  | 10:AJ:91:ASP:HB2   | 1.99                     | 0.44              |
| 28:B3:28:SER:HB3   | 28:B3:39:ARG:HH21  | 1.82                     | 0.44              |
| 35:BB:2758:A:H2'   | 35:BB:2759:G:H5'   | 1.99                     | 0.44              |
| 35:BB:841:G:C5     | 35:BB:842:U:C5     | 3.05                     | 0.44              |
| 35:BB:919:U:H2'    | 35:BB:920:A:C8     | 2.52                     | 0.44              |
| 42:BI:100:ILE:HG23 | 42:BI:104:GLN:OE1  | 2.17                     | 0.44              |
| 42:BI:138:VAL:HG12 | 42:BI:139:VAL:N    | 2.31                     | 0.44              |
| 31:B6:13:ASN:HD22  | 35:BB:125:A:H1'    | 1.83                     | 0.44              |
| 35:BB:136:G:H2'    | 35:BB:137:U:C6     | 2.52                     | 0.44              |
| 35:BB:2718:G:C6    | 35:BB:2719:G:C5    | 3.05                     | 0.44              |
| 35:BB:2897:U:H2'   | 35:BB:2898:U:C6    | 2.53                     | 0.44              |
| 38:BE:192:ALA:O    | 38:BE:196:VAL:HG23 | 2.18                     | 0.44              |
| 39:BF:109:ARG:O    | 39:BF:110:ILE:HG23 | 2.18                     | 0.44              |
| 54:BU:80:ASP:OD1   | 54:BU:95:PHE:HB3   | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:579:A:C6     | 1:AA:763:G:C6     | 3.05                     | 0.44              |
| 13:AM:15:VAL:HG13 | 13:AM:16:ILE:H    | 1.83                     | 0.44              |
| 22:AV:34:G:C6     | 22:AV:35:G:C6     | 3.05                     | 0.44              |
| 35:BB:2131:U:O2   | 35:BB:2131:U:H3'  | 2.17                     | 0.44              |
| 42:BI:70:THR:O    | 42:BI:70:THR:HG23 | 2.17                     | 0.44              |
| 1:AA:1366:C:C4    | 1:AA:1367:C:C5    | 3.06                     | 0.44              |
| 17:AQ:5:ARG:HD3   | 17:AQ:5:ARG:HA    | 1.83                     | 0.44              |
| 35:BB:1506:U:C2   | 35:BB:1507:C:C5   | 3.06                     | 0.44              |
| 35:BB:2513:A:C6   | 35:BB:2574:G:C6   | 3.05                     | 0.44              |
| 35:BB:2643:G:C5   | 35:BB:2644:G:C5   | 3.06                     | 0.44              |
| 35:BB:780:G:H2'   | 35:BB:782:A:C5    | 2.52                     | 0.44              |
| 42:BI:54:ILE:HD11 | 42:BI:71:LYS:N    | 2.33                     | 0.44              |
| 54:BU:57:ILE:HG13 | 54:BU:57:ILE:H    | 1.59                     | 0.44              |
| 1:AA:1110:A:H3'   | 1:AA:1111:A:C8    | 2.50                     | 0.44              |
| 1:AA:1442:G:C6    | 1:AA:1443:C:C4    | 3.06                     | 0.44              |
| 1:AA:232:G:H1'    | 1:AA:262:A:N1     | 2.33                     | 0.44              |
| 35:BB:1231:U:H2'  | 35:BB:1232:G:H8   | 1.83                     | 0.44              |
| 35:BB:1949:G:C6   | 35:BB:1950:G:C6   | 3.05                     | 0.44              |
| 35:BB:2284:A:C5   | 35:BB:2285:C:C5   | 3.05                     | 0.44              |
| 35:BB:2709:G:C5   | 35:BB:2710:C:C4   | 3.06                     | 0.44              |
| 35:BB:571:U:C4    | 35:BB:575:A:C5    | 3.06                     | 0.44              |
| 1:AA:151:A:C2     | 1:AA:152:A:H1'    | 2.53                     | 0.44              |
| 1:AA:796:C:H4'    | 11:AK:126:ARG:HE  | 1.83                     | 0.44              |
| 3:AC:38:VAL:HG21  | 3:AC:90:VAL:HG13  | 2.00                     | 0.44              |
| 9:AI:35:GLU:CD    | 9:AI:35:GLU:H     | 2.21                     | 0.44              |
| 11:AK:83:VAL:CG1  | 11:AK:85:VAL:HG23 | 2.48                     | 0.44              |
| 35:BB:1144:A:C6   | 35:BB:1145:C:C4   | 3.05                     | 0.44              |
| 35:BB:2870:C:C4   | 35:BB:2871:U:C4   | 3.06                     | 0.44              |
| 42:BI:59:THR:HG23 | 42:BI:59:THR:O    | 2.18                     | 0.44              |
| 42:BI:72:THR:OG1  | 42:BI:73:PRO:HD2  | 2.18                     | 0.44              |
| 53:BT:5:GLU:HA    | 53:BT:8:LEU:HD12  | 2.00                     | 0.44              |
| 1:AA:1144:G:N2    | 1:AA:1146:A:H62   | 2.16                     | 0.43              |
| 1:AA:202:G:N2     | 1:AA:216:U:C2     | 2.86                     | 0.43              |
| 1:AA:21:G:H2'     | 1:AA:22:G:C8      | 2.53                     | 0.43              |
| 1:AA:517:G:H2'    | 1:AA:531:U:C5     | 2.53                     | 0.43              |
| 1:AA:72:A:C6      | 1:AA:73:C:C4      | 3.06                     | 0.43              |
| 39:BF:35:LEU:HG   | 39:BF:90:LEU:HD11 | 2.00                     | 0.43              |
| 1:AA:1088:G:C6    | 1:AA:1089:G:C5    | 3.06                     | 0.43              |
| 1:AA:1170:A:C8    | 1:AA:1171:A:C8    | 3.06                     | 0.43              |
| 35:BB:2327:A:H2'  | 35:BB:2328:A:C8   | 2.53                     | 0.43              |
| 35:BB:773:U:H5'   | 35:BB:774:G:OP2   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:BT:43:ILE:O    | 53:BT:46:ALA:HB3   | 2.18                     | 0.43              |
| 20:AT:13:SER:O    | 20:AT:16:ALA:HB3   | 2.17                     | 0.43              |
| 22:AV:37:G:C2     | 22:AV:38:U:H1'     | 2.53                     | 0.43              |
| 35:BB:1056:G:H5'  | 35:BB:1057:A:H5'   | 2.00                     | 0.43              |
| 35:BB:1054:A:C2   | 35:BB:1106:G:C5    | 3.06                     | 0.43              |
| 35:BB:1707:G:C5   | 35:BB:1756:G:C6    | 3.07                     | 0.43              |
| 35:BB:1893:C:H2'  | 35:BB:1894:C:H5'   | 2.01                     | 0.43              |
| 35:BB:778:G:C5    | 35:BB:779:U:C4     | 3.06                     | 0.43              |
| 42:BI:35:MET:HE3  | 42:BI:39:LYS:HG2   | 2.00                     | 0.43              |
| 49:BP:45:VAL:H    | 49:BP:61:ARG:H     | 1.66                     | 0.43              |
| 1:AA:1027:C:C2    | 1:AA:1035:A:C2     | 3.07                     | 0.43              |
| 35:BB:1138:G:H2'  | 35:BB:1139:G:O4'   | 2.18                     | 0.43              |
| 35:BB:1381:G:C6   | 35:BB:1382:G:C2    | 3.06                     | 0.43              |
| 35:BB:1724:G:C6   | 35:BB:1725:U:C4    | 3.06                     | 0.43              |
| 35:BB:1838:C:C5   | 35:BB:1899:A:C5    | 3.06                     | 0.43              |
| 35:BB:200:U:C5    | 35:BB:201:C:C5     | 3.06                     | 0.43              |
| 35:BB:2104:C:H4'  | 35:BB:2104:C:OP1   | 2.18                     | 0.43              |
| 35:BB:469:G:OP1   | 38:BE:73:ILE:HD11  | 2.18                     | 0.43              |
| 1:AA:1526:G:C5    | 1:AA:1527:U:C5     | 3.06                     | 0.43              |
| 1:AA:872:A:C4     | 1:AA:874:G:C8      | 3.06                     | 0.43              |
| 6:AF:41:ASP:HA    | 6:AF:60:VAL:HA     | 2.00                     | 0.43              |
| 35:BB:1358:G:C2   | 35:BB:1372:U:H5    | 2.36                     | 0.43              |
| 35:BB:2302:U:H2'  | 35:BB:2303:G:C8    | 2.54                     | 0.43              |
| 35:BB:352:A:C2    | 35:BB:353:C:C2     | 3.05                     | 0.43              |
| 1:AA:768:A:OP1    | 1:AA:804:U:H4'     | 2.18                     | 0.43              |
| 1:AA:1108:G:OP1   | 3:AC:175:HIS:CD2   | 2.71                     | 0.43              |
| 35:BB:945:A:C5    | 35:BB:2448:A:C2    | 3.07                     | 0.43              |
| 35:BB:300:A:H1'   | 35:BB:319:G:H1'    | 2.00                     | 0.43              |
| 35:BB:287:G:C2    | 35:BB:354:A:C4     | 3.06                     | 0.43              |
| 38:BE:15:SER:HB2  | 38:BE:18:THR:HB    | 2.01                     | 0.43              |
| 42:BI:21:PRO:HB2  | 42:BI:22:PRO:CD    | 2.42                     | 0.43              |
| 44:BK:71:ARG:H    | 44:BK:105:ARG:HH21 | 1.67                     | 0.43              |
| 1:AA:627:G:C6     | 1:AA:628:G:C5      | 3.07                     | 0.43              |
| 35:BB:2117:A:H5'' | 35:BB:2148:G:H21   | 1.84                     | 0.43              |
| 35:BB:2183:A:H2'  | 35:BB:2184:A:C8    | 2.54                     | 0.43              |
| 35:BB:2648:G:H2'  | 35:BB:2649:C:C6    | 2.54                     | 0.43              |
| 42:BI:112:LYS:HB2 | 42:BI:116:MET:SD   | 2.59                     | 0.43              |
| 43:BJ:32:LEU:HD22 | 43:BJ:122:LEU:HD13 | 2.00                     | 0.43              |
| 1:AA:1249:C:O2    | 9:AI:71:ILE:HD11   | 2.18                     | 0.43              |
| 1:AA:1301:U:C2    | 1:AA:1303:C:C6     | 3.07                     | 0.43              |
| 1:AA:646:G:C4     | 1:AA:647:C:C6      | 3.06                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:825:A:C6     | 1:AA:826:C:C4      | 3.06                     | 0.43              |
| 13:AM:38:ILE:HD13 | 13:AM:51:GLN:HB2   | 2.01                     | 0.43              |
| 14:AN:26:LEU:HD23 | 14:AN:30:ILE:HD12  | 2.00                     | 0.43              |
| 34:BA:9:G:C6      | 34:BA:10:G:C5      | 3.07                     | 0.43              |
| 35:BB:2897:U:C4   | 35:BB:2898:U:C4    | 3.06                     | 0.43              |
| 1:AA:1063:C:H3'   | 1:AA:1064:G:H2'    | 2.01                     | 0.43              |
| 1:AA:246:A:C8     | 1:AA:279:A:C2      | 3.07                     | 0.43              |
| 1:AA:313:A:C6     | 1:AA:314:C:C4      | 3.06                     | 0.43              |
| 1:AA:462:G:H2'    | 1:AA:463:U:H6      | 1.83                     | 0.43              |
| 35:BB:1712:U:C4   | 35:BB:1713:A:C5    | 3.07                     | 0.43              |
| 35:BB:2511:U:H2'  | 35:BB:2512:C:O4'   | 2.19                     | 0.43              |
| 35:BB:303:G:H2'   | 35:BB:304:U:O4'    | 2.17                     | 0.43              |
| 35:BB:77:G:C2     | 35:BB:78:U:C2      | 3.07                     | 0.43              |
| 38:BE:135:ALA:HB1 | 38:BE:139:LYS:NZ   | 2.34                     | 0.43              |
| 1:AA:202:G:H21    | 1:AA:465:A:H61     | 1.67                     | 0.43              |
| 1:AA:751:U:C4     | 1:AA:752:G:C2      | 3.06                     | 0.43              |
| 35:BB:297:G:C6    | 35:BB:298:G:C4     | 3.06                     | 0.43              |
| 35:BB:98:G:N2     | 54:BU:6:ARG:HH22   | 2.16                     | 0.43              |
| 1:AA:1082:A:C5    | 1:AA:1083:U:C4     | 3.07                     | 0.42              |
| 1:AA:1309:G:C6    | 1:AA:1310:G:C5     | 3.07                     | 0.42              |
| 1:AA:473:U:H2'    | 1:AA:474:G:C8      | 2.53                     | 0.42              |
| 1:AA:842:U:H4'    | 1:AA:843:U:OP2     | 2.19                     | 0.42              |
| 35:BB:1726:C:H2'  | 35:BB:1727:C:C6    | 2.53                     | 0.42              |
| 35:BB:2734:A:H2'  | 35:BB:2735:G:H5'   | 2.00                     | 0.42              |
| 38:BE:22:ASP:HA   | 38:BE:114:ARG:HH22 | 1.83                     | 0.42              |
| 39:BF:3:LEU:HD13  | 39:BF:3:LEU:HA     | 1.88                     | 0.42              |
| 42:BI:123:ALA:HA  | 42:BI:126:ARG:NH1  | 2.33                     | 0.42              |
| 42:BI:128:ILE:HA  | 42:BI:131:THR:HG23 | 2.00                     | 0.42              |
| 42:BI:12:VAL:HG13 | 42:BI:41:PHE:CE2   | 2.54                     | 0.42              |
| 1:AA:1133:G:C2    | 1:AA:1142:G:C2     | 3.07                     | 0.42              |
| 1:AA:149:A:N6     | 1:AA:171:A:C8      | 2.87                     | 0.42              |
| 3:AC:13:ILE:HG13  | 3:AC:14:VAL:HG22   | 2.01                     | 0.42              |
| 35:BB:2305:U:H3   | 39:BF:148:VAL:CG1  | 2.32                     | 0.42              |
| 35:BB:712:G:C6    | 35:BB:713:G:C4     | 3.07                     | 0.42              |
| 35:BB:766:U:H2'   | 35:BB:767:U:C6     | 2.54                     | 0.42              |
| 35:BB:890:C:H3'   | 35:BB:891:G:H4'    | 2.01                     | 0.42              |
| 43:BJ:116:ARG:HA  | 43:BJ:119:PHE:CD2  | 2.54                     | 0.42              |
| 1:AA:202:G:H21    | 1:AA:465:A:N6      | 2.18                     | 0.42              |
| 2:AB:143:LEU:HD23 | 2:AB:143:LEU:HA    | 1.98                     | 0.42              |
| 19:AS:62:THR:HG22 | 19:AS:63:ASP:H     | 1.83                     | 0.42              |
| 35:BB:1172:C:H3'  | 35:BB:1173:U:H6    | 1.83                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BB:1880:U:H2'   | 35:BB:1881:C:C6    | 2.54                     | 0.42              |
| 35:BB:2051:A:C5    | 35:BB:2614:A:C5    | 3.07                     | 0.42              |
| 35:BB:1783:A:C2    | 35:BB:2587:A:C5    | 3.08                     | 0.42              |
| 35:BB:664:G:C5     | 35:BB:665:U:C5     | 3.07                     | 0.42              |
| 35:BB:820:A:C2     | 35:BB:821:A:C4     | 3.07                     | 0.42              |
| 35:BB:841:G:C6     | 35:BB:842:U:C4     | 3.07                     | 0.42              |
| 36:BC:206:LYS:HG3  | 36:BC:209:ALA:H    | 1.84                     | 0.42              |
| 1:AA:1130:A:C2     | 1:AA:1146:A:C4     | 3.07                     | 0.42              |
| 1:AA:1225:A:C2     | 1:AA:1226:C:C2     | 3.08                     | 0.42              |
| 1:AA:1332:A:H2'    | 1:AA:1333:A:C8     | 2.54                     | 0.42              |
| 1:AA:59:A:H3'      | 1:AA:60:A:C5'      | 2.49                     | 0.42              |
| 30:B5:37:LYS:HD2   | 35:BB:2130:U:OP2   | 2.19                     | 0.42              |
| 35:BB:1692:U:H2'   | 35:BB:1694:C:C5    | 2.55                     | 0.42              |
| 35:BB:2601:C:H4'   | 35:BB:2602:A:OP2   | 2.18                     | 0.42              |
| 35:BB:536:G:C6     | 35:BB:537:G:C4     | 3.07                     | 0.42              |
| 35:BB:941:A:H2'    | 35:BB:942:G:C8     | 2.55                     | 0.42              |
| 42:BI:72:THR:CG2   | 42:BI:112:LYS:HD2  | 2.50                     | 0.42              |
| 42:BI:73:PRO:HA    | 42:BI:74:PRO:HD3   | 1.92                     | 0.42              |
| 1:AA:673:A:H2'     | 1:AA:674:G:C8      | 2.54                     | 0.42              |
| 32:B7:29:ARG:NE    | 32:B7:29:ARG:HA    | 2.35                     | 0.42              |
| 35:BB:1283:G:H21   | 35:BB:1329:U:H3    | 1.66                     | 0.42              |
| 35:BB:1893:C:C5    | 35:BB:1894:C:C5    | 3.07                     | 0.42              |
| 35:BB:663:G:C5     | 35:BB:664:G:N7     | 2.87                     | 0.42              |
| 39:BF:69:ALA:HB3   | 39:BF:80:GLN:HA    | 2.02                     | 0.42              |
| 42:BI:89:SER:HA    | 42:BI:97:VAL:HG11  | 2.01                     | 0.42              |
| 48:BO:55:GLU:CD    | 48:BO:55:GLU:H     | 2.22                     | 0.42              |
| 1:AA:113:G:H2'     | 1:AA:114:U:C6      | 2.55                     | 0.42              |
| 1:AA:1506:U:H4'    | 11:AK:128:VAL:HG13 | 2.01                     | 0.42              |
| 34:BA:29:A:C2      | 34:BA:30:C:C2      | 3.08                     | 0.42              |
| 35:BB:1737:G:C6    | 35:BB:1738:G:N1    | 2.87                     | 0.42              |
| 35:BB:2241:A:H2'   | 35:BB:2242:G:C8    | 2.55                     | 0.42              |
| 35:BB:2898:U:H2'   | 35:BB:2899:A:H8    | 1.85                     | 0.42              |
| 37:BD:33:ARG:HB2   | 37:BD:94:GLN:H     | 1.85                     | 0.42              |
| 40:BG:87:GLN:HB3   | 40:BG:88:LEU:H     | 1.75                     | 0.42              |
| 42:BI:91:LYS:HD2   | 42:BI:91:LYS:N     | 2.35                     | 0.42              |
| 1:AA:226:G:C6      | 1:AA:227:G:C5      | 3.08                     | 0.42              |
| 35:BB:1681:G:C6    | 35:BB:1762:A:C6    | 3.07                     | 0.42              |
| 35:BB:918:A:C5     | 35:BB:919:U:H1'    | 2.55                     | 0.42              |
| 43:BJ:140:LEU:HD12 | 43:BJ:140:LEU:HA   | 1.95                     | 0.42              |
| 1:AA:448:A:C4      | 1:AA:487:A:C2      | 3.08                     | 0.42              |
| 1:AA:580:C:H2'     | 1:AA:581:G:C8      | 2.55                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:677:U:C4     | 1:AA:678:U:C5      | 3.07                     | 0.42              |
| 1:AA:814:A:H5'    | 1:AA:1511:G:H4'    | 2.01                     | 0.42              |
| 3:AC:174:LEU:HD23 | 3:AC:200:TRP:CE3   | 2.54                     | 0.42              |
| 35:BB:2352:A:H2'  | 35:BB:2353:G:H5'   | 2.00                     | 0.42              |
| 35:BB:883:G:H22   | 35:BB:894:U:H1'    | 1.85                     | 0.42              |
| 38:BE:122:GLU:HA  | 38:BE:189:THR:HG22 | 2.02                     | 0.42              |
| 42:BI:117:THR:O   | 42:BI:118:GLY:C    | 2.58                     | 0.42              |
| 42:BI:129:GLU:O   | 42:BI:133:ARG:HG3  | 2.19                     | 0.42              |
| 11:AK:20:ALA:CB   | 11:AK:81:LEU:HD22  | 2.49                     | 0.42              |
| 35:BB:1037:G:C6   | 35:BB:1038:G:N7    | 2.87                     | 0.42              |
| 35:BB:1067:A:N7   | 35:BB:1068:G:C4    | 2.88                     | 0.42              |
| 35:BB:389:G:H2'   | 35:BB:390:U:H6     | 1.84                     | 0.42              |
| 35:BB:605:G:C5    | 35:BB:606:U:C4     | 3.08                     | 0.42              |
| 35:BB:631:A:C6    | 35:BB:632:A:C6     | 3.08                     | 0.42              |
| 37:BD:67:HIS:CE1  | 37:BD:68:PHE:CE1   | 3.07                     | 0.42              |
| 38:BE:14:VAL:HG21 | 38:BE:193:VAL:HG12 | 2.02                     | 0.42              |
| 42:BI:68:PHE:N    | 42:BI:68:PHE:CD1   | 2.88                     | 0.42              |
| 1:AA:469:C:C5     | 1:AA:470:C:C4      | 3.07                     | 0.42              |
| 1:AA:942:G:C6     | 1:AA:943:U:C4      | 3.08                     | 0.42              |
| 1:AA:429:U:H3'    | 4:AD:8:LEU:HD12    | 2.02                     | 0.42              |
| 25:B0:4:CYS:O     | 25:B0:50:VAL:HA    | 2.19                     | 0.42              |
| 42:BI:131:THR:O   | 42:BI:135:MET:HG3  | 2.20                     | 0.42              |
| 42:BI:54:ILE:O    | 42:BI:54:ILE:HG23  | 2.20                     | 0.42              |
| 42:BI:53:PRO:CG   | 42:BI:77:VAL:HG11  | 2.49                     | 0.42              |
| 1:AA:1250:A:H2'   | 1:AA:1251:A:C8     | 2.55                     | 0.41              |
| 35:BB:1065:U:C5   | 35:BB:1066:U:C4    | 3.08                     | 0.41              |
| 35:BB:1886:U:H2'  | 35:BB:1887:C:C6    | 2.55                     | 0.41              |
| 35:BB:1995:U:H2'  | 35:BB:1996:C:C6    | 2.55                     | 0.41              |
| 35:BB:460:A:C2    | 35:BB:470:A:C4     | 3.08                     | 0.41              |
| 35:BB:722:A:C5    | 35:BB:723:C:C5     | 3.08                     | 0.41              |
| 1:AA:1188:A:H2'   | 1:AA:1189:U:H5'    | 2.02                     | 0.41              |
| 1:AA:1458:G:N1    | 1:AA:1459:G:C5     | 2.88                     | 0.41              |
| 1:AA:439:U:C6     | 1:AA:440:C:C5      | 3.08                     | 0.41              |
| 1:AA:1109:C:OP2   | 3:AC:175:HIS:CD2   | 2.74                     | 0.41              |
| 9:AI:51:LEU:HB2   | 9:AI:56:MET:SD     | 2.60                     | 0.41              |
| 35:BB:1082:U:O4   | 35:BB:1086:A:C2    | 2.73                     | 0.41              |
| 35:BB:1426:G:C6   | 35:BB:1427:A:C6    | 3.09                     | 0.41              |
| 35:BB:1787:A:C4   | 35:BB:1788:C:C5    | 3.08                     | 0.41              |
| 35:BB:2404:U:H2'  | 35:BB:2405:G:O4'   | 2.20                     | 0.41              |
| 35:BB:957:C:H42   | 35:BB:2494:G:H21   | 1.68                     | 0.41              |
| 1:AA:518:C:H2'    | 1:AA:530:G:C8      | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:AI:80:HIS:CE1   | 9:AI:105:ARG:HA   | 2.56                     | 0.41              |
| 17:AQ:61:ARG:HD3  | 17:AQ:75:VAL:HG22 | 2.02                     | 0.41              |
| 22:AV:36:G:N2     | 23:AX:17:C:H1'    | 2.34                     | 0.41              |
| 35:BB:195:A:H5''  | 45:BL:47:ARG:HH11 | 1.85                     | 0.41              |
| 35:BB:2038:G:C6   | 35:BB:2039:U:C4   | 3.08                     | 0.41              |
| 35:BB:2517:C:C2   | 35:BB:2542:A:N6   | 2.89                     | 0.41              |
| 41:BH:89:LYS:HD3  | 41:BH:126:GLY:HA2 | 2.01                     | 0.41              |
| 35:BB:2116:G:H4'  | 35:BB:2146:C:C6   | 2.56                     | 0.41              |
| 35:BB:45:G:C5'    | 35:BB:46:G:H5'    | 2.50                     | 0.41              |
| 1:AA:735:C:H2'    | 1:AA:736:C:H6     | 1.85                     | 0.41              |
| 35:BB:201:C:C5    | 35:BB:202:U:C5    | 3.08                     | 0.41              |
| 35:BB:2391:G:C4   | 35:BB:2424:C:C5   | 3.09                     | 0.41              |
| 35:BB:2627:G:C5   | 35:BB:2628:C:C4   | 3.08                     | 0.41              |
| 35:BB:639:U:H2'   | 35:BB:640:C:C6    | 2.55                     | 0.41              |
| 49:BP:47:ILE:HG23 | 49:BP:96:LEU:H    | 1.85                     | 0.41              |
| 52:BS:66:ILE:HA   | 52:BS:69:LEU:HD12 | 2.02                     | 0.41              |
| 1:AA:555:U:H2'    | 1:AA:556:C:C6     | 2.56                     | 0.41              |
| 6:AF:42:TRP:HB2   | 6:AF:59:TYR:HB2   | 2.03                     | 0.41              |
| 13:AM:84:CYS:HB2  | 19:AS:73:PHE:CE2  | 2.55                     | 0.41              |
| 35:BB:1951:U:C2   | 35:BB:1954:G:C8   | 3.08                     | 0.41              |
| 35:BB:2329:U:H2'  | 35:BB:2330:G:C8   | 2.55                     | 0.41              |
| 35:BB:2351:G:N1   | 35:BB:2365:G:C6   | 2.89                     | 0.41              |
| 35:BB:2731:G:C2   | 35:BB:2732:G:C6   | 3.09                     | 0.41              |
| 35:BB:568:U:O2    | 35:BB:570:G:C8    | 2.74                     | 0.41              |
| 44:BK:32:TYR:HB2  | 44:BK:33:ALA:H    | 1.73                     | 0.41              |
| 1:AA:181:A:H1'    | 1:AA:182:A:C2     | 2.55                     | 0.41              |
| 1:AA:299:G:H2'    | 1:AA:300:A:C8     | 2.55                     | 0.41              |
| 1:AA:592:G:C6     | 1:AA:593:U:C4     | 3.09                     | 0.41              |
| 5:AE:131:ASN:HA   | 5:AE:132:PRO:HD2  | 1.97                     | 0.41              |
| 13:AM:9:PRO:O     | 13:AM:44:ILE:HG21 | 2.20                     | 0.41              |
| 17:AQ:14:ASP:H    | 17:AQ:54:ILE:HD11 | 1.85                     | 0.41              |
| 35:BB:1348:C:C5   | 35:BB:1349:C:C6   | 3.09                     | 0.41              |
| 35:BB:345:A:N3    | 35:BB:346:A:N1    | 2.68                     | 0.41              |
| 35:BB:700:G:C6    | 35:BB:701:G:C5    | 3.08                     | 0.41              |
| 35:BB:945:A:H3'   | 35:BB:946:C:H5''  | 2.03                     | 0.41              |
| 42:BI:45:THR:O    | 42:BI:48:ILE:HG22 | 2.20                     | 0.41              |
| 49:BP:44:GLY:HA3  | 49:BP:60:VAL:HG13 | 2.03                     | 0.41              |
| 35:BB:297:G:H4'   | 54:BU:85:ARG:HE   | 1.86                     | 0.41              |
| 1:AA:208:U:C2     | 1:AA:212:G:N1     | 2.89                     | 0.41              |
| 8:AH:66:GLN:HE22  | 8:AH:68:LYS:HB2   | 1.86                     | 0.41              |
| 22:AV:72:G:C3'    | 22:AV:73:A:H5''   | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:B7:38:LYS:HG2  | 32:B7:42:HIS:CE1  | 2.56                     | 0.41              |
| 35:BB:1662:U:H2'  | 35:BB:1663:G:O4'  | 2.20                     | 0.41              |
| 35:BB:1674:G:H21  | 35:BB:1677:A:H61  | 1.67                     | 0.41              |
| 35:BB:2661:G:H2'  | 35:BB:2662:A:C8   | 2.55                     | 0.41              |
| 35:BB:486:C:H2'   | 35:BB:487:C:H6    | 1.86                     | 0.41              |
| 1:AA:1018:G:H2'   | 1:AA:1019:A:C8    | 2.55                     | 0.41              |
| 14:AN:81:ILE:HG13 | 14:AN:81:ILE:H    | 1.49                     | 0.41              |
| 35:BB:1081:U:H4'  | 42:BI:126:ARG:NH1 | 2.35                     | 0.41              |
| 35:BB:2298:A:C6   | 35:BB:2299:U:C2   | 3.09                     | 0.41              |
| 35:BB:2615:U:C2   | 35:BB:2616:C:C6   | 3.09                     | 0.41              |
| 35:BB:2747:G:H1   | 35:BB:2754:U:H2'  | 1.86                     | 0.41              |
| 35:BB:492:A:H2'   | 35:BB:493:G:O4'   | 2.21                     | 0.41              |
| 35:BB:950:G:C4    | 35:BB:951:C:C6    | 3.09                     | 0.41              |
| 42:BI:41:PHE:CE2  | 42:BI:45:THR:HG21 | 2.55                     | 0.41              |
| 42:BI:56:VAL:CG2  | 42:BI:68:PHE:HB2  | 2.51                     | 0.41              |
| 1:AA:1004:A:H1'   | 1:AA:1026:G:C5    | 2.56                     | 0.41              |
| 1:AA:38:G:C6      | 1:AA:397:A:C2     | 3.09                     | 0.41              |
| 1:AA:486:U:H2'    | 1:AA:487:A:H8     | 1.86                     | 0.41              |
| 1:AA:741:G:N2     | 1:AA:742:G:H1'    | 2.36                     | 0.41              |
| 1:AA:90:C:H2'     | 1:AA:91:U:C6      | 2.56                     | 0.41              |
| 27:B2:33:HIS:CE1  | 27:B2:34:THR:O    | 2.74                     | 0.41              |
| 34:BA:33:G:C2     | 34:BA:50:A:C2     | 3.08                     | 0.41              |
| 35:BB:271:G:C6    | 35:BB:367:G:C6    | 3.09                     | 0.41              |
| 42:BI:10:LEU:HD12 | 42:BI:10:LEU:C    | 2.41                     | 0.41              |
| 42:BI:99:LYS:HB2  | 42:BI:140:GLU:OE1 | 2.20                     | 0.41              |
| 1:AA:1302:C:C2    | 1:AA:1302:C:OP1   | 2.74                     | 0.41              |
| 1:AA:332:G:C4     | 1:AA:333:U:C6     | 3.09                     | 0.41              |
| 1:AA:529:G:H4'    | 1:AA:533:A:C2     | 2.56                     | 0.41              |
| 1:AA:875:U:C4     | 1:AA:876:C:C5     | 3.09                     | 0.41              |
| 7:AG:8:GLN:CD     | 7:AG:9:ARG:H      | 2.24                     | 0.41              |
| 22:AV:7:G:C6      | 22:AV:49:G:C5     | 3.09                     | 0.41              |
| 34:BA:99:A:C5     | 34:BA:100:G:C5    | 3.08                     | 0.41              |
| 35:BB:1515:A:H2'  | 35:BB:1516:G:O4'  | 2.21                     | 0.41              |
| 35:BB:165:A:C2    | 35:BB:166:U:C2    | 3.09                     | 0.41              |
| 35:BB:2266:A:H4'  | 35:BB:2267:A:O5'  | 2.21                     | 0.41              |
| 35:BB:2888:C:H2'  | 35:BB:2889:C:C6   | 2.56                     | 0.41              |
| 35:BB:833:A:H2'   | 35:BB:834:G:C8    | 2.56                     | 0.41              |
| 42:BI:11:GLN:NE2  | 42:BI:74:PRO:HG3  | 2.35                     | 0.41              |
| 51:BR:14:VAL:HG22 | 51:BR:16:GLU:H    | 1.85                     | 0.41              |
| 1:AA:557:G:C6     | 1:AA:558:G:C2     | 3.09                     | 0.40              |
| 1:AA:973:G:H3'    | 1:AA:974:A:H8     | 1.85                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BB:1432:G:H2'  | 35:BB:1433:A:C8   | 2.56                     | 0.40              |
| 35:BB:2063:C:C6   | 35:BB:2064:C:C5   | 3.10                     | 0.40              |
| 35:BB:2235:G:C2   | 35:BB:2236:U:C2   | 3.09                     | 0.40              |
| 35:BB:2547:A:H2'  | 35:BB:2548:U:C6   | 2.56                     | 0.40              |
| 35:BB:2731:G:H5'' | 35:BB:2732:G:OP2  | 2.21                     | 0.40              |
| 35:BB:2:G:C2      | 35:BB:3:U:C2      | 3.09                     | 0.40              |
| 35:BB:339:U:H2'   | 35:BB:340:A:C8    | 2.57                     | 0.40              |
| 35:BB:850:U:H2'   | 35:BB:851:C:C6    | 2.57                     | 0.40              |
| 37:BD:131:ASP:HB2 | 37:BD:139:SER:HB3 | 2.02                     | 0.40              |
| 50:BQ:13:HIS:O    | 50:BQ:17:LEU:HG   | 2.21                     | 0.40              |
| 1:AA:230:G:C6     | 1:AA:231:U:C4     | 3.09                     | 0.40              |
| 1:AA:376:G:C2     | 1:AA:389:A:C2     | 3.08                     | 0.40              |
| 1:AA:404:G:H1     | 1:AA:499:A:H62    | 1.69                     | 0.40              |
| 1:AA:57:G:C6      | 1:AA:58:C:C4      | 3.09                     | 0.40              |
| 4:AD:143:SER:HA   | 4:AD:178:GLU:HA   | 2.04                     | 0.40              |
| 13:AM:78:ARG:HD2  | 19:AS:64:GLU:HG3  | 2.03                     | 0.40              |
| 35:BB:1416:G:C4   | 35:BB:1417:C:C5   | 3.09                     | 0.40              |
| 35:BB:1481:U:H2'  | 35:BB:1482:G:H4'  | 2.03                     | 0.40              |
| 35:BB:341:C:H2'   | 35:BB:342:A:O4'   | 2.21                     | 0.40              |
| 35:BB:670:A:H4'   | 35:BB:671:C:H5'   | 2.02                     | 0.40              |
| 35:BB:811:U:H2'   | 45:BL:21:ARG:HA   | 2.03                     | 0.40              |
| 42:BI:101:SER:OG  | 42:BI:104:GLN:HG3 | 2.21                     | 0.40              |
| 1:AA:908:A:C2     | 1:AA:909:A:C4     | 3.09                     | 0.40              |
| 6:AF:74:LEU:HA    | 6:AF:74:LEU:HD23  | 1.79                     | 0.40              |
| 11:AK:83:VAL:HG12 | 11:AK:85:VAL:HG23 | 2.03                     | 0.40              |
| 35:BB:1171:G:C6   | 35:BB:1172:C:C4   | 3.09                     | 0.40              |
| 35:BB:132:G:O2'   | 35:BB:133:U:H5'   | 2.21                     | 0.40              |
| 35:BB:1378:A:C5   | 35:BB:1380:G:C5   | 3.10                     | 0.40              |
| 35:BB:1759:A:C5   | 35:BB:1760:C:C4   | 3.09                     | 0.40              |
| 35:BB:311:A:O4'   | 35:BB:332:A:C4    | 2.75                     | 0.40              |
| 35:BB:783:A:H2'   | 35:BB:784:G:H4'   | 2.02                     | 0.40              |
| 35:BB:838:C:C5    | 35:BB:941:A:N6    | 2.89                     | 0.40              |
| 36:BC:52:HIS:H    | 36:BC:216:ARG:NH2 | 2.18                     | 0.40              |
| 43:BJ:132:HIS:CD2 | 43:BJ:132:HIS:N   | 2.88                     | 0.40              |
| 51:BR:60:LYS:H    | 51:BR:100:GLY:HA3 | 1.86                     | 0.40              |
| 1:AA:109:A:H3'    | 1:AA:110:C:H5'    | 2.03                     | 0.40              |
| 1:AA:370:C:C2     | 1:AA:371:A:C8     | 3.10                     | 0.40              |
| 2:AB:22:TRP:HA    | 2:AB:188:THR:HG23 | 2.02                     | 0.40              |
| 10:AJ:23:ALA:HA   | 10:AJ:26:VAL:HG12 | 2.02                     | 0.40              |
| 12:AL:53:ARG:HA   | 12:AL:63:THR:HA   | 2.04                     | 0.40              |
| 34:BA:115:A:C2    | 34:BA:116:G:C5    | 3.09                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 35:BB:1499:C:C2  | 35:BB:1500:G:C8   | 3.09                     | 0.40              |
| 35:BB:1684:G:C6  | 35:BB:1685:C:C4   | 3.09                     | 0.40              |
| 35:BB:2051:A:C6  | 35:BB:2614:A:C4   | 3.10                     | 0.40              |
| 35:BB:2702:G:H2' | 35:BB:2703:C:C6   | 2.56                     | 0.40              |
| 35:BB:2729:G:H2' | 35:BB:2730:C:C6   | 2.56                     | 0.40              |
| 35:BB:438:G:C2   | 35:BB:439:A:C4    | 3.10                     | 0.40              |
| 35:BB:1818:U:C4  | 36:BC:152:GLN:HB2 | 2.57                     | 0.40              |
| 1:AA:1261:A:C2   | 1:AA:1262:C:H1'   | 2.57                     | 0.40              |
| 1:AA:175:C:O2    | 1:AA:1447:A:H2    | 2.04                     | 0.40              |
| 1:AA:369:G:C6    | 1:AA:370:C:C4     | 3.10                     | 0.40              |
| 1:AA:496:A:H5'   | 1:AA:497:G:OP2    | 2.22                     | 0.40              |
| 9:AI:83:THR:HA   | 9:AI:97:LEU:HD13  | 2.04                     | 0.40              |
| 22:AV:3:G:C2     | 22:AV:71:C:C2     | 3.08                     | 0.40              |
| 34:BA:24:G:C6    | 34:BA:56:G:C2     | 3.10                     | 0.40              |
| 35:BB:1427:A:H4' | 35:BB:1428:C:O4'  | 2.21                     | 0.40              |
| 35:BB:1445:G:C5  | 35:BB:1446:C:C5   | 3.09                     | 0.40              |
| 35:BB:563:A:C5   | 35:BB:2018:G:C6   | 3.10                     | 0.40              |
| 35:BB:2292:U:H2' | 35:BB:2293:G:H8   | 1.85                     | 0.40              |
| 35:BB:877:A:C6   | 35:BB:901:C:C4    | 3.09                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | AB    | 216/218 (99%) | 159 (74%) | 41 (19%) | 16 (7%)  | 1           | 18 |
| 3   | AC    | 204/206 (99%) | 158 (78%) | 31 (15%) | 15 (7%)  | 1           | 18 |
| 4   | AD    | 203/205 (99%) | 160 (79%) | 34 (17%) | 9 (4%)   | 3           | 29 |
| 5   | AE    | 148/150 (99%) | 110 (74%) | 27 (18%) | 11 (7%)  | 1           | 18 |
| 6   | AF    | 98/100 (98%)  | 73 (74%)  | 18 (18%) | 7 (7%)   | 1           | 19 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 7   | AG    | 148/150 (99%) | 109 (74%) | 33 (22%) | 6 (4%)   | 3           | 30  |
| 8   | AH    | 127/129 (98%) | 94 (74%)  | 27 (21%) | 6 (5%)   | 3           | 28  |
| 9   | AI    | 125/127 (98%) | 99 (79%)  | 21 (17%) | 5 (4%)   | 3           | 31  |
| 10  | AJ    | 96/98 (98%)   | 71 (74%)  | 14 (15%) | 11 (12%) | 0           | 8   |
| 11  | AK    | 115/117 (98%) | 96 (84%)  | 14 (12%) | 5 (4%)   | 3           | 30  |
| 12  | AL    | 121/123 (98%) | 100 (83%) | 12 (10%) | 9 (7%)   | 1           | 18  |
| 13  | AM    | 111/113 (98%) | 80 (72%)  | 19 (17%) | 12 (11%) | 0           | 10  |
| 14  | AN    | 92/96 (96%)   | 57 (62%)  | 22 (24%) | 13 (14%) | 0           | 5   |
| 15  | AO    | 86/88 (98%)   | 73 (85%)  | 11 (13%) | 2 (2%)   | 7           | 43  |
| 16  | AP    | 78/80 (98%)   | 62 (80%)  | 10 (13%) | 6 (8%)   | 1           | 17  |
| 17  | AQ    | 78/80 (98%)   | 65 (83%)  | 7 (9%)   | 6 (8%)   | 1           | 17  |
| 18  | AR    | 53/55 (96%)   | 42 (79%)  | 8 (15%)  | 3 (6%)   | 2           | 24  |
| 19  | AS    | 77/79 (98%)   | 61 (79%)  | 13 (17%) | 3 (4%)   | 3           | 31  |
| 20  | AT    | 83/85 (98%)   | 68 (82%)  | 13 (16%) | 2 (2%)   | 7           | 42  |
| 21  | AU    | 49/51 (96%)   | 41 (84%)  | 5 (10%)  | 3 (6%)   | 2           | 22  |
| 24  | AZ    | 18/20 (90%)   | 16 (89%)  | 1 (6%)   | 1 (6%)   | 2           | 24  |
| 25  | B0    | 75/77 (97%)   | 52 (69%)  | 20 (27%) | 3 (4%)   | 3           | 31  |
| 26  | B1    | 61/63 (97%)   | 45 (74%)  | 14 (23%) | 2 (3%)   | 4           | 36  |
| 27  | B2    | 56/58 (97%)   | 49 (88%)  | 7 (12%)  | 0        | 100         | 100 |
| 28  | B3    | 54/56 (96%)   | 42 (78%)  | 9 (17%)  | 3 (6%)   | 2           | 24  |
| 29  | B4    | 48/50 (96%)   | 39 (81%)  | 7 (15%)  | 2 (4%)   | 3           | 30  |
| 30  | B5    | 232/234 (99%) | 190 (82%) | 37 (16%) | 5 (2%)   | 8           | 44  |
| 31  | B6    | 44/46 (96%)   | 29 (66%)  | 11 (25%) | 4 (9%)   | 1           | 14  |
| 32  | B7    | 62/64 (97%)   | 52 (84%)  | 5 (8%)   | 5 (8%)   | 1           | 16  |
| 33  | B8    | 36/38 (95%)   | 30 (83%)  | 4 (11%)  | 2 (6%)   | 2           | 24  |
| 36  | BC    | 269/271 (99%) | 209 (78%) | 47 (18%) | 13 (5%)  | 2           | 27  |
| 37  | BD    | 207/209 (99%) | 149 (72%) | 37 (18%) | 21 (10%) | 1           | 12  |
| 38  | BE    | 199/201 (99%) | 161 (81%) | 23 (12%) | 15 (8%)  | 1           | 18  |
| 39  | BF    | 176/178 (99%) | 131 (74%) | 26 (15%) | 19 (11%) | 0           | 10  |
| 40  | BG    | 171/176 (97%) | 134 (78%) | 28 (16%) | 9 (5%)   | 2           | 25  |
| 41  | BH    | 147/149 (99%) | 111 (76%) | 31 (21%) | 5 (3%)   | 4           | 35  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 42  | BI    | 139/141 (99%)   | 113 (81%)  | 21 (15%)  | 5 (4%)   | 4           | 34 |
| 43  | BJ    | 140/142 (99%)   | 106 (76%)  | 24 (17%)  | 10 (7%)  | 1           | 19 |
| 44  | BK    | 119/121 (98%)   | 95 (80%)   | 14 (12%)  | 10 (8%)  | 1           | 15 |
| 45  | BL    | 141/143 (99%)   | 115 (82%)  | 16 (11%)  | 10 (7%)  | 1           | 19 |
| 46  | BM    | 134/136 (98%)   | 105 (78%)  | 21 (16%)  | 8 (6%)   | 2           | 22 |
| 47  | BN    | 118/120 (98%)   | 96 (81%)   | 16 (14%)  | 6 (5%)   | 2           | 26 |
| 48  | BO    | 114/116 (98%)   | 98 (86%)   | 14 (12%)  | 2 (2%)   | 10          | 49 |
| 49  | BP    | 112/114 (98%)   | 85 (76%)   | 19 (17%)  | 8 (7%)   | 1           | 19 |
| 50  | BQ    | 115/117 (98%)   | 84 (73%)   | 21 (18%)  | 10 (9%)  | 1           | 15 |
| 51  | BR    | 101/103 (98%)   | 80 (79%)   | 13 (13%)  | 8 (8%)   | 1           | 17 |
| 52  | BS    | 108/110 (98%)   | 76 (70%)   | 21 (19%)  | 11 (10%) | 1           | 11 |
| 53  | BT    | 91/93 (98%)     | 60 (66%)   | 25 (28%)  | 6 (7%)   | 1           | 21 |
| 54  | BU    | 94/102 (92%)    | 71 (76%)   | 16 (17%)  | 7 (7%)   | 1           | 18 |
| 55  | BW    | 92/94 (98%)     | 76 (83%)   | 10 (11%)  | 6 (6%)   | 1           | 21 |
| 56  | BY    | 77/79 (98%)     | 46 (60%)   | 18 (23%)  | 13 (17%) | 0           | 4  |
| All | All   | 5858/5971 (98%) | 4523 (77%) | 956 (16%) | 379 (6%) | 3           | 21 |

All (379) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AC    | 17  | TRP  |
| 3   | AC    | 116 | ALA  |
| 5   | AE    | 11  | GLN  |
| 5   | AE    | 17  | VAL  |
| 9   | AI    | 58  | GLU  |
| 10  | AJ    | 42  | LEU  |
| 10  | AJ    | 57  | VAL  |
| 10  | AJ    | 58  | ASN  |
| 10  | AJ    | 67  | ILE  |
| 10  | AJ    | 92  | LEU  |
| 12  | AL    | 32  | VAL  |
| 13  | AM    | 3   | ILE  |
| 13  | AM    | 104 | ASN  |
| 14  | AN    | 51  | PRO  |
| 14  | AN    | 80  | ARG  |
| 16  | AP    | 25  | ARG  |
| 16  | AP    | 45  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | AQ    | 71  | SER  |
| 18  | AR    | 22  | TYR  |
| 21  | AU    | 32  | ARG  |
| 26  | B1    | 37  | LEU  |
| 30  | B5    | 217 | THR  |
| 30  | B5    | 225 | ASP  |
| 37  | BD    | 31  | ALA  |
| 37  | BD    | 71  | ALA  |
| 37  | BD    | 107 | VAL  |
| 37  | BD    | 152 | PRO  |
| 38  | BE    | 4   | VAL  |
| 38  | BE    | 183 | PHE  |
| 39  | BF    | 101 | ARG  |
| 39  | BF    | 112 | ASP  |
| 40  | BG    | 2   | ARG  |
| 40  | BG    | 100 | ASN  |
| 41  | BH    | 119 | ASN  |
| 42  | BI    | 18  | ASN  |
| 43  | BJ    | 132 | HIS  |
| 43  | BJ    | 140 | LEU  |
| 44  | BK    | 53  | LYS  |
| 44  | BK    | 71  | ARG  |
| 45  | BL    | 29  | LYS  |
| 45  | BL    | 113 | ALA  |
| 47  | BN    | 72  | ASP  |
| 47  | BN    | 119 | SER  |
| 49  | BP    | 25  | VAL  |
| 50  | BQ    | 71  | ASN  |
| 50  | BQ    | 73  | ILE  |
| 50  | BQ    | 87  | VAL  |
| 50  | BQ    | 88  | GLU  |
| 51  | BR    | 42  | ALA  |
| 52  | BS    | 61  | ASN  |
| 52  | BS    | 64  | ALA  |
| 52  | BS    | 76  | VAL  |
| 52  | BS    | 89  | ALA  |
| 53  | BT    | 38  | ALA  |
| 54  | BU    | 98  | ASN  |
| 56  | BY    | 14  | ASP  |
| 56  | BY    | 58  | LEU  |
| 2   | AB    | 22  | TRP  |
| 2   | AB    | 103 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 216 | VAL  |
| 2   | AB    | 218 | ALA  |
| 2   | AB    | 224 | ARG  |
| 3   | AC    | 7   | ASN  |
| 3   | AC    | 53  | ARG  |
| 3   | AC    | 82  | ASP  |
| 3   | AC    | 164 | THR  |
| 4   | AD    | 7   | LYS  |
| 4   | AD    | 36  | ALA  |
| 4   | AD    | 146 | GLU  |
| 5   | AE    | 25  | LYS  |
| 5   | AE    | 44  | ARG  |
| 5   | AE    | 89  | THR  |
| 5   | AE    | 119 | VAL  |
| 6   | AF    | 38  | ARG  |
| 6   | AF    | 63  | ASN  |
| 6   | AF    | 85  | ILE  |
| 7   | AG    | 116 | ALA  |
| 8   | AH    | 82  | LEU  |
| 8   | AH    | 95  | MET  |
| 8   | AH    | 116 | ARG  |
| 10  | AJ    | 17  | LEU  |
| 10  | AJ    | 33  | GLY  |
| 10  | AJ    | 35  | GLN  |
| 10  | AJ    | 85  | ASP  |
| 11  | AK    | 79  | LYS  |
| 12  | AL    | 33  | CYS  |
| 12  | AL    | 46  | SER  |
| 12  | AL    | 54  | VAL  |
| 13  | AM    | 16  | ILE  |
| 13  | AM    | 29  | SER  |
| 13  | AM    | 47  | LEU  |
| 13  | AM    | 87  | GLY  |
| 14  | AN    | 30  | ILE  |
| 14  | AN    | 43  | ALA  |
| 14  | AN    | 45  | LEU  |
| 14  | AN    | 99  | SER  |
| 16  | AP    | 12  | LYS  |
| 16  | AP    | 54  | LEU  |
| 17  | AQ    | 12  | VAL  |
| 21  | AU    | 29  | ALA  |
| 26  | B1    | 2   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | B6    | 15  | SER  |
| 32  | B7    | 30  | HIS  |
| 33  | B8    | 7   | VAL  |
| 36  | BC    | 19  | VAL  |
| 36  | BC    | 35  | LYS  |
| 36  | BC    | 121 | ALA  |
| 36  | BC    | 168 | GLY  |
| 36  | BC    | 177 | SER  |
| 37  | BD    | 74  | GLU  |
| 37  | BD    | 118 | PHE  |
| 37  | BD    | 137 | SER  |
| 37  | BD    | 161 | MET  |
| 37  | BD    | 174 | SER  |
| 38  | BE    | 30  | GLN  |
| 38  | BE    | 116 | ASP  |
| 38  | BE    | 130 | LYS  |
| 39  | BF    | 44  | ALA  |
| 39  | BF    | 84  | ILE  |
| 39  | BF    | 103 | ILE  |
| 39  | BF    | 106 | ALA  |
| 39  | BF    | 145 | VAL  |
| 40  | BG    | 29  | ASN  |
| 40  | BG    | 39  | ALA  |
| 40  | BG    | 94  | ARG  |
| 41  | BH    | 91  | PHE  |
| 43  | BJ    | 47  | HIS  |
| 43  | BJ    | 111 | LYS  |
| 44  | BK    | 112 | PHE  |
| 44  | BK    | 113 | MET  |
| 46  | BM    | 55  | ARG  |
| 46  | BM    | 56  | ALA  |
| 46  | BM    | 67  | VAL  |
| 46  | BM    | 72  | PRO  |
| 46  | BM    | 73  | ILE  |
| 46  | BM    | 122 | ALA  |
| 47  | BN    | 63  | ARG  |
| 49  | BP    | 35  | SER  |
| 49  | BP    | 81  | ASP  |
| 49  | BP    | 105 | LYS  |
| 51  | BR    | 3   | ALA  |
| 51  | BR    | 16  | GLU  |
| 51  | BR    | 27  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | BR    | 53  | PHE  |
| 51  | BR    | 65  | ALA  |
| 52  | BS    | 53  | SER  |
| 53  | BT    | 36  | LYS  |
| 53  | BT    | 73  | ARG  |
| 54  | BU    | 63  | ALA  |
| 54  | BU    | 94  | PHE  |
| 55  | BW    | 44  | HIS  |
| 55  | BW    | 66  | ASP  |
| 56  | BY    | 33  | GLY  |
| 56  | BY    | 69  | GLU  |
| 56  | BY    | 74  | LYS  |
| 56  | BY    | 75  | ASN  |
| 2   | AB    | 63  | LYS  |
| 2   | AB    | 84  | LEU  |
| 3   | AC    | 106 | ARG  |
| 3   | AC    | 126 | ARG  |
| 4   | AD    | 192 | ALA  |
| 6   | AF    | 94  | HIS  |
| 6   | AF    | 99  | ALA  |
| 7   | AG    | 118 | ARG  |
| 7   | AG    | 138 | GLU  |
| 9   | AI    | 9   | GLY  |
| 10  | AJ    | 79  | PRO  |
| 11  | AK    | 101 | ALA  |
| 12  | AL    | 24  | GLU  |
| 12  | AL    | 60  | PHE  |
| 12  | AL    | 90  | PRO  |
| 13  | AM    | 30  | LYS  |
| 13  | AM    | 105 | ALA  |
| 14  | AN    | 52  | ARG  |
| 14  | AN    | 61  | ASN  |
| 17  | AQ    | 49  | ASN  |
| 17  | AQ    | 63  | CYS  |
| 17  | AQ    | 66  | LEU  |
| 18  | AR    | 26  | ALA  |
| 20  | AT    | 47  | GLN  |
| 21  | AU    | 30  | GLU  |
| 25  | B0    | 17  | ARG  |
| 28  | B3    | 49  | ARG  |
| 30  | B5    | 159 | GLY  |
| 30  | B5    | 206 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | B6    | 35  | ARG  |
| 32  | B7    | 49  | VAL  |
| 36  | BC    | 189 | ALA  |
| 36  | BC    | 205 | GLY  |
| 36  | BC    | 240 | GLY  |
| 37  | BD    | 30  | GLU  |
| 37  | BD    | 65  | ALA  |
| 37  | BD    | 175 | LEU  |
| 37  | BD    | 176 | ASP  |
| 37  | BD    | 194 | PRO  |
| 37  | BD    | 207 | VAL  |
| 38  | BE    | 2   | GLU  |
| 38  | BE    | 16  | GLU  |
| 38  | BE    | 45  | ALA  |
| 38  | BE    | 83  | VAL  |
| 38  | BE    | 106 | LYS  |
| 39  | BF    | 59  | ILE  |
| 39  | BF    | 107 | VAL  |
| 39  | BF    | 148 | VAL  |
| 40  | BG    | 136 | ASP  |
| 41  | BH    | 15  | LEU  |
| 42  | BI    | 23  | VAL  |
| 43  | BJ    | 59  | ALA  |
| 43  | BJ    | 71  | ASP  |
| 44  | BK    | 36  | GLY  |
| 44  | BK    | 92  | GLU  |
| 44  | BK    | 120 | PRO  |
| 45  | BL    | 43  | GLY  |
| 45  | BL    | 64  | PHE  |
| 47  | BN    | 42  | LYS  |
| 49  | BP    | 13  | LYS  |
| 50  | BQ    | 9   | ALA  |
| 50  | BQ    | 91  | ARG  |
| 51  | BR    | 98  | ILE  |
| 52  | BS    | 2   | GLU  |
| 52  | BS    | 30  | SER  |
| 52  | BS    | 62  | ASP  |
| 54  | BU    | 85  | ARG  |
| 54  | BU    | 99  | SER  |
| 55  | BW    | 45  | ASP  |
| 55  | BW    | 82  | TYR  |
| 56  | BY    | 40  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 33  | ALA  |
| 2   | AB    | 79  | VAL  |
| 2   | AB    | 156 | LEU  |
| 3   | AC    | 15  | LYS  |
| 3   | AC    | 107 | LYS  |
| 3   | AC    | 111 | ASP  |
| 4   | AD    | 47  | LEU  |
| 4   | AD    | 119 | HIS  |
| 4   | AD    | 147 | LYS  |
| 7   | AG    | 40  | SER  |
| 8   | AH    | 66  | GLN  |
| 8   | AH    | 72  | GLU  |
| 9   | AI    | 12  | LYS  |
| 9   | AI    | 121 | ARG  |
| 12  | AL    | 72  | ASN  |
| 13  | AM    | 7   | ASN  |
| 13  | AM    | 11  | HIS  |
| 13  | AM    | 22  | TYR  |
| 14  | AN    | 62  | ARG  |
| 14  | AN    | 66  | THR  |
| 14  | AN    | 68  | ARG  |
| 15  | AO    | 7   | THR  |
| 17  | AQ    | 5   | ARG  |
| 24  | AZ    | 18  | ALA  |
| 25  | B0    | 32  | LEU  |
| 28  | B3    | 44  | ALA  |
| 29  | B4    | 37  | LYS  |
| 31  | B6    | 33  | ARG  |
| 32  | B7    | 51  | LYS  |
| 36  | BC    | 58  | LYS  |
| 36  | BC    | 112 | GLY  |
| 36  | BC    | 132 | ARG  |
| 37  | BD    | 109 | VAL  |
| 37  | BD    | 151 | THR  |
| 38  | BE    | 96  | VAL  |
| 39  | BF    | 41  | GLU  |
| 39  | BF    | 46  | LYS  |
| 39  | BF    | 78  | ILE  |
| 39  | BF    | 82  | TYR  |
| 40  | BG    | 31  | GLU  |
| 40  | BG    | 175 | LYS  |
| 43  | BJ    | 81  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | BJ    | 84  | ILE  |
| 44  | BK    | 91  | SER  |
| 45  | BL    | 36  | LYS  |
| 45  | BL    | 117 | THR  |
| 45  | BL    | 143 | GLU  |
| 46  | BM    | 61  | GLY  |
| 47  | BN    | 98  | LEU  |
| 47  | BN    | 100 | CYS  |
| 48  | BO    | 16  | ARG  |
| 48  | BO    | 107 | ALA  |
| 49  | BP    | 47  | ILE  |
| 50  | BQ    | 78  | PHE  |
| 52  | BS    | 31  | GLN  |
| 52  | BS    | 41  | LYS  |
| 53  | BT    | 28  | ASN  |
| 54  | BU    | 12  | VAL  |
| 55  | BW    | 10  | LYS  |
| 55  | BW    | 93  | ARG  |
| 56  | BY    | 52  | CYS  |
| 56  | BY    | 61  | LYS  |
| 2   | AB    | 47  | PRO  |
| 2   | AB    | 87  | ASP  |
| 2   | AB    | 132 | GLU  |
| 2   | AB    | 165 | ALA  |
| 3   | AC    | 42  | LEU  |
| 3   | AC    | 128 | MET  |
| 3   | AC    | 175 | HIS  |
| 4   | AD    | 68  | GLU  |
| 4   | AD    | 163 | GLN  |
| 5   | AE    | 131 | ASN  |
| 5   | AE    | 137 | ARG  |
| 6   | AF    | 79  | ARG  |
| 7   | AG    | 114 | SER  |
| 10  | AJ    | 16  | ARG  |
| 12  | AL    | 118 | VAL  |
| 13  | AM    | 65  | GLU  |
| 15  | AO    | 87  | ARG  |
| 19  | AS    | 23  | GLU  |
| 19  | AS    | 31  | ARG  |
| 20  | AT    | 67  | HIS  |
| 25  | B0    | 27  | ARG  |
| 28  | B3    | 20  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | B4    | 33  | LEU  |
| 32  | B7    | 7   | ARG  |
| 32  | B7    | 43  | LEU  |
| 36  | BC    | 203 | VAL  |
| 37  | BD    | 122 | VAL  |
| 37  | BD    | 138 | LEU  |
| 38  | BE    | 164 | LEU  |
| 38  | BE    | 167 | VAL  |
| 39  | BF    | 2   | LYS  |
| 39  | BF    | 27  | VAL  |
| 39  | BF    | 74  | ALA  |
| 39  | BF    | 79  | ARG  |
| 41  | BH    | 123 | ARG  |
| 42  | BI    | 14  | ALA  |
| 43  | BJ    | 52  | ASP  |
| 44  | BK    | 6   | THR  |
| 49  | BP    | 54  | LEU  |
| 49  | BP    | 76  | HIS  |
| 53  | BT    | 21  | SER  |
| 53  | BT    | 70  | HIS  |
| 54  | BU    | 38  | ILE  |
| 2   | AB    | 72  | LYS  |
| 5   | AE    | 110 | MET  |
| 6   | AF    | 80  | PHE  |
| 8   | AH    | 43  | GLY  |
| 9   | AI    | 27  | ILE  |
| 11  | AK    | 125 | LYS  |
| 14  | AN    | 21  | ALA  |
| 14  | AN    | 31  | SER  |
| 16  | AP    | 17  | TYR  |
| 18  | AR    | 35  | SER  |
| 30  | B5    | 55  | SER  |
| 33  | B8    | 16  | ILE  |
| 37  | BD    | 203 | VAL  |
| 39  | BF    | 24  | VAL  |
| 42  | BI    | 2   | LYS  |
| 46  | BM    | 134 | THR  |
| 50  | BQ    | 81  | GLY  |
| 52  | BS    | 72  | THR  |
| 56  | BY    | 35  | ILE  |
| 56  | BY    | 73  | PRO  |
| 2   | AB    | 70  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AC    | 154 | GLY  |
| 5   | AE    | 15  | ILE  |
| 5   | AE    | 118 | GLY  |
| 16  | AP    | 36  | VAL  |
| 37  | BD    | 9   | VAL  |
| 38  | BE    | 89  | PRO  |
| 42  | BI    | 4   | VAL  |
| 43  | BJ    | 96  | ARG  |
| 45  | BL    | 122 | VAL  |
| 11  | AK    | 96  | ILE  |
| 38  | BE    | 82  | GLY  |
| 40  | BG    | 125 | PRO  |
| 45  | BL    | 100 | ILE  |
| 50  | BQ    | 33  | VAL  |
| 56  | BY    | 47  | GLY  |
| 56  | BY    | 50  | VAL  |
| 7   | AG    | 79  | VAL  |
| 11  | AK    | 15  | VAL  |
| 31  | B6    | 44  | VAL  |
| 41  | BH    | 16  | GLY  |
| 19  | AS    | 61  | VAL  |
| 36  | BC    | 125 | PRO  |
| 44  | BK    | 35  | VAL  |
| 45  | BL    | 114 | GLY  |
| 50  | BQ    | 39  | ILE  |
| 51  | BR    | 101 | ILE  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | AB    | 180/180 (100%) | 171 (95%) | 9 (5%)   | 28          | 60 |
| 3   | AC    | 170/170 (100%) | 158 (93%) | 12 (7%)  | 17          | 50 |
| 4   | AD    | 172/172 (100%) | 165 (96%) | 7 (4%)   | 35          | 65 |
| 5   | AE    | 113/113 (100%) | 103 (91%) | 10 (9%)  | 12          | 40 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 6   | AF    | 87/87 (100%)   | 85 (98%)  | 2 (2%)   | 56          | 78  |
| 7   | AG    | 123/123 (100%) | 120 (98%) | 3 (2%)   | 54          | 77  |
| 8   | AH    | 104/104 (100%) | 99 (95%)  | 5 (5%)   | 30          | 62  |
| 9   | AI    | 105/105 (100%) | 100 (95%) | 5 (5%)   | 30          | 62  |
| 10  | AJ    | 86/86 (100%)   | 81 (94%)  | 5 (6%)   | 23          | 56  |
| 11  | AK    | 90/90 (100%)   | 86 (96%)  | 4 (4%)   | 33          | 63  |
| 12  | AL    | 103/103 (100%) | 98 (95%)  | 5 (5%)   | 29          | 61  |
| 13  | AM    | 91/91 (100%)   | 89 (98%)  | 2 (2%)   | 57          | 79  |
| 14  | AN    | 79/79 (100%)   | 76 (96%)  | 3 (4%)   | 38          | 67  |
| 15  | AO    | 76/76 (100%)   | 69 (91%)  | 7 (9%)   | 11          | 38  |
| 16  | AP    | 65/65 (100%)   | 62 (95%)  | 3 (5%)   | 31          | 63  |
| 17  | AQ    | 74/74 (100%)   | 68 (92%)  | 6 (8%)   | 14          | 44  |
| 18  | AR    | 48/48 (100%)   | 44 (92%)  | 4 (8%)   | 13          | 44  |
| 19  | AS    | 70/70 (100%)   | 64 (91%)  | 6 (9%)   | 12          | 42  |
| 20  | AT    | 65/65 (100%)   | 64 (98%)  | 1 (2%)   | 70          | 85  |
| 21  | AU    | 44/44 (100%)   | 38 (86%)  | 6 (14%)  | 4           | 23  |
| 25  | B0    | 67/67 (100%)   | 65 (97%)  | 2 (3%)   | 46          | 72  |
| 26  | B1    | 55/55 (100%)   | 50 (91%)  | 5 (9%)   | 11          | 38  |
| 27  | B2    | 48/48 (100%)   | 47 (98%)  | 1 (2%)   | 59          | 80  |
| 28  | B3    | 47/47 (100%)   | 46 (98%)  | 1 (2%)   | 59          | 80  |
| 29  | B4    | 45/45 (100%)   | 42 (93%)  | 3 (7%)   | 19          | 51  |
| 30  | B5    | 181/181 (100%) | 175 (97%) | 6 (3%)   | 43          | 70  |
| 31  | B6    | 38/38 (100%)   | 33 (87%)  | 5 (13%)  | 5           | 24  |
| 32  | B7    | 51/51 (100%)   | 48 (94%)  | 3 (6%)   | 23          | 56  |
| 33  | B8    | 34/34 (100%)   | 34 (100%) | 0        | 100         | 100 |
| 36  | BC    | 216/216 (100%) | 204 (94%) | 12 (6%)  | 25          | 57  |
| 37  | BD    | 164/164 (100%) | 146 (89%) | 18 (11%) | 7           | 30  |
| 38  | BE    | 165/165 (100%) | 157 (95%) | 8 (5%)   | 30          | 62  |
| 39  | BF    | 149/149 (100%) | 143 (96%) | 6 (4%)   | 36          | 65  |
| 40  | BG    | 136/137 (99%)  | 125 (92%) | 11 (8%)  | 14          | 44  |
| 41  | BH    | 114/114 (100%) | 110 (96%) | 4 (4%)   | 41          | 69  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 42  | BI    | 109/109 (100%)   | 104 (95%)  | 5 (5%)   | 31          | 63 |
| 43  | BJ    | 116/116 (100%)   | 112 (97%)  | 4 (3%)   | 42          | 70 |
| 44  | BK    | 102/102 (100%)   | 92 (90%)   | 10 (10%) | 9           | 34 |
| 45  | BL    | 102/102 (100%)   | 98 (96%)   | 4 (4%)   | 37          | 66 |
| 46  | BM    | 109/109 (100%)   | 104 (95%)  | 5 (5%)   | 31          | 63 |
| 47  | BN    | 100/100 (100%)   | 96 (96%)   | 4 (4%)   | 36          | 65 |
| 48  | BO    | 86/86 (100%)     | 84 (98%)   | 2 (2%)   | 56          | 78 |
| 49  | BP    | 99/99 (100%)     | 96 (97%)   | 3 (3%)   | 46          | 72 |
| 50  | BQ    | 89/89 (100%)     | 83 (93%)   | 6 (7%)   | 19          | 51 |
| 51  | BR    | 84/84 (100%)     | 76 (90%)   | 8 (10%)  | 10          | 36 |
| 52  | BS    | 93/93 (100%)     | 87 (94%)   | 6 (6%)   | 20          | 53 |
| 53  | BT    | 80/80 (100%)     | 68 (85%)   | 12 (15%) | 3           | 20 |
| 54  | BU    | 81/83 (98%)      | 76 (94%)   | 5 (6%)   | 21          | 54 |
| 55  | BW    | 78/78 (100%)     | 73 (94%)   | 5 (6%)   | 20          | 53 |
| 56  | BY    | 59/59 (100%)     | 54 (92%)   | 5 (8%)   | 12          | 43 |
| All | All   | 4842/4845 (100%) | 4568 (94%) | 274 (6%) | 28          | 57 |

All (274) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 17  | HIS  |
| 2   | AB    | 38  | HIS  |
| 2   | AB    | 72  | LYS  |
| 2   | AB    | 81  | ASP  |
| 2   | AB    | 101 | THR  |
| 2   | AB    | 103 | TRP  |
| 2   | AB    | 104 | LYS  |
| 2   | AB    | 174 | GLU  |
| 2   | AB    | 186 | VAL  |
| 3   | AC    | 14  | VAL  |
| 3   | AC    | 25  | THR  |
| 3   | AC    | 27  | GLU  |
| 3   | AC    | 38  | VAL  |
| 3   | AC    | 44  | LYS  |
| 3   | AC    | 83  | VAL  |
| 3   | AC    | 106 | ARG  |
| 3   | AC    | 133 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AC    | 164 | THR  |
| 3   | AC    | 168 | ARG  |
| 3   | AC    | 171 | ARG  |
| 3   | AC    | 174 | LEU  |
| 4   | AD    | 34  | GLU  |
| 4   | AD    | 43  | ARG  |
| 4   | AD    | 71  | PHE  |
| 4   | AD    | 110 | ARG  |
| 4   | AD    | 136 | VAL  |
| 4   | AD    | 170 | LEU  |
| 4   | AD    | 198 | LEU  |
| 5   | AE    | 14  | LEU  |
| 5   | AE    | 70  | MET  |
| 5   | AE    | 85  | LYS  |
| 5   | AE    | 96  | GLN  |
| 5   | AE    | 100 | GLU  |
| 5   | AE    | 110 | MET  |
| 5   | AE    | 121 | ASN  |
| 5   | AE    | 137 | ARG  |
| 5   | AE    | 146 | MET  |
| 5   | AE    | 150 | GLU  |
| 6   | AF    | 55  | HIS  |
| 6   | AF    | 91  | ARG  |
| 7   | AG    | 2   | ARG  |
| 7   | AG    | 8   | GLN  |
| 7   | AG    | 135 | LYS  |
| 8   | AH    | 28  | SER  |
| 8   | AH    | 41  | GLU  |
| 8   | AH    | 65  | PHE  |
| 8   | AH    | 75  | GLN  |
| 8   | AH    | 117 | GLN  |
| 9   | AI    | 11  | ARG  |
| 9   | AI    | 35  | GLU  |
| 9   | AI    | 44  | ARG  |
| 9   | AI    | 60  | LEU  |
| 9   | AI    | 90  | ASP  |
| 10  | AJ    | 5   | ARG  |
| 10  | AJ    | 50  | THR  |
| 10  | AJ    | 56  | HIS  |
| 10  | AJ    | 73  | LEU  |
| 10  | AJ    | 75  | ASP  |
| 11  | AK    | 75  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | AK    | 90  | PRO  |
| 11  | AK    | 93  | GLU  |
| 11  | AK    | 122 | PRO  |
| 12  | AL    | 29  | LYS  |
| 12  | AL    | 50  | LYS  |
| 12  | AL    | 54  | VAL  |
| 12  | AL    | 93  | ARG  |
| 12  | AL    | 115 | LYS  |
| 13  | AM    | 18  | LEU  |
| 13  | AM    | 91  | ARG  |
| 14  | AN    | 23  | ARG  |
| 14  | AN    | 81  | ILE  |
| 14  | AN    | 88  | MET  |
| 15  | AO    | 2   | LEU  |
| 15  | AO    | 46  | LYS  |
| 15  | AO    | 63  | ARG  |
| 15  | AO    | 72  | LYS  |
| 15  | AO    | 76  | ARG  |
| 15  | AO    | 77  | TYR  |
| 15  | AO    | 88  | ARG  |
| 16  | AP    | 34  | GLU  |
| 16  | AP    | 59  | HIS  |
| 16  | AP    | 67  | ILE  |
| 17  | AQ    | 7   | LEU  |
| 17  | AQ    | 51  | GLU  |
| 17  | AQ    | 56  | ASP  |
| 17  | AQ    | 66  | LEU  |
| 17  | AQ    | 73  | THR  |
| 17  | AQ    | 76  | ARG  |
| 18  | AR    | 19  | GLU  |
| 18  | AR    | 52  | ARG  |
| 18  | AR    | 65  | SER  |
| 18  | AR    | 72  | ARG  |
| 19  | AS    | 9   | PHE  |
| 19  | AS    | 11  | ASP  |
| 19  | AS    | 22  | VAL  |
| 19  | AS    | 23  | GLU  |
| 19  | AS    | 52  | ASN  |
| 19  | AS    | 60  | PHE  |
| 20  | AT    | 55  | PRO  |
| 21  | AU    | 3   | ILE  |
| 21  | AU    | 7   | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AU    | 8   | ASN  |
| 21  | AU    | 16  | ARG  |
| 21  | AU    | 30  | GLU  |
| 21  | AU    | 53  | LYS  |
| 25  | B0    | 26  | ARG  |
| 25  | B0    | 47  | THR  |
| 26  | B1    | 9   | LYS  |
| 26  | B1    | 10  | SER  |
| 26  | B1    | 15  | ASN  |
| 26  | B1    | 50  | VAL  |
| 26  | B1    | 57  | LEU  |
| 27  | B2    | 3   | THR  |
| 28  | B3    | 51  | ARG  |
| 29  | B4    | 11  | VAL  |
| 29  | B4    | 32  | LYS  |
| 29  | B4    | 45  | HIS  |
| 30  | B5    | 44  | VAL  |
| 30  | B5    | 56  | ASP  |
| 30  | B5    | 166 | ASP  |
| 30  | B5    | 174 | THR  |
| 30  | B5    | 180 | PHE  |
| 30  | B5    | 213 | SER  |
| 31  | B6    | 5   | PHE  |
| 31  | B6    | 15  | SER  |
| 31  | B6    | 22  | MET  |
| 31  | B6    | 26  | ASN  |
| 31  | B6    | 34  | ARG  |
| 32  | B7    | 15  | LYS  |
| 32  | B7    | 27  | ASN  |
| 32  | B7    | 53  | ASP  |
| 36  | BC    | 10  | PRO  |
| 36  | BC    | 13  | ARG  |
| 36  | BC    | 25  | LYS  |
| 36  | BC    | 58  | LYS  |
| 36  | BC    | 120 | ASP  |
| 36  | BC    | 129 | LEU  |
| 36  | BC    | 140 | VAL  |
| 36  | BC    | 162 | GLN  |
| 36  | BC    | 164 | VAL  |
| 36  | BC    | 173 | LEU  |
| 36  | BC    | 212 | TRP  |
| 36  | BC    | 227 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | BD    | 2   | ILE  |
| 37  | BD    | 17  | GLU  |
| 37  | BD    | 30  | GLU  |
| 37  | BD    | 33  | ARG  |
| 37  | BD    | 35  | THR  |
| 37  | BD    | 45  | TYR  |
| 37  | BD    | 46  | ARG  |
| 37  | BD    | 60  | VAL  |
| 37  | BD    | 74  | GLU  |
| 37  | BD    | 84  | LEU  |
| 37  | BD    | 105 | LYS  |
| 37  | BD    | 130 | GLN  |
| 37  | BD    | 149 | ASN  |
| 37  | BD    | 151 | THR  |
| 37  | BD    | 161 | MET  |
| 37  | BD    | 183 | GLU  |
| 37  | BD    | 197 | THR  |
| 37  | BD    | 201 | LEU  |
| 38  | BE    | 1   | MET  |
| 38  | BE    | 60  | TRP  |
| 38  | BE    | 79  | ARG  |
| 38  | BE    | 89  | PRO  |
| 38  | BE    | 134 | LEU  |
| 38  | BE    | 173 | THR  |
| 38  | BE    | 176 | ASP  |
| 38  | BE    | 185 | LYS  |
| 39  | BF    | 3   | LEU  |
| 39  | BF    | 55  | ASP  |
| 39  | BF    | 111 | ARG  |
| 39  | BF    | 129 | MET  |
| 39  | BF    | 135 | ILE  |
| 39  | BF    | 151 | LEU  |
| 40  | BG    | 21  | GLN  |
| 40  | BG    | 23  | ILE  |
| 40  | BG    | 25  | ILE  |
| 40  | BG    | 34  | ARG  |
| 40  | BG    | 36  | LEU  |
| 40  | BG    | 38  | ASP  |
| 40  | BG    | 72  | ASN  |
| 40  | BG    | 88  | LEU  |
| 40  | BG    | 123 | GLU  |
| 40  | BG    | 154 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | BG    | 167 | VAL  |
| 41  | BH    | 12  | LEU  |
| 41  | BH    | 68  | ARG  |
| 41  | BH    | 97  | ARG  |
| 41  | BH    | 144 | VAL  |
| 42  | BI    | 54  | ILE  |
| 42  | BI    | 91  | LYS  |
| 42  | BI    | 99  | LYS  |
| 42  | BI    | 121 | ILE  |
| 42  | BI    | 140 | GLU  |
| 43  | BJ    | 52  | ASP  |
| 43  | BJ    | 124 | VAL  |
| 43  | BJ    | 132 | HIS  |
| 43  | BJ    | 135 | GLN  |
| 44  | BK    | 6   | THR  |
| 44  | BK    | 41  | ILE  |
| 44  | BK    | 49  | ARG  |
| 44  | BK    | 57  | VAL  |
| 44  | BK    | 61  | VAL  |
| 44  | BK    | 69  | VAL  |
| 44  | BK    | 71  | ARG  |
| 44  | BK    | 80  | ASP  |
| 44  | BK    | 89  | ASN  |
| 44  | BK    | 114 | LYS  |
| 45  | BL    | 3   | LEU  |
| 45  | BL    | 6   | LEU  |
| 45  | BL    | 51  | GLU  |
| 45  | BL    | 73  | ILE  |
| 46  | BM    | 22  | GLN  |
| 46  | BM    | 60  | GLN  |
| 46  | BM    | 66  | ARG  |
| 46  | BM    | 70  | ASP  |
| 46  | BM    | 71  | LYS  |
| 47  | BN    | 50  | PRO  |
| 47  | BN    | 85  | PRO  |
| 47  | BN    | 99  | LYS  |
| 47  | BN    | 112 | TYR  |
| 48  | BO    | 48  | LEU  |
| 48  | BO    | 69  | ASP  |
| 49  | BP    | 13  | LYS  |
| 49  | BP    | 42  | PHE  |
| 49  | BP    | 88  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | BQ    | 14  | LYS  |
| 50  | BQ    | 18  | LYS  |
| 50  | BQ    | 33  | VAL  |
| 50  | BQ    | 38  | VAL  |
| 50  | BQ    | 40  | LYS  |
| 50  | BQ    | 99  | VAL  |
| 51  | BR    | 13  | ARG  |
| 51  | BR    | 21  | ARG  |
| 51  | BR    | 22  | LEU  |
| 51  | BR    | 64  | VAL  |
| 51  | BR    | 72  | VAL  |
| 51  | BR    | 78  | ARG  |
| 51  | BR    | 80  | ARG  |
| 51  | BR    | 86  | GLN  |
| 52  | BS    | 7   | HIS  |
| 52  | BS    | 20  | VAL  |
| 52  | BS    | 22  | ASP  |
| 52  | BS    | 31  | GLN  |
| 52  | BS    | 48  | LYS  |
| 52  | BS    | 82  | MET  |
| 53  | BT    | 3   | ARG  |
| 53  | BT    | 5   | GLU  |
| 53  | BT    | 7   | LEU  |
| 53  | BT    | 16  | VAL  |
| 53  | BT    | 29  | THR  |
| 53  | BT    | 32  | LEU  |
| 53  | BT    | 34  | VAL  |
| 53  | BT    | 61  | LEU  |
| 53  | BT    | 72  | GLN  |
| 53  | BT    | 86  | THR  |
| 53  | BT    | 91  | GLN  |
| 53  | BT    | 92  | ASN  |
| 54  | BU    | 3   | LYS  |
| 54  | BU    | 14  | THR  |
| 54  | BU    | 81  | ARG  |
| 54  | BU    | 85  | ARG  |
| 54  | BU    | 98  | ASN  |
| 55  | BW    | 1   | MET  |
| 55  | BW    | 29  | ILE  |
| 55  | BW    | 42  | LEU  |
| 55  | BW    | 68  | LYS  |
| 55  | BW    | 75  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | BY    | 19  | ARG  |
| 56  | BY    | 25  | PHE  |
| 56  | BY    | 34  | SER  |
| 56  | BY    | 35  | ILE  |
| 56  | BY    | 65  | LYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 17  | HIS  |
| 2   | AB    | 92  | ASN  |
| 2   | AB    | 167 | HIS  |
| 2   | AB    | 189 | ASN  |
| 3   | AC    | 139 | ASN  |
| 3   | AC    | 175 | HIS  |
| 4   | AD    | 88  | ASN  |
| 5   | AE    | 88  | HIS  |
| 5   | AE    | 96  | GLN  |
| 5   | AE    | 120 | HIS  |
| 5   | AE    | 134 | ASN  |
| 5   | AE    | 147 | ASN  |
| 6   | AF    | 3   | HIS  |
| 6   | AF    | 37  | HIS  |
| 6   | AF    | 68  | GLN  |
| 6   | AF    | 81  | ASN  |
| 8   | AH    | 66  | GLN  |
| 8   | AH    | 117 | GLN  |
| 9   | AI    | 80  | HIS  |
| 9   | AI    | 125 | GLN  |
| 11  | AK    | 23  | HIS  |
| 13  | AM    | 99  | GLN  |
| 14  | AN    | 65  | GLN  |
| 15  | AO    | 41  | HIS  |
| 15  | AO    | 45  | HIS  |
| 15  | AO    | 50  | HIS  |
| 16  | AP    | 59  | HIS  |
| 17  | AQ    | 46  | HIS  |
| 19  | AS    | 55  | GLN  |
| 20  | AT    | 19  | HIS  |
| 20  | AT    | 67  | HIS  |
| 25  | B0    | 15  | ASN  |
| 25  | B0    | 16  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | B0    | 35  | HIS  |
| 26  | B1    | 36  | GLN  |
| 26  | B1    | 41  | HIS  |
| 27  | B2    | 33  | HIS  |
| 28  | B3    | 41  | HIS  |
| 29  | B4    | 18  | HIS  |
| 29  | B4    | 45  | HIS  |
| 30  | B5    | 103 | GLN  |
| 30  | B5    | 129 | GLN  |
| 31  | B6    | 6   | GLN  |
| 32  | B7    | 25  | HIS  |
| 32  | B7    | 42  | HIS  |
| 36  | BC    | 141 | HIS  |
| 36  | BC    | 225 | ASN  |
| 37  | BD    | 32  | ASN  |
| 37  | BD    | 67  | HIS  |
| 38  | BE    | 92  | HIS  |
| 38  | BE    | 163 | ASN  |
| 38  | BE    | 165 | HIS  |
| 39  | BF    | 134 | GLN  |
| 40  | BG    | 103 | ASN  |
| 42  | BI    | 11  | GLN  |
| 42  | BI    | 33  | ASN  |
| 42  | BI    | 93  | ASN  |
| 43  | BJ    | 40  | HIS  |
| 43  | BJ    | 77  | HIS  |
| 43  | BJ    | 80  | HIS  |
| 43  | BJ    | 132 | HIS  |
| 44  | BK    | 29  | HIS  |
| 44  | BK    | 89  | ASN  |
| 47  | BN    | 16  | HIS  |
| 47  | BN    | 31  | HIS  |
| 49  | BP    | 76  | HIS  |
| 50  | BQ    | 13  | HIS  |
| 50  | BQ    | 36  | GLN  |
| 51  | BR    | 66  | HIS  |
| 51  | BR    | 87  | GLN  |
| 51  | BR    | 89  | HIS  |
| 51  | BR    | 91  | GLN  |
| 52  | BS    | 61  | ASN  |
| 52  | BS    | 102 | HIS  |
| 53  | BT    | 15  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | BU    | 39  | ASN  |
| 54  | BU    | 45  | GLN  |
| 54  | BU    | 98  | ASN  |
| 55  | BW    | 44  | HIS  |
| 55  | BW    | 88  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1529/1530 (99%) | 269 (17%)         | 34 (2%)         |
| 22  | AV    | 76/77 (98%)     | 15 (19%)          | 0               |
| 23  | AX    | 10/11 (90%)     | 8 (80%)           | 0               |
| 34  | BA    | 112/117 (95%)   | 16 (14%)          | 2 (1%)          |
| 35  | BB    | 2902/2903 (99%) | 471 (16%)         | 56 (1%)         |
| All | All   | 4629/4638 (99%) | 779 (16%)         | 92 (1%)         |

All (779) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 7   | A    |
| 1   | AA    | 9   | G    |
| 1   | AA    | 15  | G    |
| 1   | AA    | 31  | G    |
| 1   | AA    | 32  | A    |
| 1   | AA    | 39  | G    |
| 1   | AA    | 47  | C    |
| 1   | AA    | 48  | C    |
| 1   | AA    | 50  | A    |
| 1   | AA    | 51  | A    |
| 1   | AA    | 52  | C    |
| 1   | AA    | 55  | A    |
| 1   | AA    | 60  | A    |
| 1   | AA    | 61  | G    |
| 1   | AA    | 67  | C    |
| 1   | AA    | 70  | U    |
| 1   | AA    | 71  | A    |
| 1   | AA    | 75  | G    |
| 1   | AA    | 79  | G    |
| 1   | AA    | 80  | A    |
| 1   | AA    | 83  | C    |
| 1   | AA    | 84  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 85  | U    |
| 1   | AA    | 86  | G    |
| 1   | AA    | 88  | U    |
| 1   | AA    | 91  | U    |
| 1   | AA    | 101 | A    |
| 1   | AA    | 130 | A    |
| 1   | AA    | 144 | G    |
| 1   | AA    | 149 | A    |
| 1   | AA    | 155 | A    |
| 1   | AA    | 182 | A    |
| 1   | AA    | 197 | A    |
| 1   | AA    | 204 | G    |
| 1   | AA    | 205 | A    |
| 1   | AA    | 209 | U    |
| 1   | AA    | 210 | C    |
| 1   | AA    | 211 | G    |
| 1   | AA    | 239 | U    |
| 1   | AA    | 240 | G    |
| 1   | AA    | 243 | A    |
| 1   | AA    | 244 | U    |
| 1   | AA    | 245 | U    |
| 1   | AA    | 247 | G    |
| 1   | AA    | 252 | U    |
| 1   | AA    | 253 | A    |
| 1   | AA    | 257 | G    |
| 1   | AA    | 258 | G    |
| 1   | AA    | 266 | G    |
| 1   | AA    | 267 | C    |
| 1   | AA    | 280 | C    |
| 1   | AA    | 289 | G    |
| 1   | AA    | 306 | A    |
| 1   | AA    | 308 | C    |
| 1   | AA    | 328 | C    |
| 1   | AA    | 329 | A    |
| 1   | AA    | 332 | G    |
| 1   | AA    | 345 | C    |
| 1   | AA    | 352 | C    |
| 1   | AA    | 354 | G    |
| 1   | AA    | 367 | U    |
| 1   | AA    | 373 | A    |
| 1   | AA    | 374 | A    |
| 1   | AA    | 382 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 397 | A    |
| 1   | AA    | 398 | U    |
| 1   | AA    | 406 | G    |
| 1   | AA    | 408 | A    |
| 1   | AA    | 409 | U    |
| 1   | AA    | 411 | A    |
| 1   | AA    | 412 | A    |
| 1   | AA    | 413 | G    |
| 1   | AA    | 414 | A    |
| 1   | AA    | 416 | G    |
| 1   | AA    | 424 | G    |
| 1   | AA    | 429 | U    |
| 1   | AA    | 430 | A    |
| 1   | AA    | 435 | A    |
| 1   | AA    | 438 | U    |
| 1   | AA    | 451 | A    |
| 1   | AA    | 453 | G    |
| 1   | AA    | 456 | A    |
| 1   | AA    | 459 | A    |
| 1   | AA    | 460 | A    |
| 1   | AA    | 461 | A    |
| 1   | AA    | 462 | G    |
| 1   | AA    | 463 | U    |
| 1   | AA    | 465 | A    |
| 1   | AA    | 466 | A    |
| 1   | AA    | 468 | A    |
| 1   | AA    | 471 | U    |
| 1   | AA    | 482 | A    |
| 1   | AA    | 484 | G    |
| 1   | AA    | 485 | U    |
| 1   | AA    | 486 | U    |
| 1   | AA    | 493 | A    |
| 1   | AA    | 499 | A    |
| 1   | AA    | 508 | U    |
| 1   | AA    | 511 | C    |
| 1   | AA    | 512 | U    |
| 1   | AA    | 518 | C    |
| 1   | AA    | 524 | G    |
| 1   | AA    | 527 | G    |
| 1   | AA    | 533 | A    |
| 1   | AA    | 547 | A    |
| 1   | AA    | 562 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 563 | A    |
| 1   | AA    | 572 | A    |
| 1   | AA    | 573 | A    |
| 1   | AA    | 575 | G    |
| 1   | AA    | 576 | C    |
| 1   | AA    | 577 | G    |
| 1   | AA    | 596 | A    |
| 1   | AA    | 631 | C    |
| 1   | AA    | 632 | U    |
| 1   | AA    | 633 | G    |
| 1   | AA    | 653 | U    |
| 1   | AA    | 665 | A    |
| 1   | AA    | 666 | G    |
| 1   | AA    | 700 | G    |
| 1   | AA    | 702 | A    |
| 1   | AA    | 703 | G    |
| 1   | AA    | 721 | G    |
| 1   | AA    | 724 | G    |
| 1   | AA    | 731 | G    |
| 1   | AA    | 747 | A    |
| 1   | AA    | 748 | G    |
| 1   | AA    | 752 | G    |
| 1   | AA    | 755 | G    |
| 1   | AA    | 781 | A    |
| 1   | AA    | 782 | A    |
| 1   | AA    | 793 | U    |
| 1   | AA    | 794 | A    |
| 1   | AA    | 812 | G    |
| 1   | AA    | 815 | A    |
| 1   | AA    | 817 | C    |
| 1   | AA    | 819 | A    |
| 1   | AA    | 821 | G    |
| 1   | AA    | 828 | U    |
| 1   | AA    | 841 | C    |
| 1   | AA    | 842 | U    |
| 1   | AA    | 843 | U    |
| 1   | AA    | 844 | G    |
| 1   | AA    | 845 | A    |
| 1   | AA    | 846 | G    |
| 1   | AA    | 847 | G    |
| 1   | AA    | 849 | G    |
| 1   | AA    | 873 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 914  | A    |
| 1   | AA    | 926  | G    |
| 1   | AA    | 927  | G    |
| 1   | AA    | 934  | C    |
| 1   | AA    | 935  | A    |
| 1   | AA    | 945  | G    |
| 1   | AA    | 960  | U    |
| 1   | AA    | 961  | U    |
| 1   | AA    | 968  | A    |
| 1   | AA    | 969  | A    |
| 1   | AA    | 971  | G    |
| 1   | AA    | 974  | A    |
| 1   | AA    | 975  | A    |
| 1   | AA    | 976  | G    |
| 1   | AA    | 977  | A    |
| 1   | AA    | 981  | U    |
| 1   | AA    | 993  | G    |
| 1   | AA    | 994  | A    |
| 1   | AA    | 996  | A    |
| 1   | AA    | 1004 | A    |
| 1   | AA    | 1018 | G    |
| 1   | AA    | 1020 | G    |
| 1   | AA    | 1028 | C    |
| 1   | AA    | 1030 | U    |
| 1   | AA    | 1032 | G    |
| 1   | AA    | 1034 | G    |
| 1   | AA    | 1035 | A    |
| 1   | AA    | 1036 | A    |
| 1   | AA    | 1050 | G    |
| 1   | AA    | 1053 | G    |
| 1   | AA    | 1055 | A    |
| 1   | AA    | 1065 | U    |
| 1   | AA    | 1066 | C    |
| 1   | AA    | 1070 | U    |
| 1   | AA    | 1085 | U    |
| 1   | AA    | 1086 | U    |
| 1   | AA    | 1094 | G    |
| 1   | AA    | 1095 | U    |
| 1   | AA    | 1101 | A    |
| 1   | AA    | 1112 | C    |
| 1   | AA    | 1118 | U    |
| 1   | AA    | 1119 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1124 | G    |
| 1   | AA    | 1125 | U    |
| 1   | AA    | 1130 | A    |
| 1   | AA    | 1133 | G    |
| 1   | AA    | 1134 | G    |
| 1   | AA    | 1135 | U    |
| 1   | AA    | 1136 | C    |
| 1   | AA    | 1137 | C    |
| 1   | AA    | 1139 | G    |
| 1   | AA    | 1140 | C    |
| 1   | AA    | 1144 | G    |
| 1   | AA    | 1145 | A    |
| 1   | AA    | 1146 | A    |
| 1   | AA    | 1159 | U    |
| 1   | AA    | 1160 | G    |
| 1   | AA    | 1167 | A    |
| 1   | AA    | 1168 | U    |
| 1   | AA    | 1169 | A    |
| 1   | AA    | 1181 | G    |
| 1   | AA    | 1184 | G    |
| 1   | AA    | 1191 | A    |
| 1   | AA    | 1196 | A    |
| 1   | AA    | 1197 | A    |
| 1   | AA    | 1202 | U    |
| 1   | AA    | 1212 | U    |
| 1   | AA    | 1213 | A    |
| 1   | AA    | 1215 | G    |
| 1   | AA    | 1225 | A    |
| 1   | AA    | 1226 | C    |
| 1   | AA    | 1227 | A    |
| 1   | AA    | 1228 | C    |
| 1   | AA    | 1238 | A    |
| 1   | AA    | 1241 | G    |
| 1   | AA    | 1249 | C    |
| 1   | AA    | 1250 | A    |
| 1   | AA    | 1258 | G    |
| 1   | AA    | 1270 | G    |
| 1   | AA    | 1278 | G    |
| 1   | AA    | 1279 | G    |
| 1   | AA    | 1280 | A    |
| 1   | AA    | 1285 | A    |
| 1   | AA    | 1286 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1287 | A    |
| 1   | AA    | 1297 | G    |
| 1   | AA    | 1300 | G    |
| 1   | AA    | 1301 | U    |
| 1   | AA    | 1303 | C    |
| 1   | AA    | 1305 | G    |
| 1   | AA    | 1316 | G    |
| 1   | AA    | 1320 | C    |
| 1   | AA    | 1321 | U    |
| 1   | AA    | 1323 | G    |
| 1   | AA    | 1331 | G    |
| 1   | AA    | 1336 | C    |
| 1   | AA    | 1346 | A    |
| 1   | AA    | 1353 | G    |
| 1   | AA    | 1363 | A    |
| 1   | AA    | 1364 | U    |
| 1   | AA    | 1380 | U    |
| 1   | AA    | 1381 | U    |
| 1   | AA    | 1399 | C    |
| 1   | AA    | 1419 | G    |
| 1   | AA    | 1432 | G    |
| 1   | AA    | 1446 | A    |
| 1   | AA    | 1448 | C    |
| 1   | AA    | 1451 | U    |
| 1   | AA    | 1452 | C    |
| 1   | AA    | 1454 | G    |
| 1   | AA    | 1493 | A    |
| 1   | AA    | 1494 | G    |
| 1   | AA    | 1497 | G    |
| 1   | AA    | 1499 | A    |
| 1   | AA    | 1503 | A    |
| 1   | AA    | 1506 | U    |
| 1   | AA    | 1517 | G    |
| 1   | AA    | 1520 | C    |
| 1   | AA    | 1528 | U    |
| 1   | AA    | 1529 | G    |
| 1   | AA    | 1530 | G    |
| 22  | AV    | 4    | C    |
| 22  | AV    | 5    | A    |
| 22  | AV    | 8    | U    |
| 22  | AV    | 19   | G    |
| 22  | AV    | 21   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | AV    | 31  | C    |
| 22  | AV    | 33  | U    |
| 22  | AV    | 43  | G    |
| 22  | AV    | 48  | C    |
| 22  | AV    | 49  | G    |
| 22  | AV    | 53  | G    |
| 22  | AV    | 67  | G    |
| 22  | AV    | 71  | C    |
| 22  | AV    | 73  | A    |
| 22  | AV    | 76  | A    |
| 23  | AX    | 13  | A    |
| 23  | AX    | 14  | A    |
| 23  | AX    | 16  | C    |
| 23  | AX    | 17  | C    |
| 23  | AX    | 18  | C    |
| 23  | AX    | 19  | A    |
| 23  | AX    | 20  | G    |
| 23  | AX    | 22  | A    |
| 34  | BA    | 9   | G    |
| 34  | BA    | 14  | U    |
| 34  | BA    | 16  | G    |
| 34  | BA    | 26  | C    |
| 34  | BA    | 29  | A    |
| 34  | BA    | 30  | C    |
| 34  | BA    | 42  | C    |
| 34  | BA    | 45  | A    |
| 34  | BA    | 52  | A    |
| 34  | BA    | 53  | A    |
| 34  | BA    | 66  | A    |
| 34  | BA    | 67  | G    |
| 34  | BA    | 90  | C    |
| 34  | BA    | 91  | C    |
| 34  | BA    | 99  | A    |
| 34  | BA    | 109 | A    |
| 35  | BB    | 34  | U    |
| 35  | BB    | 35  | G    |
| 35  | BB    | 46  | G    |
| 35  | BB    | 71  | A    |
| 35  | BB    | 74  | A    |
| 35  | BB    | 75  | G    |
| 35  | BB    | 84  | A    |
| 35  | BB    | 91  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | BB    | 95  | A    |
| 35  | BB    | 100 | U    |
| 35  | BB    | 101 | A    |
| 35  | BB    | 102 | U    |
| 35  | BB    | 103 | A    |
| 35  | BB    | 118 | A    |
| 35  | BB    | 120 | U    |
| 35  | BB    | 126 | A    |
| 35  | BB    | 128 | C    |
| 35  | BB    | 136 | G    |
| 35  | BB    | 137 | U    |
| 35  | BB    | 139 | U    |
| 35  | BB    | 140 | C    |
| 35  | BB    | 141 | G    |
| 35  | BB    | 143 | C    |
| 35  | BB    | 144 | A    |
| 35  | BB    | 160 | A    |
| 35  | BB    | 180 | G    |
| 35  | BB    | 181 | A    |
| 35  | BB    | 196 | A    |
| 35  | BB    | 199 | A    |
| 35  | BB    | 216 | A    |
| 35  | BB    | 221 | A    |
| 35  | BB    | 222 | A    |
| 35  | BB    | 233 | A    |
| 35  | BB    | 241 | A    |
| 35  | BB    | 248 | G    |
| 35  | BB    | 249 | C    |
| 35  | BB    | 255 | A    |
| 35  | BB    | 265 | A    |
| 35  | BB    | 266 | G    |
| 35  | BB    | 268 | C    |
| 35  | BB    | 271 | G    |
| 35  | BB    | 273 | G    |
| 35  | BB    | 276 | U    |
| 35  | BB    | 277 | G    |
| 35  | BB    | 281 | C    |
| 35  | BB    | 283 | G    |
| 35  | BB    | 285 | G    |
| 35  | BB    | 286 | U    |
| 35  | BB    | 294 | A    |
| 35  | BB    | 299 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | BB    | 311 | A    |
| 35  | BB    | 321 | U    |
| 35  | BB    | 322 | A    |
| 35  | BB    | 329 | G    |
| 35  | BB    | 330 | A    |
| 35  | BB    | 333 | G    |
| 35  | BB    | 346 | A    |
| 35  | BB    | 352 | A    |
| 35  | BB    | 353 | C    |
| 35  | BB    | 362 | A    |
| 35  | BB    | 363 | G    |
| 35  | BB    | 364 | C    |
| 35  | BB    | 369 | U    |
| 35  | BB    | 371 | A    |
| 35  | BB    | 372 | G    |
| 35  | BB    | 386 | G    |
| 35  | BB    | 387 | U    |
| 35  | BB    | 406 | G    |
| 35  | BB    | 411 | G    |
| 35  | BB    | 412 | A    |
| 35  | BB    | 424 | G    |
| 35  | BB    | 451 | U    |
| 35  | BB    | 455 | C    |
| 35  | BB    | 456 | C    |
| 35  | BB    | 457 | A    |
| 35  | BB    | 479 | A    |
| 35  | BB    | 481 | G    |
| 35  | BB    | 490 | C    |
| 35  | BB    | 491 | G    |
| 35  | BB    | 504 | A    |
| 35  | BB    | 505 | A    |
| 35  | BB    | 508 | A    |
| 35  | BB    | 509 | C    |
| 35  | BB    | 512 | G    |
| 35  | BB    | 531 | C    |
| 35  | BB    | 532 | A    |
| 35  | BB    | 544 | C    |
| 35  | BB    | 545 | U    |
| 35  | BB    | 546 | U    |
| 35  | BB    | 547 | A    |
| 35  | BB    | 548 | G    |
| 35  | BB    | 549 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | BB    | 550 | C    |
| 35  | BB    | 555 | G    |
| 35  | BB    | 563 | A    |
| 35  | BB    | 573 | U    |
| 35  | BB    | 575 | A    |
| 35  | BB    | 586 | A    |
| 35  | BB    | 588 | U    |
| 35  | BB    | 603 | A    |
| 35  | BB    | 613 | A    |
| 35  | BB    | 615 | U    |
| 35  | BB    | 627 | A    |
| 35  | BB    | 637 | A    |
| 35  | BB    | 646 | U    |
| 35  | BB    | 647 | G    |
| 35  | BB    | 653 | U    |
| 35  | BB    | 654 | A    |
| 35  | BB    | 655 | A    |
| 35  | BB    | 671 | C    |
| 35  | BB    | 686 | U    |
| 35  | BB    | 730 | A    |
| 35  | BB    | 746 | U    |
| 35  | BB    | 747 | U    |
| 35  | BB    | 757 | G    |
| 35  | BB    | 762 | U    |
| 35  | BB    | 764 | A    |
| 35  | BB    | 775 | G    |
| 35  | BB    | 782 | A    |
| 35  | BB    | 784 | G    |
| 35  | BB    | 785 | G    |
| 35  | BB    | 788 | A    |
| 35  | BB    | 793 | A    |
| 35  | BB    | 805 | G    |
| 35  | BB    | 812 | C    |
| 35  | BB    | 819 | A    |
| 35  | BB    | 827 | U    |
| 35  | BB    | 828 | U    |
| 35  | BB    | 846 | U    |
| 35  | BB    | 847 | U    |
| 35  | BB    | 858 | G    |
| 35  | BB    | 859 | G    |
| 35  | BB    | 869 | G    |
| 35  | BB    | 871 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | BB    | 875  | G    |
| 35  | BB    | 876  | C    |
| 35  | BB    | 881  | G    |
| 35  | BB    | 887  | U    |
| 35  | BB    | 888  | C    |
| 35  | BB    | 891  | G    |
| 35  | BB    | 896  | A    |
| 35  | BB    | 897  | C    |
| 35  | BB    | 900  | A    |
| 35  | BB    | 901  | C    |
| 35  | BB    | 910  | A    |
| 35  | BB    | 912  | C    |
| 35  | BB    | 919  | U    |
| 35  | BB    | 931  | U    |
| 35  | BB    | 932  | U    |
| 35  | BB    | 941  | A    |
| 35  | BB    | 946  | C    |
| 35  | BB    | 958  | U    |
| 35  | BB    | 961  | C    |
| 35  | BB    | 973  | A    |
| 35  | BB    | 974  | G    |
| 35  | BB    | 983  | A    |
| 35  | BB    | 991  | C    |
| 35  | BB    | 995  | C    |
| 35  | BB    | 996  | A    |
| 35  | BB    | 1005 | C    |
| 35  | BB    | 1012 | U    |
| 35  | BB    | 1013 | C    |
| 35  | BB    | 1022 | G    |
| 35  | BB    | 1023 | U    |
| 35  | BB    | 1025 | G    |
| 35  | BB    | 1033 | U    |
| 35  | BB    | 1054 | A    |
| 35  | BB    | 1056 | G    |
| 35  | BB    | 1057 | A    |
| 35  | BB    | 1061 | U    |
| 35  | BB    | 1067 | A    |
| 35  | BB    | 1070 | A    |
| 35  | BB    | 1071 | G    |
| 35  | BB    | 1078 | U    |
| 35  | BB    | 1088 | A    |
| 35  | BB    | 1090 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | BB    | 1095 | A    |
| 35  | BB    | 1096 | A    |
| 35  | BB    | 1104 | C    |
| 35  | BB    | 1112 | G    |
| 35  | BB    | 1116 | G    |
| 35  | BB    | 1130 | U    |
| 35  | BB    | 1132 | U    |
| 35  | BB    | 1133 | A    |
| 35  | BB    | 1134 | A    |
| 35  | BB    | 1135 | C    |
| 35  | BB    | 1136 | G    |
| 35  | BB    | 1139 | G    |
| 35  | BB    | 1142 | A    |
| 35  | BB    | 1176 | U    |
| 35  | BB    | 1205 | A    |
| 35  | BB    | 1206 | G    |
| 35  | BB    | 1238 | G    |
| 35  | BB    | 1241 | A    |
| 35  | BB    | 1242 | U    |
| 35  | BB    | 1248 | G    |
| 35  | BB    | 1250 | G    |
| 35  | BB    | 1253 | A    |
| 35  | BB    | 1256 | G    |
| 35  | BB    | 1266 | G    |
| 35  | BB    | 1271 | G    |
| 35  | BB    | 1272 | A    |
| 35  | BB    | 1273 | U    |
| 35  | BB    | 1275 | A    |
| 35  | BB    | 1276 | A    |
| 35  | BB    | 1300 | G    |
| 35  | BB    | 1301 | A    |
| 35  | BB    | 1312 | U    |
| 35  | BB    | 1313 | U    |
| 35  | BB    | 1321 | A    |
| 35  | BB    | 1325 | U    |
| 35  | BB    | 1332 | G    |
| 35  | BB    | 1337 | G    |
| 35  | BB    | 1341 | G    |
| 35  | BB    | 1352 | U    |
| 35  | BB    | 1365 | A    |
| 35  | BB    | 1368 | G    |
| 35  | BB    | 1374 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | BB    | 1379 | U    |
| 35  | BB    | 1383 | A    |
| 35  | BB    | 1394 | U    |
| 35  | BB    | 1396 | U    |
| 35  | BB    | 1416 | G    |
| 35  | BB    | 1419 | A    |
| 35  | BB    | 1420 | A    |
| 35  | BB    | 1421 | G    |
| 35  | BB    | 1427 | A    |
| 35  | BB    | 1428 | C    |
| 35  | BB    | 1451 | C    |
| 35  | BB    | 1453 | A    |
| 35  | BB    | 1458 | U    |
| 35  | BB    | 1459 | G    |
| 35  | BB    | 1460 | U    |
| 35  | BB    | 1461 | C    |
| 35  | BB    | 1469 | A    |
| 35  | BB    | 1476 | U    |
| 35  | BB    | 1477 | A    |
| 35  | BB    | 1478 | G    |
| 35  | BB    | 1482 | G    |
| 35  | BB    | 1490 | A    |
| 35  | BB    | 1497 | U    |
| 35  | BB    | 1504 | A    |
| 35  | BB    | 1505 | A    |
| 35  | BB    | 1507 | C    |
| 35  | BB    | 1508 | A    |
| 35  | BB    | 1509 | A    |
| 35  | BB    | 1510 | G    |
| 35  | BB    | 1523 | U    |
| 35  | BB    | 1524 | G    |
| 35  | BB    | 1532 | A    |
| 35  | BB    | 1535 | A    |
| 35  | BB    | 1536 | C    |
| 35  | BB    | 1538 | G    |
| 35  | BB    | 1552 | A    |
| 35  | BB    | 1569 | A    |
| 35  | BB    | 1578 | U    |
| 35  | BB    | 1585 | C    |
| 35  | BB    | 1608 | A    |
| 35  | BB    | 1609 | A    |
| 35  | BB    | 1610 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | BB    | 1618 | A    |
| 35  | BB    | 1634 | A    |
| 35  | BB    | 1635 | A    |
| 35  | BB    | 1640 | A    |
| 35  | BB    | 1647 | U    |
| 35  | BB    | 1648 | U    |
| 35  | BB    | 1654 | A    |
| 35  | BB    | 1674 | G    |
| 35  | BB    | 1699 | G    |
| 35  | BB    | 1700 | A    |
| 35  | BB    | 1714 | U    |
| 35  | BB    | 1715 | G    |
| 35  | BB    | 1729 | U    |
| 35  | BB    | 1731 | G    |
| 35  | BB    | 1733 | G    |
| 35  | BB    | 1738 | G    |
| 35  | BB    | 1756 | G    |
| 35  | BB    | 1758 | U    |
| 35  | BB    | 1761 | C    |
| 35  | BB    | 1762 | A    |
| 35  | BB    | 1764 | C    |
| 35  | BB    | 1773 | A    |
| 35  | BB    | 1776 | G    |
| 35  | BB    | 1781 | U    |
| 35  | BB    | 1800 | C    |
| 35  | BB    | 1801 | A    |
| 35  | BB    | 1808 | A    |
| 35  | BB    | 1809 | A    |
| 35  | BB    | 1816 | C    |
| 35  | BB    | 1829 | A    |
| 35  | BB    | 1870 | C    |
| 35  | BB    | 1884 | G    |
| 35  | BB    | 1896 | G    |
| 35  | BB    | 1906 | G    |
| 35  | BB    | 1913 | A    |
| 35  | BB    | 1914 | C    |
| 35  | BB    | 1929 | G    |
| 35  | BB    | 1930 | G    |
| 35  | BB    | 1937 | A    |
| 35  | BB    | 1938 | A    |
| 35  | BB    | 1940 | U    |
| 35  | BB    | 1955 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | BB    | 1966 | A    |
| 35  | BB    | 1967 | C    |
| 35  | BB    | 1970 | A    |
| 35  | BB    | 1971 | U    |
| 35  | BB    | 1972 | G    |
| 35  | BB    | 1991 | U    |
| 35  | BB    | 1993 | U    |
| 35  | BB    | 1997 | C    |
| 35  | BB    | 2020 | A    |
| 35  | BB    | 2021 | C    |
| 35  | BB    | 2022 | U    |
| 35  | BB    | 2023 | C    |
| 35  | BB    | 2031 | A    |
| 35  | BB    | 2032 | G    |
| 35  | BB    | 2033 | A    |
| 35  | BB    | 2043 | C    |
| 35  | BB    | 2055 | C    |
| 35  | BB    | 2056 | G    |
| 35  | BB    | 2059 | A    |
| 35  | BB    | 2060 | A    |
| 35  | BB    | 2061 | G    |
| 35  | BB    | 2062 | A    |
| 35  | BB    | 2065 | C    |
| 35  | BB    | 2069 | G    |
| 35  | BB    | 2076 | U    |
| 35  | BB    | 2077 | A    |
| 35  | BB    | 2102 | G    |
| 35  | BB    | 2104 | C    |
| 35  | BB    | 2111 | U    |
| 35  | BB    | 2113 | U    |
| 35  | BB    | 2117 | A    |
| 35  | BB    | 2119 | A    |
| 35  | BB    | 2128 | G    |
| 35  | BB    | 2130 | U    |
| 35  | BB    | 2131 | U    |
| 35  | BB    | 2132 | U    |
| 35  | BB    | 2133 | G    |
| 35  | BB    | 2134 | A    |
| 35  | BB    | 2135 | A    |
| 35  | BB    | 2136 | G    |
| 35  | BB    | 2137 | U    |
| 35  | BB    | 2144 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | BB    | 2145 | C    |
| 35  | BB    | 2146 | C    |
| 35  | BB    | 2148 | G    |
| 35  | BB    | 2149 | U    |
| 35  | BB    | 2152 | G    |
| 35  | BB    | 2153 | C    |
| 35  | BB    | 2155 | U    |
| 35  | BB    | 2158 | A    |
| 35  | BB    | 2159 | G    |
| 35  | BB    | 2160 | C    |
| 35  | BB    | 2163 | A    |
| 35  | BB    | 2164 | C    |
| 35  | BB    | 2165 | C    |
| 35  | BB    | 2166 | U    |
| 35  | BB    | 2167 | U    |
| 35  | BB    | 2176 | A    |
| 35  | BB    | 2179 | C    |
| 35  | BB    | 2181 | U    |
| 35  | BB    | 2187 | U    |
| 35  | BB    | 2192 | U    |
| 35  | BB    | 2198 | A    |
| 35  | BB    | 2203 | U    |
| 35  | BB    | 2204 | G    |
| 35  | BB    | 2212 | A    |
| 35  | BB    | 2213 | U    |
| 35  | BB    | 2214 | C    |
| 35  | BB    | 2225 | A    |
| 35  | BB    | 2226 | C    |
| 35  | BB    | 2238 | G    |
| 35  | BB    | 2239 | G    |
| 35  | BB    | 2250 | G    |
| 35  | BB    | 2251 | G    |
| 35  | BB    | 2266 | A    |
| 35  | BB    | 2278 | A    |
| 35  | BB    | 2279 | G    |
| 35  | BB    | 2283 | C    |
| 35  | BB    | 2286 | G    |
| 35  | BB    | 2287 | A    |
| 35  | BB    | 2288 | A    |
| 35  | BB    | 2297 | A    |
| 35  | BB    | 2305 | U    |
| 35  | BB    | 2307 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | BB    | 2308 | G    |
| 35  | BB    | 2311 | A    |
| 35  | BB    | 2322 | A    |
| 35  | BB    | 2324 | U    |
| 35  | BB    | 2325 | G    |
| 35  | BB    | 2333 | A    |
| 35  | BB    | 2335 | A    |
| 35  | BB    | 2336 | A    |
| 35  | BB    | 2337 | G    |
| 35  | BB    | 2347 | C    |
| 35  | BB    | 2383 | G    |
| 35  | BB    | 2385 | C    |
| 35  | BB    | 2388 | A    |
| 35  | BB    | 2396 | G    |
| 35  | BB    | 2402 | U    |
| 35  | BB    | 2403 | C    |
| 35  | BB    | 2406 | A    |
| 35  | BB    | 2407 | A    |
| 35  | BB    | 2423 | U    |
| 35  | BB    | 2425 | A    |
| 35  | BB    | 2426 | A    |
| 35  | BB    | 2429 | G    |
| 35  | BB    | 2430 | A    |
| 35  | BB    | 2434 | A    |
| 35  | BB    | 2441 | U    |
| 35  | BB    | 2448 | A    |
| 35  | BB    | 2458 | G    |
| 35  | BB    | 2472 | G    |
| 35  | BB    | 2473 | U    |
| 35  | BB    | 2476 | A    |
| 35  | BB    | 2478 | A    |
| 35  | BB    | 2491 | U    |
| 35  | BB    | 2492 | U    |
| 35  | BB    | 2498 | C    |
| 35  | BB    | 2502 | G    |
| 35  | BB    | 2503 | A    |
| 35  | BB    | 2505 | G    |
| 35  | BB    | 2506 | U    |
| 35  | BB    | 2518 | A    |
| 35  | BB    | 2529 | G    |
| 35  | BB    | 2530 | A    |
| 35  | BB    | 2534 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | BB    | 2535 | G    |
| 35  | BB    | 2554 | U    |
| 35  | BB    | 2555 | U    |
| 35  | BB    | 2566 | A    |
| 35  | BB    | 2567 | G    |
| 35  | BB    | 2573 | C    |
| 35  | BB    | 2586 | U    |
| 35  | BB    | 2602 | A    |
| 35  | BB    | 2609 | U    |
| 35  | BB    | 2613 | U    |
| 35  | BB    | 2629 | U    |
| 35  | BB    | 2630 | G    |
| 35  | BB    | 2682 | A    |
| 35  | BB    | 2689 | U    |
| 35  | BB    | 2713 | U    |
| 35  | BB    | 2714 | G    |
| 35  | BB    | 2726 | A    |
| 35  | BB    | 2744 | G    |
| 35  | BB    | 2748 | A    |
| 35  | BB    | 2751 | G    |
| 35  | BB    | 2757 | A    |
| 35  | BB    | 2765 | A    |
| 35  | BB    | 2778 | A    |
| 35  | BB    | 2791 | G    |
| 35  | BB    | 2793 | C    |
| 35  | BB    | 2796 | U    |
| 35  | BB    | 2797 | U    |
| 35  | BB    | 2798 | U    |
| 35  | BB    | 2799 | A    |
| 35  | BB    | 2800 | A    |
| 35  | BB    | 2808 | G    |
| 35  | BB    | 2809 | A    |
| 35  | BB    | 2820 | A    |
| 35  | BB    | 2821 | A    |
| 35  | BB    | 2832 | U    |
| 35  | BB    | 2836 | U    |
| 35  | BB    | 2849 | U    |
| 35  | BB    | 2850 | A    |
| 35  | BB    | 2867 | G    |
| 35  | BB    | 2872 | A    |
| 35  | BB    | 2873 | A    |
| 35  | BB    | 2883 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | BB    | 2893 | A    |

All (92) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 7    | A    |
| 1   | AA    | 51   | A    |
| 1   | AA    | 60   | A    |
| 1   | AA    | 85   | U    |
| 1   | AA    | 243  | A    |
| 1   | AA    | 279  | A    |
| 1   | AA    | 328  | C    |
| 1   | AA    | 366  | A    |
| 1   | AA    | 372  | C    |
| 1   | AA    | 381  | C    |
| 1   | AA    | 412  | A    |
| 1   | AA    | 428  | G    |
| 1   | AA    | 429  | U    |
| 1   | AA    | 461  | A    |
| 1   | AA    | 484  | G    |
| 1   | AA    | 485  | U    |
| 1   | AA    | 632  | U    |
| 1   | AA    | 815  | A    |
| 1   | AA    | 843  | U    |
| 1   | AA    | 845  | A    |
| 1   | AA    | 960  | U    |
| 1   | AA    | 976  | G    |
| 1   | AA    | 1049 | U    |
| 1   | AA    | 1065 | U    |
| 1   | AA    | 1137 | C    |
| 1   | AA    | 1168 | U    |
| 1   | AA    | 1201 | A    |
| 1   | AA    | 1214 | C    |
| 1   | AA    | 1226 | C    |
| 1   | AA    | 1257 | A    |
| 1   | AA    | 1278 | G    |
| 1   | AA    | 1300 | G    |
| 1   | AA    | 1319 | A    |
| 1   | AA    | 1529 | G    |
| 34  | BA    | 25   | U    |
| 34  | BA    | 66   | A    |
| 35  | BB    | 91   | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | BB    | 241  | A    |
| 35  | BB    | 320  | A    |
| 35  | BB    | 321  | U    |
| 35  | BB    | 455  | C    |
| 35  | BB    | 670  | A    |
| 35  | BB    | 827  | U    |
| 35  | BB    | 829  | A    |
| 35  | BB    | 858  | G    |
| 35  | BB    | 876  | C    |
| 35  | BB    | 880  | G    |
| 35  | BB    | 887  | U    |
| 35  | BB    | 889  | C    |
| 35  | BB    | 890  | C    |
| 35  | BB    | 891  | G    |
| 35  | BB    | 973  | A    |
| 35  | BB    | 1088 | A    |
| 35  | BB    | 1174 | U    |
| 35  | BB    | 1205 | A    |
| 35  | BB    | 1272 | A    |
| 35  | BB    | 1312 | U    |
| 35  | BB    | 1332 | G    |
| 35  | BB    | 1458 | U    |
| 35  | BB    | 1459 | G    |
| 35  | BB    | 1509 | A    |
| 35  | BB    | 1608 | A    |
| 35  | BB    | 1617 | C    |
| 35  | BB    | 1699 | G    |
| 35  | BB    | 1730 | C    |
| 35  | BB    | 1808 | A    |
| 35  | BB    | 1938 | A    |
| 35  | BB    | 1944 | U    |
| 35  | BB    | 1966 | A    |
| 35  | BB    | 2076 | U    |
| 35  | BB    | 2130 | U    |
| 35  | BB    | 2131 | U    |
| 35  | BB    | 2132 | U    |
| 35  | BB    | 2133 | G    |
| 35  | BB    | 2144 | G    |
| 35  | BB    | 2145 | C    |
| 35  | BB    | 2152 | G    |
| 35  | BB    | 2159 | G    |
| 35  | BB    | 2172 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | BB    | 2282 | G    |
| 35  | BB    | 2286 | G    |
| 35  | BB    | 2307 | G    |
| 35  | BB    | 2308 | G    |
| 35  | BB    | 2336 | A    |
| 35  | BB    | 2402 | U    |
| 35  | BB    | 2406 | A    |
| 35  | BB    | 2423 | U    |
| 35  | BB    | 2425 | A    |
| 35  | BB    | 2491 | U    |
| 35  | BB    | 2601 | C    |
| 35  | BB    | 2602 | A    |
| 35  | BB    | 2756 | U    |

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | 5MU  | AV    | 54  | 22   | 14,21,23     | 1.48 | 2 (14%)  | 15,30,35    | 4.17 | 3 (20%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 22  | 5MU  | AV    | 54  | 22   | -       | 0/3/25/26 | 0/2/2/2 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 22  | AV    | 54  | 5MU  | C6-N1 | 2.18 | 1.38        | 1.35     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 22  | AV    | 54  | 5MU  | C4-N3 | 4.29 | 1.40        | 1.33     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 22  | AV    | 54  | 5MU  | C5-C4-N3   | -3.99 | 113.59      | 123.12   |
| 22  | AV    | 54  | 5MU  | O4'-C1'-N1 | 2.91  | 113.90      | 108.08   |
| 22  | AV    | 54  | 5MU  | C4-N3-C2   | 15.26 | 127.24      | 114.13   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 54  | BU    | 1                |
| 14  | AN    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | BU    | 4:ILE     | C      | 6:ARG     | N      | 4.65         |
| 1     | AN    | 35:ALA    | C      | 40:ARG    | N      | 4.56         |