



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

Mar 2, 2017 – 12:38 pm GMT

PDB ID : 4V6M  
EMDB ID: : EMD-1858  
Title : Structure of the ribosome-SecYE complex in the membrane environment  
Authors : Frauenfeld, J.; Gumbart, J.; van der Sluis, E.O.; Funes, S.; Gartmann, M.;  
Beatrix, B.; Mielke, T.; Berninghausen, O.; Becker, T.; Schulten, K.; Beck-  
mann, R.  
Deposited on : 2011-02-08  
Resolution : 7.10 Å(reported)

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) : recalc29047

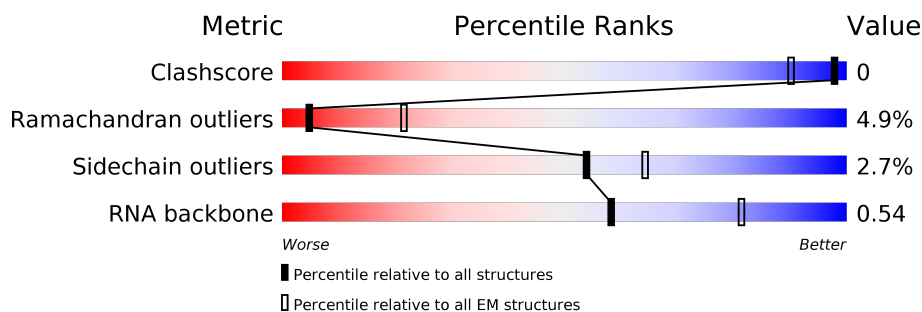
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.10 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.




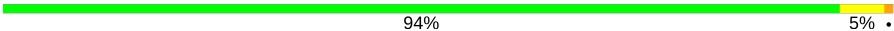

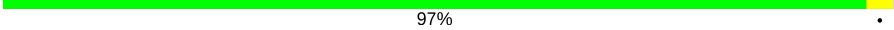
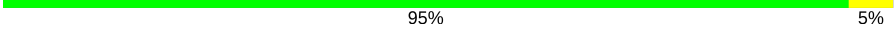


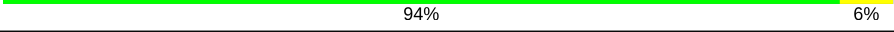
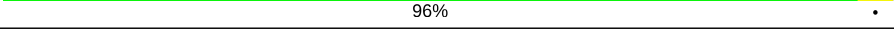


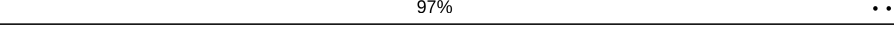
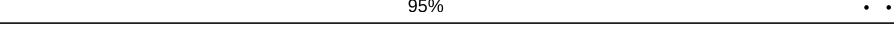


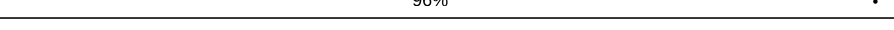
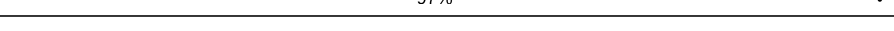
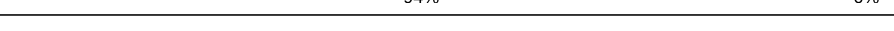
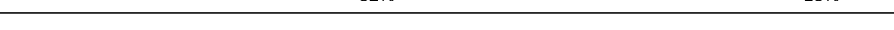
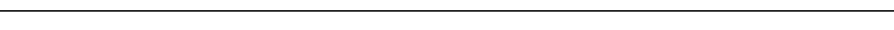
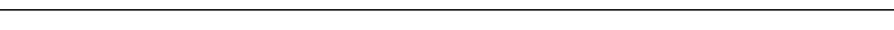
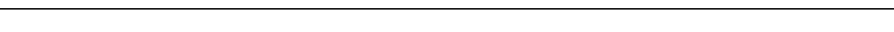
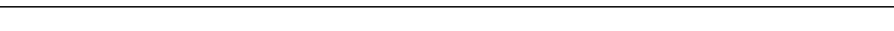
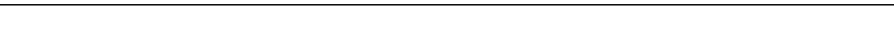

| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 125131                      | 1336                        |
| Ramachandran outliers | 121729                      | 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    | 1542   | 78% 19% .        |
| 2   | AX    | 11     | 9% 45% 45%       |
| 3   | AV    | 77     | 77% 23%          |
| 4   | AZ    | 98     | 76% 23% .        |
| 5   | A0    | 200    | 96% 5%           |
| 5   | A1    | 200    | 95% 5% .         |
| 6   | AB    | 240    | 94% 5% .         |
| 7   | AC    | 232    | 90% 9% .         |





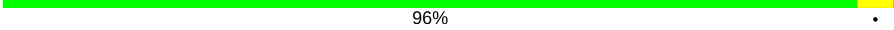
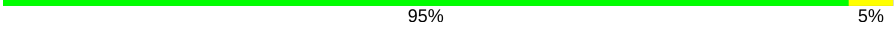

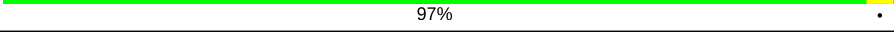


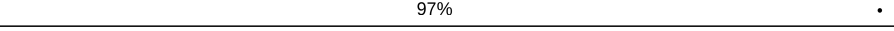

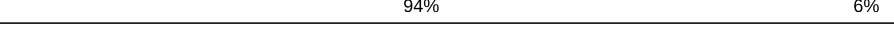
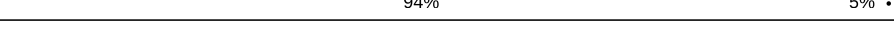


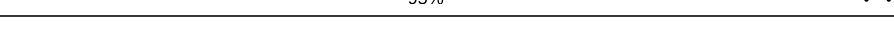
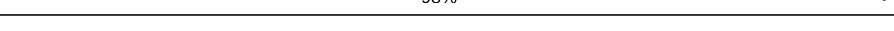
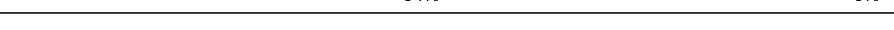
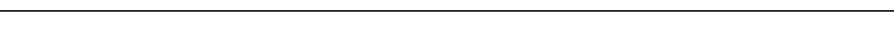
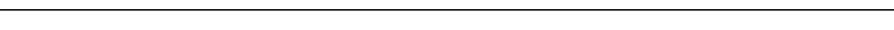
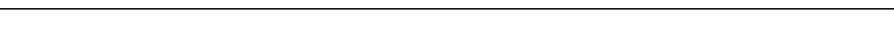
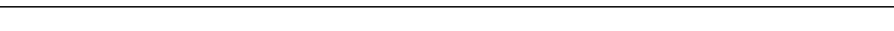
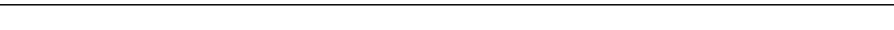

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 8   | AD    | 205    |  91% 9%        |
| 9   | AE    | 166    |  94% 5% .      |
| 10  | AF    | 135    |  93% 7%        |
| 11  | AG    | 178    |  97% .         |
| 12  | AH    | 129    |  95% 5%        |
| 13  | AI    | 129    |  90% 9% .      |
| 14  | AJ    | 103    |  88% 12%       |
| 15  | AK    | 128    |  94% 6%        |
| 16  | AL    | 123    |  96% .         |
| 17  | AM    | 117    |  92% 7% .      |
| 18  | AN    | 100    |  88% 12%       |
| 19  | AO    | 88     |  97% ..       |
| 20  | AP    | 82     |  95% . .     |
| 21  | AQ    | 83     |  87% 13%     |
| 22  | AR    | 74     |  92% 8%      |
| 23  | AS    | 91     |  96% .       |
| 24  | AT    | 86     |  97% .       |
| 25  | AU    | 70     |  94% 6%      |
| 26  | B7    | 120    |  . 82% 18%   |
| 27  | B8    | 2904   |  . 80% 18% . |
| 28  | BA    | 435    |  80% 16% .   |
| 29  | BB    | 116    |  89% 10% .   |
| 30  | B5    | 234    |  95% 5%      |
| 31  | B6    | 272    |  93% 6% .    |
| 32  | BD    | 209    |  90% 10%     |

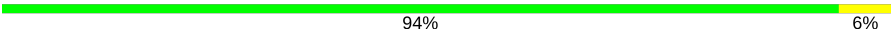

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 33  | BE    | 201    |  94% 6%      |
| 34  | BF    | 178    |  90% 9% .    |
| 35  | BG    | 176    |  93% 7% .    |
| 36  | BH    | 149    |  88% 11% .   |
| 37  | BI    | 141    |  96% . .     |
| 38  | BJ    | 142    |  95% 5%      |
| 39  | BK    | 123    |  91% 9%      |
| 40  | BL    | 144    |  97% . .     |
| 41  | BM    | 136    |  92% 7% .    |
| 42  | BN    | 127    |  89% 11%     |
| 43  | BO    | 117    |  97% .       |
| 44  | BP    | 114    |  91% 9%     |
| 45  | BQ    | 117    |  94% 6%    |
| 46  | BR    | 103    |  94% 5% .  |
| 47  | BS    | 110    |  92% 7% .  |
| 48  | BT    | 100    |  89% 9% .  |
| 49  | BU    | 103    |  95% . .   |
| 50  | BV    | 94     |  98% .     |
| 51  | BW    | 84     |  94% 6%    |
| 52  | BX    | 77     |  91% 9%    |
| 53  | BY    | 63     |  95% 5%    |
| 54  | BZ    | 58     |  93% 7%    |
| 55  | B0    | 56     |  96% .     |
| 56  | B1    | 54     |  94% 6%    |
| 57  | B2    | 46     |  87% 11% . |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 58  | B3    | 64     |  94%6% |
| 59  | B4    | 38     |  92%8% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60  | PEV  | A0    | 308  | X         | -        | -       | -                |
| 60  | PEV  | A0    | 314  | X         | -        | -       | -                |
| 60  | PEV  | A0    | 323  | X         | -        | -       | -                |
| 60  | PEV  | A1    | 301  | X         | -        | -       | -                |
| 60  | PEV  | A1    | 305  | X         | -        | -       | -                |
| 60  | PEV  | A1    | 313  | X         | -        | -       | -                |
| 60  | PEV  | A1    | 317  | X         | -        | -       | -                |
| 60  | PEV  | AZ    | 204  | X         | -        | -       | -                |
| 60  | PEV  | B8    | 3001 | X         | -        | -       | -                |
| 60  | PEV  | BA    | 502  | X         | -        | -       | -                |
| 60  | PEV  | BA    | 508  | X         | -        | -       | -                |
| 60  | PEV  | BA    | 526  | X         | -        | -       | -                |
| 60  | PEV  | BA    | 530  | X         | -        | -       | -                |
| 60  | PEV  | BA    | 533  | -         | -        | X       | -                |
| 60  | PEV  | BA    | 535  | X         | -        | -       | -                |
| 60  | PEV  | BA    | 537  | X         | -        | -       | -                |
| 60  | PEV  | BA    | 538  | X         | -        | -       | -                |
| 60  | PEV  | BB    | 202  | X         | -        | -       | -                |
| 60  | PEV  | BB    | 206  | X         | -        | -       | -                |
| 61  | PGV  | A0    | 304  | X         | -        | -       | -                |
| 61  | PGV  | A0    | 305  | X         | -        | -       | -                |
| 61  | PGV  | A0    | 306  | X         | -        | -       | -                |
| 61  | PGV  | A0    | 317  | X         | -        | -       | -                |
| 61  | PGV  | A0    | 318  | X         | -        | -       | -                |
| 61  | PGV  | A0    | 325  | X         | -        | -       | -                |
| 61  | PGV  | A0    | 327  | X         | -        | -       | -                |
| 61  | PGV  | A0    | 328  | X         | -        | -       | -                |
| 61  | PGV  | A0    | 331  | X         | -        | -       | -                |
| 61  | PGV  | A0    | 332  | X         | -        | -       | -                |
| 61  | PGV  | A1    | 303  | X         | -        | -       | -                |
| 61  | PGV  | A1    | 311  | X         | -        | -       | -                |
| 61  | PGV  | A1    | 315  | X         | -        | -       | -                |
| 61  | PGV  | A1    | 318  | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 61  | PGV  | AZ    | 205  | X         | -        | -       | -                |
| 61  | PGV  | AZ    | 207  | X         | -        | -       | -                |
| 61  | PGV  | B8    | 3005 | X         | -        | -       | -                |
| 61  | PGV  | BA    | 501  | X         | -        | -       | -                |
| 61  | PGV  | BA    | 505  | X         | -        | -       | -                |
| 61  | PGV  | BA    | 512  | X         | -        | -       | -                |
| 61  | PGV  | BA    | 515  | X         | -        | -       | -                |
| 61  | PGV  | BA    | 516  | X         | -        | -       | -                |
| 61  | PGV  | BA    | 522  | X         | -        | -       | -                |
| 61  | PGV  | BA    | 536  | X         | -        | -       | -                |
| 61  | PGV  | BA    | 540  | X         | -        | -       | -                |
| 61  | PGV  | BB    | 203  | X         | -        | -       | -                |
| 61  | PGV  | BB    | 204  | X         | -        | -       | -                |
| 61  | PGV  | BB    | 205  | X         | -        | -       | -                |
| 61  | PGV  | BB    | 207  | X         | -        | -       | -                |
| 61  | PGV  | BB    | 208  | X         | -        | -       | -                |
| 61  | PGV  | BB    | 213  | X         | -        | -       | -                |
| 61  | PGV  | BB    | 217  | X         | -        | -       | -                |

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 163040 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    | 1542     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 33080 | 14754 | 6064 | 10720 | 1542 |         |       |

- Molecule 2 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 2   | AX    | 11       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 231   | 103 | 39 | 78 | 11 |         |       |

- Molecule 3 is a RNA chain called FtsQ nascent chain.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | AV    | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1649  | 733 | 297 | 542 | 77 |         |       |

- Molecule 4 is a protein called Cell division protein FtsQ.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | AZ    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 779   | 496 | 142 | 138 | 3 |         |       |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| AZ    | 104     | GLN      | -      | EXPRESSION TAG | UNP Q8X9Y5 |
| AZ    | 105     | HIS      | -      | EXPRESSION TAG | UNP Q8X9Y5 |
| AZ    | 106     | ALA      | -      | EXPRESSION TAG | UNP Q8X9Y5 |
| AZ    | 107     | ARG      | -      | EXPRESSION TAG | UNP Q8X9Y5 |
| AZ    | 108     | LEU      | -      | EXPRESSION TAG | UNP Q8X9Y5 |
| AZ    | 109     | ASP      | -      | EXPRESSION TAG | UNP Q8X9Y5 |
| AZ    | 110     | LYS      | -      | EXPRESSION TAG | UNP Q8X9Y5 |
| AZ    | 111     | PRO      | -      | EXPRESSION TAG | UNP Q8X9Y5 |
| AZ    | 112     | GLY      | -      | EXPRESSION TAG | UNP Q8X9Y5 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| AZ    | 113     | ALA      | -      | EXPRESSION TAG | UNP Q8X9Y5 |
| AZ    | 114     | ARG      | -      | EXPRESSION TAG | UNP Q8X9Y5 |
| AZ    | 115     | HIS      | -      | EXPRESSION TAG | UNP Q8X9Y5 |
| AZ    | 116     | PRO      | -      | EXPRESSION TAG | UNP Q8X9Y5 |
| AZ    | 117     | CYS      | -      | EXPRESSION TAG | UNP Q8X9Y5 |
| AZ    | 118     | TRP      | -      | EXPRESSION TAG | UNP Q8X9Y5 |
| AZ    | 119     | PRO      | -      | EXPRESSION TAG | UNP Q8X9Y5 |

- Molecule 5 is a protein called Apolipoprotein A-I.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | A0    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1640  | 1028 | 290 | 319 | 3 |         |       |
| 5   | A1    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1640  | 1028 | 290 | 319 | 3 |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | AB    | 240      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1872  | 1180 | 332 | 352 | 8 |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | AC    | 232      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1822  | 1149 | 346 | 323 | 4 |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | AD    | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | AE    | 166      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1225  | 761 | 232 | 226 | 6 |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S6.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | AF    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1101  | 677 | 198 | 219 | 7 |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | AG    | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1400  | 874 | 269 | 253 | 4 |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | AH    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | AI    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1036  | 642 | 208 | 183 | 3 |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | AJ    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 825   | 514 | 158 | 151 | 2 |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | AK    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 965   | 595 | 196 | 171 | 3 |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | AL    | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | AM    | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 910   | 564 | 183 | 160 | 3 |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | AN    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | AO    | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 716   | 440 | 146 | 129 | 1 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| AO    | 79      | ARG      | GLN    | CONFLICT | UNP P0ADZ4 |

- Molecule 20 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | AP    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | AQ    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 672   | 425 | 124 | 120 | 3 |         |       |

- Molecule 22 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | AR    | 74       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 626   | 395 | 123 | 107 | 1 |         |       |

- Molecule 23 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | AS    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 727   | 464 | 139 | 122 | 2 |         |       |

- Molecule 24 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | AT    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 414 | 138 | 115 | 3 |         |       |

- Molecule 25 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 25  | AU    | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 590   | 366 | 125 | 98 | 1 |         |       |

- Molecule 26 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 26  | B7    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2570  | 1144 | 468 | 838 | 120 |         |       |

- Molecule 27 is a RNA chain called 23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 27  | B8    | 2904     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62341 | 27810 | 11469 | 20158 | 2904 |         |       |

- Molecule 28 is a protein called Preprotein translocase secY subunit.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 28  | BA    | 435      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3362  | 2221 | 553 | 571 | 17 |         |       |

- Molecule 29 is a protein called Preprotein translocase secE subunit.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | BB    | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 889   | 587 | 154 | 145 | 3 |         |       |

- 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 L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 31  | B6    | 272      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2092  | 1294 | 425 | 366 | 7 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | BD    | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | BE    | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | BF    | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1420  | 905 | 251 | 258 | 6 |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | BG    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | BH    | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | BI    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | BJ    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | BK    | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 947   | 593 | 181 | 167 | 6 |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | BL    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 654 | 207 | 190 | 2 |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | BM    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | BN    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1008  | 621 | 204 | 178 | 5 |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | BO    | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 900   | 557 | 179 | 163 | 1 |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | BP    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | BQ    | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |   |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | BR    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | BS    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | BT    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 787   | 496 | 146 | 143 | 2 |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | BU    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 789   | 498 | 148 | 143 |   |         |       |

- Molecule 50 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | BV    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | BW    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 634   | 391 | 129 | 113 | 1 |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | BX    | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 53  | BY    | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 54  | BZ    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 55  | B0    | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

- Molecule 56 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 56  | B1    | 54       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 441   | 284 | 81 | 76 |         |       |

- Molecule 57 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 57  | B2    | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

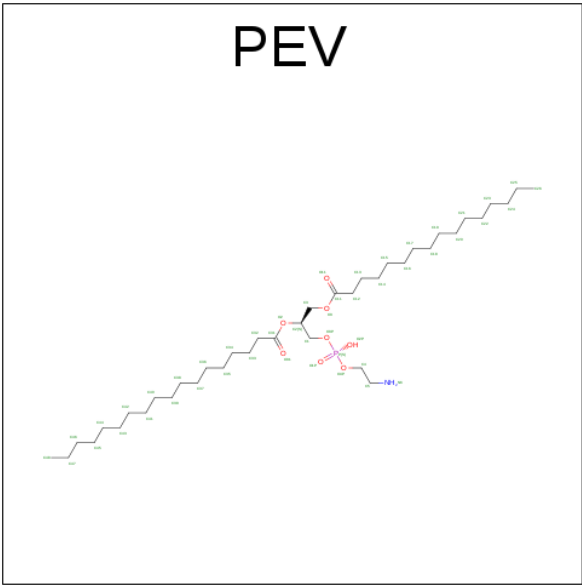
- Molecule 58 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 58  | B3    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 59 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 59  | B4    | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 60 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: C<sub>39</sub>H<sub>78</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf |
|-----|-------|----------|-------|-----|----|-----|----|---------|
| 60  | AZ    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 245   | 195 | 5  | 40  | 5  |         |
| 60  | AZ    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 245   | 195 | 5  | 40  | 5  |         |
| 60  | AZ    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 245   | 195 | 5  | 40  | 5  |         |
| 60  | AZ    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 245   | 195 | 5  | 40  | 5  |         |
| 60  | AZ    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 245   | 195 | 5  | 40  | 5  |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |

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| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf |
|-----|-------|----------|-------|-----|----|-----|----|---------|
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A0    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1078  | 858 | 22 | 176 | 22 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |

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| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf |
|-----|-------|----------|-------|-----|----|-----|----|---------|
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C   | N  | O   | P  | 0       |
|     |       |          | 1225  | 975 | 25 | 200 | 25 |         |

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| Mol | Chain | Residues | Atoms |      |    |     |    | AltConf |
|-----|-------|----------|-------|------|----|-----|----|---------|
| 60  | A1    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1225  | 975  | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1225  | 975  | 25 | 200 | 25 |         |
| 60  | A1    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1225  | 975  | 25 | 200 | 25 |         |
| 60  | B8    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 294   | 234  | 6  | 48  | 6  |         |
| 60  | B8    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 294   | 234  | 6  | 48  | 6  |         |
| 60  | B8    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 294   | 234  | 6  | 48  | 6  |         |
| 60  | B8    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 294   | 234  | 6  | 48  | 6  |         |
| 60  | B8    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 294   | 234  | 6  | 48  | 6  |         |
| 60  | B8    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 294   | 234  | 6  | 48  | 6  |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |

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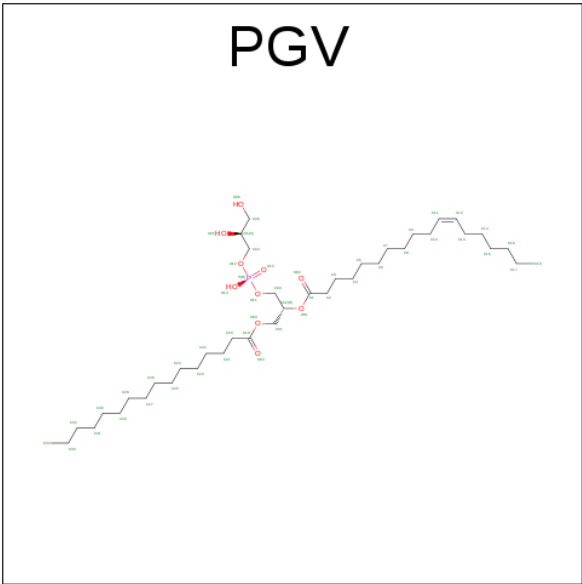
| Mol | Chain | Residues | Atoms |      |    |     |    | AltConf |
|-----|-------|----------|-------|------|----|-----|----|---------|
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BA    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 1568  | 1248 | 32 | 256 | 32 |         |
| 60  | BB    | 1        | Total | C    | N  | O   | P  | 0       |
|     |       |          | 539   | 429  | 11 | 88  | 11 |         |

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| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf |
|-----|-------|----------|-------|-----|----|----|----|---------|
| 60  | BB    | 1        | Total | C   | N  | O  | P  | 0       |
|     |       |          | 539   | 429 | 11 | 88 | 11 |         |
| 60  | BB    | 1        | Total | C   | N  | O  | P  | 0       |
|     |       |          | 539   | 429 | 11 | 88 | 11 |         |
| 60  | BB    | 1        | Total | C   | N  | O  | P  | 0       |
|     |       |          | 539   | 429 | 11 | 88 | 11 |         |
| 60  | BB    | 1        | Total | C   | N  | O  | P  | 0       |
|     |       |          | 539   | 429 | 11 | 88 | 11 |         |
| 60  | BB    | 1        | Total | C   | N  | O  | P  | 0       |
|     |       |          | 539   | 429 | 11 | 88 | 11 |         |
| 60  | BB    | 1        | Total | C   | N  | O  | P  | 0       |
|     |       |          | 539   | 429 | 11 | 88 | 11 |         |
| 60  | BB    | 1        | Total | C   | N  | O  | P  | 0       |
|     |       |          | 539   | 429 | 11 | 88 | 11 |         |
| 60  | BB    | 1        | Total | C   | N  | O  | P  | 0       |
|     |       |          | 539   | 429 | 11 | 88 | 11 |         |

- Molecule 61 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



| Mol | Chain | Residues | Atoms |     |     |    | AltConf |
|-----|-------|----------|-------|-----|-----|----|---------|
| 61  | AZ    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 102   | 80  | 20  | 2  |         |
| 61  | AZ    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 102   | 80  | 20  | 2  |         |
| 61  | A0    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 510   | 400 | 100 | 10 |         |
| 61  | A0    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 510   | 400 | 100 | 10 |         |
| 61  | A0    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 510   | 400 | 100 | 10 |         |
| 61  | A0    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 510   | 400 | 100 | 10 |         |
| 61  | A0    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 510   | 400 | 100 | 10 |         |
| 61  | A0    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 510   | 400 | 100 | 10 |         |
| 61  | A0    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 510   | 400 | 100 | 10 |         |
| 61  | A0    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 510   | 400 | 100 | 10 |         |
| 61  | A0    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 510   | 400 | 100 | 10 |         |
| 61  | A1    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 204   | 160 | 40  | 4  |         |
| 61  | A1    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 204   | 160 | 40  | 4  |         |
| 61  | A1    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 204   | 160 | 40  | 4  |         |
| 61  | A1    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 204   | 160 | 40  | 4  |         |
| 61  | B8    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 51    | 40  | 10  | 1  |         |
| 61  | BA    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 408   | 320 | 80  | 8  |         |
| 61  | BA    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 408   | 320 | 80  | 8  |         |
| 61  | BA    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 408   | 320 | 80  | 8  |         |
| 61  | BA    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 408   | 320 | 80  | 8  |         |
| 61  | BA    | 1        | Total | C   | O   | P  | 0       |
|     |       |          | 408   | 320 | 80  | 8  |         |

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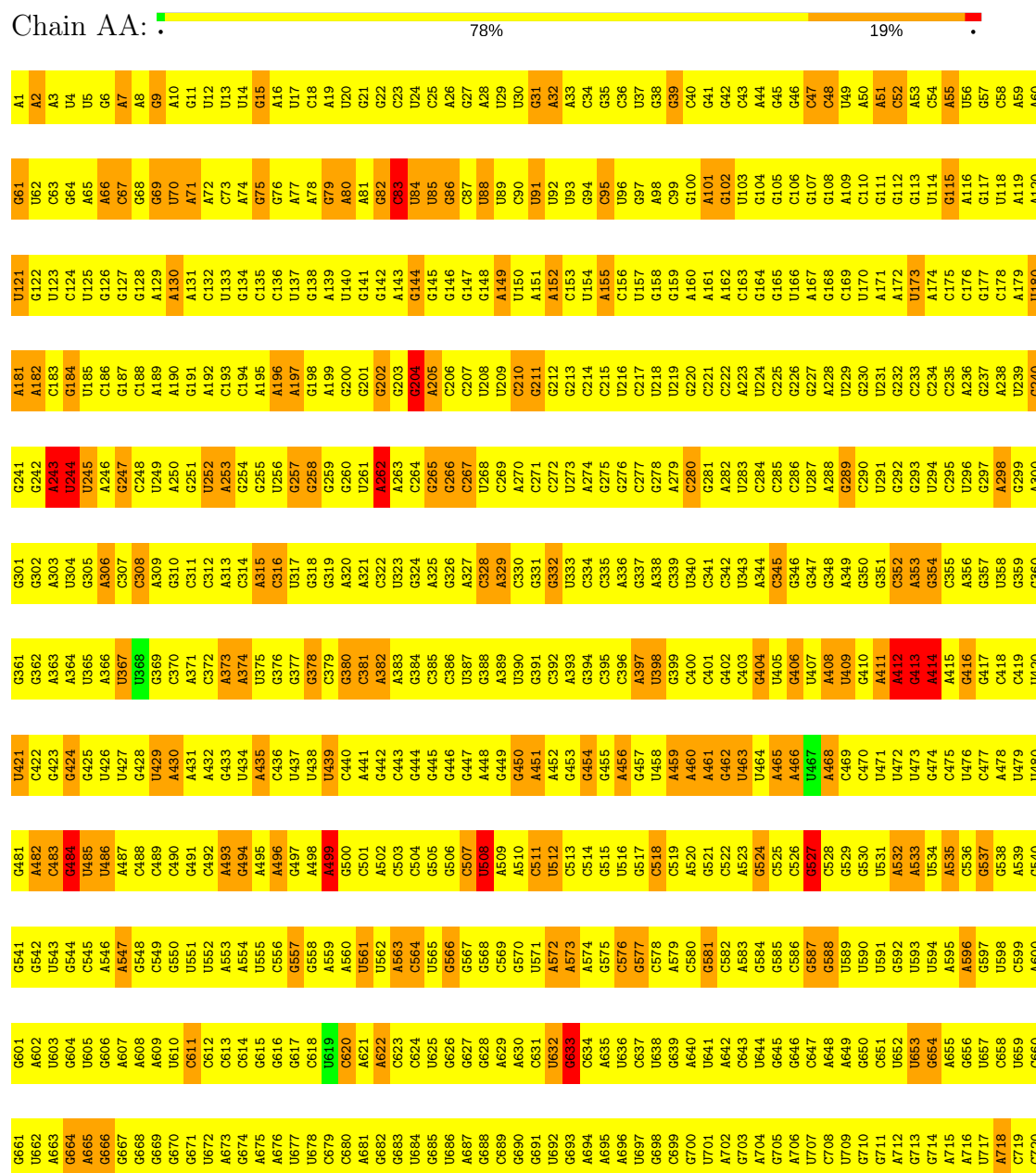
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| Mol | Chain | Residues | Atoms |     |    |   | AltConf |
|-----|-------|----------|-------|-----|----|---|---------|
| 61  | BA    | 1        | Total | C   | O  | P | 0       |
|     |       |          | 408   | 320 | 80 | 8 |         |
| 61  | BA    | 1        | Total | C   | O  | P | 0       |
|     |       |          | 408   | 320 | 80 | 8 |         |
| 61  | BA    | 1        | Total | C   | O  | P | 0       |
|     |       |          | 408   | 320 | 80 | 8 |         |
| 61  | BB    | 1        | Total | C   | O  | P | 0       |
|     |       |          | 357   | 280 | 70 | 7 |         |
| 61  | BB    | 1        | Total | C   | O  | P | 0       |
|     |       |          | 357   | 280 | 70 | 7 |         |
| 61  | BB    | 1        | Total | C   | O  | P | 0       |
|     |       |          | 357   | 280 | 70 | 7 |         |
| 61  | BB    | 1        | Total | C   | O  | P | 0       |
|     |       |          | 357   | 280 | 70 | 7 |         |
| 61  | BB    | 1        | Total | C   | O  | P | 0       |
|     |       |          | 357   | 280 | 70 | 7 |         |
| 61  | BB    | 1        | Total | C   | O  | P | 0       |
|     |       |          | 357   | 280 | 70 | 7 |         |

### 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





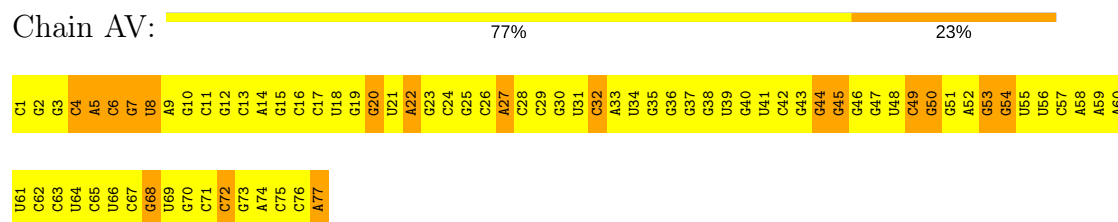
|       |       |       |       |       |       |       |       |       |       |      |      |      |      |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|
| A1502 | G1442 | C1382 | C1322 | C1262 | U1202 | G1142 | A1082 | A1022 | C962  | G902 | C841 | A781 | G721 |
| A1503 | C1443 | C1383 | G1323 | C1263 | C1203 | G1143 | U1083 | U1023 | G963  | G903 | U842 | A782 | G722 |
| G1504 | U1444 | C1384 | A1324 | U1264 | A1204 | G1144 | G1084 | G1024 | U964  | U904 | U843 | C783 | G723 |
| U1505 | U1445 | G1385 | C1325 | C1265 | U1205 | U1145 | U1085 | U1025 | U965  | U905 | G844 | A784 | G724 |
| A1506 | A1446 | G1386 | U1326 | G1266 | G1206 | A1146 | U1086 | G1026 | G966  | A906 | A845 | G785 | G725 |
| A1507 | A1447 | G1387 | C1327 | G1267 | G1207 | C1147 | G1087 | G1027 | C967  | A907 | G846 | G786 | G726 |
| A1508 | C1448 | C1388 | C1328 | G1268 | C1208 | U1148 | G1088 | U1028 | A968  | A908 | G847 | A787 | G727 |
| U1509 | C1449 | C1389 | A1329 | A1269 | C1209 | C1149 | G1089 | C1029 | A969  | A909 | C848 | U788 | A728 |
| C1510 | U1450 | U1390 | U1330 | G1270 | C1210 | A1150 | U1090 | U1030 | C970  | C910 | G849 | U789 | A729 |
| U1511 | U1451 | G1391 | A1331 | A1271 | U1211 | A1151 | U1091 | C1031 | G971  | U850 | U790 | A790 | G730 |
| U1512 | C1452 | G1392 | A1332 | G1272 | U1212 | A1152 | A1092 | G1032 | C972  | C912 | G851 | G791 | G731 |
| A1513 | G1453 | U1393 | A1333 | A1273 | A1213 | G1153 | A1093 | G1033 | G973  | A913 | G852 | A792 | C732 |
| G1514 | A1454 | A1394 | A1334 | A1274 | C1214 | G1154 | G1094 | G1034 | A974  | A914 | C853 | U793 | C733 |
| G1515 | G1455 | C1395 | U1335 | A1275 | G1215 | A1155 | U1095 | A1035 | A975  | A915 | U854 | A794 | G734 |
| G1516 | A1456 | A1396 | C1336 | G1276 | A1216 | G1156 | C1096 | A1036 | G976  | U916 | U855 | C795 | C735 |
| G1517 | G1457 | C1397 | G1337 | C1277 | C1217 | A1157 | C1097 | C1037 | A977  | G917 | C856 | C796 | C736 |
| A1518 | G1458 | A1398 | G1338 | G1278 | C1218 | U1158 | C1098 | A1038 | A978  | A918 | C857 | C797 | C737 |
| A1519 | G1459 | C1399 | A1339 | G1279 | A1219 | U1159 | G1099 | G1039 | C979  | A919 | G858 | U798 | C738 |
| C1520 | C1460 | U1400 | A1340 | A1280 | G1220 | G1160 | C1100 | U1040 | C980  | U920 | G859 | G799 | C739 |
| C1521 | G1461 | G1401 | U1341 | C1281 | G1221 | C1161 | A1101 | G1041 | U981  | U921 | A860 | G800 | U740 |
| U1522 | C1462 | C1402 | G1342 | U1282 | G1222 | C1162 | A1102 | A1042 | U982  | G922 | G861 | U801 | G741 |
| G1523 | U1463 | G1403 | G1343 | U1283 | C1223 | A1163 | C1103 | G1043 | A983  | A923 | C862 | A802 | G742 |
| C1524 | U1464 | C1404 | C1344 | C1284 | U1224 | G1164 | G1104 | A1044 | C984  | C924 | U863 | G803 | A743 |
| G1525 | A1465 | U1405 | A1345 | A1285 | A1225 | U1165 | A1105 | C1045 | C985  | G925 | A864 | U804 | C744 |
| G1526 | C1466 | G1406 | G1346 | U1286 | G1226 | G1166 | G1106 | A1046 | U986  | G926 | A865 | C805 | G745 |
| U1527 | C1467 | C1407 | G1347 | A1287 | A1227 | A1167 | C1107 | G1047 | C987  | G927 | C866 | C806 | A746 |
| U1528 | A1468 | A1408 | U1348 | U1288 | C1228 | U1168 | G1108 | G1048 | G988  | G928 | G867 | A807 | A747 |
| G1529 | C1469 | C1409 | A1349 | A1289 | A1229 | U1169 | C1109 | U1049 | U989  | G929 | C868 | C808 | G748 |
| G1530 | U1470 | A1410 | A1350 | G1290 | C1230 | A1170 | A1110 | G1050 | C990  | C930 | G869 | C809 | A749 |
| A1531 | A1471 | C1411 | U1351 | U1291 | G1231 | A1171 | A1111 | C1051 | U991  | C931 | C810 | C750 | C750 |
| U1532 | U1472 | C1412 | C1352 | G1292 | U1232 | C1172 | G1112 | U1052 | U992  | C932 | C811 | C751 | U751 |
| C1533 | G1473 | A1413 | G1353 | C1293 | G1233 | U1173 | C1113 | G1053 | G993  | C933 | A872 | G752 | G752 |
| A1534 | U1474 | U1414 | U1354 | G1294 | C1234 | C1174 | C1114 | C1054 | A994  | C934 | A873 | A753 | A753 |
| C1535 | G1475 | G1415 | G1355 | U1295 | C1235 | G1175 | U1115 | A1055 | C995  | A935 | U875 | A814 | G754 |
| C1536 | A1476 | G1416 | G1356 | C1296 | A1236 | U1176 | U1116 | U1056 | C996  | C936 | C876 | A815 | G755 |
| U1537 | U1477 | G1417 | A1357 | G1297 | C1237 | G1177 | A1117 | G1057 | U997  | A937 | G877 | A816 | C756 |
| G1538 | U1478 | A1418 | U1358 | U1298 | A1238 | G1178 | U1118 | G1058 | C998  | A938 | A878 | C817 | U757 |
| C1539 | C1479 | G1419 | C1359 | A1299 | A1239 | A1179 | C1119 | C1059 | C999  | C939 | G818 | G818 | C758 |
| U1540 | A1480 | U1420 | A1360 | G1300 | U1240 | A1180 | C1120 | U1060 | A1000 | C940 | C880 | A819 | A759 |
| U1541 | U1481 | G1421 | G1361 | U1301 | G1241 | G1181 | U1121 | G1061 | C1001 | G941 | G881 | U820 | G760 |
| A1542 | G1482 | G1422 | A1362 | C1302 | G1242 | G1182 | U1122 | U1062 | G1002 | G942 | C882 | G821 | U761 |
|       | A1483 | G1423 | A1363 | C1303 | C1243 | U1183 | U1123 | C1063 | G1003 | U943 | C883 | U822 | U762 |
|       | C1484 | U1424 | G1364 | G1304 | G1244 | G1184 | G1124 | G1064 | A1004 | G944 | U884 | C823 | G763 |
|       | U1485 | U1425 | G1365 | G1305 | C1245 | G1185 | U1125 | U1065 | A1005 | G945 | G885 | G824 | C764 |
|       | G1486 | G1426 | C1366 | A1306 | A1246 | G1186 | U1126 | C1066 | G886  | A946 | G886 | A825 | G765 |
|       | G1487 | C1427 | C1367 | U1307 | U1247 | G1187 | A1067 | A1067 | G887  | G947 | G887 | C826 | A766 |
|       | G1488 | A1428 | A1368 | U1308 | A1248 | A1188 | G1068 | U1008 | C888  | C948 | G888 | U827 | A767 |
|       | G1489 | C1429 | C1369 | G1309 | C1249 | U1189 | C1069 | U1009 | A889  | A949 | A889 | U828 | A768 |
|       | U1490 | A1430 | G1370 | G1310 | A1250 | G1190 | A1130 | U1010 | G890  | U950 | G890 | G829 | G769 |
|       | G1491 | C1431 | G1371 | A1311 | A1251 | A1191 | G1131 | C1071 | U891  | G951 | U891 | G830 | C770 |
|       | A1492 | G1432 | U1372 | G1312 | A1252 | C1192 | C1132 | G1072 | A892  | U952 | A892 | A831 | G771 |
|       | A1493 | A1433 | G1373 | U1313 | G1253 | G1193 | G1133 | U1073 | C893  | G953 | C893 | G832 | G772 |
|       | G1494 | A1434 | A1374 | C1314 | A1254 | U1194 | G1134 | G1074 | A894  | G954 | G894 | G833 | G773 |
|       | U1495 | G1435 | A1375 | U1315 | G1255 | C1195 | U1135 | U1075 | G895  | U955 | G895 | U834 | G774 |
|       | C1496 | U1436 | G1376 | G1316 | A1256 | A1196 | C1136 | U1076 | A896  | U956 | C896 | U835 | G775 |
|       | G1497 | A1437 | U1377 | C1317 | A1257 | A1197 | C1137 | G1077 | C897  | U957 | C897 | G836 | G776 |
|       | U1498 | G1438 | C1378 | A1318 | G1258 | G1198 | G1138 | U1078 | A898  | A958 | G898 | U837 | A777 |
|       | A1499 | U1439 | G1379 | C1319 | C1259 | U1199 | G1139 | G1079 | C899  | A959 | C899 | G838 | G778 |
|       | U1500 | U1440 | U1380 | C1320 | G1260 | C1200 | A1080 | A1080 | A900  | U960 | A900 | C779 | C779 |
|       | C1501 | A1441 | U1381 | U1321 | A1261 | A1201 | C1141 | A1081 | A1021 | U961 | A901 | C840 | A780 |

• Molecule 2: mRNA

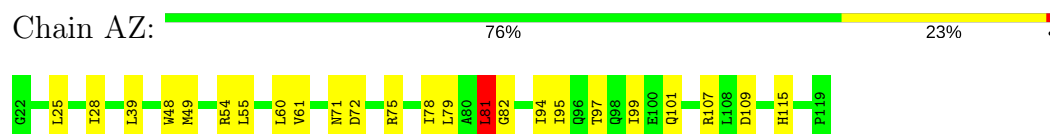
Chain AX: 9% 45% 45%

|     |
|-----|
| U12 |
| C13 |
| G14 |
| C15 |
| C16 |
| C17 |
| C18 |
| U19 |
| G20 |
| A21 |
| A22 |

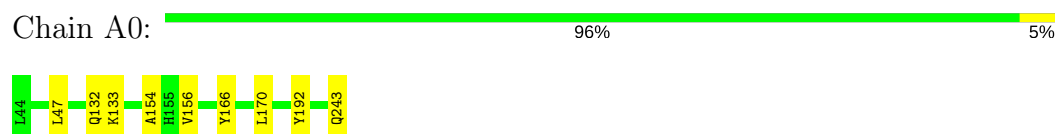
- Molecule 3: FtsQ nascent chain



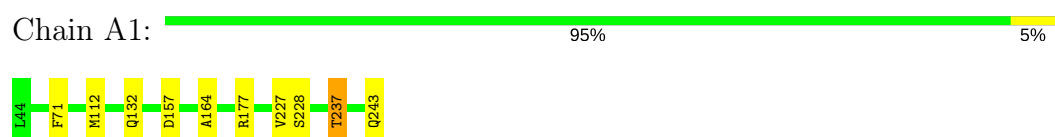
- Molecule 4: Cell division protein FtsQ



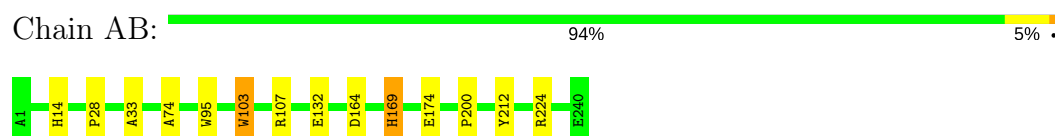
- Molecule 5: Apolipoprotein A-I



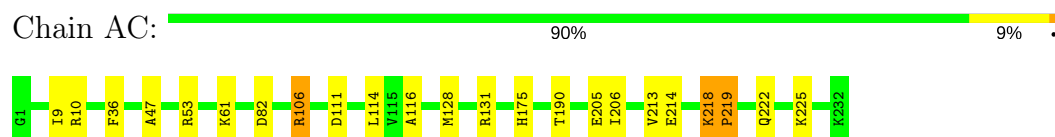
- Molecule 5: Apolipoprotein A-I



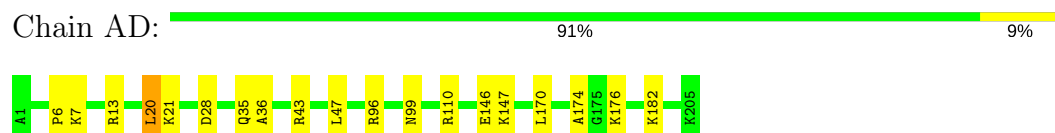
- Molecule 6: 30S ribosomal protein S2



- Molecule 7: 30S ribosomal protein S3



- Molecule 8: 30S ribosomal protein S4



## • Molecule 9: 30S ribosomal protein S5

Chain AE:  94% 5%

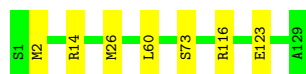
## • Molecule 10: 30S ribosomal protein S6

Chain AF:  93% 7%

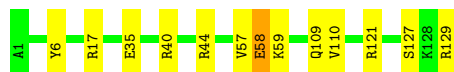
## • Molecule 11: 30S ribosomal protein S7

Chain AG:  97%


## • Molecule 12: 30S ribosomal protein S8

Chain AH:  95% 5%

## • Molecule 13: 30S ribosomal protein S9

Chain AI:  90% 9%

## • Molecule 14: 30S ribosomal protein S10

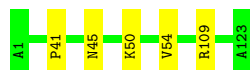
Chain AJ:  88% 12%

## • Molecule 15: 30S ribosomal protein S11

Chain AK:  94% 6%

## • Molecule 16: 30S ribosomal protein S12

Chain AL:  96% .



- Molecule 17: 30S ribosomal protein S13

Chain AM:  92% 7% .



- Molecule 18: 30S ribosomal protein S14

Chain AN:  88% 12%



- Molecule 19: 30S ribosomal protein S15

Chain AO:  97% ..




- Molecule 20: 30S ribosomal protein S16

Chain AP:  95% ..



- Molecule 21: 30S ribosomal protein S17

Chain AQ:  87% 13%



- Molecule 22: 30S ribosomal protein S18

Chain AR:  92% 8%



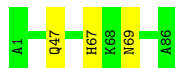
- Molecule 23: 30S ribosomal protein S19

Chain AS:  96% .



- Molecule 24: 30S ribosomal protein S20

Chain AT: 97%



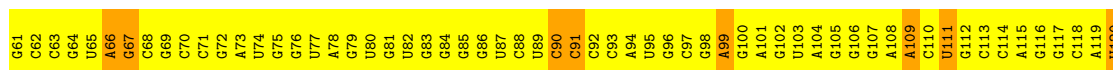
- Molecule 25: 30S ribosomal protein S21

Chain AU: 94%



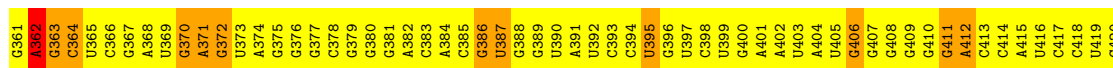
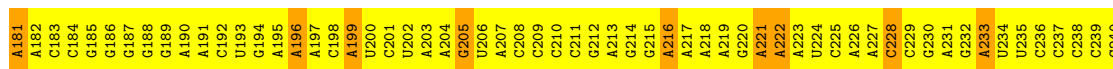
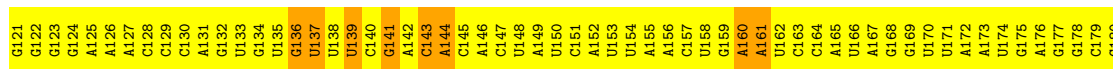
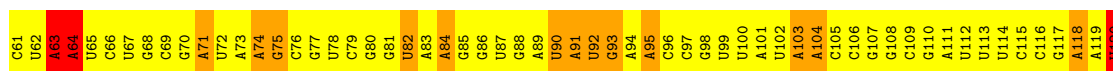
- Molecule 26: 5S RIBOSOMAL RNA

Chain B7: 82%



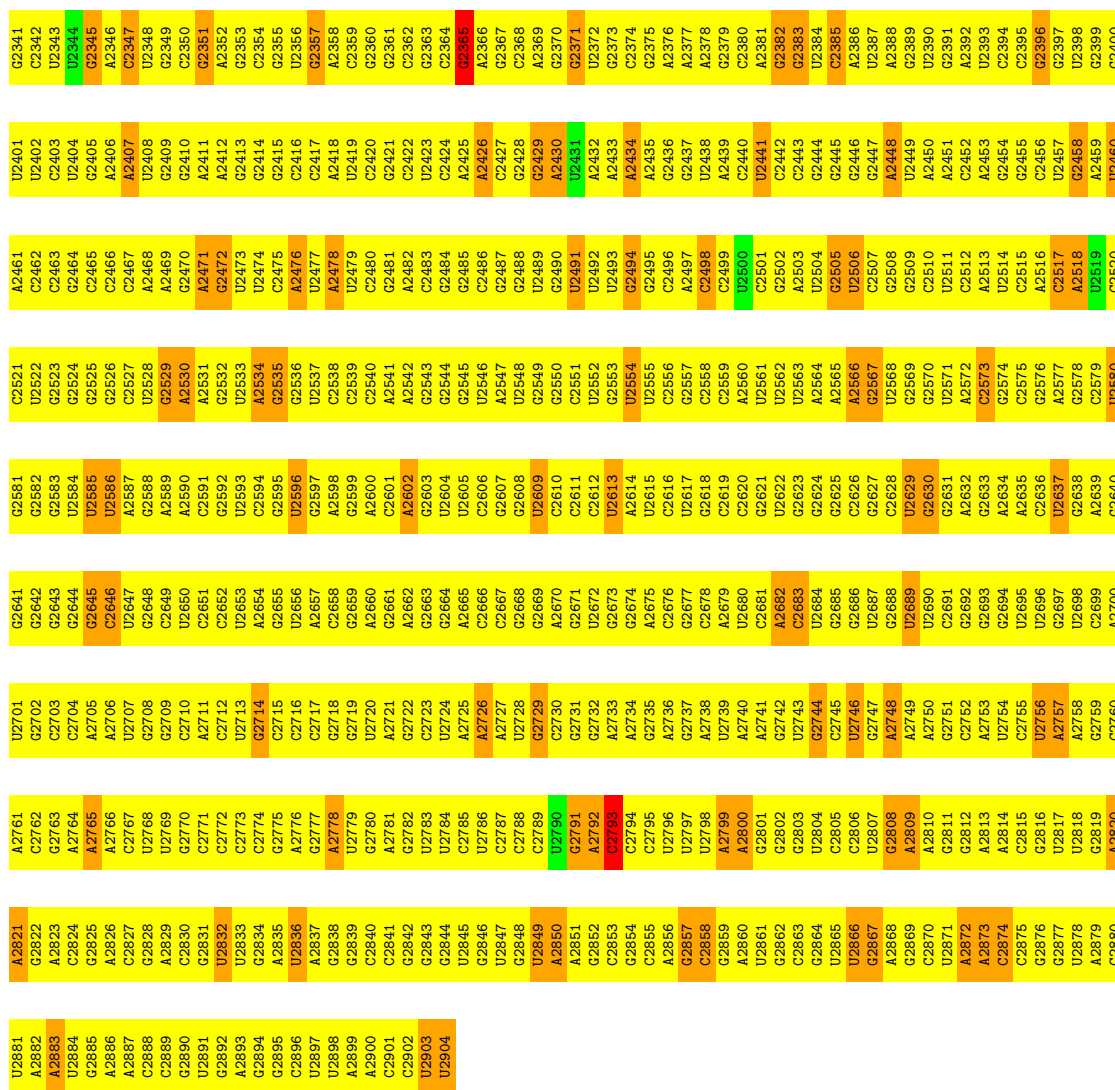
- Molecule 27: 23S RIBOSOMAL RNA

Chain B8: 80%



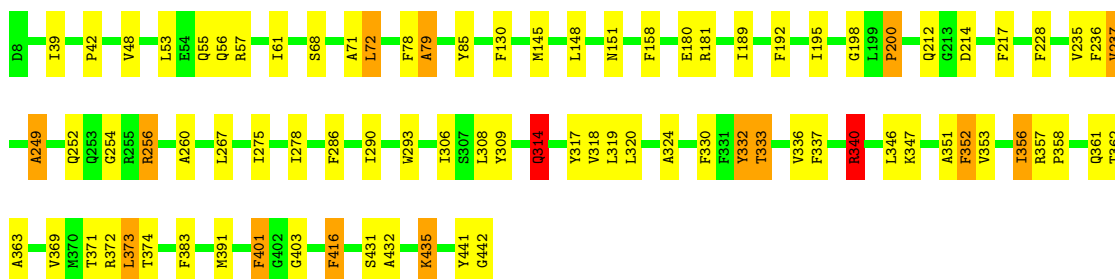
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| A1321 | C1261 | U1201 | U1141 | U1081 | A1021 | C961  | C901 | G841 | A781 | A721 | A661 | G601 | A541 | C481 | C421 |
| A1322 | A1262 | G1202 | A1142 | U1082 | G1022 | G962  | C902 | U842 | A782 | A722 | G662 | A602 | C942 | A482 | A422 |
| C1323 | A1263 | A1203 | A1143 | U1083 | G1023 | U963  | C903 | G843 | A783 | C723 | G663 | A603 | C943 | A483 | A423 |
| G1324 | A1264 | A1204 | A1144 | U1084 | G1024 | U964  | C904 | A844 | G784 | C724 | G664 | G604 | C944 | A484 | G424 |
| U1325 | A1265 | A1205 | C1145 | A1085 | G1025 | C965  | A905 | U845 | G785 | C725 | U665 | U606 | U546 | C485 | G426 |
| U1326 | G1266 | G1206 | C1146 | U1086 | G1026 | G966  | U906 | U846 | G786 | C726 | A666 | U607 | U547 | C486 | C427 |
| A1327 | U1267 | C1207 | A1147 | G1087 | A1027 | U967  | G907 | U847 | C787 | A727 | U667 | U607 | A547 | C487 | U427 |
| A1328 | A1268 | C1208 | U1148 | A1088 | A1028 | C968  | C908 | C848 | A788 | C728 | A668 | A608 | G548 | C488 | A428 |
| U1329 | A1269 | U1209 | G1149 | U1089 | A1029 | G969  | U909 | A849 | A789 | C729 | G669 | A609 | G549 | C489 | A429 |
| C1330 | C1270 | G1210 | A1150 | U1090 | C1030 | U970  | A910 | U850 | U790 | A730 | A670 | C610 | C550 | C490 | U430 |
| G1331 | G1271 | C1211 | A1151 | G1091 | G1031 | G971  | A911 | C851 | C791 | C731 | C671 | C611 | C551 | C491 | U431 |
| C1332 | A1272 | G1212 | C1152 | C1092 | A1032 | A972  | C912 | U852 | A792 | C732 | C672 | G612 | U552 | A492 | A432 |
| U1333 | U1273 | A1213 | C1153 | G1093 | U1033 | A973  | C913 | U853 | A793 | C733 | C673 | A613 | C553 | C493 | C433 |
| G1334 | A1274 | A1214 | G1154 | U1094 | G1034 | G974  | G914 | C854 | A794 | A734 | G674 | A614 | U554 | C494 | U434 |
| C1335 | A1275 | G1215 | A1155 | A1095 | U1035 | A975  | C915 | G855 | C795 | A735 | A675 | U615 | G555 | C495 | C435 |
| A1336 | A1276 | G1216 | A1156 | U1096 | G1036 | G976  | G916 | G856 | A676 | C736 | A676 | A616 | A556 | C496 | C436 |
| G1337 | G1277 | U1217 | U1157 | U1097 | G1037 | G977  | A917 | G857 | G797 | C737 | A677 | C617 | C557 | A497 | U437 |
| C1338 | C1278 | G1218 | C1158 | U1098 | G1038 | G978  | A918 | G858 | G798 | C738 | C678 | G618 | U558 | C498 | C438 |
| U1339 | G1279 | U1219 | U1159 | G1099 | A1039 | A979  | U919 | G859 | G799 | A739 | C679 | G619 | G559 | U499 | A439 |
| U1340 | G1280 | G1220 | G1160 | C1100 | A1040 | A980  | A920 | U860 | A800 | C740 | C680 | G620 | C560 | G500 | C440 |
| G1341 | G1281 | C1221 | C1161 | U1101 | G1041 | A981  | C921 | A861 | G801 | C741 | C681 | A621 | G561 | A501 | U441 |
| A1342 | U1282 | U1222 | G1162 | C1102 | G1042 | C982  | C922 | G862 | A802 | A742 | G682 | G622 | U562 | A502 | G442 |
| C1343 | G1283 | G1223 | G1163 | A1103 | C1043 | A983  | G923 | A863 | U803 | C743 | U683 | C623 | A563 | A503 | A443 |
| U1344 | A1284 | U1224 | C1164 | C1104 | C1044 | A984  | G924 | G864 | A804 | C744 | G684 | C624 | C564 | A504 | C444 |
| C1345 | A1285 | G1225 | A1165 | U1105 | C1045 | C985  | A925 | C865 | G805 | C745 | A685 | G625 | C565 | A505 | C445 |
| A1346 | A1286 | A1226 | G1166 | G1106 | A1046 | C986  | G926 | A866 | C906 | C746 | U686 | A626 | U566 | G506 | G446 |
| A1347 | G1287 | G1227 | C1167 | U1107 | G1047 | C987  | A927 | C867 | U807 | C747 | C687 | A627 | U567 | A507 | A447 |
| C1348 | A1288 | G1228 | G1168 | U1108 | A1048 | A988  | A928 | U868 | G808 | C748 | U688 | G628 | U568 | A508 | U448 |
| G1349 | C1289 | C1229 | A1169 | C1109 | C1049 | G989  | U929 | G869 | G809 | A749 | A689 | G629 | U569 | C509 | A449 |
| C1350 | C1290 | G1170 | C1170 | G1110 | A1050 | A990  | G930 | U870 | U810 | C750 | G690 | G630 | C570 | C510 | C450 |
| U1351 | C1291 | U1231 | G1171 | A1111 | G1051 | C991  | U931 | U871 | U811 | C751 | C691 | A631 | U571 | U511 | U451 |
| U1352 | G1292 | G1232 | C1172 | G1112 | C1052 | C992  | U932 | U872 | C812 | C752 | C692 | A632 | A572 | G512 | G452 |
| A1353 | C1293 | C1233 | U1173 | U1113 | G993  | C993  | A933 | G873 | C813 | C753 | U693 | A633 | U573 | A513 | A453 |
| U1354 | A1294 | U1234 | A1174 | C1114 | A1054 | C994  | G934 | G874 | C814 | C754 | U694 | C634 | A574 | A514 | A454 |
| G1355 | C1295 | G1235 | A1175 | G1115 | G1055 | C995  | C935 | G875 | C815 | C755 | G695 | C635 | A575 | A515 | C455 |
| C1356 | G1296 | U1236 | U1176 | G1116 | G1056 | A996  | A936 | C876 | C816 | C756 | G696 | G636 | U576 | C516 | C456 |
| U1357 | A1297 | G1237 | G1177 | U1177 | A1057 | G997  | C937 | A877 | C817 | C757 | G697 | A637 | G577 | C517 | A457 |
| G1358 | C1298 | G1238 | C1178 | C1118 | U1058 | C998  | G938 | A878 | G818 | C758 | C698 | G638 | G578 | G518 | G458 |
| A1359 | G1299 | G1239 | G1179 | U1119 | G1059 | U999  | G939 | G879 | A819 | C759 | A699 | U639 | G579 | U519 | U459 |
| C1360 | G1300 | U1240 | U1180 | G1120 | U1060 | A1000 | G940 | G880 | A820 | C760 | G700 | C640 | U580 | G520 | A460 |
| G1361 | A1301 | A1241 | U1181 | C1121 | U1061 | A1001 | A941 | G881 | A821 | C761 | G701 | U641 | C581 | U521 | C461 |
| C1362 | A1302 | U1242 | G1182 | G1122 | G1062 | G1002 | G942 | G882 | G822 | C762 | U702 | A582 | A582 | A522 | C462 |
| G1363 | C1303 | C1243 | U1183 | C1123 | G1063 | G1003 | A943 | G883 | C823 | C763 | U703 | A643 | G583 | C523 | G463 |
| A1364 | A1304 | A1244 | U1184 | G1124 | C1064 | U1004 | C944 | U884 | U824 | C764 | G704 | A644 | C584 | G524 | U464 |
| C1365 | C1305 | G1245 | G1185 | G1125 | U1065 | C1005 | A945 | C885 | A825 | C765 | A705 | C645 | G585 | U525 | G465 |
| A1366 | C1306 | A1246 | G1186 | A1126 | U1066 | C1006 | C946 | A886 | U826 | C766 | A706 | U646 | A586 | A526 | A466 |
| A1367 | A1307 | A1247 | U1187 | A1127 | A1067 | C1007 | A947 | U887 | U827 | C767 | G707 | G647 | C587 | C527 | G467 |
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| A1373 | U1313 | A1253 | A1193 | A1133 | C1073 | C1013 | G953 | C893 | A833 | C773 | G713 | U653 | U593 | G533 | G473 |
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| U1379 | C1319 | G1259 | U1199 | U1139 | U1079 | U1019 | A959 | C899 | U839 | C779 | A719 | G659 | A599 | A479 | A479 |
| G1380 | C1320 | A1260 | C1200 | C1140 | A1080 | A1020 | A960 | A900 | C940 | C780 | U720 | C660 | G600 | C540 | A480 |

|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
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| A2284 | G2224 | C2164 | C2104 | C2044 | G1984 | C1924 | U1864 | C1804 | A1744 | U1684 | U1624 | C1564 | A1504 | G1444 | A1384 |
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| A2297 | G2237 | C2177 | A2117 | G2057 | C1997 | A1937 | A1877 | G1817 | A1757 | G1697 | A1637 | U1577 | G1517 | U1457 | U1397 |
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| A2301 | A2241 | U2181 | G2121 | G2061 | C2001 | A1941 | C1881 | A1821 | C1761 | A1701 | A1641 | G1581 | U1521 | C1461 | G1401 |
| U2302 | G2242 | U2182 | U2122 | A2062 | G2002 | C1942 | U1882 | G1822 | A1762 | G1702 | G1642 | C1582 | A1522 | C1462 | U1402 |
| G2303 | C2243 | A2183 | G2123 | C2063 | A2003 | U1943 | U1883 | G1823 | G1763 | C1703 | G1643 | A1583 | U1523 | C1463 | A1403 |
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| U2305 | U2245 | U2185 | G2125 | C2065 | A2005 | G1945 | A1885 | U1825 | U1765 | A1705 | G1645 | C1585 | A1525 | G1465 | U1405 |
| G2306 | G2246 | G2186 | A2126 | C2066 | C2006 | U1946 | U1886 | G1826 | G1766 | C1706 | C1646 | A1586 | C1526 | U1466 | U1406 |
| G2307 | A2247 | U2187 | G2127 | G2067 | U2007 | G1947 | G1887 | U1827 | G1767 | U1707 | U1647 | G1587 | G1527 | U1467 | G1407 |
| G2308 | C2248 | U2188 | G2128 | U2068 | C2008 | G1948 | G1888 | G1828 | C1768 | C1708 | U1648 | A1588 | A1528 | U1468 | A1408 |
| A2309 | U2249 | U2189 | C2129 | G2069 | A2009 | G1949 | A1889 | A1829 | U1769 | U1709 | G1649 | U1589 | G1529 | A1469 | U1409 |
| C2310 | G2250 | G2190 | U2130 | A2070 | C2010 | G1950 | A1890 | C1830 | G1770 | G1710 | A1650 | A1590 | G1530 | C1470 | U1410 |
| A2311 | G2251 | A2191 | U2131 | A2071 | U2011 | U1951 | G1891 | G1831 | C1771 | U1711 | G1651 | A1591 | C1531 | G1471 | U1411 |
| G2252 | C2252 | U2192 | U2132 | C2072 | A1952 | A1952 | C1892 | G1832 | A1772 | U1712 | A1652 | C1592 | A1532 | C1472 | U1412 |
| G2313 | G2253 | C2193 | C2133 | C2073 | G2013 | A1953 | C1893 | G1833 | A1773 | U1713 | G1653 | A1593 | C1533 | C1473 | A1413 |
| A2314 | C2254 | U2194 | A2134 | U2074 | G1954 | A1954 | C1894 | G1834 | C1774 | U1714 | A1654 | U1594 | A1534 | U1474 | A1414 |
| G2315 | G2255 | U2195 | A2135 | U2075 | A2015 | G1955 | C1895 | G1835 | U1775 | G1715 | A1655 | C1595 | A1535 | G1475 | U1415 |
| G2316 | G2256 | C2196 | G2136 | U2076 | U2016 | U1956 | G1896 | C1836 | G1776 | U1716 | C1656 | A1596 | C1536 | U1476 | G1416 |
| A2317 | U2257 | U2197 | U2137 | A2077 | U2017 | G1957 | G1897 | C1837 | U1777 | U1717 | U1657 | A1597 | G1537 | U1477 | C1417 |
| G2318 | C2258 | A2198 | G2138 | C2078 | G2018 | C1958 | U1898 | C1838 | U1778 | G1718 | C1658 | A1598 | G1538 | G1478 | A1418 |
| G2319 | U2259 | A2199 | U2139 | U2079 | A2019 | G1959 | A1899 | G1839 | U1779 | G1719 | G1659 | U1599 | U1539 | G1479 | A1419 |
| C2320 | C2260 | C2200 | G2140 | A2080 | A2020 | A1960 | A1900 | G1840 | A1780 | U1720 | G1660 | C1600 | G1540 | C1480 | A1420 |
| U2321 | G2261 | G2201 | G2141 | U2081 | C2021 | C1961 | A1901 | U1841 | U1781 | G1721 | G1661 | G1601 | C1541 | U1481 | G1421 |
| U2322 | U2262 | U2202 | A2142 | A2082 | U2022 | C1962 | C1902 | G1842 | U1782 | A1722 | G1662 | U1602 | U1542 | G1482 | G1422 |
| G2323 | C2263 | G2203 | C2143 | G2083 | C2023 | U1963 | G1903 | C1843 | A1783 | G1723 | G1663 | A1603 | G1543 | G1483 | G1423 |
| C2324 | G2264 | U2204 | G2144 | C2084 | G2024 | G1964 | G1904 | C1844 | A1784 | G1724 | A1664 | C1604 | A1544 | U1484 | G1424 |
| G2325 | U2265 | A2205 | C2145 | U2085 | C2025 | C1965 | C1905 | G1845 | A1785 | U1725 | A1665 | C1605 | A1545 | U1485 | G1425 |
| A2266 | C2266 | C2206 | C2146 | U2086 | U2026 | A1966 | G1906 | G1846 | A1786 | G1726 | G1666 | C1606 | A1546 | U1486 | G1426 |
| A2327 | A2267 | C2207 | A2147 | G2087 | G2027 | C1967 | G1907 | A1847 | A1787 | G1727 | G1667 | C1607 | C1547 | U1487 | A1427 |
| A2328 | A2268 | C2208 | G2148 | A2088 | U2028 | G1968 | C1908 | A1848 | C1788 | G1728 | A1668 | A1608 | A1548 | C1488 | A1428 |
| G2329 | G2269 | G2209 | U2149 | C2089 | G2029 | A1969 | C1909 | G1849 | A1789 | U1729 | A1669 | A1609 | A1549 | G1489 | G1429 |
| G2330 | A2270 | U2210 | C2150 | A2090 | A2030 | U1970 | G1910 | G1850 | C1790 | G1730 | C1670 | A1610 | A1550 | A1490 | G1430 |
| G2331 | G2271 | A2211 | U2151 | C2091 | A2031 | U1971 | U1911 | U1851 | A1791 | G1731 | U1671 | C1611 | A1551 | G1491 | A1431 |
| C2332 | U2272 | A2212 | G2152 | U2092 | G2032 | A1972 | A1912 | U1852 | A1792 | C1732 | A1672 | C1612 | A1552 | G1492 | G1432 |
| A2333 | A2273 | U2213 | C2153 | A2093 | A2033 | G1973 | A1913 | A1853 | G1793 | G1733 | G1673 | C1613 | A1553 | C1493 | A1433 |
| U2334 | A2274 | C2214 | A2154 | A2094 | U2034 | C1974 | A1914 | A1854 | A1794 | G1734 | G1674 | A1614 | U1554 | A1494 | A1434 |
| G2335 | C2275 | G2215 | A2155 | A2095 | G2035 | G1975 | U1915 | U1855 | A1795 | A1735 | C1675 | G1615 | C1555 | A1495 | G1435 |
| A2336 | G2276 | G2216 | U2156 | C2096 | G2036 | U1976 | A1916 | U1856 | U1796 | U1736 | A1676 | A1616 | C1556 | A1496 | G1436 |
| G2337 | G2277 | G2217 | G2157 | A2097 | A2037 | A1977 | U1917 | G1857 | G1797 | G1737 | A1677 | C1617 | C1557 | U1497 | C1437 |
| C2338 | A2278 | G2218 | A2158 | U2098 | G2038 | A1978 | A1918 | A1858 | U1798 | G1738 | A1678 | A1618 | C1558 | C1498 | U1438 |
| G2339 | G2279 | U2219 | C2159 | U2099 | U2039 | A1979 | A1919 | U1859 | G1799 | A1739 | A1679 | U1559 | U1559 | A1439 | G1439 |
| A2340 | G2280 | U2220 | C2160 | G2100 | G2040 | G1980 | G1860 | G1800 | G1740 | G1680 | G1620 | G1560 | G1500 | G1440 |       |



- Molecule 28: Preprotein translocase secY subunit

Chain BA:  80% 16% 4%



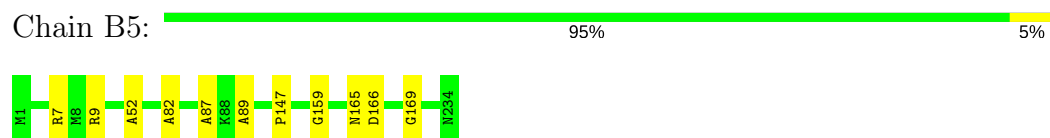
- Molecule 29: Preprotein translocase secE subunit

Chain BB:  89% 10%

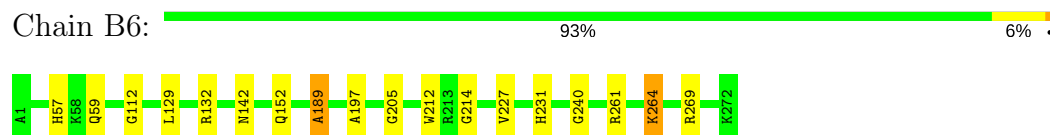




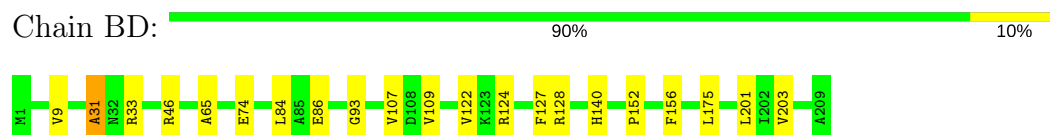
- Molecule 30: 50S ribosomal protein L1



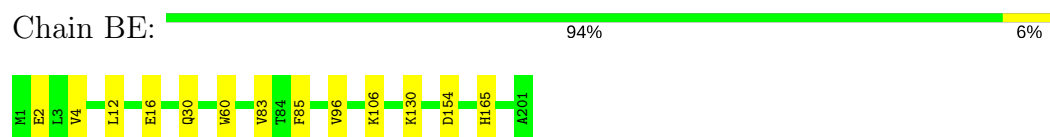
- Molecule 31: 50S ribosomal protein L2



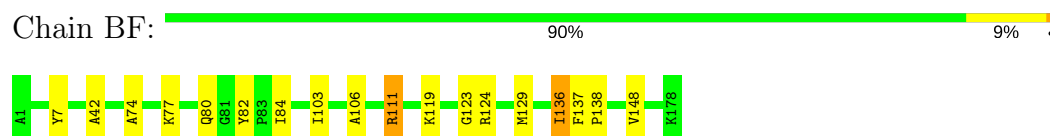
- Molecule 32: 50S ribosomal protein L3



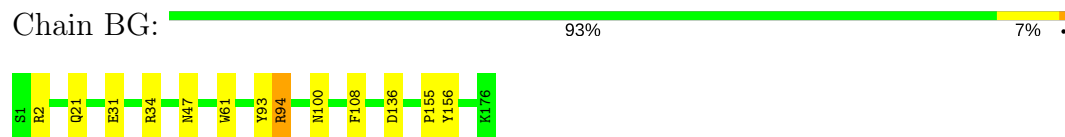
- Molecule 33: 50S ribosomal protein L4



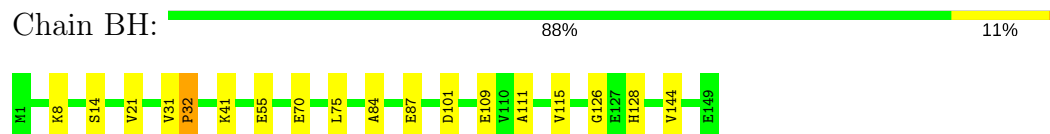
- Molecule 34: 50S ribosomal protein L5



- Molecule 35: 50S ribosomal protein L6

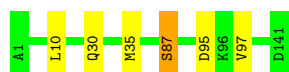


- Molecule 36: 50S ribosomal protein L9



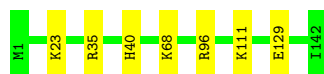
- Molecule 37: 50S ribosomal protein L11

Chain BI:  96% ..



- Molecule 38: 50S ribosomal protein L13

Chain BJ:  95% 5%



- Molecule 39: 50S ribosomal protein L14

Chain BK:  91% 9%



- Molecule 40: 50S ribosomal protein L15

Chain BL:  97% ..



- Molecule 41: 50S ribosomal protein L16

Chain BM:  92% 7% .



- Molecule 42: 50S ribosomal protein L17

Chain BN:  89% 11%



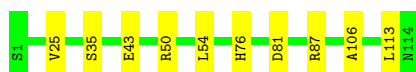
- Molecule 43: 50S ribosomal protein L18

Chain BO:  97% .



- Molecule 44: 50S ribosomal protein L19

Chain BP:  91% 9%



- Molecule 45: 50S ribosomal protein L20

Chain BQ: 94% 6%



- Molecule 46: 50S ribosomal protein L21

Chain BR: 94% 5%



- Molecule 47: 50S ribosomal protein L22

Chain BS: 92% 7%



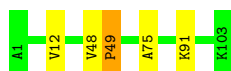
- Molecule 48: 50S ribosomal protein L23

Chain BT: 89% 9%



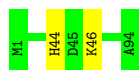
- Molecule 49: 50S ribosomal protein L24

Chain BU: 95%



- Molecule 50: 50S ribosomal protein L25

Chain BV: 98%



- Molecule 51: 50S ribosomal protein L27

Chain BW: 94% 6%



- Molecule 52: 50S ribosomal protein L28

Chain BX:  91% 9%



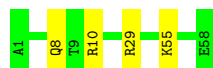
- Molecule 53: 50S ribosomal protein L29

Chain BY:  95% 5%



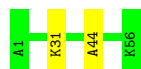
- Molecule 54: 50S ribosomal protein L30

Chain BZ:  93% 7%



- Molecule 55: 50S ribosomal protein L32

Chain B0:  96% 4%




- Molecule 56: 50S ribosomal protein L33

Chain B1:  94% 6%



- Molecule 57: 50S ribosomal protein L34

Chain B2:  87% 11% 2%



- Molecule 58: 50S ribosomal protein L35

Chain B3:  94% 6%



- Molecule 59: 50S ribosomal protein L36

Chain B4:  92% 8%



## 4 Experimental information

| Property                             | Value                 | Source    |
|--------------------------------------|-----------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE       | Depositor |
| Imposed symmetry                     | POINT, Not provided   | Depositor |
| Number of particles used             | 85664                 | Depositor |
| Resolution determination method      | Not provided          | Depositor |
| CTF correction method                | DEFOCUS GROUP VOLUMES | Depositor |
| Microscope                           | FEI Polara 300        | Depositor |
| Voltage (kV)                         | 300                   | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 22                    | Depositor |
| Minimum defocus (nm)                 | 1000                  | Depositor |
| Maximum defocus (nm)                 | 4500                  | Depositor |
| Magnification                        | 38000                 | Depositor |
| Image detector                       | Kodak SO163           | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PGV, PEV

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    | 1.60         | 46/37039 (0.1%)  | 2.50        | 4339/57778 (7.5%)  |
| 10  | AF    | 0.99         | 0/1121           | 1.06        | 0/1509             |
| 11  | AG    | 1.03         | 0/1422           | 1.01        | 2/1908 (0.1%)      |
| 12  | AH    | 0.96         | 0/989            | 1.01        | 0/1326             |
| 13  | AI    | 1.12         | 0/1048           | 1.01        | 0/1394             |
| 14  | AJ    | 1.03         | 0/835            | 1.03        | 0/1127             |
| 15  | AK    | 1.05         | 0/982            | 1.05        | 0/1323             |
| 16  | AL    | 1.07         | 0/969            | 1.01        | 0/1300             |
| 17  | AM    | 1.05         | 0/919            | 0.99        | 1/1226 (0.1%)      |
| 18  | AN    | 1.07         | 0/817            | 1.05        | 1/1088 (0.1%)      |
| 19  | AO    | 1.06         | 0/724            | 0.92        | 0/966              |
| 2   | AX    | 1.56         | 0/256            | 2.32        | 28/394 (7.1%)      |
| 20  | AP    | 1.07         | 0/659            | 1.03        | 0/884              |
| 21  | AQ    | 0.99         | 0/681            | 1.05        | 0/913              |
| 22  | AR    | 1.14         | 0/637            | 1.05        | 2/851 (0.2%)       |
| 23  | AS    | 0.96         | 0/744            | 0.96        | 0/995              |
| 24  | AT    | 0.96         | 0/676            | 0.94        | 0/895              |
| 25  | AU    | 1.18         | 0/598            | 0.99        | 0/792              |
| 26  | B7    | 1.59         | 2/2873 (0.1%)    | 2.49        | 325/4478 (7.3%)    |
| 27  | B8    | 1.60         | 100/69822 (0.1%) | 2.50        | 8171/108926 (7.5%) |
| 28  | BA    | 1.68         | 7/3439 (0.2%)    | 1.14        | 15/4662 (0.3%)     |
| 29  | BB    | 0.98         | 1/902 (0.1%)     | 1.05        | 1/1228 (0.1%)      |
| 3   | AV    | 1.61         | 1/1842 (0.1%)    | 2.43        | 211/2870 (7.4%)    |
| 30  | B5    | 0.92         | 0/1748           | 0.97        | 0/2355             |
| 31  | B6    | 1.04         | 0/2131           | 1.03        | 1/2863 (0.0%)      |
| 32  | BD    | 0.97         | 0/1586           | 1.08        | 4/2134 (0.2%)      |
| 33  | BE    | 0.95         | 0/1571           | 1.01        | 2/2113 (0.1%)      |
| 34  | BF    | 1.01         | 0/1444           | 1.06        | 1/1937 (0.1%)      |
| 35  | BG    | 0.96         | 0/1343           | 1.06        | 4/1816 (0.2%)      |
| 36  | BH    | 0.93         | 0/1122           | 1.05        | 0/1515             |
| 37  | BI    | 0.86         | 0/1046           | 1.00        | 1/1410 (0.1%)      |
| 38  | BJ    | 0.97         | 0/1152           | 1.01        | 0/1551             |

| Mol | Chain | Bond lengths |                   | Bond angles |                     |
|-----|-------|--------------|-------------------|-------------|---------------------|
|     |       | RMSZ         | # Z  >2           | RMSZ        | # Z  >2             |
| 39  | BK    | 1.03         | 0/956             | 1.03        | 0/1279              |
| 4   | AZ    | 0.98         | 0/795             | 1.16        | 0/1082              |
| 40  | BL    | 1.04         | 0/1062            | 0.98        | 1/1413 (0.1%)       |
| 41  | BM    | 1.03         | 0/1093            | 1.06        | 2/1460 (0.1%)       |
| 42  | BN    | 1.10         | 0/1021            | 1.03        | 1/1364 (0.1%)       |
| 43  | BO    | 1.07         | 0/910             | 0.98        | 0/1219              |
| 44  | BP    | 1.06         | 0/929             | 1.03        | 0/1242              |
| 45  | BQ    | 1.09         | 0/960             | 1.00        | 2/1278 (0.2%)       |
| 46  | BR    | 1.01         | 0/829             | 1.07        | 1/1107 (0.1%)       |
| 47  | BS    | 0.99         | 0/864             | 1.04        | 1/1156 (0.1%)       |
| 48  | BT    | 0.98         | 0/794             | 1.09        | 1/1060 (0.1%)       |
| 49  | BU    | 0.96         | 0/797             | 1.04        | 0/1062              |
| 5   | A0    | 0.96         | 1/1667 (0.1%)     | 0.95        | 3/2240 (0.1%)       |
| 5   | A1    | 0.97         | 1/1667 (0.1%)     | 0.95        | 0/2240              |
| 50  | BV    | 0.96         | 0/766             | 1.02        | 0/1025              |
| 51  | BW    | 1.04         | 0/642             | 1.05        | 0/848               |
| 52  | BX    | 1.09         | 0/635             | 1.04        | 0/848               |
| 53  | BY    | 1.00         | 0/510             | 0.90        | 0/677               |
| 54  | BZ    | 0.99         | 0/453             | 0.99        | 0/605               |
| 55  | B0    | 1.05         | 0/450             | 0.97        | 0/599               |
| 56  | B1    | 0.93         | 0/448             | 1.01        | 0/594               |
| 57  | B2    | 1.25         | 0/380             | 1.06        | 0/498               |
| 58  | B3    | 0.98         | 0/513             | 0.98        | 0/676               |
| 59  | B4    | 1.20         | 2/303 (0.7%)      | 1.03        | 0/397               |
| 6   | AB    | 0.92         | 0/1904            | 0.98        | 1/2565 (0.0%)       |
| 7   | AC    | 1.00         | 0/1852            | 1.06        | 1/2490 (0.0%)       |
| 8   | AD    | 1.04         | 0/1665            | 0.99        | 0/2227              |
| 9   | AE    | 0.97         | 0/1239            | 1.03        | 0/1664              |
| All | All   | 1.44         | 161/169241 (0.1%) | 2.16        | 13123/251442 (5.2%) |

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                   | 72                  |
| 12  | AH    | 0                   | 1                   |
| 13  | AI    | 0                   | 1                   |
| 26  | B7    | 0                   | 2                   |
| 27  | B8    | 0                   | 100                 |
| 28  | BA    | 0                   | 5                   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | AV    | 0                   | 2                   |
| 34  | BF    | 0                   | 1                   |
| 36  | BH    | 0                   | 1                   |
| 49  | BU    | 0                   | 1                   |
| 5   | A1    | 0                   | 1                   |
| 57  | B2    | 0                   | 1                   |
| 7   | AC    | 0                   | 1                   |
| All | All   | 0                   | 189                 |

All (161) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 28  | BA    | 416  | PHE  | CG-CD2  | 41.52 | 2.01        | 1.38     |
| 28  | BA    | 416  | PHE  | CG-CD1  | 39.62 | 1.98        | 1.38     |
| 28  | BA    | 416  | PHE  | CE2-CZ  | 30.78 | 1.95        | 1.37     |
| 28  | BA    | 416  | PHE  | CE1-CZ  | 30.54 | 1.95        | 1.37     |
| 28  | BA    | 416  | PHE  | CD2-CE2 | 27.89 | 1.95        | 1.39     |
| 28  | BA    | 416  | PHE  | CD1-CE1 | 26.46 | 1.92        | 1.39     |
| 27  | B8    | 2860 | A    | N7-C5   | -7.97 | 1.34        | 1.39     |
| 27  | B8    | 2378 | A    | N7-C5   | -7.45 | 1.34        | 1.39     |
| 1   | AA    | 1016 | A    | N7-C5   | -7.37 | 1.34        | 1.39     |
| 27  | B8    | 2111 | U    | C2-N3   | 7.37  | 1.43        | 1.37     |
| 5   | A0    | 243  | GLN  | C-OXT   | 7.34  | 1.37        | 1.23     |
| 28  | BA    | 442  | GLY  | C-OXT   | 7.34  | 1.37        | 1.23     |
| 5   | A1    | 243  | GLN  | C-OXT   | 7.32  | 1.37        | 1.23     |
| 29  | BB    | 127  | PHE  | C-OXT   | 7.29  | 1.37        | 1.23     |
| 27  | B8    | 1571 | A    | N7-C5   | -7.16 | 1.34        | 1.39     |
| 27  | B8    | 1213 | A    | N7-C5   | -7.09 | 1.34        | 1.39     |
| 1   | AA    | 190  | A    | N7-C5   | -7.09 | 1.34        | 1.39     |
| 1   | AA    | 162  | A    | N7-C5   | -6.95 | 1.35        | 1.39     |
| 27  | B8    | 633  | A    | N7-C5   | -6.93 | 1.35        | 1.39     |
| 1   | AA    | 487  | A    | N7-C5   | -6.92 | 1.35        | 1.39     |
| 27  | B8    | 1641 | A    | N7-C5   | -6.54 | 1.35        | 1.39     |
| 1   | AA    | 1005 | A    | N7-C5   | -6.34 | 1.35        | 1.39     |
| 27  | B8    | 705  | A    | N7-C5   | -6.32 | 1.35        | 1.39     |
| 1   | AA    | 1339 | A    | N7-C5   | -6.25 | 1.35        | 1.39     |
| 1   | AA    | 1468 | A    | N7-C5   | -6.24 | 1.35        | 1.39     |
| 26  | B7    | 73   | A    | N7-C5   | -6.23 | 1.35        | 1.39     |
| 27  | B8    | 1608 | A    | N7-C5   | -6.18 | 1.35        | 1.39     |
| 27  | B8    | 402  | A    | N7-C5   | -6.18 | 1.35        | 1.39     |
| 27  | B8    | 216  | A    | N7-C5   | -6.17 | 1.35        | 1.39     |
| 27  | B8    | 471  | A    | N7-C5   | -6.08 | 1.35        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 27  | B8    | 2225 | A    | N7-C5 | -6.08 | 1.35        | 1.39     |
| 1   | AA    | 495  | A    | N7-C5 | -6.06 | 1.35        | 1.39     |
| 1   | AA    | 119  | A    | N7-C5 | -6.05 | 1.35        | 1.39     |
| 27  | B8    | 820  | A    | N7-C5 | -6.03 | 1.35        | 1.39     |
| 1   | AA    | 1014 | A    | O3'-P | -6.01 | 1.53        | 1.61     |
| 27  | B8    | 2412 | A    | N7-C5 | -6.00 | 1.35        | 1.39     |
| 27  | B8    | 1469 | A    | N7-C5 | -5.99 | 1.35        | 1.39     |
| 27  | B8    | 1722 | A    | N7-C5 | -5.95 | 1.35        | 1.39     |
| 27  | B8    | 2366 | A    | N7-C5 | -5.95 | 1.35        | 1.39     |
| 27  | B8    | 1029 | A    | N7-C5 | -5.94 | 1.35        | 1.39     |
| 27  | B8    | 374  | A    | N7-C5 | -5.85 | 1.35        | 1.39     |
| 27  | B8    | 2082 | A    | N7-C5 | -5.84 | 1.35        | 1.39     |
| 27  | B8    | 1001 | A    | N7-C5 | -5.83 | 1.35        | 1.39     |
| 27  | B8    | 877  | A    | N7-C5 | -5.82 | 1.35        | 1.39     |
| 27  | B8    | 2352 | A    | N7-C5 | -5.82 | 1.35        | 1.39     |
| 27  | B8    | 310  | A    | N7-C5 | -5.82 | 1.35        | 1.39     |
| 27  | B8    | 1866 | A    | N7-C5 | -5.79 | 1.35        | 1.39     |
| 27  | B8    | 513  | A    | N7-C5 | -5.78 | 1.35        | 1.39     |
| 27  | B8    | 52   | A    | N7-C5 | -5.78 | 1.35        | 1.39     |
| 27  | B8    | 1572 | A    | N7-C5 | -5.75 | 1.35        | 1.39     |
| 27  | B8    | 1744 | A    | N7-C5 | -5.75 | 1.35        | 1.39     |
| 1   | AA    | 533  | A    | N7-C5 | -5.74 | 1.35        | 1.39     |
| 27  | B8    | 2435 | A    | N7-C5 | -5.70 | 1.35        | 1.39     |
| 1   | AA    | 327  | A    | N7-C5 | -5.69 | 1.35        | 1.39     |
| 1   | AA    | 1375 | A    | N7-C5 | -5.68 | 1.35        | 1.39     |
| 27  | B8    | 2587 | A    | N7-C5 | -5.67 | 1.35        | 1.39     |
| 27  | B8    | 371  | A    | N7-C5 | -5.66 | 1.35        | 1.39     |
| 1   | AA    | 909  | A    | N7-C5 | -5.64 | 1.35        | 1.39     |
| 1   | AA    | 151  | A    | N7-C5 | -5.63 | 1.35        | 1.39     |
| 27  | B8    | 2013 | A    | N7-C5 | -5.61 | 1.35        | 1.39     |
| 27  | B8    | 2335 | A    | N7-C5 | -5.60 | 1.35        | 1.39     |
| 27  | B8    | 2662 | A    | N7-C5 | -5.59 | 1.35        | 1.39     |
| 1   | AA    | 1170 | A    | N7-C5 | -5.58 | 1.35        | 1.39     |
| 59  | B4    | 27   | CYS  | CB-SG | 5.56  | 1.91        | 1.82     |
| 27  | B8    | 1286 | A    | N7-C5 | -5.55 | 1.35        | 1.39     |
| 27  | B8    | 1477 | A    | N7-C5 | -5.52 | 1.35        | 1.39     |
| 27  | B8    | 340  | A    | N7-C5 | -5.52 | 1.35        | 1.39     |
| 27  | B8    | 190  | A    | N7-C5 | -5.50 | 1.35        | 1.39     |
| 27  | B8    | 2268 | A    | N7-C5 | -5.50 | 1.35        | 1.39     |
| 27  | B8    | 1021 | A    | N7-C5 | -5.48 | 1.35        | 1.39     |
| 27  | B8    | 256  | A    | N7-C5 | -5.46 | 1.35        | 1.39     |
| 27  | B8    | 1872 | A    | N7-C5 | -5.46 | 1.35        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 59  | B4    | 11   | CYS  | CB-SG | 5.45  | 1.91        | 1.82     |
| 1   | AA    | 873  | A    | N7-C5 | -5.45 | 1.35        | 1.39     |
| 27  | B8    | 191  | A    | N7-C5 | -5.45 | 1.35        | 1.39     |
| 27  | B8    | 251  | A    | N7-C5 | -5.42 | 1.35        | 1.39     |
| 27  | B8    | 2430 | A    | N7-C5 | -5.42 | 1.35        | 1.39     |
| 27  | B8    | 1373 | A    | N7-C5 | -5.41 | 1.36        | 1.39     |
| 1   | AA    | 468  | A    | N7-C5 | -5.41 | 1.36        | 1.39     |
| 1   | AA    | 1055 | A    | N7-C5 | -5.41 | 1.36        | 1.39     |
| 1   | AA    | 383  | A    | N7-C5 | -5.39 | 1.36        | 1.39     |
| 27  | B8    | 973  | A    | N7-C5 | -5.39 | 1.36        | 1.39     |
| 27  | B8    | 1717 | A    | N7-C5 | -5.39 | 1.36        | 1.39     |
| 27  | B8    | 609  | A    | N7-C5 | -5.38 | 1.36        | 1.39     |
| 1   | AA    | 919  | A    | N7-C5 | -5.38 | 1.36        | 1.39     |
| 27  | B8    | 278  | A    | N7-C5 | -5.38 | 1.36        | 1.39     |
| 1   | AA    | 781  | A    | N7-C5 | -5.36 | 1.36        | 1.39     |
| 27  | B8    | 1802 | A    | N7-C5 | -5.36 | 1.36        | 1.39     |
| 27  | B8    | 1378 | A    | N7-C5 | -5.34 | 1.36        | 1.39     |
| 27  | B8    | 918  | A    | N7-C5 | -5.34 | 1.36        | 1.39     |
| 27  | B8    | 447  | A    | N7-C5 | -5.32 | 1.36        | 1.39     |
| 27  | B8    | 1970 | A    | N7-C5 | -5.32 | 1.36        | 1.39     |
| 1   | AA    | 171  | A    | N7-C5 | -5.31 | 1.36        | 1.39     |
| 27  | B8    | 556  | A    | N7-C5 | -5.30 | 1.36        | 1.39     |
| 27  | B8    | 2297 | A    | N7-C5 | -5.29 | 1.36        | 1.39     |
| 27  | B8    | 279  | A    | N7-C5 | -5.28 | 1.36        | 1.39     |
| 1   | AA    | 908  | A    | N7-C5 | -5.27 | 1.36        | 1.39     |
| 1   | AA    | 439  | U    | C2-N3 | 5.26  | 1.41        | 1.37     |
| 27  | B8    | 138  | U    | C2-N3 | 5.26  | 1.41        | 1.37     |
| 27  | B8    | 266  | G    | C2-N3 | 5.26  | 1.36        | 1.32     |
| 27  | B8    | 1439 | A    | N7-C5 | -5.26 | 1.36        | 1.39     |
| 27  | B8    | 1890 | A    | N7-C5 | -5.26 | 1.36        | 1.39     |
| 27  | B8    | 412  | A    | N7-C5 | -5.25 | 1.36        | 1.39     |
| 27  | B8    | 49   | A    | N7-C5 | -5.25 | 1.36        | 1.39     |
| 27  | B8    | 1470 | A    | N7-C5 | -5.25 | 1.36        | 1.39     |
| 1   | AA    | 55   | A    | N7-C5 | -5.25 | 1.36        | 1.39     |
| 27  | B8    | 917  | A    | N7-C5 | -5.24 | 1.36        | 1.39     |
| 26  | B7    | 99   | A    | N7-C5 | -5.24 | 1.36        | 1.39     |
| 27  | B8    | 1354 | A    | N7-C5 | -5.24 | 1.36        | 1.39     |
| 27  | B8    | 1237 | A    | N7-C5 | -5.23 | 1.36        | 1.39     |
| 27  | B8    | 428  | A    | N7-C5 | -5.22 | 1.36        | 1.39     |
| 27  | B8    | 2903 | U    | C2-N3 | 5.22  | 1.41        | 1.37     |
| 1   | AA    | 262  | A    | N7-C5 | -5.21 | 1.36        | 1.39     |
| 27  | B8    | 975  | A    | N7-C5 | -5.21 | 1.36        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | AA    | 498  | A    | N7-C5 | -5.21 | 1.36        | 1.39     |
| 1   | AA    | 1401 | G    | C2-N3 | 5.20  | 1.36        | 1.32     |
| 1   | AA    | 1306 | A    | N7-C5 | -5.17 | 1.36        | 1.39     |
| 27  | B8    | 879  | G    | C2-N3 | 5.17  | 1.36        | 1.32     |
| 27  | B8    | 1419 | A    | N7-C5 | -5.17 | 1.36        | 1.39     |
| 27  | B8    | 1580 | A    | N7-C5 | -5.16 | 1.36        | 1.39     |
| 27  | B8    | 1254 | A    | N7-C5 | -5.16 | 1.36        | 1.39     |
| 1   | AA    | 696  | A    | N7-C5 | -5.15 | 1.36        | 1.39     |
| 27  | B8    | 1340 | U    | C2-N3 | 5.15  | 1.41        | 1.37     |
| 27  | B8    | 2741 | A    | N7-C5 | -5.14 | 1.36        | 1.39     |
| 1   | AA    | 860  | A    | N7-C5 | -5.14 | 1.36        | 1.39     |
| 27  | B8    | 470  | A    | N7-C5 | -5.13 | 1.36        | 1.39     |
| 1   | AA    | 759  | A    | N7-C5 | -5.13 | 1.36        | 1.39     |
| 27  | B8    | 713  | G    | C2-N3 | 5.13  | 1.36        | 1.32     |
| 1   | AA    | 69   | G    | N1-C2 | 5.13  | 1.41        | 1.37     |
| 1   | AA    | 1483 | A    | N7-C5 | -5.12 | 1.36        | 1.39     |
| 1   | AA    | 753  | A    | N7-C5 | -5.12 | 1.36        | 1.39     |
| 27  | B8    | 2029 | G    | C2-N3 | 5.12  | 1.36        | 1.32     |
| 1   | AA    | 653  | U    | C2-N3 | 5.12  | 1.41        | 1.37     |
| 1   | AA    | 115  | G    | C2-N3 | 5.12  | 1.36        | 1.32     |
| 27  | B8    | 1    | G    | C2-N3 | 5.12  | 1.36        | 1.32     |
| 27  | B8    | 699  | A    | N7-C5 | -5.11 | 1.36        | 1.39     |
| 27  | B8    | 2748 | A    | N7-C5 | -5.10 | 1.36        | 1.39     |
| 1   | AA    | 1261 | A    | N7-C5 | -5.10 | 1.36        | 1.39     |
| 27  | B8    | 2171 | A    | N7-C5 | -5.10 | 1.36        | 1.39     |
| 27  | B8    | 2077 | A    | N7-C5 | -5.10 | 1.36        | 1.39     |
| 1   | AA    | 116  | A    | N7-C5 | -5.09 | 1.36        | 1.39     |
| 27  | B8    | 1690 | A    | N7-C5 | -5.09 | 1.36        | 1.39     |
| 1   | AA    | 1077 | G    | N1-C2 | 5.08  | 1.41        | 1.37     |
| 1   | AA    | 1288 | A    | N7-C5 | -5.08 | 1.36        | 1.39     |
| 27  | B8    | 1395 | A    | N7-C5 | -5.07 | 1.36        | 1.39     |
| 27  | B8    | 1932 | A    | N7-C5 | -5.07 | 1.36        | 1.39     |
| 1   | AA    | 1255 | G    | C2-N3 | 5.07  | 1.36        | 1.32     |
| 27  | B8    | 2511 | U    | C2-N3 | 5.06  | 1.41        | 1.37     |
| 1   | AA    | 282  | A    | N7-C5 | -5.06 | 1.36        | 1.39     |
| 27  | B8    | 1634 | A    | N7-C5 | -5.06 | 1.36        | 1.39     |
| 27  | B8    | 1848 | A    | N7-C5 | -5.05 | 1.36        | 1.39     |
| 1   | AA    | 1316 | G    | C2-N3 | 5.05  | 1.36        | 1.32     |
| 27  | B8    | 1027 | A    | N7-C5 | -5.04 | 1.36        | 1.39     |
| 27  | B8    | 2199 | A    | N7-C5 | -5.03 | 1.36        | 1.39     |
| 27  | B8    | 1803 | A    | N7-C5 | -5.03 | 1.36        | 1.39     |
| 1   | AA    | 1365 | G    | C2-N3 | 5.03  | 1.36        | 1.32     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 27  | B8    | 2566 | A    | N7-C5 | -5.02 | 1.36        | 1.39     |
| 27  | B8    | 2033 | A    | N7-C5 | -5.01 | 1.36        | 1.39     |
| 3   | AV    | 40   | G    | N1-C2 | 5.01  | 1.41        | 1.37     |
| 27  | B8    | 2405 | G    | C2-N3 | 5.00  | 1.36        | 1.32     |
| 27  | B8    | 2592 | G    | C2-N3 | 5.00  | 1.36        | 1.32     |

All (13123) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | AA    | 85   | U    | P-O3'-C3' | 19.51 | 143.11      | 119.70   |
| 27  | B8    | 670  | A    | P-O3'-C3' | 17.35 | 140.52      | 119.70   |
| 27  | B8    | 2076 | U    | P-O3'-C3' | 15.69 | 138.53      | 119.70   |
| 27  | B8    | 6    | A    | N1-C6-N6  | 14.72 | 127.43      | 118.60   |
| 1   | AA    | 1252 | A    | N1-C6-N6  | 14.43 | 127.26      | 118.60   |
| 27  | B8    | 449  | A    | N1-C6-N6  | 14.43 | 127.26      | 118.60   |
| 1   | AA    | 328  | C    | P-O3'-C3' | 14.42 | 137.00      | 119.70   |
| 27  | B8    | 2766 | A    | N1-C6-N6  | 14.36 | 127.21      | 118.60   |
| 27  | B8    | 677  | A    | N1-C6-N6  | 14.21 | 127.12      | 118.60   |
| 27  | B8    | 890  | C    | P-O3'-C3' | 14.20 | 136.75      | 119.70   |
| 1   | AA    | 1036 | A    | N1-C6-N6  | 14.12 | 127.07      | 118.60   |
| 27  | B8    | 1977 | A    | N1-C6-N6  | 14.11 | 127.07      | 118.60   |
| 27  | B8    | 2899 | A    | N1-C6-N6  | 14.10 | 127.06      | 118.60   |
| 27  | B8    | 863  | A    | N1-C6-N6  | 14.04 | 127.02      | 118.60   |
| 1   | AA    | 262  | A    | N1-C6-N6  | 14.02 | 127.01      | 118.60   |
| 1   | AA    | 937  | A    | N1-C6-N6  | 14.01 | 127.01      | 118.60   |
| 27  | B8    | 1745 | A    | N1-C6-N6  | 13.97 | 126.98      | 118.60   |
| 1   | AA    | 1014 | A    | P-O3'-C3' | 13.90 | 136.38      | 119.70   |
| 27  | B8    | 880  | G    | P-O3'-C3' | 13.88 | 136.36      | 119.70   |
| 27  | B8    | 1784 | A    | N1-C6-N6  | 13.85 | 126.91      | 118.60   |
| 1   | AA    | 174  | A    | N1-C6-N6  | 13.84 | 126.91      | 118.60   |
| 26  | B7    | 66   | A    | N1-C6-N6  | 13.79 | 126.88      | 118.60   |
| 1   | AA    | 780  | A    | N1-C6-N6  | 13.79 | 126.87      | 118.60   |
| 1   | AA    | 16   | A    | N1-C6-N6  | 13.75 | 126.85      | 118.60   |
| 1   | AA    | 181  | A    | N1-C6-N6  | 13.74 | 126.84      | 118.60   |
| 26  | B7    | 109  | A    | N1-C6-N6  | 13.73 | 126.84      | 118.60   |
| 27  | B8    | 959  | A    | N1-C6-N6  | 13.71 | 126.83      | 118.60   |
| 27  | B8    | 1713 | A    | N1-C6-N6  | 13.71 | 126.82      | 118.60   |
| 27  | B8    | 330  | A    | N1-C6-N6  | 13.68 | 126.81      | 118.60   |
| 1   | AA    | 906  | A    | N1-C6-N6  | 13.66 | 126.80      | 118.60   |
| 27  | B8    | 5    | A    | N1-C6-N6  | 13.64 | 126.78      | 118.60   |
| 27  | B8    | 2171 | A    | N1-C6-N6  | 13.64 | 126.78      | 118.60   |
| 1   | AA    | 1465 | A    | N1-C6-N6  | 13.62 | 126.77      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | AA    | 1500 | A    | N1-C6-N6  | 13.62 | 126.77      | 118.60   |
| 1   | AA    | 1035 | A    | N1-C6-N6  | 13.61 | 126.77      | 118.60   |
| 27  | B8    | 2662 | A    | N1-C6-N6  | 13.54 | 126.72      | 118.60   |
| 1   | AA    | 1111 | A    | N1-C6-N6  | 13.54 | 126.72      | 118.60   |
| 27  | B8    | 1598 | A    | N1-C6-N6  | 13.51 | 126.71      | 118.60   |
| 1   | AA    | 71   | A    | N1-C6-N6  | 13.47 | 126.68      | 118.60   |
| 1   | AA    | 288  | A    | N1-C6-N6  | 13.46 | 126.68      | 118.60   |
| 27  | B8    | 689  | A    | N1-C6-N6  | 13.46 | 126.67      | 118.60   |
| 1   | AA    | 901  | A    | N1-C6-N6  | 13.44 | 126.66      | 118.60   |
| 1   | AA    | 1492 | A    | N1-C6-N6  | 13.44 | 126.66      | 118.60   |
| 1   | AA    | 192  | A    | N1-C6-N6  | 13.43 | 126.66      | 118.60   |
| 27  | B8    | 2163 | A    | N1-C6-N6  | 13.41 | 126.65      | 118.60   |
| 27  | B8    | 2826 | A    | N1-C6-N6  | 13.39 | 126.64      | 118.60   |
| 1   | AA    | 923  | A    | N1-C6-N6  | 13.38 | 126.63      | 118.60   |
| 27  | B8    | 1205 | A    | P-O3'-C3' | 13.38 | 135.75      | 119.70   |
| 27  | B8    | 1899 | A    | N1-C6-N6  | 13.38 | 126.63      | 118.60   |
| 27  | B8    | 2090 | A    | N1-C6-N6  | 13.37 | 126.62      | 118.60   |
| 27  | B8    | 219  | A    | N1-C6-N6  | 13.36 | 126.61      | 118.60   |
| 26  | B7    | 108  | A    | N1-C6-N6  | 13.34 | 126.60      | 118.60   |
| 27  | B8    | 928  | A    | N1-C6-N6  | 13.33 | 126.60      | 118.60   |
| 27  | B8    | 718  | A    | N1-C6-N6  | 13.32 | 126.59      | 118.60   |
| 27  | B8    | 794  | A    | N1-C6-N6  | 13.32 | 126.59      | 118.60   |
| 27  | B8    | 443  | A    | N1-C6-N6  | 13.31 | 126.59      | 118.60   |
| 27  | B8    | 1532 | A    | N1-C6-N6  | 13.31 | 126.58      | 118.60   |
| 27  | B8    | 1127 | A    | N1-C6-N6  | 13.29 | 126.57      | 118.60   |
| 27  | B8    | 56   | A    | N1-C6-N6  | 13.28 | 126.57      | 118.60   |
| 1   | AA    | 199  | A    | N1-C6-N6  | 13.26 | 126.56      | 118.60   |
| 27  | B8    | 233  | A    | N1-C6-N6  | 13.25 | 126.55      | 118.60   |
| 3   | AV    | 9    | A    | N1-C6-N6  | 13.24 | 126.54      | 118.60   |
| 27  | B8    | 911  | A    | N1-C6-N6  | 13.24 | 126.54      | 118.60   |
| 1   | AA    | 1437 | A    | N1-C6-N6  | 13.22 | 126.53      | 118.60   |
| 1   | AA    | 595  | A    | N1-C6-N6  | 13.22 | 126.53      | 118.60   |
| 27  | B8    | 734  | A    | N1-C6-N6  | 13.20 | 126.52      | 118.60   |
| 27  | B8    | 2734 | A    | N1-C6-N6  | 13.20 | 126.52      | 118.60   |
| 1   | AA    | 1236 | A    | N1-C6-N6  | 13.18 | 126.51      | 118.60   |
| 1   | AA    | 996  | A    | N1-C6-N6  | 13.17 | 126.50      | 118.60   |
| 1   | AA    | 1226 | C    | P-O3'-C3' | 13.17 | 135.51      | 119.70   |
| 1   | AA    | 1513 | A    | N1-C6-N6  | 13.17 | 126.50      | 118.60   |
| 27  | B8    | 947  | A    | N1-C6-N6  | 13.16 | 126.50      | 118.60   |
| 1   | AA    | 746  | A    | N1-C6-N6  | 13.16 | 126.50      | 118.60   |
| 1   | AA    | 155  | A    | N1-C6-N6  | 13.13 | 126.48      | 118.60   |
| 27  | B8    | 1027 | A    | N1-C6-N6  | 13.12 | 126.47      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | AA    | 814  | A    | N1-C6-N6  | 13.11 | 126.47      | 118.60   |
| 27  | B8    | 213  | A    | N1-C6-N6  | 13.11 | 126.47      | 118.60   |
| 1   | AA    | 1360 | A    | N1-C6-N6  | 13.10 | 126.46      | 118.60   |
| 27  | B8    | 19   | A    | N1-C6-N6  | 13.07 | 126.44      | 118.60   |
| 27  | B8    | 2154 | A    | N1-C6-N6  | 13.07 | 126.44      | 118.60   |
| 1   | AA    | 1014 | A    | N1-C6-N6  | 13.06 | 126.44      | 118.60   |
| 27  | B8    | 1791 | A    | N1-C6-N6  | 13.06 | 126.44      | 118.60   |
| 27  | B8    | 13   | A    | N1-C6-N6  | 13.06 | 126.43      | 118.60   |
| 27  | B8    | 1431 | A    | N1-C6-N6  | 13.04 | 126.42      | 118.60   |
| 27  | B8    | 1787 | A    | N1-C6-N6  | 13.03 | 126.42      | 118.60   |
| 27  | B8    | 2051 | A    | N1-C6-N6  | 13.03 | 126.42      | 118.60   |
| 1   | AA    | 1080 | A    | N1-C6-N6  | 13.03 | 126.42      | 118.60   |
| 27  | B8    | 104  | A    | N1-C6-N6  | 13.03 | 126.42      | 118.60   |
| 27  | B8    | 2453 | A    | N1-C6-N6  | 13.01 | 126.41      | 118.60   |
| 1   | AA    | 1398 | A    | N1-C6-N6  | 13.01 | 126.41      | 118.60   |
| 27  | B8    | 2879 | A    | N1-C6-N6  | 13.00 | 126.40      | 118.60   |
| 27  | B8    | 2284 | A    | N1-C6-N6  | 13.00 | 126.40      | 118.60   |
| 27  | B8    | 1144 | A    | N1-C6-N6  | 12.99 | 126.39      | 118.60   |
| 1   | AA    | 1197 | A    | N1-C6-N6  | 12.99 | 126.39      | 118.60   |
| 27  | B8    | 199  | A    | N1-C6-N6  | 12.98 | 126.39      | 118.60   |
| 27  | B8    | 1700 | A    | N1-C6-N6  | 12.98 | 126.39      | 118.60   |
| 27  | B8    | 1084 | A    | N1-C6-N6  | 12.97 | 126.38      | 118.60   |
| 27  | B8    | 1603 | A    | N1-C6-N6  | 12.97 | 126.38      | 118.60   |
| 27  | B8    | 1918 | A    | N1-C6-N6  | 12.97 | 126.38      | 118.60   |
| 27  | B8    | 685  | A    | N1-C6-N6  | 12.96 | 126.38      | 118.60   |
| 27  | B8    | 756  | A    | N1-C6-N6  | 12.95 | 126.37      | 118.60   |
| 1   | AA    | 502  | A    | N1-C6-N6  | 12.95 | 126.37      | 118.60   |
| 27  | B8    | 28   | A    | N1-C6-N6  | 12.95 | 126.37      | 118.60   |
| 27  | B8    | 849  | A    | N1-C6-N6  | 12.94 | 126.37      | 118.60   |
| 26  | B7    | 101  | A    | N1-C6-N6  | 12.94 | 126.36      | 118.60   |
| 27  | B8    | 1590 | A    | N1-C6-N6  | 12.93 | 126.36      | 118.60   |
| 27  | B8    | 599  | A    | N1-C6-N6  | 12.93 | 126.36      | 118.60   |
| 1   | AA    | 451  | A    | N1-C6-N6  | 12.90 | 126.34      | 118.60   |
| 27  | B8    | 152  | A    | N1-C6-N6  | 12.90 | 126.34      | 118.60   |
| 27  | B8    | 1095 | A    | N1-C6-N6  | 12.89 | 126.33      | 118.60   |
| 27  | B8    | 1927 | A    | N1-C6-N6  | 12.88 | 126.33      | 118.60   |
| 27  | B8    | 322  | A    | N1-C6-N6  | 12.87 | 126.32      | 118.60   |
| 1   | AA    | 563  | A    | N1-C6-N6  | 12.87 | 126.32      | 118.60   |
| 27  | B8    | 2800 | A    | N1-C6-N6  | 12.84 | 126.30      | 118.60   |
| 27  | B8    | 1269 | A    | N1-C6-N6  | 12.84 | 126.30      | 118.60   |
| 27  | B8    | 1354 | A    | N1-C6-N6  | 12.83 | 126.30      | 118.60   |
| 27  | B8    | 1061 | U    | P-O3'-C3' | 12.82 | 135.09      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 27  | B8    | 503  | A    | N1-C6-N6 | 12.81 | 126.29      | 118.60   |
| 27  | B8    | 582  | A    | N1-C6-N6 | 12.80 | 126.28      | 118.60   |
| 27  | B8    | 221  | A    | N1-C6-N6 | 12.77 | 126.26      | 118.60   |
| 1   | AA    | 1044 | A    | N1-C6-N6 | 12.77 | 126.26      | 118.60   |
| 27  | B8    | 1677 | A    | N1-C6-N6 | 12.76 | 126.25      | 118.60   |
| 27  | B8    | 2184 | A    | N1-C6-N6 | 12.75 | 126.25      | 118.60   |
| 1   | AA    | 673  | A    | N1-C6-N6 | 12.75 | 126.25      | 118.60   |
| 27  | B8    | 515  | A    | N1-C6-N6 | 12.75 | 126.25      | 118.60   |
| 27  | B8    | 502  | A    | N1-C6-N6 | 12.74 | 126.25      | 118.60   |
| 27  | B8    | 1275 | A    | N1-C6-N6 | 12.74 | 126.25      | 118.60   |
| 27  | B8    | 2873 | A    | N1-C6-N6 | 12.74 | 126.25      | 118.60   |
| 27  | B8    | 899  | A    | N1-C6-N6 | 12.74 | 126.24      | 118.60   |
| 1   | AA    | 915  | A    | N1-C6-N6 | 12.73 | 126.24      | 118.60   |
| 27  | B8    | 1433 | A    | N1-C6-N6 | 12.72 | 126.23      | 118.60   |
| 1   | AA    | 320  | A    | N1-C6-N6 | 12.72 | 126.23      | 118.60   |
| 27  | B8    | 1936 | A    | N1-C6-N6 | 12.72 | 126.23      | 118.60   |
| 27  | B8    | 155  | A    | N1-C6-N6 | 12.71 | 126.23      | 118.60   |
| 27  | B8    | 1496 | A    | N1-C6-N6 | 12.71 | 126.22      | 118.60   |
| 27  | B8    | 429  | A    | N1-C6-N6 | 12.71 | 126.22      | 118.60   |
| 1   | AA    | 81   | A    | N1-C6-N6 | 12.70 | 126.22      | 118.60   |
| 1   | AA    | 1229 | A    | N1-C6-N6 | 12.70 | 126.22      | 118.60   |
| 27  | B8    | 878  | A    | N1-C6-N6 | 12.69 | 126.22      | 118.60   |
| 1   | AA    | 77   | A    | N1-C6-N6 | 12.69 | 126.22      | 118.60   |
| 27  | B8    | 1634 | A    | N1-C6-N6 | 12.69 | 126.21      | 118.60   |
| 1   | AA    | 478  | A    | N1-C6-N6 | 12.68 | 126.21      | 118.60   |
| 27  | B8    | 1264 | A    | N1-C6-N6 | 12.68 | 126.21      | 118.60   |
| 1   | AA    | 371  | A    | N1-C6-N6 | 12.67 | 126.20      | 118.60   |
| 27  | B8    | 2430 | A    | N1-C6-N6 | 12.67 | 126.20      | 118.60   |
| 27  | B8    | 262  | A    | N1-C6-N6 | 12.67 | 126.20      | 118.60   |
| 27  | B8    | 182  | A    | N1-C6-N6 | 12.65 | 126.19      | 118.60   |
| 27  | B8    | 226  | A    | N1-C6-N6 | 12.65 | 126.19      | 118.60   |
| 1   | AA    | 98   | A    | N1-C6-N6 | 12.65 | 126.19      | 118.60   |
| 27  | B8    | 522  | A    | N1-C6-N6 | 12.65 | 126.19      | 118.60   |
| 27  | B8    | 2037 | A    | N1-C6-N6 | 12.65 | 126.19      | 118.60   |
| 27  | B8    | 2042 | A    | N1-C6-N6 | 12.65 | 126.19      | 118.60   |
| 27  | B8    | 2352 | A    | N1-C6-N6 | 12.65 | 126.19      | 118.60   |
| 27  | B8    | 693  | A    | N1-C6-N6 | 12.65 | 126.19      | 118.60   |
| 1   | AA    | 1269 | A    | N1-C6-N6 | 12.64 | 126.19      | 118.60   |
| 27  | B8    | 532  | A    | N1-C6-N6 | 12.64 | 126.19      | 118.60   |
| 27  | B8    | 255  | A    | N1-C6-N6 | 12.64 | 126.18      | 118.60   |
| 1   | AA    | 10   | A    | N1-C6-N6 | 12.64 | 126.18      | 118.60   |
| 1   | AA    | 1219 | A    | N1-C6-N6 | 12.64 | 126.18      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26  | B7    | 58   | A    | N1-C6-N6  | 12.63 | 126.18      | 118.60   |
| 1   | AA    | 162  | A    | N1-C6-N6  | 12.63 | 126.18      | 118.60   |
| 1   | AA    | 336  | A    | N1-C6-N6  | 12.63 | 126.17      | 118.60   |
| 1   | AA    | 964  | A    | N1-C6-N6  | 12.62 | 126.17      | 118.60   |
| 27  | B8    | 342  | A    | N1-C6-N6  | 12.62 | 126.17      | 118.60   |
| 1   | AA    | 456  | A    | N1-C6-N6  | 12.62 | 126.17      | 118.60   |
| 27  | B8    | 1244 | A    | N1-C6-N6  | 12.61 | 126.17      | 118.60   |
| 27  | B8    | 2281 | A    | N1-C6-N6  | 12.61 | 126.17      | 118.60   |
| 3   | AV    | 27   | A    | N1-C6-N6  | 12.61 | 126.17      | 118.60   |
| 27  | B8    | 190  | A    | N1-C6-N6  | 12.61 | 126.17      | 118.60   |
| 27  | B8    | 666  | A    | N1-C6-N6  | 12.61 | 126.16      | 118.60   |
| 26  | B7    | 29   | A    | N1-C6-N6  | 12.60 | 126.16      | 118.60   |
| 27  | B8    | 2267 | A    | N1-C6-N6  | 12.60 | 126.16      | 118.60   |
| 1   | AA    | 1306 | A    | N1-C6-N6  | 12.60 | 126.16      | 118.60   |
| 1   | AA    | 309  | A    | N1-C6-N6  | 12.60 | 126.16      | 118.60   |
| 27  | B8    | 1773 | A    | N1-C6-N6  | 12.60 | 126.16      | 118.60   |
| 27  | B8    | 2013 | A    | N1-C6-N6  | 12.60 | 126.16      | 118.60   |
| 27  | B8    | 761  | A    | N1-C6-N6  | 12.59 | 126.16      | 118.60   |
| 27  | B8    | 2369 | A    | N1-C6-N6  | 12.59 | 126.16      | 118.60   |
| 27  | B8    | 347  | A    | N1-C6-N6  | 12.59 | 126.16      | 118.60   |
| 27  | B8    | 655  | A    | N1-C6-N6  | 12.58 | 126.15      | 118.60   |
| 27  | B8    | 1260 | A    | N1-C6-N6  | 12.58 | 126.15      | 118.60   |
| 1   | AA    | 675  | A    | N1-C6-N6  | 12.58 | 126.15      | 118.60   |
| 27  | B8    | 195  | A    | N1-C6-N6  | 12.58 | 126.15      | 118.60   |
| 27  | B8    | 2600 | A    | N1-C6-N6  | 12.58 | 126.15      | 118.60   |
| 1   | AA    | 139  | A    | N1-C6-N6  | 12.57 | 126.14      | 118.60   |
| 1   | AA    | 205  | A    | N1-C6-N6  | 12.57 | 126.14      | 118.60   |
| 1   | AA    | 1016 | A    | N1-C6-N6  | 12.57 | 126.14      | 118.60   |
| 26  | B7    | 39   | A    | N1-C6-N6  | 12.57 | 126.14      | 118.60   |
| 27  | B8    | 2336 | A    | P-O3'-C3' | 12.57 | 134.78      | 119.70   |
| 27  | B8    | 2412 | A    | N1-C6-N6  | 12.57 | 126.14      | 118.60   |
| 1   | AA    | 974  | A    | N1-C6-N6  | 12.56 | 126.14      | 118.60   |
| 27  | B8    | 1039 | A    | N1-C6-N6  | 12.56 | 126.14      | 118.60   |
| 27  | B8    | 730  | A    | N1-C6-N6  | 12.56 | 126.14      | 118.60   |
| 1   | AA    | 1167 | A    | N1-C6-N6  | 12.56 | 126.14      | 118.60   |
| 27  | B8    | 83   | A    | N1-C6-N6  | 12.56 | 126.14      | 118.60   |
| 27  | B8    | 592  | A    | N1-C6-N6  | 12.56 | 126.14      | 118.60   |
| 27  | B8    | 637  | A    | N1-C6-N6  | 12.56 | 126.14      | 118.60   |
| 27  | B8    | 2516 | A    | N1-C6-N6  | 12.56 | 126.14      | 118.60   |
| 27  | B8    | 2278 | A    | N1-C6-N6  | 12.56 | 126.14      | 118.60   |
| 27  | B8    | 1637 | A    | N1-C6-N6  | 12.56 | 126.13      | 118.60   |
| 27  | B8    | 721  | A    | N1-C6-N6  | 12.54 | 126.13      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | AA    | 33   | A    | N1-C6-N6 | 12.54 | 126.12      | 118.60   |
| 1   | AA    | 300  | A    | N1-C6-N6 | 12.54 | 126.12      | 118.60   |
| 1   | AA    | 1110 | A    | N1-C6-N6 | 12.54 | 126.13      | 118.60   |
| 1   | AA    | 1151 | A    | N1-C6-N6 | 12.54 | 126.12      | 118.60   |
| 27  | B8    | 492  | A    | N1-C6-N6 | 12.54 | 126.12      | 118.60   |
| 27  | B8    | 1387 | A    | N1-C6-N6 | 12.54 | 126.12      | 118.60   |
| 27  | B8    | 743  | A    | N1-C6-N6 | 12.54 | 126.12      | 118.60   |
| 27  | B8    | 2311 | A    | N1-C6-N6 | 12.54 | 126.12      | 118.60   |
| 27  | B8    | 749  | A    | N1-C6-N6 | 12.53 | 126.12      | 118.60   |
| 27  | B8    | 1213 | A    | N1-C6-N6 | 12.53 | 126.12      | 118.60   |
| 1   | AA    | 1000 | A    | N1-C6-N6 | 12.53 | 126.11      | 118.60   |
| 27  | B8    | 497  | A    | N1-C6-N6 | 12.53 | 126.12      | 118.60   |
| 27  | B8    | 2381 | A    | N1-C6-N6 | 12.52 | 126.11      | 118.60   |
| 27  | B8    | 95   | A    | N1-C6-N6 | 12.52 | 126.11      | 118.60   |
| 1   | AA    | 238  | A    | N1-C6-N6 | 12.52 | 126.11      | 118.60   |
| 1   | AA    | 1081 | A    | N1-C6-N6 | 12.51 | 126.11      | 118.60   |
| 27  | B8    | 2317 | A    | N1-C6-N6 | 12.51 | 126.10      | 118.60   |
| 27  | B8    | 2333 | A    | N1-C6-N6 | 12.51 | 126.10      | 118.60   |
| 27  | B8    | 2541 | A    | N1-C6-N6 | 12.51 | 126.10      | 118.60   |
| 27  | B8    | 2274 | A    | N1-C6-N6 | 12.50 | 126.10      | 118.60   |
| 27  | B8    | 2860 | A    | N1-C6-N6 | 12.50 | 126.10      | 118.60   |
| 27  | B8    | 1551 | A    | N1-C6-N6 | 12.49 | 126.10      | 118.60   |
| 1   | AA    | 655  | A    | N1-C6-N6 | 12.49 | 126.09      | 118.60   |
| 1   | AA    | 468  | A    | N1-C6-N6 | 12.48 | 126.09      | 118.60   |
| 27  | B8    | 644  | A    | N1-C6-N6 | 12.48 | 126.09      | 118.60   |
| 27  | B8    | 2378 | A    | N1-C6-N6 | 12.48 | 126.09      | 118.60   |
| 27  | B8    | 265  | A    | N1-C6-N6 | 12.48 | 126.09      | 118.60   |
| 27  | B8    | 1204 | A    | N1-C6-N6 | 12.48 | 126.09      | 118.60   |
| 27  | B8    | 1810 | A    | N1-C6-N6 | 12.48 | 126.09      | 118.60   |
| 27  | B8    | 575  | A    | N1-C6-N6 | 12.48 | 126.08      | 118.60   |
| 27  | B8    | 742  | A    | N1-C6-N6 | 12.47 | 126.08      | 118.60   |
| 1   | AA    | 716  | A    | N1-C6-N6 | 12.47 | 126.08      | 118.60   |
| 1   | AA    | 263  | A    | N1-C6-N6 | 12.47 | 126.08      | 118.60   |
| 1   | AA    | 865  | A    | N1-C6-N6 | 12.47 | 126.08      | 118.60   |
| 1   | AA    | 1171 | A    | N1-C6-N6 | 12.47 | 126.08      | 118.60   |
| 1   | AA    | 53   | A    | N1-C6-N6 | 12.46 | 126.08      | 118.60   |
| 27  | B8    | 2727 | A    | N1-C6-N6 | 12.46 | 126.08      | 118.60   |
| 1   | AA    | 1357 | A    | N1-C6-N6 | 12.46 | 126.08      | 118.60   |
| 27  | B8    | 2386 | A    | N1-C6-N6 | 12.46 | 126.08      | 118.60   |
| 1   | AA    | 1434 | A    | N1-C6-N6 | 12.46 | 126.07      | 118.60   |
| 27  | B8    | 1143 | A    | N1-C6-N6 | 12.46 | 126.07      | 118.60   |
| 1   | AA    | 228  | A    | N1-C6-N6 | 12.45 | 126.07      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 26  | B7    | 115  | A    | N1-C6-N6  | 12.45 | 126.07      | 118.60   |
| 27  | B8    | 705  | A    | N1-C6-N6  | 12.45 | 126.07      | 118.60   |
| 27  | B8    | 1794 | A    | N1-C6-N6  | 12.44 | 126.07      | 118.60   |
| 27  | B8    | 127  | A    | N1-C6-N6  | 12.44 | 126.06      | 118.60   |
| 1   | AA    | 629  | A    | N1-C6-N6  | 12.44 | 126.06      | 118.60   |
| 27  | B8    | 2753 | A    | N1-C6-N6  | 12.44 | 126.06      | 118.60   |
| 1   | AA    | 1065 | U    | P-O3'-C3' | 12.43 | 134.62      | 119.70   |
| 27  | B8    | 149  | A    | N1-C6-N6  | 12.43 | 126.06      | 118.60   |
| 27  | B8    | 2482 | A    | N1-C6-N6  | 12.43 | 126.06      | 118.60   |
| 1   | AA    | 482  | A    | N1-C6-N6  | 12.43 | 126.06      | 118.60   |
| 27  | B8    | 299  | A    | N1-C6-N6  | 12.43 | 126.06      | 118.60   |
| 27  | B8    | 382  | A    | N1-C6-N6  | 12.43 | 126.06      | 118.60   |
| 27  | B8    | 300  | A    | N1-C6-N6  | 12.43 | 126.06      | 118.60   |
| 27  | B8    | 466  | A    | N1-C6-N6  | 12.43 | 126.06      | 118.60   |
| 1   | AA    | 270  | A    | N1-C6-N6  | 12.42 | 126.06      | 118.60   |
| 27  | B8    | 633  | A    | N1-C6-N6  | 12.42 | 126.05      | 118.60   |
| 27  | B8    | 2670 | A    | N1-C6-N6  | 12.42 | 126.05      | 118.60   |
| 27  | B8    | 2598 | A    | N1-C6-N6  | 12.42 | 126.05      | 118.60   |
| 1   | AA    | 223  | A    | N1-C6-N6  | 12.41 | 126.05      | 118.60   |
| 1   | AA    | 1418 | A    | N1-C6-N6  | 12.41 | 126.05      | 118.60   |
| 1   | AA    | 459  | A    | N1-C6-N6  | 12.41 | 126.05      | 118.60   |
| 27  | B8    | 2094 | A    | N1-C6-N6  | 12.41 | 126.05      | 118.60   |
| 27  | B8    | 415  | A    | N1-C6-N6  | 12.41 | 126.05      | 118.60   |
| 27  | B8    | 1285 | A    | N1-C6-N6  | 12.41 | 126.05      | 118.60   |
| 27  | B8    | 1654 | A    | N1-C6-N6  | 12.41 | 126.05      | 118.60   |
| 1   | AA    | 960  | U    | P-O3'-C3' | 12.40 | 134.59      | 119.70   |
| 27  | B8    | 1664 | A    | N1-C6-N6  | 12.40 | 126.04      | 118.60   |
| 27  | B8    | 89   | A    | N1-C6-N6  | 12.40 | 126.04      | 118.60   |
| 27  | B8    | 2147 | A    | N1-C6-N6  | 12.40 | 126.04      | 118.60   |
| 1   | AA    | 695  | A    | N1-C6-N6  | 12.40 | 126.04      | 118.60   |
| 1   | AA    | 253  | A    | N1-C6-N6  | 12.39 | 126.04      | 118.60   |
| 27  | B8    | 1579 | A    | N1-C6-N6  | 12.39 | 126.04      | 118.60   |
| 27  | B8    | 84   | A    | N1-C6-N6  | 12.39 | 126.03      | 118.60   |
| 27  | B8    | 2088 | A    | N1-C6-N6  | 12.38 | 126.03      | 118.60   |
| 1   | AA    | 80   | A    | N1-C6-N6  | 12.38 | 126.03      | 118.60   |
| 1   | AA    | 694  | A    | N1-C6-N6  | 12.38 | 126.03      | 118.60   |
| 1   | AA    | 1155 | A    | N1-C6-N6  | 12.38 | 126.03      | 118.60   |
| 27  | B8    | 1755 | A    | N1-C6-N6  | 12.38 | 126.03      | 118.60   |
| 27  | B8    | 1194 | A    | N1-C6-N6  | 12.38 | 126.03      | 118.60   |
| 27  | B8    | 2781 | A    | N1-C6-N6  | 12.38 | 126.03      | 118.60   |
| 1   | AA    | 28   | A    | N1-C6-N6  | 12.38 | 126.03      | 118.60   |
| 26  | B7    | 94   | A    | N1-C6-N6  | 12.38 | 126.03      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 27  | B8    | 2711 | A    | N1-C6-N6 | 12.38 | 126.03      | 118.60   |
| 1   | AA    | 959  | A    | N1-C6-N6 | 12.37 | 126.02      | 118.60   |
| 27  | B8    | 2031 | A    | N1-C6-N6 | 12.37 | 126.02      | 118.60   |
| 27  | B8    | 943  | A    | N1-C6-N6 | 12.37 | 126.02      | 118.60   |
| 27  | B8    | 1384 | A    | N1-C6-N6 | 12.37 | 126.02      | 118.60   |
| 26  | B7    | 50   | A    | N1-C6-N6 | 12.36 | 126.02      | 118.60   |
| 27  | B8    | 2900 | A    | N1-C6-N6 | 12.37 | 126.02      | 118.60   |
| 27  | B8    | 368  | A    | N1-C6-N6 | 12.36 | 126.02      | 118.60   |
| 27  | B8    | 513  | A    | N1-C6-N6 | 12.36 | 126.02      | 118.60   |
| 27  | B8    | 1502 | A    | N1-C6-N6 | 12.36 | 126.02      | 118.60   |
| 1   | AA    | 600  | A    | N1-C6-N6 | 12.36 | 126.02      | 118.60   |
| 27  | B8    | 1640 | A    | N1-C6-N6 | 12.36 | 126.02      | 118.60   |
| 27  | B8    | 2211 | A    | N1-C6-N6 | 12.36 | 126.02      | 118.60   |
| 27  | B8    | 1253 | A    | N1-C6-N6 | 12.36 | 126.01      | 118.60   |
| 1   | AA    | 768  | A    | N1-C6-N6 | 12.35 | 126.01      | 118.60   |
| 27  | B8    | 111  | A    | N1-C6-N6 | 12.35 | 126.01      | 118.60   |
| 27  | B8    | 1528 | A    | N1-C6-N6 | 12.35 | 126.01      | 118.60   |
| 1   | AA    | 1105 | A    | N1-C6-N6 | 12.34 | 126.00      | 118.60   |
| 27  | B8    | 227  | A    | N1-C6-N6 | 12.34 | 126.00      | 118.60   |
| 27  | B8    | 1928 | A    | N1-C6-N6 | 12.34 | 126.00      | 118.60   |
| 1   | AA    | 460  | A    | N1-C6-N6 | 12.34 | 126.00      | 118.60   |
| 1   | AA    | 676  | A    | N1-C6-N6 | 12.34 | 126.00      | 118.60   |
| 27  | B8    | 1366 | A    | N1-C6-N6 | 12.34 | 126.00      | 118.60   |
| 1   | AA    | 994  | A    | N1-C6-N6 | 12.34 | 126.00      | 118.60   |
| 27  | B8    | 2700 | A    | N1-C6-N6 | 12.34 | 126.00      | 118.60   |
| 27  | B8    | 2411 | A    | N1-C6-N6 | 12.33 | 126.00      | 118.60   |
| 27  | B8    | 626  | A    | N1-C6-N6 | 12.33 | 126.00      | 118.60   |
| 27  | B8    | 1548 | A    | N1-C6-N6 | 12.33 | 126.00      | 118.60   |
| 27  | B8    | 1705 | A    | N1-C6-N6 | 12.33 | 126.00      | 118.60   |
| 27  | B8    | 2170 | A    | N1-C6-N6 | 12.32 | 125.99      | 118.60   |
| 27  | B8    | 2665 | A    | N1-C6-N6 | 12.32 | 126.00      | 118.60   |
| 27  | B8    | 716  | A    | N1-C6-N6 | 12.32 | 125.99      | 118.60   |
| 27  | B8    | 1998 | A    | N1-C6-N6 | 12.32 | 125.99      | 118.60   |
| 27  | B8    | 1525 | A    | N1-C6-N6 | 12.32 | 125.99      | 118.60   |
| 1   | AA    | 236  | A    | N1-C6-N6 | 12.31 | 125.99      | 118.60   |
| 1   | AA    | 573  | A    | N1-C6-N6 | 12.31 | 125.99      | 118.60   |
| 27  | B8    | 1490 | A    | N1-C6-N6 | 12.31 | 125.99      | 118.60   |
| 27  | B8    | 38   | A    | N1-C6-N6 | 12.31 | 125.99      | 118.60   |
| 27  | B8    | 1969 | A    | N1-C6-N6 | 12.31 | 125.99      | 118.60   |
| 27  | B8    | 2198 | A    | N1-C6-N6 | 12.31 | 125.98      | 118.60   |
| 27  | B8    | 2434 | A    | N1-C6-N6 | 12.31 | 125.98      | 118.60   |
| 1   | AA    | 1377 | A    | N1-C6-N6 | 12.30 | 125.98      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 27  | B8    | 251  | A    | N1-C6-N6 | 12.30 | 125.98      | 118.60   |
| 27  | B8    | 1586 | A    | N1-C6-N6 | 12.30 | 125.98      | 118.60   |
| 27  | B8    | 1757 | A    | N1-C6-N6 | 12.30 | 125.98      | 118.60   |
| 1   | AA    | 784  | A    | N1-C6-N6 | 12.30 | 125.98      | 118.60   |
| 27  | B8    | 167  | A    | N1-C6-N6 | 12.30 | 125.98      | 118.60   |
| 27  | B8    | 1913 | A    | N1-C6-N6 | 12.30 | 125.98      | 118.60   |
| 1   | AA    | 831  | A    | N1-C6-N6 | 12.30 | 125.98      | 118.60   |
| 27  | B8    | 2589 | A    | N1-C6-N6 | 12.30 | 125.98      | 118.60   |
| 1   | AA    | 8    | A    | N1-C6-N6 | 12.30 | 125.98      | 118.60   |
| 1   | AA    | 32   | A    | N1-C6-N6 | 12.30 | 125.98      | 118.60   |
| 27  | B8    | 2632 | A    | N1-C6-N6 | 12.30 | 125.98      | 118.60   |
| 27  | B8    | 1669 | A    | N1-C6-N6 | 12.29 | 125.98      | 118.60   |
| 27  | B8    | 1591 | A    | N1-C6-N6 | 12.29 | 125.97      | 118.60   |
| 1   | AA    | 131  | A    | N1-C6-N6 | 12.29 | 125.97      | 118.60   |
| 1   | AA    | 1004 | A    | N1-C6-N6 | 12.28 | 125.97      | 118.60   |
| 1   | AA    | 1188 | A    | N1-C6-N6 | 12.28 | 125.97      | 118.60   |
| 27  | B8    | 1077 | A    | N1-C6-N6 | 12.28 | 125.97      | 118.60   |
| 1   | AA    | 1280 | A    | N1-C6-N6 | 12.28 | 125.97      | 118.60   |
| 27  | B8    | 1650 | A    | N1-C6-N6 | 12.28 | 125.97      | 118.60   |
| 27  | B8    | 1286 | A    | N1-C6-N6 | 12.28 | 125.97      | 118.60   |
| 27  | B8    | 2887 | A    | N1-C6-N6 | 12.28 | 125.97      | 118.60   |
| 1   | AA    | 935  | A    | N1-C6-N6 | 12.27 | 125.96      | 118.60   |
| 27  | B8    | 1413 | A    | N1-C6-N6 | 12.27 | 125.96      | 118.60   |
| 1   | AA    | 983  | A    | N1-C6-N6 | 12.27 | 125.96      | 118.60   |
| 27  | B8    | 2183 | A    | N1-C6-N6 | 12.27 | 125.96      | 118.60   |
| 1   | AA    | 574  | A    | N1-C6-N6 | 12.27 | 125.96      | 118.60   |
| 27  | B8    | 2158 | A    | N1-C6-N6 | 12.27 | 125.96      | 118.60   |
| 1   | AA    | 1287 | A    | N1-C6-N6 | 12.27 | 125.96      | 118.60   |
| 27  | B8    | 782  | A    | N1-C6-N6 | 12.26 | 125.96      | 118.60   |
| 27  | B8    | 632  | A    | N1-C6-N6 | 12.26 | 125.96      | 118.60   |
| 27  | B8    | 1952 | A    | N1-C6-N6 | 12.26 | 125.96      | 118.60   |
| 1   | AA    | 559  | A    | N1-C6-N6 | 12.26 | 125.95      | 118.60   |
| 1   | AA    | 706  | A    | N1-C6-N6 | 12.26 | 125.95      | 118.60   |
| 1   | AA    | 1374 | A    | N1-C6-N6 | 12.26 | 125.95      | 118.60   |
| 3   | AV    | 22   | A    | N1-C6-N6 | 12.25 | 125.95      | 118.60   |
| 1   | AA    | 182  | A    | N1-C6-N6 | 12.25 | 125.95      | 118.60   |
| 27  | B8    | 1274 | A    | N1-C6-N6 | 12.25 | 125.95      | 118.60   |
| 27  | B8    | 1819 | A    | N1-C6-N6 | 12.25 | 125.95      | 118.60   |
| 27  | B8    | 2503 | A    | N1-C6-N6 | 12.25 | 125.95      | 118.60   |
| 1   | AA    | 66   | A    | N1-C6-N6 | 12.25 | 125.95      | 118.60   |
| 3   | AV    | 77   | A    | N1-C6-N6 | 12.24 | 125.95      | 118.60   |
| 27  | B8    | 845  | A    | N1-C6-N6 | 12.24 | 125.95      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 27  | B8    | 2679 | A    | N1-C6-N6 | 12.24 | 125.95      | 118.60   |
| 27  | B8    | 1226 | A    | N1-C6-N6 | 12.24 | 125.94      | 118.60   |
| 1   | AA    | 907  | A    | N1-C6-N6 | 12.24 | 125.94      | 118.60   |
| 1   | AA    | 1250 | A    | N1-C6-N6 | 12.24 | 125.94      | 118.60   |
| 27  | B8    | 1735 | A    | N1-C6-N6 | 12.24 | 125.94      | 118.60   |
| 1   | AA    | 3    | A    | N1-C6-N6 | 12.24 | 125.94      | 118.60   |
| 1   | AA    | 1251 | A    | N1-C6-N6 | 12.24 | 125.94      | 118.60   |
| 27  | B8    | 2439 | A    | N1-C6-N6 | 12.24 | 125.94      | 118.60   |
| 27  | B8    | 1009 | A    | N1-C6-N6 | 12.23 | 125.94      | 118.60   |
| 27  | B8    | 608  | A    | N1-C6-N6 | 12.23 | 125.94      | 118.60   |
| 27  | B8    | 2328 | A    | N1-C6-N6 | 12.23 | 125.94      | 118.60   |
| 27  | B8    | 203  | A    | N1-C6-N6 | 12.22 | 125.93      | 118.60   |
| 27  | B8    | 996  | A    | N1-C6-N6 | 12.22 | 125.93      | 118.60   |
| 27  | B8    | 2340 | A    | N1-C6-N6 | 12.22 | 125.93      | 118.60   |
| 27  | B8    | 2660 | A    | N1-C6-N6 | 12.22 | 125.93      | 118.60   |
| 27  | B8    | 1367 | A    | N1-C6-N6 | 12.22 | 125.93      | 118.60   |
| 27  | B8    | 2837 | A    | N1-C6-N6 | 12.22 | 125.93      | 118.60   |
| 27  | B8    | 354  | A    | N1-C6-N6 | 12.21 | 125.93      | 118.60   |
| 1   | AA    | 190  | A    | N1-C6-N6 | 12.21 | 125.92      | 118.60   |
| 1   | AA    | 787  | A    | N1-C6-N6 | 12.21 | 125.92      | 118.60   |
| 27  | B8    | 2675 | A    | N1-C6-N6 | 12.21 | 125.92      | 118.60   |
| 3   | AV    | 5    | A    | N1-C6-N6 | 12.21 | 125.92      | 118.60   |
| 27  | B8    | 2738 | A    | N1-C6-N6 | 12.20 | 125.92      | 118.60   |
| 27  | B8    | 91   | A    | N1-C6-N6 | 12.20 | 125.92      | 118.60   |
| 27  | B8    | 892  | A    | N1-C6-N6 | 12.20 | 125.92      | 118.60   |
| 27  | B8    | 925  | A    | N1-C6-N6 | 12.20 | 125.92      | 118.60   |
| 27  | B8    | 2376 | A    | N1-C6-N6 | 12.20 | 125.92      | 118.60   |
| 27  | B8    | 2406 | A    | N1-C6-N6 | 12.20 | 125.92      | 118.60   |
| 1   | AA    | 919  | A    | N1-C6-N6 | 12.20 | 125.92      | 118.60   |
| 26  | B7    | 119  | A    | N1-C6-N6 | 12.20 | 125.92      | 118.60   |
| 1   | AA    | 383  | A    | N1-C6-N6 | 12.19 | 125.92      | 118.60   |
| 1   | AA    | 1152 | A    | N1-C6-N6 | 12.19 | 125.92      | 118.60   |
| 1   | AA    | 1447 | A    | N1-C6-N6 | 12.19 | 125.92      | 118.60   |
| 27  | B8    | 2821 | A    | N1-C6-N6 | 12.19 | 125.92      | 118.60   |
| 1   | AA    | 143  | A    | N1-C6-N6 | 12.19 | 125.91      | 118.60   |
| 27  | B8    | 294  | A    | N1-C6-N6 | 12.19 | 125.91      | 118.60   |
| 27  | B8    | 1618 | A    | N1-C6-N6 | 12.19 | 125.91      | 118.60   |
| 27  | B8    | 2126 | A    | N1-C6-N6 | 12.19 | 125.91      | 118.60   |
| 1   | AA    | 560  | A    | N1-C6-N6 | 12.18 | 125.91      | 118.60   |
| 27  | B8    | 602  | A    | N1-C6-N6 | 12.18 | 125.91      | 118.60   |
| 27  | B8    | 1134 | A    | N1-C6-N6 | 12.18 | 125.91      | 118.60   |
| 27  | B8    | 2358 | A    | N1-C6-N6 | 12.18 | 125.91      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | AA    | 120  | A    | N1-C6-N6 | 12.18 | 125.91      | 118.60   |
| 1   | AA    | 1456 | A    | N1-C6-N6 | 12.18 | 125.91      | 118.60   |
| 27  | B8    | 1866 | A    | N1-C6-N6 | 12.18 | 125.91      | 118.60   |
| 27  | B8    | 1829 | A    | N1-C6-N6 | 12.18 | 125.91      | 118.60   |
| 1   | AA    | 59   | A    | N1-C6-N6 | 12.18 | 125.91      | 118.60   |
| 27  | B8    | 2314 | A    | N1-C6-N6 | 12.18 | 125.91      | 118.60   |
| 1   | AA    | 648  | A    | N1-C6-N6 | 12.17 | 125.91      | 118.60   |
| 1   | AA    | 1519 | A    | N1-C6-N6 | 12.17 | 125.90      | 118.60   |
| 27  | B8    | 2893 | A    | N1-C6-N6 | 12.17 | 125.90      | 118.60   |
| 1   | AA    | 1196 | A    | N1-C6-N6 | 12.16 | 125.90      | 118.60   |
| 27  | B8    | 423  | A    | N1-C6-N6 | 12.16 | 125.90      | 118.60   |
| 27  | B8    | 430  | A    | N1-C6-N6 | 12.16 | 125.90      | 118.60   |
| 27  | B8    | 482  | A    | N1-C6-N6 | 12.16 | 125.90      | 118.60   |
| 1   | AA    | 1396 | A    | N1-C6-N6 | 12.16 | 125.90      | 118.60   |
| 27  | B8    | 53   | A    | N1-C6-N6 | 12.16 | 125.90      | 118.60   |
| 27  | B8    | 1495 | A    | N1-C6-N6 | 12.16 | 125.89      | 118.60   |
| 1   | AA    | 303  | A    | N1-C6-N6 | 12.15 | 125.89      | 118.60   |
| 27  | B8    | 1953 | A    | N1-C6-N6 | 12.15 | 125.89      | 118.60   |
| 1   | AA    | 366  | A    | N1-C6-N6 | 12.15 | 125.89      | 118.60   |
| 1   | AA    | 546  | A    | N1-C6-N6 | 12.15 | 125.89      | 118.60   |
| 27  | B8    | 332  | A    | N1-C6-N6 | 12.14 | 125.89      | 118.60   |
| 27  | B8    | 789  | A    | N1-C6-N6 | 12.14 | 125.88      | 118.60   |
| 1   | AA    | 630  | A    | N1-C6-N6 | 12.13 | 125.88      | 118.60   |
| 27  | B8    | 1420 | A    | N1-C6-N6 | 12.13 | 125.88      | 118.60   |
| 27  | B8    | 1609 | A    | N1-C6-N6 | 12.13 | 125.88      | 118.60   |
| 27  | B8    | 1987 | A    | N1-C6-N6 | 12.13 | 125.88      | 118.60   |
| 27  | B8    | 981  | A    | N1-C6-N6 | 12.13 | 125.88      | 118.60   |
| 27  | B8    | 2792 | A    | N1-C6-N6 | 12.13 | 125.88      | 118.60   |
| 27  | B8    | 2471 | A    | N1-C6-N6 | 12.13 | 125.88      | 118.60   |
| 27  | B8    | 217  | A    | N1-C6-N6 | 12.13 | 125.88      | 118.60   |
| 1   | AA    | 1201 | A    | N1-C6-N6 | 12.12 | 125.87      | 118.60   |
| 1   | AA    | 149  | A    | N1-C6-N6 | 12.12 | 125.87      | 118.60   |
| 27  | B8    | 14   | A    | N1-C6-N6 | 12.12 | 125.87      | 118.60   |
| 1   | AA    | 349  | A    | N1-C6-N6 | 12.12 | 125.87      | 118.60   |
| 1   | AA    | 635  | A    | N1-C6-N6 | 12.12 | 125.87      | 118.60   |
| 1   | AA    | 1170 | A    | N1-C6-N6 | 12.12 | 125.87      | 118.60   |
| 1   | AA    | 815  | A    | N1-C6-N6 | 12.12 | 125.87      | 118.60   |
| 1   | AA    | 900  | A    | N1-C6-N6 | 12.12 | 125.87      | 118.60   |
| 27  | B8    | 320  | A    | N1-C6-N6 | 12.12 | 125.87      | 118.60   |
| 1   | AA    | 539  | A    | N1-C6-N6 | 12.12 | 125.87      | 118.60   |
| 1   | AA    | 1507 | A    | N1-C6-N6 | 12.12 | 125.87      | 118.60   |
| 27  | B8    | 2810 | A    | N1-C6-N6 | 12.11 | 125.87      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | AA    | 1324 | A    | N1-C6-N6 | 12.11 | 125.87      | 118.60   |
| 27  | B8    | 146  | A    | N1-C6-N6 | 12.11 | 125.86      | 118.60   |
| 27  | B8    | 2706 | A    | N1-C6-N6 | 12.11 | 125.86      | 118.60   |
| 1   | AA    | 493  | A    | N1-C6-N6 | 12.10 | 125.86      | 118.60   |
| 1   | AA    | 1274 | A    | N1-C6-N6 | 12.10 | 125.86      | 118.60   |
| 27  | B8    | 1762 | A    | N1-C6-N6 | 12.10 | 125.86      | 118.60   |
| 27  | B8    | 272  | A    | N1-C6-N6 | 12.10 | 125.86      | 118.60   |
| 27  | B8    | 802  | A    | N1-C6-N6 | 12.10 | 125.86      | 118.60   |
| 27  | B8    | 945  | A    | N1-C6-N6 | 12.10 | 125.86      | 118.60   |
| 1   | AA    | 510  | A    | N1-C6-N6 | 12.10 | 125.86      | 118.60   |
| 1   | AA    | 1169 | A    | N1-C6-N6 | 12.10 | 125.86      | 118.60   |
| 27  | B8    | 352  | A    | N1-C6-N6 | 12.10 | 125.86      | 118.60   |
| 27  | B8    | 1073 | A    | N1-C6-N6 | 12.10 | 125.86      | 118.60   |
| 27  | B8    | 2518 | A    | N1-C6-N6 | 12.10 | 125.86      | 118.60   |
| 27  | B8    | 2572 | A    | N1-C6-N6 | 12.10 | 125.86      | 118.60   |
| 1   | AA    | 119  | A    | N1-C6-N6 | 12.09 | 125.86      | 118.60   |
| 27  | B8    | 2823 | A    | N1-C6-N6 | 12.09 | 125.86      | 118.60   |
| 1   | AA    | 873  | A    | N1-C6-N6 | 12.09 | 125.86      | 118.60   |
| 27  | B8    | 833  | A    | N1-C6-N6 | 12.09 | 125.85      | 118.60   |
| 1   | AA    | 499  | A    | N1-C6-N6 | 12.09 | 125.85      | 118.60   |
| 27  | B8    | 2101 | A    | N1-C6-N6 | 12.09 | 125.85      | 118.60   |
| 27  | B8    | 2191 | A    | N1-C6-N6 | 12.09 | 125.85      | 118.60   |
| 27  | B8    | 2461 | A    | N1-C6-N6 | 12.09 | 125.85      | 118.60   |
| 27  | B8    | 792  | A    | N1-C6-N6 | 12.09 | 125.85      | 118.60   |
| 1   | AA    | 465  | A    | N1-C6-N6 | 12.09 | 125.85      | 118.60   |
| 27  | B8    | 819  | A    | N1-C6-N6 | 12.09 | 125.85      | 118.60   |
| 27  | B8    | 1085 | A    | N1-C6-N6 | 12.09 | 125.85      | 118.60   |
| 27  | B8    | 1593 | A    | N1-C6-N6 | 12.09 | 125.85      | 118.60   |
| 1   | AA    | 44   | A    | N1-C6-N6 | 12.08 | 125.85      | 118.60   |
| 27  | B8    | 1978 | A    | N1-C6-N6 | 12.08 | 125.85      | 118.60   |
| 27  | B8    | 160  | A    | N1-C6-N6 | 12.08 | 125.85      | 118.60   |
| 27  | B8    | 1096 | A    | N1-C6-N6 | 12.08 | 125.85      | 118.60   |
| 27  | B8    | 1877 | A    | N1-C6-N6 | 12.08 | 125.85      | 118.60   |
| 27  | B8    | 2432 | A    | N1-C6-N6 | 12.08 | 125.85      | 118.60   |
| 27  | B8    | 2682 | A    | N1-C6-N6 | 12.08 | 125.85      | 118.60   |
| 1   | AA    | 1163 | A    | N1-C6-N6 | 12.07 | 125.84      | 118.60   |
| 27  | B8    | 706  | A    | N1-C6-N6 | 12.07 | 125.84      | 118.60   |
| 27  | B8    | 2377 | A    | N1-C6-N6 | 12.07 | 125.84      | 118.60   |
| 27  | B8    | 1805 | A    | N1-C6-N6 | 12.07 | 125.84      | 118.60   |
| 27  | B8    | 627  | A    | N1-C6-N6 | 12.06 | 125.84      | 118.60   |
| 27  | B8    | 2142 | A    | N1-C6-N6 | 12.06 | 125.84      | 118.60   |
| 27  | B8    | 2241 | A    | N1-C6-N6 | 12.06 | 125.84      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 27  | B8    | 2407 | A    | N1-C6-N6 | 12.06 | 125.84      | 118.60   |
| 1   | AA    | 435  | A    | N1-C6-N6 | 12.06 | 125.84      | 118.60   |
| 1   | AA    | 1022 | A    | N1-C6-N6 | 12.06 | 125.84      | 118.60   |
| 1   | AA    | 496  | A    | N1-C6-N6 | 12.06 | 125.83      | 118.60   |
| 1   | AA    | 1254 | A    | N1-C6-N6 | 12.06 | 125.84      | 118.60   |
| 27  | B8    | 979  | A    | N1-C6-N6 | 12.06 | 125.84      | 118.60   |
| 27  | B8    | 1069 | A    | N1-C6-N6 | 12.06 | 125.83      | 118.60   |
| 27  | B8    | 1566 | A    | N1-C6-N6 | 12.06 | 125.83      | 118.60   |
| 27  | B8    | 1403 | A    | N1-C6-N6 | 12.06 | 125.83      | 118.60   |
| 27  | B8    | 1503 | A    | N1-C6-N6 | 12.06 | 125.83      | 118.60   |
| 27  | B8    | 2560 | A    | N1-C6-N6 | 12.06 | 125.83      | 118.60   |
| 3   | AV    | 14   | A    | N1-C6-N6 | 12.05 | 125.83      | 118.60   |
| 27  | B8    | 1090 | A    | N1-C6-N6 | 12.05 | 125.83      | 118.60   |
| 1   | AA    | 743  | A    | N1-C6-N6 | 12.05 | 125.83      | 118.60   |
| 27  | B8    | 1676 | A    | N1-C6-N6 | 12.05 | 125.83      | 118.60   |
| 27  | B8    | 2814 | A    | N1-C6-N6 | 12.05 | 125.83      | 118.60   |
| 1   | AA    | 938  | A    | N1-C6-N6 | 12.05 | 125.83      | 118.60   |
| 27  | B8    | 1050 | A    | N1-C6-N6 | 12.05 | 125.83      | 118.60   |
| 27  | B8    | 1570 | A    | N1-C6-N6 | 12.04 | 125.83      | 118.60   |
| 27  | B8    | 2602 | A    | N1-C6-N6 | 12.04 | 125.83      | 118.60   |
| 27  | B8    | 1230 | A    | N1-C6-N6 | 12.04 | 125.83      | 118.60   |
| 27  | B8    | 2850 | A    | N1-C6-N6 | 12.04 | 125.83      | 118.60   |
| 27  | B8    | 590  | A    | N1-C6-N6 | 12.04 | 125.82      | 118.60   |
| 27  | B8    | 804  | A    | N1-C6-N6 | 12.04 | 125.82      | 118.60   |
| 27  | B8    | 1678 | A    | N1-C6-N6 | 12.04 | 125.82      | 118.60   |
| 27  | B8    | 10   | A    | N1-C6-N6 | 12.03 | 125.82      | 118.60   |
| 27  | B8    | 2005 | A    | N1-C6-N6 | 12.03 | 125.82      | 118.60   |
| 1   | AA    | 321  | A    | N1-C6-N6 | 12.03 | 125.82      | 118.60   |
| 26  | B7    | 46   | A    | N1-C6-N6 | 12.03 | 125.82      | 118.60   |
| 27  | B8    | 1722 | A    | N1-C6-N6 | 12.03 | 125.82      | 118.60   |
| 1   | AA    | 553  | A    | N1-C6-N6 | 12.03 | 125.82      | 118.60   |
| 27  | B8    | 480  | A    | N1-C6-N6 | 12.03 | 125.81      | 118.60   |
| 27  | B8    | 2388 | A    | N1-C6-N6 | 12.03 | 125.82      | 118.60   |
| 27  | B8    | 1938 | A    | N1-C6-N6 | 12.02 | 125.81      | 118.60   |
| 1   | AA    | 1311 | A    | N1-C6-N6 | 12.02 | 125.81      | 118.60   |
| 1   | AA    | 306  | A    | N1-C6-N6 | 12.02 | 125.81      | 118.60   |
| 27  | B8    | 1353 | A    | N1-C6-N6 | 12.02 | 125.81      | 118.60   |
| 27  | B8    | 1014 | A    | N1-C6-N6 | 12.01 | 125.81      | 118.60   |
| 27  | B8    | 2080 | A    | N1-C6-N6 | 12.01 | 125.81      | 118.60   |
| 27  | B8    | 2346 | A    | N1-C6-N6 | 12.01 | 125.81      | 118.60   |
| 27  | B8    | 2309 | A    | N1-C6-N6 | 12.01 | 125.80      | 118.60   |
| 27  | B8    | 223  | A    | N1-C6-N6 | 12.00 | 125.80      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 27  | B8    | 1020 | A    | N1-C6-N6 | 12.00 | 125.80      | 118.60   |
| 27  | B8    | 2448 | A    | N1-C6-N6 | 12.00 | 125.80      | 118.60   |
| 27  | B8    | 764  | A    | N1-C6-N6 | 12.00 | 125.80      | 118.60   |
| 1   | AA    | 958  | A    | N1-C6-N6 | 12.00 | 125.80      | 118.60   |
| 27  | B8    | 2097 | A    | N1-C6-N6 | 12.00 | 125.80      | 118.60   |
| 1   | AA    | 189  | A    | N1-C6-N6 | 12.00 | 125.80      | 118.60   |
| 1   | AA    | 1350 | A    | N1-C6-N6 | 12.00 | 125.80      | 118.60   |
| 27  | B8    | 563  | A    | N1-C6-N6 | 12.00 | 125.80      | 118.60   |
| 1   | AA    | 579  | A    | N1-C6-N6 | 11.99 | 125.80      | 118.60   |
| 1   | AA    | 363  | A    | N1-C6-N6 | 11.99 | 125.80      | 118.60   |
| 1   | AA    | 1021 | A    | N1-C6-N6 | 11.99 | 125.80      | 118.60   |
| 27  | B8    | 1008 | A    | N1-C6-N6 | 11.99 | 125.80      | 118.60   |
| 27  | B8    | 1057 | A    | N1-C6-N6 | 11.99 | 125.80      | 118.60   |
| 27  | B8    | 472  | A    | N1-C6-N6 | 11.99 | 125.79      | 118.60   |
| 27  | B8    | 1970 | A    | N1-C6-N6 | 11.99 | 125.79      | 118.60   |
| 27  | B8    | 2288 | A    | N1-C6-N6 | 11.99 | 125.79      | 118.60   |
| 27  | B8    | 1754 | A    | N1-C6-N6 | 11.99 | 125.79      | 118.60   |
| 27  | B8    | 2425 | A    | N1-C6-N6 | 11.98 | 125.79      | 118.60   |
| 1   | AA    | 532  | A    | N1-C6-N6 | 11.98 | 125.79      | 118.60   |
| 27  | B8    | 1029 | A    | N1-C6-N6 | 11.98 | 125.79      | 118.60   |
| 27  | B8    | 1048 | A    | N1-C6-N6 | 11.98 | 125.79      | 118.60   |
| 27  | B8    | 1241 | A    | N1-C6-N6 | 11.98 | 125.79      | 118.60   |
| 1   | AA    | 1180 | A    | N1-C6-N6 | 11.98 | 125.79      | 118.60   |
| 27  | B8    | 668  | A    | N1-C6-N6 | 11.98 | 125.79      | 118.60   |
| 27  | B8    | 2019 | A    | N1-C6-N6 | 11.98 | 125.79      | 118.60   |
| 27  | B8    | 311  | A    | N1-C6-N6 | 11.97 | 125.78      | 118.60   |
| 27  | B8    | 345  | A    | N1-C6-N6 | 11.97 | 125.78      | 118.60   |
| 27  | B8    | 1169 | A    | N1-C6-N6 | 11.97 | 125.78      | 118.60   |
| 27  | B8    | 1665 | A    | N1-C6-N6 | 11.97 | 125.78      | 118.60   |
| 1   | AA    | 1092 | A    | N1-C6-N6 | 11.97 | 125.78      | 118.60   |
| 27  | B8    | 1246 | A    | N1-C6-N6 | 11.97 | 125.78      | 118.60   |
| 27  | B8    | 1597 | A    | N1-C6-N6 | 11.97 | 125.78      | 118.60   |
| 27  | B8    | 1802 | A    | N1-C6-N6 | 11.97 | 125.78      | 118.60   |
| 1   | AA    | 728  | A    | N1-C6-N6 | 11.97 | 125.78      | 118.60   |
| 1   | AA    | 1542 | A    | N1-C6-N6 | 11.97 | 125.78      | 118.60   |
| 27  | B8    | 603  | A    | N1-C6-N6 | 11.96 | 125.78      | 118.60   |
| 27  | B8    | 1262 | A    | N1-C6-N6 | 11.96 | 125.78      | 118.60   |
| 1   | AA    | 781  | A    | N1-C6-N6 | 11.96 | 125.78      | 118.60   |
| 3   | AV    | 52   | A    | N1-C6-N6 | 11.96 | 125.78      | 118.60   |
| 27  | B8    | 2776 | A    | N1-C6-N6 | 11.96 | 125.78      | 118.60   |
| 27  | B8    | 52   | A    | N1-C6-N6 | 11.96 | 125.78      | 118.60   |
| 27  | B8    | 218  | A    | N1-C6-N6 | 11.96 | 125.78      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 27  | B8    | 1672 | A    | N1-C6-N6 | 11.96 | 125.77      | 118.60   |
| 27  | B8    | 2426 | A    | N1-C6-N6 | 11.96 | 125.77      | 118.60   |
| 27  | B8    | 2809 | A    | N1-C6-N6 | 11.96 | 125.77      | 118.60   |
| 27  | B8    | 1327 | A    | N1-C6-N6 | 11.95 | 125.77      | 118.60   |
| 27  | B8    | 1383 | A    | N1-C6-N6 | 11.95 | 125.77      | 118.60   |
| 27  | B8    | 1385 | A    | N1-C6-N6 | 11.95 | 125.77      | 118.60   |
| 27  | B8    | 1871 | A    | N1-C6-N6 | 11.95 | 125.77      | 118.60   |
| 1   | AA    | 1493 | A    | N1-C6-N6 | 11.95 | 125.77      | 118.60   |
| 27  | B8    | 980  | A    | N1-C6-N6 | 11.95 | 125.77      | 118.60   |
| 27  | B8    | 1847 | A    | N1-C6-N6 | 11.95 | 125.77      | 118.60   |
| 27  | B8    | 2740 | A    | N1-C6-N6 | 11.95 | 125.77      | 118.60   |
| 1   | AA    | 101  | A    | N1-C6-N6 | 11.94 | 125.77      | 118.60   |
| 1   | AA    | 816  | A    | N1-C6-N6 | 11.94 | 125.77      | 118.60   |
| 27  | B8    | 2531 | A    | N1-C6-N6 | 11.94 | 125.77      | 118.60   |
| 27  | B8    | 1046 | A    | N1-C6-N6 | 11.94 | 125.76      | 118.60   |
| 1   | AA    | 602  | A    | N1-C6-N6 | 11.94 | 125.76      | 118.60   |
| 27  | B8    | 905  | A    | N1-C6-N6 | 11.94 | 125.76      | 118.60   |
| 1   | AA    | 621  | A    | N1-C6-N6 | 11.94 | 125.76      | 118.60   |
| 1   | AA    | 1431 | A    | N1-C6-N6 | 11.94 | 125.76      | 118.60   |
| 27  | B8    | 631  | A    | N1-C6-N6 | 11.94 | 125.76      | 118.60   |
| 1   | AA    | 807  | A    | N1-C6-N6 | 11.93 | 125.76      | 118.60   |
| 27  | B8    | 191  | A    | N1-C6-N6 | 11.93 | 125.76      | 118.60   |
| 27  | B8    | 348  | A    | N1-C6-N6 | 11.93 | 125.76      | 118.60   |
| 27  | B8    | 2205 | A    | N1-C6-N6 | 11.93 | 125.76      | 118.60   |
| 1   | AA    | 1117 | A    | N1-C6-N6 | 11.93 | 125.76      | 118.60   |
| 1   | AA    | 1271 | A    | N1-C6-N6 | 11.93 | 125.76      | 118.60   |
| 1   | AA    | 1480 | A    | N1-C6-N6 | 11.93 | 125.76      | 118.60   |
| 27  | B8    | 2247 | A    | N1-C6-N6 | 11.93 | 125.76      | 118.60   |
| 1   | AA    | 338  | A    | N1-C6-N6 | 11.93 | 125.76      | 118.60   |
| 1   | AA    | 596  | A    | N1-C6-N6 | 11.93 | 125.76      | 118.60   |
| 1   | AA    | 946  | A    | N1-C6-N6 | 11.93 | 125.76      | 118.60   |
| 27  | B8    | 572  | A    | N1-C6-N6 | 11.92 | 125.75      | 118.60   |
| 1   | AA    | 1257 | A    | N1-C6-N6 | 11.92 | 125.75      | 118.60   |
| 27  | B8    | 793  | A    | N1-C6-N6 | 11.92 | 125.75      | 118.60   |
| 27  | B8    | 983  | A    | N1-C6-N6 | 11.92 | 125.75      | 118.60   |
| 27  | B8    | 1966 | A    | N1-C6-N6 | 11.92 | 125.75      | 118.60   |
| 1   | AA    | 1019 | A    | N1-C6-N6 | 11.91 | 125.75      | 118.60   |
| 27  | B8    | 752  | A    | N1-C6-N6 | 11.91 | 125.75      | 118.60   |
| 27  | B8    | 172  | A    | N1-C6-N6 | 11.91 | 125.75      | 118.60   |
| 1   | AA    | 715  | A    | N1-C6-N6 | 11.91 | 125.75      | 118.60   |
| 27  | B8    | 1759 | A    | N1-C6-N6 | 11.91 | 125.75      | 118.60   |
| 27  | B8    | 739  | A    | N1-C6-N6 | 11.91 | 125.74      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 27  | B8    | 2071 | A    | N1-C6-N6 | 11.91 | 125.75      | 118.60   |
| 27  | B8    | 2058 | A    | N1-C6-N6 | 11.91 | 125.74      | 118.60   |
| 1   | AA    | 51   | A    | N1-C6-N6 | 11.90 | 125.74      | 118.60   |
| 1   | AA    | 1067 | A    | N1-C6-N6 | 11.90 | 125.74      | 118.60   |
| 1   | AA    | 1468 | A    | N1-C6-N6 | 11.90 | 125.74      | 118.60   |
| 27  | B8    | 1504 | A    | N1-C6-N6 | 11.90 | 125.74      | 118.60   |
| 27  | B8    | 1392 | A    | N1-C6-N6 | 11.90 | 125.74      | 118.60   |
| 1   | AA    | 1093 | A    | N1-C6-N6 | 11.89 | 125.74      | 118.60   |
| 27  | B8    | 173  | A    | N1-C6-N6 | 11.89 | 125.74      | 118.60   |
| 27  | B8    | 1000 | A    | N1-C6-N6 | 11.89 | 125.74      | 118.60   |
| 27  | B8    | 2565 | A    | N1-C6-N6 | 11.89 | 125.73      | 118.60   |
| 27  | B8    | 2799 | A    | N1-C6-N6 | 11.89 | 125.73      | 118.60   |
| 1   | AA    | 1394 | A    | N1-C6-N6 | 11.88 | 125.73      | 118.60   |
| 1   | AA    | 1446 | A    | N1-C6-N6 | 11.88 | 125.73      | 118.60   |
| 27  | B8    | 44   | A    | N1-C6-N6 | 11.88 | 125.73      | 118.60   |
| 27  | B8    | 216  | A    | N1-C6-N6 | 11.88 | 125.73      | 118.60   |
| 27  | B8    | 270  | A    | N1-C6-N6 | 11.88 | 125.73      | 118.60   |
| 27  | B8    | 2322 | A    | N1-C6-N6 | 11.88 | 125.73      | 118.60   |
| 1   | AA    | 1082 | A    | N1-C6-N6 | 11.88 | 125.73      | 118.60   |
| 1   | AA    | 1430 | A    | N1-C6-N6 | 11.88 | 125.73      | 118.60   |
| 27  | B8    | 1129 | A    | N1-C6-N6 | 11.88 | 125.73      | 118.60   |
| 27  | B8    | 1470 | A    | N1-C6-N6 | 11.88 | 125.73      | 118.60   |
| 2   | AX    | 21   | A    | N1-C6-N6 | 11.87 | 125.72      | 118.60   |
| 27  | B8    | 125  | A    | N1-C6-N6 | 11.87 | 125.72      | 118.60   |
| 1   | AA    | 918  | A    | N1-C6-N6 | 11.87 | 125.72      | 118.60   |
| 27  | B8    | 2758 | A    | N1-C6-N6 | 11.87 | 125.72      | 118.60   |
| 1   | AA    | 344  | A    | N1-C6-N6 | 11.87 | 125.72      | 118.60   |
| 1   | AA    | 749  | A    | N1-C6-N6 | 11.87 | 125.72      | 118.60   |
| 27  | B8    | 936  | A    | N1-C6-N6 | 11.87 | 125.72      | 118.60   |
| 27  | B8    | 2003 | A    | N1-C6-N6 | 11.87 | 125.72      | 118.60   |
| 1   | AA    | 1213 | A    | N1-C6-N6 | 11.87 | 125.72      | 118.60   |
| 1   | AA    | 19   | A    | N1-C6-N6 | 11.86 | 125.72      | 118.60   |
| 1   | AA    | 1499 | A    | N1-C6-N6 | 11.86 | 125.72      | 118.60   |
| 27  | B8    | 788  | A    | N1-C6-N6 | 11.87 | 125.72      | 118.60   |
| 27  | B8    | 960  | A    | N1-C6-N6 | 11.86 | 125.72      | 118.60   |
| 27  | B8    | 984  | A    | N1-C6-N6 | 11.86 | 125.72      | 118.60   |
| 27  | B8    | 877  | A    | N1-C6-N6 | 11.86 | 125.71      | 118.60   |
| 27  | B8    | 861  | A    | N1-C6-N6 | 11.86 | 125.71      | 118.60   |
| 27  | B8    | 197  | A    | N1-C6-N6 | 11.85 | 125.71      | 118.60   |
| 27  | B8    | 1302 | A    | N1-C6-N6 | 11.85 | 125.71      | 118.60   |
| 27  | B8    | 1151 | A    | N1-C6-N6 | 11.85 | 125.71      | 118.60   |
| 27  | B8    | 2634 | A    | N1-C6-N6 | 11.85 | 125.71      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | AA    | 572  | A    | N1-C6-N6 | 11.85 | 125.71      | 118.60   |
| 3   | AV    | 59   | A    | N1-C6-N6 | 11.85 | 125.71      | 118.60   |
| 27  | B8    | 1900 | A    | N1-C6-N6 | 11.85 | 125.71      | 118.60   |
| 1   | AA    | 607  | A    | N1-C6-N6 | 11.84 | 125.71      | 118.60   |
| 1   | AA    | 389  | A    | N1-C6-N6 | 11.84 | 125.70      | 118.60   |
| 27  | B8    | 309  | A    | N1-C6-N6 | 11.84 | 125.70      | 118.60   |
| 27  | B8    | 1549 | A    | N1-C6-N6 | 11.84 | 125.70      | 118.60   |
| 27  | B8    | 1981 | A    | N1-C6-N6 | 11.84 | 125.70      | 118.60   |
| 27  | B8    | 2459 | A    | N1-C6-N6 | 11.84 | 125.70      | 118.60   |
| 1   | AA    | 1    | A    | N1-C6-N6 | 11.84 | 125.70      | 118.60   |
| 1   | AA    | 161  | A    | N1-C6-N6 | 11.84 | 125.70      | 118.60   |
| 27  | B8    | 1347 | A    | N1-C6-N6 | 11.84 | 125.70      | 118.60   |
| 1   | AA    | 1476 | A    | N1-C6-N6 | 11.83 | 125.70      | 118.60   |
| 27  | B8    | 1626 | A    | N1-C6-N6 | 11.83 | 125.70      | 118.60   |
| 27  | B8    | 504  | A    | N1-C6-N6 | 11.83 | 125.70      | 118.60   |
| 27  | B8    | 2547 | A    | N1-C6-N6 | 11.82 | 125.69      | 118.60   |
| 1   | AA    | 851  | G    | N1-C6-O6 | 11.82 | 126.99      | 119.90   |
| 1   | AA    | 1046 | A    | N1-C6-N6 | 11.82 | 125.69      | 118.60   |
| 27  | B8    | 101  | A    | N1-C6-N6 | 11.82 | 125.69      | 118.60   |
| 27  | B8    | 231  | A    | N1-C6-N6 | 11.82 | 125.69      | 118.60   |
| 27  | B8    | 2813 | A    | N1-C6-N6 | 11.82 | 125.69      | 118.60   |
| 27  | B8    | 49   | A    | N1-C6-N6 | 11.82 | 125.69      | 118.60   |
| 27  | B8    | 384  | A    | N1-C6-N6 | 11.82 | 125.69      | 118.60   |
| 1   | AA    | 197  | A    | N1-C6-N6 | 11.82 | 125.69      | 118.60   |
| 1   | AA    | 2    | A    | N1-C6-N6 | 11.82 | 125.69      | 118.60   |
| 1   | AA    | 415  | A    | N1-C6-N6 | 11.82 | 125.69      | 118.60   |
| 27  | B8    | 844  | A    | N1-C6-N6 | 11.82 | 125.69      | 118.60   |
| 27  | B8    | 1808 | A    | N1-C6-N6 | 11.81 | 125.69      | 118.60   |
| 1   | AA    | 315  | A    | N1-C6-N6 | 11.81 | 125.69      | 118.60   |
| 1   | AA    | 356  | A    | N1-C6-N6 | 11.81 | 125.69      | 118.60   |
| 27  | B8    | 917  | A    | N1-C6-N6 | 11.81 | 125.69      | 118.60   |
| 2   | AX    | 22   | A    | N1-C6-N6 | 11.80 | 125.68      | 118.60   |
| 27  | B8    | 470  | A    | N1-C6-N6 | 11.80 | 125.68      | 118.60   |
| 1   | AA    | 777  | A    | N1-C6-N6 | 11.80 | 125.68      | 118.60   |
| 26  | B7    | 104  | A    | N1-C6-N6 | 11.80 | 125.68      | 118.60   |
| 27  | B8    | 422  | A    | N1-C6-N6 | 11.80 | 125.68      | 118.60   |
| 1   | AA    | 1216 | A    | N1-C6-N6 | 11.80 | 125.68      | 118.60   |
| 27  | B8    | 1789 | A    | N1-C6-N6 | 11.80 | 125.68      | 118.60   |
| 27  | B8    | 196  | A    | N1-C6-N6 | 11.80 | 125.68      | 118.60   |
| 27  | B8    | 1328 | A    | N1-C6-N6 | 11.80 | 125.68      | 118.60   |
| 1   | AA    | 466  | A    | N1-C6-N6 | 11.79 | 125.68      | 118.60   |
| 1   | AA    | 1102 | A    | N1-C6-N6 | 11.79 | 125.68      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | AA    | 1518 | A    | N1-C6-N6 | 11.79 | 125.67      | 118.60   |
| 27  | B8    | 1156 | A    | N1-C6-N6 | 11.79 | 125.67      | 118.60   |
| 27  | B8    | 2009 | A    | N1-C6-N6 | 11.79 | 125.67      | 118.60   |
| 27  | B8    | 1508 | A    | N1-C6-N6 | 11.79 | 125.67      | 118.60   |
| 27  | B8    | 1632 | A    | N1-C6-N6 | 11.79 | 125.67      | 118.60   |
| 1   | AA    | 495  | A    | N1-C6-N6 | 11.78 | 125.67      | 118.60   |
| 1   | AA    | 1227 | A    | N1-C6-N6 | 11.78 | 125.67      | 118.60   |
| 27  | B8    | 1175 | A    | N1-C6-N6 | 11.78 | 125.67      | 118.60   |
| 1   | AA    | 767  | A    | N1-C6-N6 | 11.78 | 125.67      | 118.60   |
| 27  | B8    | 507  | A    | N1-C6-N6 | 11.78 | 125.67      | 118.60   |
| 27  | B8    | 972  | A    | N1-C6-N6 | 11.78 | 125.67      | 118.60   |
| 27  | B8    | 1571 | A    | N1-C6-N6 | 11.78 | 125.67      | 118.60   |
| 27  | B8    | 1505 | A    | N1-C6-N6 | 11.78 | 125.67      | 118.60   |
| 1   | AA    | 640  | A    | N1-C6-N6 | 11.77 | 125.66      | 118.60   |
| 27  | B8    | 344  | A    | N1-C6-N6 | 11.77 | 125.66      | 118.60   |
| 27  | B8    | 439  | A    | N1-C6-N6 | 11.77 | 125.66      | 118.60   |
| 27  | B8    | 1801 | A    | N1-C6-N6 | 11.77 | 125.66      | 118.60   |
| 27  | B8    | 2270 | A    | N1-C6-N6 | 11.77 | 125.66      | 118.60   |
| 27  | B8    | 2736 | A    | N1-C6-N6 | 11.77 | 125.66      | 118.60   |
| 1   | AA    | 1503 | A    | N1-C6-N6 | 11.76 | 125.66      | 118.60   |
| 1   | AA    | 712  | A    | N1-C6-N6 | 11.76 | 125.66      | 118.60   |
| 27  | B8    | 1322 | A    | N1-C6-N6 | 11.76 | 125.66      | 118.60   |
| 27  | B8    | 1821 | A    | N1-C6-N6 | 11.76 | 125.66      | 118.60   |
| 1   | AA    | 1483 | A    | N1-C6-N6 | 11.76 | 125.66      | 118.60   |
| 27  | B8    | 1635 | A    | N1-C6-N6 | 11.76 | 125.66      | 118.60   |
| 27  | B8    | 1477 | A    | N1-C6-N6 | 11.76 | 125.66      | 118.60   |
| 1   | AA    | 1375 | A    | N1-C6-N6 | 11.76 | 125.65      | 118.60   |
| 1   | AA    | 622  | A    | N1-C6-N6 | 11.75 | 125.65      | 118.60   |
| 27  | B8    | 156  | A    | N1-C6-N6 | 11.75 | 125.65      | 118.60   |
| 27  | B8    | 1744 | A    | N1-C6-N6 | 11.75 | 125.65      | 118.60   |
| 1   | AA    | 397  | A    | N1-C6-N6 | 11.75 | 125.65      | 118.60   |
| 1   | AA    | 968  | A    | N1-C6-N6 | 11.75 | 125.65      | 118.60   |
| 27  | B8    | 722  | A    | N1-C6-N6 | 11.74 | 125.64      | 118.60   |
| 27  | B8    | 1054 | A    | N1-C6-N6 | 11.74 | 125.64      | 118.60   |
| 27  | B8    | 1509 | A    | N1-C6-N6 | 11.74 | 125.64      | 118.60   |
| 27  | B8    | 478  | A    | N1-C6-N6 | 11.74 | 125.64      | 118.60   |
| 27  | B8    | 896  | A    | N1-C6-N6 | 11.74 | 125.64      | 118.60   |
| 1   | AA    | 790  | A    | N1-C6-N6 | 11.74 | 125.64      | 118.60   |
| 27  | B8    | 2266 | A    | N1-C6-N6 | 11.74 | 125.64      | 118.60   |
| 27  | B8    | 1535 | A    | N1-C6-N6 | 11.73 | 125.64      | 118.60   |
| 1   | AA    | 975  | A    | N1-C6-N6 | 11.73 | 125.64      | 118.60   |
| 1   | AA    | 1179 | A    | N1-C6-N6 | 11.73 | 125.64      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | AA    | 1248 | A    | N1-C6-N6  | 11.73 | 125.64      | 118.60   |
| 27  | B8    | 1080 | A    | N1-C6-N6  | 11.73 | 125.64      | 118.60   |
| 1   | AA    | 729  | A    | N1-C6-N6  | 11.73 | 125.64      | 118.60   |
| 3   | AV    | 58   | A    | N1-C6-N6  | 11.73 | 125.64      | 118.60   |
| 27  | B8    | 975  | A    | N1-C6-N6  | 11.72 | 125.63      | 118.60   |
| 27  | B8    | 1960 | A    | N1-C6-N6  | 11.72 | 125.63      | 118.60   |
| 27  | B8    | 2577 | A    | N1-C6-N6  | 11.72 | 125.63      | 118.60   |
| 1   | AA    | 243  | A    | N1-C6-N6  | 11.72 | 125.63      | 118.60   |
| 1   | AA    | 250  | A    | N1-C6-N6  | 11.72 | 125.63      | 118.60   |
| 27  | B8    | 715  | A    | N1-C6-N6  | 11.72 | 125.63      | 118.60   |
| 1   | AA    | 74   | A    | N1-C6-N6  | 11.71 | 125.63      | 118.60   |
| 27  | B8    | 1889 | A    | N1-C6-N6  | 11.71 | 125.63      | 118.60   |
| 27  | B8    | 2614 | A    | N1-C6-N6  | 11.71 | 125.63      | 118.60   |
| 1   | AA    | 845  | A    | N1-C6-N6  | 11.71 | 125.63      | 118.60   |
| 27  | B8    | 176  | A    | N1-C6-N6  | 11.71 | 125.63      | 118.60   |
| 27  | B8    | 1010 | A    | N1-C6-N6  | 11.71 | 125.63      | 118.60   |
| 27  | B8    | 2327 | A    | N1-C6-N6  | 11.71 | 125.63      | 118.60   |
| 1   | AA    | 1130 | A    | N1-C6-N6  | 11.71 | 125.62      | 118.60   |
| 27  | B8    | 2820 | A    | N1-C6-N6  | 11.71 | 125.62      | 118.60   |
| 27  | B8    | 282  | A    | N1-C6-N6  | 11.71 | 125.62      | 118.60   |
| 1   | AA    | 484  | G    | P-O3'-C3' | 11.70 | 133.74      | 119.70   |
| 27  | B8    | 547  | A    | N1-C6-N6  | 11.70 | 125.62      | 118.60   |
| 1   | AA    | 909  | A    | N1-C6-N6  | 11.70 | 125.62      | 118.60   |
| 1   | AA    | 1408 | A    | N1-C6-N6  | 11.70 | 125.62      | 118.60   |
| 1   | AA    | 1502 | A    | N1-C6-N6  | 11.70 | 125.62      | 118.60   |
| 27  | B8    | 1419 | A    | N1-C6-N6  | 11.70 | 125.62      | 118.60   |
| 27  | B8    | 2070 | A    | N1-C6-N6  | 11.70 | 125.62      | 118.60   |
| 27  | B8    | 2534 | A    | N1-C6-N6  | 11.70 | 125.62      | 118.60   |
| 1   | AA    | 78   | A    | N1-C6-N6  | 11.69 | 125.62      | 118.60   |
| 27  | B8    | 1746 | A    | N1-C6-N6  | 11.69 | 125.62      | 118.60   |
| 27  | B8    | 508  | A    | N1-C6-N6  | 11.69 | 125.62      | 118.60   |
| 27  | B8    | 910  | A    | N1-C6-N6  | 11.69 | 125.62      | 118.60   |
| 1   | AA    | 663  | A    | N1-C6-N6  | 11.69 | 125.61      | 118.60   |
| 1   | AA    | 130  | A    | N1-C6-N6  | 11.69 | 125.61      | 118.60   |
| 27  | B8    | 918  | A    | N1-C6-N6  | 11.69 | 125.61      | 118.60   |
| 27  | B8    | 2433 | A    | N1-C6-N6  | 11.69 | 125.61      | 118.60   |
| 1   | AA    | 167  | A    | N1-C6-N6  | 11.69 | 125.61      | 118.60   |
| 27  | B8    | 1365 | A    | N1-C6-N6  | 11.69 | 125.61      | 118.60   |
| 1   | AA    | 1363 | A    | N1-C6-N6  | 11.68 | 125.61      | 118.60   |
| 27  | B8    | 1359 | A    | N1-C6-N6  | 11.68 | 125.61      | 118.60   |
| 27  | B8    | 1772 | A    | N1-C6-N6  | 11.68 | 125.61      | 118.60   |
| 27  | B8    | 2117 | A    | N1-C6-N6  | 11.68 | 125.61      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 27  | B8    | 2497 | A    | N1-C6-N6 | 11.68 | 125.61      | 118.60   |
| 27  | B8    | 432  | A    | N1-C6-N6 | 11.68 | 125.61      | 118.60   |
| 27  | B8    | 1608 | A    | N1-C6-N6 | 11.68 | 125.61      | 118.60   |
| 27  | B8    | 310  | A    | N1-C6-N6 | 11.68 | 125.61      | 118.60   |
| 1   | AA    | 461  | A    | N1-C6-N6 | 11.68 | 125.61      | 118.60   |
| 27  | B8    | 73   | A    | N1-C6-N6 | 11.68 | 125.61      | 118.60   |
| 27  | B8    | 661  | A    | N1-C6-N6 | 11.68 | 125.61      | 118.60   |
| 27  | B8    | 2468 | A    | N1-C6-N6 | 11.68 | 125.61      | 118.60   |
| 1   | AA    | 412  | A    | N1-C6-N6 | 11.67 | 125.60      | 118.60   |
| 1   | AA    | 681  | A    | N1-C6-N6 | 11.67 | 125.60      | 118.60   |
| 1   | AA    | 704  | A    | N1-C6-N6 | 11.67 | 125.60      | 118.60   |
| 1   | AA    | 298  | A    | N1-C6-N6 | 11.67 | 125.60      | 118.60   |
| 27  | B8    | 643  | A    | N1-C6-N6 | 11.67 | 125.60      | 118.60   |
| 27  | B8    | 1284 | A    | N1-C6-N6 | 11.67 | 125.60      | 118.60   |
| 27  | B8    | 2082 | A    | N1-C6-N6 | 11.67 | 125.60      | 118.60   |
| 27  | B8    | 1572 | A    | N1-C6-N6 | 11.66 | 125.60      | 118.60   |
| 1   | AA    | 747  | A    | N1-C6-N6 | 11.66 | 125.60      | 118.60   |
| 27  | B8    | 866  | A    | N1-C6-N6 | 11.66 | 125.60      | 118.60   |
| 1   | AA    | 1340 | A    | N1-C6-N6 | 11.66 | 125.59      | 118.60   |
| 27  | B8    | 404  | A    | N1-C6-N6 | 11.66 | 125.59      | 118.60   |
| 27  | B8    | 1912 | A    | N1-C6-N6 | 11.65 | 125.59      | 118.60   |
| 27  | B8    | 2476 | A    | N1-C6-N6 | 11.65 | 125.59      | 118.60   |
| 27  | B8    | 391  | A    | N1-C6-N6 | 11.65 | 125.59      | 118.60   |
| 27  | B8    | 1089 | A    | N1-C6-N6 | 11.65 | 125.59      | 118.60   |
| 1   | AA    | 1145 | A    | N1-C6-N6 | 11.64 | 125.59      | 118.60   |
| 27  | B8    | 753  | A    | N1-C6-N6 | 11.64 | 125.58      | 118.60   |
| 26  | B7    | 53   | A    | N1-C6-N6 | 11.64 | 125.58      | 118.60   |
| 27  | B8    | 2513 | A    | N1-C6-N6 | 11.64 | 125.58      | 118.60   |
| 27  | B8    | 2062 | A    | N1-C6-N6 | 11.63 | 125.58      | 118.60   |
| 1   | AA    | 1410 | A    | N1-C6-N6 | 11.63 | 125.58      | 118.60   |
| 1   | AA    | 1534 | A    | N1-C6-N6 | 11.63 | 125.58      | 118.60   |
| 27  | B8    | 1916 | A    | N1-C6-N6 | 11.63 | 125.58      | 118.60   |
| 27  | B8    | 2059 | A    | N1-C6-N6 | 11.63 | 125.58      | 118.60   |
| 27  | B8    | 2590 | A    | N1-C6-N6 | 11.63 | 125.58      | 118.60   |
| 27  | B8    | 2705 | A    | N1-C6-N6 | 11.63 | 125.58      | 118.60   |
| 27  | B8    | 1749 | A    | N1-C6-N6 | 11.63 | 125.58      | 118.60   |
| 27  | B8    | 144  | A    | N1-C6-N6 | 11.62 | 125.57      | 118.60   |
| 1   | AA    | 374  | A    | N1-C6-N6 | 11.62 | 125.57      | 118.60   |
| 1   | AA    | 977  | A    | N1-C6-N6 | 11.62 | 125.57      | 118.60   |
| 1   | AA    | 1318 | A    | N1-C6-N6 | 11.62 | 125.57      | 118.60   |
| 1   | AA    | 393  | A    | N1-C6-N6 | 11.62 | 125.57      | 118.60   |
| 27  | B8    | 278  | A    | N1-C6-N6 | 11.61 | 125.57      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | AA    | 408  | A    | N1-C6-N6 | 11.61 | 125.56      | 118.60   |
| 27  | B8    | 131  | A    | N1-C6-N6 | 11.61 | 125.57      | 118.60   |
| 27  | B8    | 1614 | A    | N1-C6-N6 | 11.60 | 125.56      | 118.60   |
| 27  | B8    | 1265 | A    | N1-C6-N6 | 11.60 | 125.56      | 118.60   |
| 27  | B8    | 1544 | A    | N1-C6-N6 | 11.60 | 125.56      | 118.60   |
| 1   | AA    | 7    | A    | N1-C6-N6 | 11.60 | 125.56      | 118.60   |
| 1   | AA    | 1042 | A    | N1-C6-N6 | 11.60 | 125.56      | 118.60   |
| 27  | B8    | 2883 | A    | N1-C6-N6 | 11.60 | 125.56      | 118.60   |
| 27  | B8    | 2418 | A    | N1-C6-N6 | 11.59 | 125.56      | 118.60   |
| 27  | B8    | 2886 | A    | N1-C6-N6 | 11.59 | 125.55      | 118.60   |
| 27  | B8    | 1247 | A    | N1-C6-N6 | 11.59 | 125.55      | 118.60   |
| 27  | B8    | 1304 | A    | N1-C6-N6 | 11.59 | 125.55      | 118.60   |
| 1   | AA    | 327  | A    | N1-C6-N6 | 11.58 | 125.55      | 118.60   |
| 27  | B8    | 1254 | A    | N1-C6-N6 | 11.58 | 125.55      | 118.60   |
| 27  | B8    | 1919 | A    | N1-C6-N6 | 11.58 | 125.55      | 118.60   |
| 27  | B8    | 2287 | A    | N1-C6-N6 | 11.58 | 125.55      | 118.60   |
| 1   | AA    | 50   | A    | N1-C6-N6 | 11.58 | 125.55      | 118.60   |
| 27  | B8    | 71   | A    | N1-C6-N6 | 11.58 | 125.55      | 118.60   |
| 27  | B8    | 165  | A    | N1-C6-N6 | 11.58 | 125.55      | 118.60   |
| 1   | AA    | 72   | A    | N1-C6-N6 | 11.57 | 125.55      | 118.60   |
| 27  | B8    | 1040 | A    | N1-C6-N6 | 11.57 | 125.54      | 118.60   |
| 27  | B8    | 2114 | A    | N1-C6-N6 | 11.57 | 125.54      | 118.60   |
| 27  | B8    | 2765 | A    | N1-C6-N6 | 11.57 | 125.54      | 118.60   |
| 1   | AA    | 913  | A    | N1-C6-N6 | 11.57 | 125.54      | 118.60   |
| 27  | B8    | 2176 | A    | N1-C6-N6 | 11.57 | 125.54      | 118.60   |
| 27  | B8    | 2721 | A    | N1-C6-N6 | 11.57 | 125.54      | 118.60   |
| 1   | AA    | 1246 | A    | N1-C6-N6 | 11.57 | 125.54      | 118.60   |
| 1   | AA    | 1339 | A    | N1-C6-N6 | 11.56 | 125.54      | 118.60   |
| 27  | B8    | 750  | A    | N1-C6-N6 | 11.56 | 125.54      | 118.60   |
| 27  | B8    | 1336 | A    | N1-C6-N6 | 11.56 | 125.54      | 118.60   |
| 27  | B8    | 2664 | G    | N1-C6-O6 | 11.56 | 126.84      | 119.90   |
| 27  | B8    | 1133 | A    | N1-C6-N6 | 11.56 | 125.53      | 118.60   |
| 27  | B8    | 2077 | A    | N1-C6-N6 | 11.56 | 125.53      | 118.60   |
| 1   | AA    | 702  | A    | N1-C6-N6 | 11.55 | 125.53      | 118.60   |
| 1   | AA    | 1531 | A    | N1-C6-N6 | 11.55 | 125.53      | 118.60   |
| 1   | AA    | 452  | A    | N1-C6-N6 | 11.55 | 125.53      | 118.60   |
| 27  | B8    | 1569 | A    | N1-C6-N6 | 11.55 | 125.53      | 118.60   |
| 27  | B8    | 614  | A    | N1-C6-N6 | 11.54 | 125.53      | 118.60   |
| 27  | B8    | 1711 | A    | N1-C6-N6 | 11.54 | 125.53      | 118.60   |
| 27  | B8    | 1276 | A    | N1-C6-N6 | 11.54 | 125.53      | 118.60   |
| 27  | B8    | 1434 | A    | N1-C6-N6 | 11.54 | 125.52      | 118.60   |
| 27  | B8    | 2835 | A    | N1-C6-N6 | 11.54 | 125.52      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | AA    | 160  | A    | N1-C6-N6 | 11.53 | 125.52      | 118.60   |
| 1   | AA    | 411  | A    | N1-C6-N6 | 11.53 | 125.52      | 118.60   |
| 1   | AA    | 1204 | A    | N1-C6-N6 | 11.53 | 125.52      | 118.60   |
| 27  | B8    | 2733 | A    | N1-C6-N6 | 11.53 | 125.52      | 118.60   |
| 1   | AA    | 523  | A    | N1-C6-N6 | 11.52 | 125.51      | 118.60   |
| 27  | B8    | 2199 | A    | N1-C6-N6 | 11.52 | 125.51      | 118.60   |
| 27  | B8    | 2566 | A    | N1-C6-N6 | 11.51 | 125.51      | 118.60   |
| 27  | B8    | 2882 | A    | N1-C6-N6 | 11.51 | 125.51      | 118.60   |
| 1   | AA    | 609  | A    | N1-C6-N6 | 11.51 | 125.51      | 118.60   |
| 27  | B8    | 2095 | A    | N1-C6-N6 | 11.51 | 125.50      | 118.60   |
| 27  | B8    | 1272 | A    | N1-C6-N6 | 11.51 | 125.50      | 118.60   |
| 27  | B8    | 1583 | A    | N1-C6-N6 | 11.51 | 125.50      | 118.60   |
| 27  | B8    | 74   | A    | N1-C6-N6 | 11.50 | 125.50      | 118.60   |
| 27  | B8    | 1616 | A    | N1-C6-N6 | 11.50 | 125.50      | 118.60   |
| 1   | AA    | 364  | A    | N1-C6-N6 | 11.50 | 125.50      | 118.60   |
| 27  | B8    | 21   | A    | N1-C6-N6 | 11.50 | 125.50      | 118.60   |
| 27  | B8    | 2030 | A    | N1-C6-N6 | 11.50 | 125.50      | 118.60   |
| 1   | AA    | 1428 | A    | N1-C6-N6 | 11.49 | 125.50      | 118.60   |
| 27  | B8    | 988  | A    | N1-C6-N6 | 11.49 | 125.50      | 118.60   |
| 1   | AA    | 649  | A    | N1-C6-N6 | 11.48 | 125.49      | 118.60   |
| 27  | B8    | 2530 | A    | N1-C6-N6 | 11.48 | 125.49      | 118.60   |
| 27  | B8    | 920  | A    | N1-C6-N6 | 11.48 | 125.49      | 118.60   |
| 27  | B8    | 927  | A    | N1-C6-N6 | 11.48 | 125.49      | 118.60   |
| 1   | AA    | 313  | A    | N1-C6-N6 | 11.48 | 125.49      | 118.60   |
| 1   | AA    | 819  | A    | N1-C6-N6 | 11.48 | 125.49      | 118.60   |
| 1   | AA    | 1413 | A    | N1-C6-N6 | 11.47 | 125.48      | 118.60   |
| 1   | AA    | 535  | A    | N1-C6-N6 | 11.47 | 125.48      | 118.60   |
| 1   | AA    | 949  | A    | N1-C6-N6 | 11.47 | 125.48      | 118.60   |
| 27  | B8    | 126  | A    | N1-C6-N6 | 11.47 | 125.48      | 118.60   |
| 27  | B8    | 453  | A    | N1-C6-N6 | 11.47 | 125.48      | 118.60   |
| 27  | B8    | 1067 | A    | N1-C6-N6 | 11.47 | 125.48      | 118.60   |
| 1   | AA    | 382  | A    | N1-C6-N6 | 11.47 | 125.48      | 118.60   |
| 1   | AA    | 449  | G    | N1-C6-O6 | 11.47 | 126.78      | 119.90   |
| 27  | B8    | 2134 | A    | N1-C6-N6 | 11.46 | 125.48      | 118.60   |
| 1   | AA    | 1225 | A    | N1-C6-N6 | 11.46 | 125.48      | 118.60   |
| 27  | B8    | 2336 | A    | N1-C6-N6 | 11.46 | 125.48      | 118.60   |
| 1   | AA    | 969  | A    | N1-C6-N6 | 11.46 | 125.47      | 118.60   |
| 1   | AA    | 792  | A    | N1-C6-N6 | 11.46 | 125.47      | 118.60   |
| 1   | AA    | 441  | A    | N1-C6-N6 | 11.45 | 125.47      | 118.60   |
| 27  | B8    | 1321 | A    | N1-C6-N6 | 11.45 | 125.47      | 118.60   |
| 27  | B8    | 1910 | G    | N1-C6-O6 | 11.45 | 126.77      | 119.90   |
| 1   | AA    | 1256 | A    | N1-C6-N6 | 11.45 | 125.47      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 27  | B8    | 64   | A    | N1-C6-N6 | 11.44 | 125.47      | 118.60   |
| 27  | B8    | 1395 | A    | N1-C6-N6 | 11.44 | 125.46      | 118.60   |
| 27  | B8    | 2635 | A    | N1-C6-N6 | 11.44 | 125.46      | 118.60   |
| 1   | AA    | 1508 | A    | N1-C6-N6 | 11.44 | 125.46      | 118.60   |
| 1   | AA    | 547  | A    | N1-C6-N6 | 11.44 | 125.46      | 118.60   |
| 1   | AA    | 878  | A    | N1-C6-N6 | 11.43 | 125.46      | 118.60   |
| 1   | AA    | 1429 | A    | N1-C6-N6 | 11.43 | 125.46      | 118.60   |
| 27  | B8    | 1510 | G    | N1-C6-O6 | 11.42 | 126.75      | 119.90   |
| 27  | B8    | 2726 | A    | N1-C6-N6 | 11.42 | 125.45      | 118.60   |
| 27  | B8    | 1147 | A    | N1-C6-N6 | 11.42 | 125.45      | 118.60   |
| 1   | AA    | 1368 | A    | N1-C6-N6 | 11.42 | 125.45      | 118.60   |
| 3   | AV    | 33   | A    | N1-C6-N6 | 11.42 | 125.45      | 118.60   |
| 27  | B8    | 1469 | A    | N1-C6-N6 | 11.42 | 125.45      | 118.60   |
| 27  | B8    | 340  | A    | N1-C6-N6 | 11.41 | 125.45      | 118.60   |
| 27  | B8    | 613  | A    | N1-C6-N6 | 11.41 | 125.45      | 118.60   |
| 1   | AA    | 1012 | A    | N1-C6-N6 | 11.41 | 125.45      | 118.60   |
| 27  | B8    | 2020 | A    | N1-C6-N6 | 11.41 | 125.44      | 118.60   |
| 27  | B8    | 526  | A    | N1-C6-N6 | 11.41 | 125.44      | 118.60   |
| 27  | B8    | 781  | A    | N1-C6-N6 | 11.41 | 125.44      | 118.60   |
| 27  | B8    | 2542 | A    | N1-C6-N6 | 11.41 | 125.44      | 118.60   |
| 1   | AA    | 665  | A    | N1-C6-N6 | 11.40 | 125.44      | 118.60   |
| 27  | B8    | 1103 | A    | N1-C6-N6 | 11.40 | 125.44      | 118.60   |
| 27  | B8    | 751  | A    | N1-C6-N6 | 11.40 | 125.44      | 118.60   |
| 27  | B8    | 1165 | A    | N1-C6-N6 | 11.40 | 125.44      | 118.60   |
| 3   | AV    | 74   | A    | N1-C6-N6 | 11.40 | 125.44      | 118.60   |
| 27  | B8    | 1237 | A    | N1-C6-N6 | 11.40 | 125.44      | 118.60   |
| 27  | B8    | 2108 | A    | N1-C6-N6 | 11.40 | 125.44      | 118.60   |
| 26  | B7    | 99   | A    | N1-C6-N6 | 11.39 | 125.44      | 118.60   |
| 27  | B8    | 1142 | A    | N1-C6-N6 | 11.39 | 125.44      | 118.60   |
| 27  | B8    | 1596 | A    | N1-C6-N6 | 11.39 | 125.44      | 118.60   |
| 1   | AA    | 325  | A    | N1-C6-N6 | 11.39 | 125.43      | 118.60   |
| 27  | B8    | 142  | A    | N1-C6-N6 | 11.39 | 125.43      | 118.60   |
| 27  | B8    | 800  | A    | N1-C6-N6 | 11.39 | 125.43      | 118.60   |
| 27  | B8    | 1373 | A    | N1-C6-N6 | 11.39 | 125.43      | 118.60   |
| 27  | B8    | 42   | A    | N1-C6-N6 | 11.39 | 125.43      | 118.60   |
| 26  | B7    | 52   | A    | N1-C6-N6 | 11.38 | 125.43      | 118.60   |
| 27  | B8    | 1786 | A    | N1-C6-N6 | 11.38 | 125.43      | 118.60   |
| 1   | AA    | 1332 | A    | N1-C6-N6 | 11.37 | 125.42      | 118.60   |
| 27  | B8    | 2872 | A    | N1-C6-N6 | 11.37 | 125.42      | 118.60   |
| 26  | B7    | 59   | A    | N1-C6-N6 | 11.36 | 125.42      | 118.60   |
| 27  | B8    | 529  | A    | N1-C6-N6 | 11.36 | 125.42      | 118.60   |
| 27  | B8    | 1494 | A    | N1-C6-N6 | 11.36 | 125.41      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 27  | B8    | 222  | A    | N1-C6-N6  | 11.35 | 125.41      | 118.60   |
| 1   | AA    | 1346 | A    | N1-C6-N6  | 11.35 | 125.41      | 118.60   |
| 1   | AA    | 825  | A    | N1-C6-N6  | 11.35 | 125.41      | 118.60   |
| 27  | B8    | 783  | A    | N1-C6-N6  | 11.35 | 125.41      | 118.60   |
| 27  | B8    | 1848 | A    | N1-C6-N6  | 11.34 | 125.41      | 118.60   |
| 27  | B8    | 2425 | A    | P-O3'-C3' | 11.34 | 133.31      | 119.70   |
| 3   | AV    | 60   | A    | N1-C6-N6  | 11.34 | 125.40      | 118.60   |
| 27  | B8    | 1086 | A    | N1-C6-N6  | 11.34 | 125.40      | 118.60   |
| 27  | B8    | 1111 | A    | N1-C6-N6  | 11.34 | 125.40      | 118.60   |
| 27  | B8    | 541  | A    | N1-C6-N6  | 11.33 | 125.40      | 118.60   |
| 1   | AA    | 864  | A    | N1-C6-N6  | 11.33 | 125.40      | 118.60   |
| 27  | B8    | 2029 | G    | N1-C6-O6  | 11.33 | 126.70      | 119.90   |
| 27  | B8    | 941  | A    | N1-C6-N6  | 11.32 | 125.39      | 118.60   |
| 27  | B8    | 2060 | A    | N1-C6-N6  | 11.31 | 125.39      | 118.60   |
| 27  | B8    | 2451 | A    | N1-C6-N6  | 11.31 | 125.38      | 118.60   |
| 26  | B7    | 73   | A    | N1-C6-N6  | 11.30 | 125.38      | 118.60   |
| 27  | B8    | 2761 | A    | N1-C6-N6  | 11.31 | 125.38      | 118.60   |
| 1   | AA    | 432  | A    | N1-C6-N6  | 11.30 | 125.38      | 118.60   |
| 27  | B8    | 1189 | A    | N1-C6-N6  | 11.30 | 125.38      | 118.60   |
| 27  | B8    | 479  | A    | N1-C6-N6  | 11.28 | 125.37      | 118.60   |
| 27  | B8    | 63   | A    | N1-C6-N6  | 11.28 | 125.37      | 118.60   |
| 27  | B8    | 362  | A    | N1-C6-N6  | 11.28 | 125.37      | 118.60   |
| 1   | AA    | 794  | A    | N1-C6-N6  | 11.28 | 125.37      | 118.60   |
| 27  | B8    | 1088 | A    | N1-C6-N6  | 11.28 | 125.37      | 118.60   |
| 27  | B8    | 621  | A    | N1-C6-N6  | 11.27 | 125.36      | 118.60   |
| 27  | B8    | 1580 | A    | N1-C6-N6  | 11.27 | 125.36      | 118.60   |
| 27  | B8    | 886  | A    | N1-C6-N6  | 11.27 | 125.36      | 118.60   |
| 1   | AA    | 60   | A    | P-O3'-C3' | 11.27 | 133.22      | 119.70   |
| 27  | B8    | 477  | A    | N1-C6-N6  | 11.27 | 125.36      | 118.60   |
| 1   | AA    | 1362 | A    | N1-C6-N6  | 11.27 | 125.36      | 118.60   |
| 27  | B8    | 574  | A    | N1-C6-N6  | 11.27 | 125.36      | 118.60   |
| 1   | AA    | 1176 | A    | N1-C6-N6  | 11.26 | 125.36      | 118.60   |
| 27  | B8    | 1287 | A    | N1-C6-N6  | 11.26 | 125.36      | 118.60   |
| 27  | B8    | 2543 | G    | N1-C6-O6  | 11.26 | 126.66      | 119.90   |
| 26  | B7    | 15   | A    | N1-C6-N6  | 11.26 | 125.35      | 118.60   |
| 27  | B8    | 94   | A    | N1-C6-N6  | 11.26 | 125.35      | 118.60   |
| 1   | AA    | 60   | A    | N1-C6-N6  | 11.25 | 125.35      | 118.60   |
| 27  | B8    | 2856 | A    | N1-C6-N6  | 11.24 | 125.34      | 118.60   |
| 1   | AA    | 908  | A    | N1-C6-N6  | 11.23 | 125.34      | 118.60   |
| 1   | AA    | 1157 | A    | N1-C6-N6  | 11.23 | 125.34      | 118.60   |
| 1   | AA    | 129  | A    | N1-C6-N6  | 11.22 | 125.33      | 118.60   |
| 1   | AA    | 1150 | A    | N1-C6-N6  | 11.22 | 125.33      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 27  | B8    | 324  | A    | N1-C6-N6  | 11.22 | 125.33      | 118.60   |
| 27  | B8    | 1679 | A    | N1-C6-N6  | 11.21 | 125.33      | 118.60   |
| 27  | B8    | 1315 | C    | P-O3'-C3' | 11.21 | 133.15      | 119.70   |
| 27  | B8    | 1070 | A    | N1-C6-N6  | 11.21 | 125.32      | 118.60   |
| 1   | AA    | 608  | A    | N1-C6-N6  | 11.20 | 125.32      | 118.60   |
| 27  | B8    | 675  | A    | N1-C6-N6  | 11.20 | 125.32      | 118.60   |
| 27  | B8    | 2750 | A    | N1-C6-N6  | 11.20 | 125.32      | 118.60   |
| 1   | AA    | 1055 | A    | N1-C6-N6  | 11.19 | 125.32      | 118.60   |
| 1   | AA    | 274  | A    | N1-C6-N6  | 11.18 | 125.31      | 118.60   |
| 27  | B8    | 2829 | A    | N1-C6-N6  | 11.18 | 125.31      | 118.60   |
| 27  | B8    | 118  | A    | N1-C6-N6  | 11.17 | 125.30      | 118.60   |
| 27  | B8    | 1630 | A    | N1-C6-N6  | 11.16 | 125.30      | 118.60   |
| 1   | AA    | 246  | A    | N1-C6-N6  | 11.16 | 125.30      | 118.60   |
| 27  | B8    | 2564 | A    | N1-C6-N6  | 11.16 | 125.30      | 118.60   |
| 27  | B8    | 1301 | A    | N1-C6-N6  | 11.15 | 125.29      | 118.60   |
| 27  | B8    | 1307 | A    | N1-C6-N6  | 11.15 | 125.29      | 118.60   |
| 27  | B8    | 1028 | A    | N1-C6-N6  | 11.15 | 125.29      | 118.60   |
| 27  | B8    | 1690 | A    | N1-C6-N6  | 11.15 | 125.29      | 118.60   |
| 27  | B8    | 727  | A    | N1-C6-N6  | 11.14 | 125.29      | 118.60   |
| 27  | B8    | 1453 | A    | N1-C6-N6  | 11.14 | 125.29      | 118.60   |
| 1   | AA    | 1206 | G    | N1-C6-O6  | 11.14 | 126.58      | 119.90   |
| 27  | B8    | 2297 | A    | N1-C6-N6  | 11.13 | 125.28      | 118.60   |
| 27  | B8    | 1021 | A    | N1-C6-N6  | 11.13 | 125.28      | 118.60   |
| 1   | AA    | 1329 | A    | N1-C6-N6  | 11.13 | 125.28      | 118.60   |
| 1   | AA    | 179  | A    | N1-C6-N6  | 11.12 | 125.27      | 118.60   |
| 27  | B8    | 2764 | A    | N1-C6-N6  | 11.12 | 125.27      | 118.60   |
| 27  | B8    | 2868 | A    | N1-C6-N6  | 11.12 | 125.27      | 118.60   |
| 27  | B8    | 1853 | A    | N1-C6-N6  | 11.11 | 125.27      | 118.60   |
| 27  | B8    | 2748 | A    | N1-C6-N6  | 11.11 | 125.27      | 118.60   |
| 27  | B8    | 1854 | A    | N1-C6-N6  | 11.11 | 125.26      | 118.60   |
| 1   | AA    | 554  | A    | N1-C6-N6  | 11.10 | 125.26      | 118.60   |
| 27  | B8    | 279  | A    | N1-C6-N6  | 11.10 | 125.26      | 118.60   |
| 27  | B8    | 1780 | A    | N1-C6-N6  | 11.10 | 125.26      | 118.60   |
| 27  | B8    | 2015 | A    | N1-C6-N6  | 11.10 | 125.26      | 118.60   |
| 1   | AA    | 1285 | A    | N1-C6-N6  | 11.10 | 125.26      | 118.60   |
| 27  | B8    | 2119 | A    | N1-C6-N6  | 11.09 | 125.25      | 118.60   |
| 27  | B8    | 1032 | A    | N1-C6-N6  | 11.08 | 125.25      | 118.60   |
| 1   | AA    | 55   | A    | N1-C6-N6  | 11.07 | 125.24      | 118.60   |
| 27  | B8    | 829  | A    | N1-C6-N6  | 11.07 | 125.24      | 118.60   |
| 1   | AA    | 151  | A    | N1-C6-N6  | 11.05 | 125.23      | 118.60   |
| 3   | AV    | 70   | G    | N1-C6-O6  | 11.05 | 126.53      | 119.90   |
| 27  | B8    | 1126 | A    | N1-C6-N6  | 11.05 | 125.23      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 27  | B8    | 1439 | A    | N1-C6-N6 | 11.05 | 125.23      | 118.60   |
| 1   | AA    | 148  | G    | N1-C6-O6 | 11.04 | 126.52      | 119.90   |
| 27  | B8    | 1393 | A    | N1-C6-N6 | 11.04 | 125.22      | 118.60   |
| 1   | AA    | 428  | G    | N1-C6-O6 | 11.04 | 126.52      | 119.90   |
| 1   | AA    | 860  | A    | N1-C6-N6 | 11.04 | 125.22      | 118.60   |
| 1   | AA    | 195  | A    | N1-C6-N6 | 11.03 | 125.22      | 118.60   |
| 27  | B8    | 181  | A    | N1-C6-N6 | 11.02 | 125.21      | 118.60   |
| 27  | B8    | 528  | A    | N1-C6-N6 | 11.01 | 125.21      | 118.60   |
| 1   | AA    | 753  | A    | N1-C6-N6 | 11.01 | 125.21      | 118.60   |
| 27  | B8    | 1872 | A    | N1-C6-N6 | 11.01 | 125.20      | 118.60   |
| 1   | AA    | 171  | A    | N1-C6-N6 | 11.01 | 125.20      | 118.60   |
| 27  | B8    | 1668 | A    | N1-C6-N6 | 11.01 | 125.20      | 118.60   |
| 27  | B8    | 1641 | A    | N1-C6-N6 | 11.00 | 125.20      | 118.60   |
| 27  | B8    | 1652 | A    | N1-C6-N6 | 11.00 | 125.20      | 118.60   |
| 27  | B8    | 2225 | A    | N1-C6-N6 | 11.00 | 125.20      | 118.60   |
| 27  | B8    | 825  | A    | N1-C6-N6 | 10.99 | 125.19      | 118.60   |
| 1   | AA    | 696  | A    | N1-C6-N6 | 10.99 | 125.19      | 118.60   |
| 27  | B8    | 900  | A    | N1-C6-N6 | 10.99 | 125.19      | 118.60   |
| 1   | AA    | 26   | A    | N1-C6-N6 | 10.98 | 125.19      | 118.60   |
| 27  | B8    | 2335 | A    | N1-C6-N6 | 10.97 | 125.18      | 118.60   |
| 1   | AA    | 766  | A    | N1-C6-N6 | 10.95 | 125.17      | 118.60   |
| 1   | AA    | 65   | A    | N1-C6-N6 | 10.94 | 125.16      | 118.60   |
| 27  | B8    | 768  | G    | N1-C6-O6 | 10.94 | 126.46      | 119.90   |
| 27  | B8    | 256  | A    | N1-C6-N6 | 10.94 | 125.16      | 118.60   |
| 27  | B8    | 1803 | A    | N1-C6-N6 | 10.94 | 125.16      | 118.60   |
| 1   | AA    | 533  | A    | N1-C6-N6 | 10.93 | 125.16      | 118.60   |
| 27  | B8    | 1381 | G    | N1-C6-O6 | 10.93 | 126.46      | 119.90   |
| 27  | B8    | 2273 | A    | N1-C6-N6 | 10.93 | 125.16      | 118.60   |
| 26  | B7    | 57   | A    | N1-C6-N6 | 10.93 | 125.16      | 118.60   |
| 1   | AA    | 520  | A    | N1-C6-N6 | 10.92 | 125.15      | 118.60   |
| 27  | B8    | 2366 | A    | N1-C6-N6 | 10.92 | 125.15      | 118.60   |
| 1   | AA    | 22   | G    | N1-C6-O6 | 10.90 | 126.44      | 119.90   |
| 1   | AA    | 109  | A    | N1-C6-N6 | 10.90 | 125.14      | 118.60   |
| 1   | AA    | 116  | A    | N1-C6-N6 | 10.90 | 125.14      | 118.60   |
| 1   | AA    | 1333 | A    | N1-C6-N6 | 10.90 | 125.14      | 118.60   |
| 1   | AA    | 914  | A    | N1-C6-N6 | 10.90 | 125.14      | 118.60   |
| 27  | B8    | 1205 | A    | N1-C6-N6 | 10.90 | 125.14      | 118.60   |
| 27  | B8    | 654  | A    | N1-C6-N6 | 10.89 | 125.14      | 118.60   |
| 27  | B8    | 2435 | A    | N1-C6-N6 | 10.89 | 125.13      | 118.60   |
| 1   | AA    | 76   | G    | N1-C6-O6 | 10.88 | 126.43      | 119.90   |
| 27  | B8    | 1701 | A    | N1-C6-N6 | 10.87 | 125.12      | 118.60   |
| 1   | AA    | 329  | A    | N1-C6-N6 | 10.86 | 125.11      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 27  | B8    | 933  | A    | N1-C6-N6  | 10.86 | 125.11      | 118.60   |
| 1   | AA    | 301  | G    | N1-C6-O6  | 10.85 | 126.41      | 119.90   |
| 1   | AA    | 509  | A    | N1-C6-N6  | 10.85 | 125.11      | 118.60   |
| 1   | AA    | 1101 | A    | N1-C6-N6  | 10.85 | 125.11      | 118.60   |
| 26  | B7    | 34   | A    | N1-C6-N6  | 10.83 | 125.10      | 118.60   |
| 27  | B8    | 2747 | G    | N1-C6-O6  | 10.83 | 126.40      | 119.90   |
| 27  | B8    | 556  | A    | N1-C6-N6  | 10.82 | 125.09      | 118.60   |
| 1   | AA    | 1005 | A    | N1-C6-N6  | 10.81 | 125.08      | 118.60   |
| 27  | B8    | 2135 | A    | N1-C6-N6  | 10.81 | 125.08      | 118.60   |
| 26  | B7    | 78   | A    | N1-C6-N6  | 10.80 | 125.08      | 118.60   |
| 27  | B8    | 1552 | A    | N1-C6-N6  | 10.80 | 125.08      | 118.60   |
| 27  | B8    | 266  | G    | N1-C6-O6  | 10.80 | 126.38      | 119.90   |
| 27  | B8    | 2014 | A    | N1-C6-N6  | 10.79 | 125.08      | 118.60   |
| 27  | B8    | 559  | G    | N1-C6-O6  | 10.79 | 126.38      | 119.90   |
| 27  | B8    | 990  | A    | N1-C6-N6  | 10.79 | 125.07      | 118.60   |
| 27  | B8    | 670  | A    | N1-C6-N6  | 10.79 | 125.07      | 118.60   |
| 1   | AA    | 487  | A    | N1-C6-N6  | 10.78 | 125.07      | 118.60   |
| 1   | AA    | 1392 | G    | N1-C6-O6  | 10.76 | 126.36      | 119.90   |
| 1   | AA    | 431  | A    | N1-C6-N6  | 10.75 | 125.05      | 118.60   |
| 1   | AA    | 674  | G    | N1-C6-O6  | 10.75 | 126.35      | 119.90   |
| 1   | AA    | 1486 | G    | N1-C6-O6  | 10.75 | 126.35      | 119.90   |
| 1   | AA    | 1034 | G    | N1-C6-O6  | 10.74 | 126.34      | 119.90   |
| 27  | B8    | 2169 | A    | N1-C6-N6  | 10.74 | 125.04      | 118.60   |
| 1   | AA    | 414  | A    | N1-C6-N6  | 10.74 | 125.04      | 118.60   |
| 27  | B8    | 663  | G    | N1-C6-O6  | 10.74 | 126.34      | 119.90   |
| 27  | B8    | 2033 | A    | N1-C6-N6  | 10.73 | 125.04      | 118.60   |
| 27  | B8    | 916  | G    | N1-C6-O6  | 10.73 | 126.34      | 119.90   |
| 27  | B8    | 1445 | G    | N1-C6-O6  | 10.72 | 126.33      | 119.90   |
| 27  | B8    | 161  | A    | N1-C6-N6  | 10.71 | 125.03      | 118.60   |
| 27  | B8    | 374  | A    | N1-C6-N6  | 10.71 | 125.03      | 118.60   |
| 1   | AA    | 184  | G    | N1-C6-O6  | 10.71 | 126.32      | 119.90   |
| 1   | AA    | 718  | A    | N1-C6-N6  | 10.71 | 125.02      | 118.60   |
| 27  | B8    | 1783 | A    | N1-C6-N6  | 10.70 | 125.02      | 118.60   |
| 27  | B8    | 2124 | G    | N1-C6-O6  | 10.70 | 126.32      | 119.90   |
| 1   | AA    | 366  | A    | P-O3'-C3' | 10.69 | 132.53      | 119.70   |
| 27  | B8    | 505  | A    | N1-C6-N6  | 10.69 | 125.02      | 118.60   |
| 27  | B8    | 2201 | G    | N1-C6-O6  | 10.69 | 126.31      | 119.90   |
| 27  | B8    | 194  | G    | N1-C6-O6  | 10.69 | 126.31      | 119.90   |
| 27  | B8    | 2778 | A    | N1-C6-N6  | 10.67 | 125.00      | 118.60   |
| 1   | AA    | 584  | G    | N1-C6-O6  | 10.66 | 126.30      | 119.90   |
| 1   | AA    | 1319 | A    | N1-C6-N6  | 10.66 | 125.00      | 118.60   |
| 27  | B8    | 1885 | A    | N1-C6-N6  | 10.66 | 125.00      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 353  | A    | N1-C6-N6   | 10.63 | 124.98      | 118.60   |
| 27  | B8    | 1717 | A    | N1-C6-N6   | 10.63 | 124.98      | 118.60   |
| 27  | B8    | 2469 | A    | N1-C6-N6   | 10.63 | 124.98      | 118.60   |
| 27  | B8    | 2298 | A    | N1-C6-N6   | 10.62 | 124.97      | 118.60   |
| 27  | B8    | 1378 | A    | N1-C6-N6   | 10.62 | 124.97      | 118.60   |
| 27  | B8    | 1975 | G    | N1-C6-O6   | 10.62 | 126.27      | 119.90   |
| 27  | B8    | 2903 | U    | O4'-C1'-N1 | 10.61 | 116.69      | 108.20   |
| 27  | B8    | 248  | G    | N1-C6-O6   | 10.61 | 126.26      | 119.90   |
| 27  | B8    | 616  | A    | N1-C6-N6   | 10.59 | 124.96      | 118.60   |
| 1   | AA    | 258  | G    | N1-C6-O6   | 10.59 | 126.25      | 119.90   |
| 1   | AA    | 1275 | A    | N1-C6-N6   | 10.58 | 124.95      | 118.60   |
| 27  | B8    | 1907 | G    | N1-C6-O6   | 10.58 | 126.25      | 119.90   |
| 27  | B8    | 2234 | G    | N1-C6-O6   | 10.58 | 126.25      | 119.90   |
| 1   | AA    | 168  | G    | N1-C6-O6   | 10.57 | 126.24      | 119.90   |
| 1   | AA    | 484  | G    | N1-C6-O6   | 10.56 | 126.23      | 119.90   |
| 27  | B8    | 820  | A    | N1-C6-N6   | 10.56 | 124.93      | 118.60   |
| 27  | B8    | 2212 | A    | N1-C6-N6   | 10.55 | 124.93      | 118.60   |
| 1   | AA    | 1289 | A    | N1-C6-N6   | 10.55 | 124.93      | 118.60   |
| 1   | AA    | 1290 | G    | N1-C6-O6   | 10.55 | 126.23      | 119.90   |
| 27  | B8    | 2052 | A    | N1-C6-N6   | 10.55 | 124.93      | 118.60   |
| 1   | AA    | 973  | G    | N1-C6-O6   | 10.55 | 126.23      | 119.90   |
| 27  | B8    | 2268 | A    | N1-C6-N6   | 10.54 | 124.92      | 118.60   |
| 27  | B8    | 1522 | A    | N1-C6-N6   | 10.53 | 124.92      | 118.60   |
| 1   | AA    | 687  | A    | N1-C6-N6   | 10.53 | 124.92      | 118.60   |
| 27  | B8    | 1001 | A    | N1-C6-N6   | 10.52 | 124.91      | 118.60   |
| 27  | B8    | 2054 | A    | N1-C6-N6   | 10.52 | 124.91      | 118.60   |
| 27  | B8    | 2535 | G    | N1-C6-O6   | 10.52 | 126.21      | 119.90   |
| 27  | B8    | 2485 | G    | N1-C6-O6   | 10.51 | 126.21      | 119.90   |
| 1   | AA    | 1435 | G    | N1-C6-O6   | 10.49 | 126.19      | 119.90   |
| 27  | B8    | 2392 | A    | N1-C6-N6   | 10.49 | 124.89      | 118.60   |
| 1   | AA    | 782  | A    | N1-C6-N6   | 10.48 | 124.89      | 118.60   |
| 27  | B8    | 103  | A    | N1-C6-N6   | 10.48 | 124.89      | 118.60   |
| 27  | B8    | 2447 | G    | N1-C6-O6   | 10.48 | 126.19      | 119.90   |
| 1   | AA    | 99   | C    | O4'-C1'-N1 | 10.48 | 116.58      | 108.20   |
| 1   | AA    | 570  | G    | N1-C6-O6   | 10.48 | 126.19      | 119.90   |
| 27  | B8    | 350  | G    | N1-C6-O6   | 10.48 | 126.19      | 119.90   |
| 27  | B8    | 2024 | G    | N1-C6-O6   | 10.48 | 126.19      | 119.90   |
| 1   | AA    | 417  | G    | N1-C6-O6   | 10.47 | 126.19      | 119.90   |
| 27  | B8    | 2587 | A    | N1-C6-N6   | 10.47 | 124.88      | 118.60   |
| 27  | B8    | 2673 | G    | N1-C6-O6   | 10.47 | 126.18      | 119.90   |
| 27  | B8    | 1342 | A    | N1-C6-N6   | 10.47 | 124.88      | 118.60   |
| 27  | B8    | 514  | A    | N1-C6-N6   | 10.46 | 124.88      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 27  | B8    | 2741 | A    | N1-C6-N6 | 10.46 | 124.88      | 118.60   |
| 27  | B8    | 1553 | A    | N1-C6-N6 | 10.46 | 124.88      | 118.60   |
| 27  | B8    | 2027 | G    | N1-C6-O6 | 10.46 | 126.17      | 119.90   |
| 1   | AA    | 275  | G    | N1-C6-O6 | 10.45 | 126.17      | 119.90   |
| 27  | B8    | 1106 | G    | N1-C6-O6 | 10.45 | 126.17      | 119.90   |
| 27  | B8    | 954  | G    | N1-C6-O6 | 10.45 | 126.17      | 119.90   |
| 27  | B8    | 2624 | G    | N1-C6-O6 | 10.45 | 126.17      | 119.90   |
| 27  | B8    | 346  | A    | N1-C6-N6 | 10.44 | 124.86      | 118.60   |
| 27  | B8    | 2895 | G    | N1-C6-O6 | 10.43 | 126.16      | 119.90   |
| 1   | AA    | 1033 | G    | N1-C6-O6 | 10.43 | 126.16      | 119.90   |
| 1   | AA    | 1441 | A    | N1-C6-N6 | 10.43 | 124.86      | 118.60   |
| 1   | AA    | 541  | G    | N1-C6-O6 | 10.42 | 126.15      | 119.90   |
| 27  | B8    | 2227 | A    | N1-C6-N6 | 10.41 | 124.84      | 118.60   |
| 1   | AA    | 1184 | G    | N1-C6-O6 | 10.40 | 126.14      | 119.90   |
| 27  | B8    | 409  | G    | N1-C6-O6 | 10.40 | 126.14      | 119.90   |
| 27  | B8    | 609  | A    | N1-C6-N6 | 10.40 | 124.84      | 118.60   |
| 1   | AA    | 669  | G    | N1-C6-O6 | 10.39 | 126.13      | 119.90   |
| 27  | B8    | 2279 | G    | N1-C6-O6 | 10.39 | 126.13      | 119.90   |
| 27  | B8    | 424  | G    | N1-C6-O6 | 10.38 | 126.13      | 119.90   |
| 27  | B8    | 538  | A    | N1-C6-N6 | 10.38 | 124.83      | 118.60   |
| 1   | AA    | 454  | G    | N1-C6-O6 | 10.38 | 126.13      | 119.90   |
| 1   | AA    | 259  | G    | N1-C6-O6 | 10.37 | 126.12      | 119.90   |
| 27  | B8    | 2421 | G    | N1-C6-O6 | 10.37 | 126.12      | 119.90   |
| 26  | B7    | 112  | G    | N1-C6-O6 | 10.36 | 126.12      | 119.90   |
| 27  | B8    | 428  | A    | N1-C6-N6 | 10.36 | 124.82      | 118.60   |
| 1   | AA    | 1191 | A    | N1-C6-N6 | 10.35 | 124.81      | 118.60   |
| 27  | B8    | 1268 | A    | N1-C6-N6 | 10.35 | 124.81      | 118.60   |
| 1   | AA    | 145  | G    | N1-C6-O6 | 10.34 | 126.11      | 119.90   |
| 27  | B8    | 2304 | G    | N1-C6-O6 | 10.33 | 126.10      | 119.90   |
| 1   | AA    | 457  | G    | N1-C6-O6 | 10.31 | 126.09      | 119.90   |
| 27  | B8    | 757  | G    | N1-C6-O6 | 10.31 | 126.09      | 119.90   |
| 1   | AA    | 616  | G    | N1-C6-O6 | 10.30 | 126.08      | 119.90   |
| 1   | AA    | 1020 | G    | N1-C6-O6 | 10.30 | 126.08      | 119.90   |
| 27  | B8    | 1743 | G    | N1-C6-O6 | 10.29 | 126.07      | 119.90   |
| 1   | AA    | 1523 | G    | N1-C6-O6 | 10.28 | 126.07      | 119.90   |
| 27  | B8    | 1422 | G    | N1-C6-O6 | 10.26 | 126.06      | 119.90   |
| 1   | AA    | 778  | G    | N1-C6-O6 | 10.24 | 126.05      | 119.90   |
| 1   | AA    | 1058 | G    | N1-C6-O6 | 10.24 | 126.05      | 119.90   |
| 1   | AA    | 359  | G    | N1-C6-O6 | 10.24 | 126.04      | 119.90   |
| 27  | B8    | 442  | G    | N1-C6-O6 | 10.24 | 126.04      | 119.90   |
| 1   | AA    | 104  | G    | N1-C6-O6 | 10.23 | 126.04      | 119.90   |
| 27  | B8    | 460  | A    | N1-C6-N6 | 10.23 | 124.74      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 628  | G    | N1-C6-O6   | 10.23 | 126.04      | 119.90   |
| 27  | B8    | 1937 | A    | N1-C6-N6   | 10.23 | 124.74      | 118.60   |
| 1   | AA    | 122  | G    | N1-C6-O6   | 10.22 | 126.03      | 119.90   |
| 27  | B8    | 676  | A    | N1-C6-N6   | 10.22 | 124.73      | 118.60   |
| 26  | B7    | 81   | G    | N1-C6-O6   | 10.21 | 126.03      | 119.90   |
| 27  | B8    | 978  | G    | N1-C6-O6   | 10.21 | 126.03      | 119.90   |
| 1   | AA    | 15   | G    | N1-C6-O6   | 10.21 | 126.03      | 119.90   |
| 1   | AA    | 626  | G    | N1-C6-O6   | 10.21 | 126.03      | 119.90   |
| 27  | B8    | 1492 | G    | N1-C6-O6   | 10.21 | 126.03      | 119.90   |
| 1   | AA    | 1433 | A    | N1-C6-N6   | 10.19 | 124.72      | 118.60   |
| 27  | B8    | 2363 | G    | N1-C6-O6   | 10.19 | 126.02      | 119.90   |
| 27  | B8    | 1689 | A    | N1-C6-N6   | 10.19 | 124.71      | 118.60   |
| 1   | AA    | 372  | C    | P-O3'-C3'  | 10.18 | 131.92      | 119.70   |
| 1   | AA    | 1201 | A    | P-O3'-C3'  | 10.18 | 131.92      | 119.70   |
| 27  | B8    | 735  | A    | N1-C6-N6   | 10.18 | 124.71      | 118.60   |
| 27  | B8    | 1098 | A    | N1-C6-N6   | 10.18 | 124.70      | 118.60   |
| 27  | B8    | 2601 | C    | P-O3'-C3'  | 10.18 | 131.91      | 119.70   |
| 27  | B8    | 1785 | A    | N1-C6-N6   | 10.16 | 124.70      | 118.60   |
| 27  | B8    | 1076 | C    | O4'-C1'-N1 | 10.15 | 116.32      | 108.20   |
| 27  | B8    | 1627 | G    | N1-C6-O6   | 10.15 | 125.99      | 119.90   |
| 27  | B8    | 2046 | G    | N1-C6-O6   | 10.15 | 125.99      | 119.90   |
| 27  | B8    | 401  | A    | N1-C6-N6   | 10.15 | 124.69      | 118.60   |
| 27  | B8    | 1655 | A    | N1-C6-N6   | 10.15 | 124.69      | 118.60   |
| 27  | B8    | 2057 | G    | N1-C6-O6   | 10.15 | 125.99      | 119.90   |
| 27  | B8    | 2714 | G    | N1-C6-O6   | 10.14 | 125.98      | 119.90   |
| 27  | B8    | 244  | A    | N1-C6-N6   | 10.14 | 124.68      | 118.60   |
| 1   | AA    | 164  | G    | N1-C6-O6   | 10.12 | 125.97      | 119.90   |
| 1   | AA    | 1405 | G    | N1-C6-O6   | 10.12 | 125.97      | 119.90   |
| 27  | B8    | 1157 | G    | N1-C6-O6   | 10.12 | 125.97      | 119.90   |
| 27  | B8    | 2639 | A    | N1-C6-N6   | 10.12 | 124.67      | 118.60   |
| 1   | AA    | 147  | G    | N1-C6-O6   | 10.12 | 125.97      | 119.90   |
| 27  | B8    | 1649 | G    | N1-C6-O6   | 10.12 | 125.97      | 119.90   |
| 1   | AA    | 933  | G    | N1-C6-O6   | 10.12 | 125.97      | 119.90   |
| 27  | B8    | 501  | A    | N1-C6-N6   | 10.11 | 124.67      | 118.60   |
| 1   | AA    | 601  | G    | N1-C6-O6   | 10.11 | 125.96      | 119.90   |
| 27  | B8    | 784  | G    | N1-C6-O6   | 10.11 | 125.96      | 119.90   |
| 1   | AA    | 1284 | C    | P-O3'-C3'  | 10.11 | 131.83      | 119.70   |
| 27  | B8    | 1826 | G    | N1-C6-O6   | 10.11 | 125.96      | 119.90   |
| 1   | AA    | 1048 | G    | N1-C6-O6   | 10.10 | 125.96      | 119.90   |
| 1   | AA    | 424  | G    | N1-C6-O6   | 10.09 | 125.95      | 119.90   |
| 27  | B8    | 2648 | G    | N1-C6-O6   | 10.09 | 125.95      | 119.90   |
| 1   | AA    | 1338 | G    | O4'-C1'-N9 | 10.09 | 116.27      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 27  | B8    | 2544 | G    | N1-C6-O6  | 10.08 | 125.95      | 119.90   |
| 27  | B8    | 2692 | G    | N1-C6-O6  | 10.08 | 125.95      | 119.90   |
| 1   | AA    | 627  | G    | N1-C6-O6  | 10.08 | 125.95      | 119.90   |
| 1   | AA    | 1455 | G    | N1-C6-O6  | 10.07 | 125.94      | 119.90   |
| 27  | B8    | 1059 | G    | N1-C6-O6  | 10.07 | 125.94      | 119.90   |
| 27  | B8    | 524  | G    | N1-C6-O6  | 10.07 | 125.94      | 119.90   |
| 1   | AA    | 1006 | G    | N1-C6-O6  | 10.07 | 125.94      | 119.90   |
| 1   | AA    | 279  | A    | P-O3'-C3' | 10.06 | 131.78      | 119.70   |
| 27  | B8    | 1038 | G    | N1-C6-O6  | 10.06 | 125.94      | 119.90   |
| 1   | AA    | 1072 | G    | N1-C6-O6  | 10.05 | 125.93      | 119.90   |
| 27  | B8    | 108  | G    | N1-C6-O6  | 10.05 | 125.93      | 119.90   |
| 27  | B8    | 2409 | G    | N1-C6-O6  | 10.05 | 125.93      | 119.90   |
| 1   | AA    | 413  | G    | N1-C6-O6  | 10.04 | 125.92      | 119.90   |
| 27  | B8    | 701  | G    | N1-C6-O6  | 10.04 | 125.92      | 119.90   |
| 27  | B8    | 1479 | G    | N1-C6-O6  | 10.04 | 125.92      | 119.90   |
| 27  | B8    | 2839 | G    | N1-C6-O6  | 10.04 | 125.92      | 119.90   |
| 27  | B8    | 496  | G    | N1-C6-O6  | 10.03 | 125.92      | 119.90   |
| 27  | B8    | 1338 | G    | N1-C6-O6  | 10.03 | 125.92      | 119.90   |
| 27  | B8    | 141  | G    | N1-C6-O6  | 10.03 | 125.92      | 119.90   |
| 27  | B8    | 533  | G    | N1-C6-O6  | 10.03 | 125.92      | 119.90   |
| 1   | AA    | 786  | G    | N1-C6-O6  | 10.03 | 125.92      | 119.90   |
| 1   | AA    | 724  | G    | N1-C6-O6  | 10.03 | 125.92      | 119.90   |
| 27  | B8    | 864  | G    | N1-C6-O6  | 10.03 | 125.92      | 119.90   |
| 27  | B8    | 1421 | G    | N1-C6-O6  | 10.03 | 125.92      | 119.90   |
| 27  | B8    | 2400 | G    | N1-C6-O6  | 10.03 | 125.92      | 119.90   |
| 1   | AA    | 667  | G    | N1-C6-O6  | 10.02 | 125.91      | 119.90   |
| 27  | B8    | 471  | A    | N1-C6-N6  | 10.02 | 124.61      | 118.60   |
| 27  | B8    | 777  | G    | N1-C6-O6  | 10.02 | 125.91      | 119.90   |
| 27  | B8    | 2819 | G    | N1-C6-O6  | 10.02 | 125.91      | 119.90   |
| 27  | B8    | 953  | G    | N1-C6-O6  | 10.02 | 125.91      | 119.90   |
| 27  | B8    | 2478 | A    | N1-C6-N6  | 10.02 | 124.61      | 118.60   |
| 1   | AA    | 1497 | G    | N1-C6-O6  | 10.01 | 125.91      | 119.90   |
| 27  | B8    | 699  | A    | N1-C6-N6  | 10.01 | 124.61      | 118.60   |
| 1   | AA    | 450  | G    | N1-C6-O6  | 10.01 | 125.90      | 119.90   |
| 27  | B8    | 2472 | G    | N1-C6-O6  | 10.01 | 125.90      | 119.90   |
| 26  | B7    | 45   | A    | N1-C6-N6  | 10.00 | 124.60      | 118.60   |
| 27  | B8    | 371  | A    | N1-C6-N6  | 10.00 | 124.60      | 118.60   |
| 27  | B8    | 2056 | G    | N1-C6-O6  | 10.00 | 125.90      | 119.90   |
| 1   | AA    | 302  | G    | N1-C6-O6  | 9.99  | 125.89      | 119.90   |
| 27  | B8    | 412  | A    | N1-C6-N6  | 9.98  | 124.59      | 118.60   |
| 27  | B8    | 2894 | G    | N1-C6-O6  | 9.98  | 125.89      | 119.90   |
| 27  | B8    | 1901 | A    | N1-C6-N6  | 9.98  | 124.59      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 26  | B7    | 54   | G    | N1-C6-O6   | 9.97 | 125.89      | 119.90   |
| 1   | AA    | 75   | G    | N1-C6-O6   | 9.97 | 125.88      | 119.90   |
| 27  | B8    | 662  | G    | N1-C6-O6   | 9.97 | 125.88      | 119.90   |
| 1   | AA    | 849  | G    | N1-C6-O6   | 9.96 | 125.88      | 119.90   |
| 1   | AA    | 889  | A    | N1-C6-N6   | 9.96 | 124.58      | 118.60   |
| 27  | B8    | 81   | G    | N1-C6-O6   | 9.96 | 125.88      | 119.90   |
| 27  | B8    | 2694 | G    | N1-C6-O6   | 9.96 | 125.88      | 119.90   |
| 27  | B8    | 2147 | A    | P-O3'-C3'  | 9.96 | 131.65      | 119.70   |
| 27  | B8    | 273  | G    | N1-C6-O6   | 9.96 | 125.87      | 119.90   |
| 1   | AA    | 642  | A    | N1-C6-N6   | 9.96 | 124.57      | 118.60   |
| 1   | AA    | 1323 | G    | N1-C6-O6   | 9.96 | 125.87      | 119.90   |
| 1   | AA    | 951  | G    | N1-C6-O6   | 9.95 | 125.87      | 119.90   |
| 27  | B8    | 1389 | G    | N1-C6-O6   | 9.95 | 125.87      | 119.90   |
| 1   | AA    | 521  | G    | N1-C6-O6   | 9.95 | 125.87      | 119.90   |
| 27  | B8    | 1465 | G    | N1-C6-O6   | 9.95 | 125.87      | 119.90   |
| 27  | B8    | 1154 | G    | N1-C6-O6   | 9.95 | 125.87      | 119.90   |
| 27  | B8    | 2414 | G    | N1-C6-O6   | 9.95 | 125.87      | 119.90   |
| 1   | AA    | 138  | G    | N1-C6-O6   | 9.94 | 125.87      | 119.90   |
| 27  | B8    | 1232 | G    | N1-C6-O6   | 9.94 | 125.87      | 119.90   |
| 27  | B8    | 1515 | A    | O4'-C1'-N9 | 9.94 | 116.16      | 108.20   |
| 27  | B8    | 1215 | G    | N1-C6-O6   | 9.94 | 125.87      | 119.90   |
| 1   | AA    | 200  | G    | N1-C6-O6   | 9.94 | 125.86      | 119.90   |
| 26  | B7    | 33   | G    | N1-C6-O6   | 9.94 | 125.86      | 119.90   |
| 26  | B7    | 15   | A    | O4'-C1'-N9 | 9.94 | 116.15      | 108.20   |
| 1   | AA    | 105  | G    | N1-C6-O6   | 9.94 | 125.86      | 119.90   |
| 1   | AA    | 685  | G    | N1-C6-O6   | 9.92 | 125.86      | 119.90   |
| 27  | B8    | 1815 | A    | N1-C6-N6   | 9.92 | 124.55      | 118.60   |
| 27  | B8    | 2012 | G    | N1-C6-O6   | 9.92 | 125.85      | 119.90   |
| 27  | B8    | 9    | G    | N1-C6-O6   | 9.92 | 125.85      | 119.90   |
| 27  | B8    | 1896 | G    | N1-C6-O6   | 9.92 | 125.85      | 119.90   |
| 1   | AA    | 279  | A    | N1-C6-N6   | 9.91 | 124.55      | 118.60   |
| 27  | B8    | 1540 | G    | N1-C6-O6   | 9.91 | 125.85      | 119.90   |
| 27  | B8    | 86   | G    | N1-C6-O6   | 9.91 | 125.84      | 119.90   |
| 1   | AA    | 1133 | G    | N1-C6-O6   | 9.91 | 125.84      | 119.90   |
| 27  | B8    | 2623 | G    | N1-C6-O6   | 9.91 | 125.84      | 119.90   |
| 27  | B8    | 2583 | G    | N1-C6-O6   | 9.90 | 125.84      | 119.90   |
| 27  | B8    | 2621 | G    | N1-C6-O6   | 9.90 | 125.84      | 119.90   |
| 27  | B8    | 2383 | G    | N1-C6-O6   | 9.90 | 125.84      | 119.90   |
| 27  | B8    | 520  | G    | N1-C6-O6   | 9.90 | 125.84      | 119.90   |
| 1   | AA    | 39   | G    | N1-C6-O6   | 9.90 | 125.84      | 119.90   |
| 1   | AA    | 1061 | G    | N1-C6-O6   | 9.90 | 125.84      | 119.90   |
| 27  | B8    | 2803 | G    | N1-C6-O6   | 9.90 | 125.84      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 27  | B8    | 949  | G    | N1-C6-O6 | 9.89 | 125.84      | 119.90   |
| 27  | B8    | 454  | A    | N1-C6-N6 | 9.89 | 124.54      | 118.60   |
| 27  | B8    | 1182 | G    | N1-C6-O6 | 9.89 | 125.83      | 119.90   |
| 27  | B8    | 2757 | A    | N1-C6-N6 | 9.89 | 124.53      | 118.60   |
| 1   | AA    | 1164 | G    | N1-C6-O6 | 9.89 | 125.83      | 119.90   |
| 27  | B8    | 875  | G    | N1-C6-O6 | 9.89 | 125.83      | 119.90   |
| 1   | AA    | 57   | G    | N1-C6-O6 | 9.88 | 125.83      | 119.90   |
| 27  | B8    | 659  | G    | N1-C6-O6 | 9.88 | 125.83      | 119.90   |
| 27  | B8    | 2445 | G    | N1-C6-O6 | 9.88 | 125.83      | 119.90   |
| 26  | B7    | 9    | G    | N1-C6-O6 | 9.88 | 125.83      | 119.90   |
| 27  | B8    | 1435 | G    | N1-C6-O6 | 9.88 | 125.83      | 119.90   |
| 1   | AA    | 838  | G    | N1-C6-O6 | 9.87 | 125.82      | 119.90   |
| 1   | AA    | 711  | G    | N1-C6-O6 | 9.87 | 125.82      | 119.90   |
| 27  | B8    | 2053 | G    | N1-C6-O6 | 9.87 | 125.82      | 119.90   |
| 27  | B8    | 2574 | G    | N1-C6-O6 | 9.87 | 125.82      | 119.90   |
| 27  | B8    | 2437 | G    | N1-C6-O6 | 9.87 | 125.82      | 119.90   |
| 27  | B8    | 2140 | G    | N1-C6-O6 | 9.86 | 125.82      | 119.90   |
| 1   | AA    | 812  | G    | N1-C6-O6 | 9.86 | 125.82      | 119.90   |
| 27  | B8    | 291  | G    | N1-C6-O6 | 9.86 | 125.82      | 119.90   |
| 27  | B8    | 1517 | G    | N1-C6-O6 | 9.86 | 125.82      | 119.90   |
| 27  | B8    | 617  | G    | N1-C6-O6 | 9.86 | 125.82      | 119.90   |
| 1   | AA    | 373  | A    | N1-C6-N6 | 9.86 | 124.51      | 118.60   |
| 27  | B8    | 2709 | G    | N1-C6-O6 | 9.85 | 125.81      | 119.90   |
| 1   | AA    | 617  | G    | N1-C6-O6 | 9.85 | 125.81      | 119.90   |
| 1   | AA    | 1233 | G    | N1-C6-O6 | 9.85 | 125.81      | 119.90   |
| 1   | AA    | 27   | G    | N1-C6-O6 | 9.85 | 125.81      | 119.90   |
| 1   | AA    | 785  | G    | N1-C6-O6 | 9.85 | 125.81      | 119.90   |
| 27  | B8    | 1034 | G    | N1-C6-O6 | 9.84 | 125.81      | 119.90   |
| 27  | B8    | 1973 | G    | N1-C6-O6 | 9.84 | 125.81      | 119.90   |
| 1   | AA    | 240  | G    | N1-C6-O6 | 9.84 | 125.81      | 119.90   |
| 1   | AA    | 645  | G    | N1-C6-O6 | 9.84 | 125.80      | 119.90   |
| 1   | AA    | 917  | G    | N1-C6-O6 | 9.84 | 125.80      | 119.90   |
| 27  | B8    | 230  | G    | N1-C6-O6 | 9.83 | 125.80      | 119.90   |
| 27  | B8    | 312  | G    | N1-C6-O6 | 9.83 | 125.80      | 119.90   |
| 27  | B8    | 649  | G    | N1-C6-O6 | 9.83 | 125.80      | 119.90   |
| 1   | AA    | 1419 | G    | N1-C6-O6 | 9.83 | 125.80      | 119.90   |
| 27  | B8    | 2217 | G    | N1-C6-O6 | 9.83 | 125.80      | 119.90   |
| 27  | B8    | 2702 | G    | N1-C6-O6 | 9.83 | 125.80      | 119.90   |
| 27  | B8    | 1424 | G    | N1-C6-O6 | 9.82 | 125.80      | 119.90   |
| 27  | B8    | 2631 | G    | N1-C6-O6 | 9.82 | 125.79      | 119.90   |
| 27  | B8    | 483  | A    | N1-C6-N6 | 9.82 | 124.49      | 118.60   |
| 1   | AA    | 117  | G    | N1-C6-O6 | 9.82 | 125.79      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | AA    | 448  | A    | N1-C6-N6 | 9.82  | 124.49      | 118.60   |
| 27  | B8    | 729  | G    | N1-C6-O6 | 9.82  | 125.79      | 119.90   |
| 1   | AA    | 61   | G    | N1-C6-O6 | 9.81  | 125.79      | 119.90   |
| 27  | B8    | 682  | G    | N1-C6-O6 | 9.81  | 125.79      | 119.90   |
| 27  | B8    | 1193 | G    | N1-C6-O6 | 9.81  | 125.79      | 119.90   |
| 1   | AA    | 115  | G    | N1-C6-O6 | 9.81  | 125.78      | 119.90   |
| 1   | AA    | 1300 | G    | N1-C6-O6 | 9.81  | 125.78      | 119.90   |
| 27  | B8    | 1809 | A    | N1-C6-N6 | 9.81  | 124.48      | 118.60   |
| 1   | AA    | 1457 | G    | N1-C6-O6 | 9.81  | 125.78      | 119.90   |
| 27  | B8    | 1538 | G    | N1-C6-O6 | 9.81  | 125.78      | 119.90   |
| 27  | B8    | 1418 | G    | N1-C6-O6 | 9.80  | 125.78      | 119.90   |
| 27  | B8    | 1797 | G    | N1-C6-O6 | 9.80  | 125.78      | 119.90   |
| 27  | B8    | 2657 | A    | N1-C6-N6 | 9.80  | 124.48      | 118.60   |
| 27  | B8    | 2221 | G    | N1-C6-O6 | 9.79  | 125.78      | 119.90   |
| 27  | B8    | 1643 | G    | N1-C6-O6 | 9.79  | 125.78      | 119.90   |
| 1   | AA    | 954  | G    | N1-C6-O6 | 9.79  | 125.77      | 119.90   |
| 26  | B7    | 21   | G    | N1-C6-O6 | 9.78  | 125.77      | 119.90   |
| 27  | B8    | 2722 | G    | N1-C6-O6 | 9.78  | 125.77      | 119.90   |
| 1   | AA    | 45   | G    | N1-C6-O6 | 9.78  | 125.77      | 119.90   |
| 1   | AA    | 1334 | G    | N1-C6-O6 | 9.78  | 125.77      | 119.90   |
| 27  | B8    | 2093 | G    | N1-C6-O6 | 9.78  | 125.77      | 119.90   |
| 1   | AA    | 1261 | A    | N1-C6-N6 | 9.77  | 124.46      | 118.60   |
| 27  | B8    | 977  | G    | N1-C6-O6 | 9.77  | 125.76      | 119.90   |
| 27  | B8    | 809  | G    | N1-C6-O6 | 9.77  | 125.76      | 119.90   |
| 27  | B8    | 2654 | A    | N1-C6-N6 | 9.77  | 124.46      | 118.60   |
| 1   | AA    | 1034 | G    | C5-C6-O6 | -9.77 | 122.74      | 128.60   |
| 27  | B8    | 2136 | G    | N1-C6-O6 | 9.77  | 125.76      | 119.90   |
| 1   | AA    | 1511 | G    | N1-C6-O6 | 9.76  | 125.76      | 119.90   |
| 27  | B8    | 123  | G    | N1-C6-O6 | 9.76  | 125.76      | 119.90   |
| 27  | B8    | 2141 | G    | N1-C6-O6 | 9.76  | 125.76      | 119.90   |
| 27  | B8    | 1239 | G    | N1-C6-O6 | 9.76  | 125.76      | 119.90   |
| 1   | AA    | 1385 | G    | N1-C6-O6 | 9.76  | 125.75      | 119.90   |
| 27  | B8    | 407  | G    | N1-C6-O6 | 9.76  | 125.75      | 119.90   |
| 1   | AA    | 1193 | G    | N1-C6-O6 | 9.76  | 125.75      | 119.90   |
| 27  | B8    | 400  | G    | N1-C6-O6 | 9.75  | 125.75      | 119.90   |
| 27  | B8    | 2069 | G    | N1-C6-O6 | 9.75  | 125.75      | 119.90   |
| 27  | B8    | 2123 | G    | N1-C6-O6 | 9.75  | 125.75      | 119.90   |
| 26  | B7    | 10   | G    | N1-C6-O6 | 9.75  | 125.75      | 119.90   |
| 27  | B8    | 1734 | G    | N1-C6-O6 | 9.75  | 125.75      | 119.90   |
| 27  | B8    | 1218 | G    | N1-C6-O6 | 9.75  | 125.75      | 119.90   |
| 26  | B7    | 86   | G    | N1-C6-O6 | 9.74  | 125.75      | 119.90   |
| 27  | B8    | 1478 | G    | N1-C6-O6 | 9.74  | 125.75      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2812 | G    | N1-C6-O6   | 9.74  | 125.75      | 119.90   |
| 27  | B8    | 1099 | G    | N1-C6-O6   | 9.74  | 125.74      | 119.90   |
| 27  | B8    | 1191 | G    | N1-C6-O6   | 9.74  | 125.74      | 119.90   |
| 1   | AA    | 455  | G    | N1-C6-O6   | 9.74  | 125.74      | 119.90   |
| 27  | B8    | 326  | G    | N1-C6-O6   | 9.74  | 125.74      | 119.90   |
| 1   | AA    | 1220 | G    | N1-C6-O6   | 9.73  | 125.74      | 119.90   |
| 27  | B8    | 2315 | G    | N1-C6-O6   | 9.73  | 125.74      | 119.90   |
| 1   | AA    | 1423 | G    | N1-C6-O6   | 9.73  | 125.74      | 119.90   |
| 1   | AA    | 402  | G    | N1-C6-O6   | 9.73  | 125.74      | 119.90   |
| 27  | B8    | 260  | G    | N1-C6-O6   | 9.73  | 125.74      | 119.90   |
| 27  | B8    | 1055 | G    | N1-C6-O6   | 9.73  | 125.74      | 119.90   |
| 1   | AA    | 497  | G    | N1-C6-O6   | 9.73  | 125.74      | 119.90   |
| 26  | B7    | 106  | G    | N1-C6-O6   | 9.73  | 125.74      | 119.90   |
| 27  | B8    | 1107 | G    | N1-C6-O6   | 9.73  | 125.74      | 119.90   |
| 1   | AA    | 668  | G    | N1-C6-O6   | 9.72  | 125.73      | 119.90   |
| 27  | B8    | 1308 | A    | N1-C6-N6   | 9.72  | 124.43      | 118.60   |
| 1   | AA    | 1353 | G    | N1-C6-O6   | 9.72  | 125.73      | 119.90   |
| 27  | B8    | 1016 | G    | N1-C6-O6   | 9.72  | 125.73      | 119.90   |
| 27  | B8    | 1682 | G    | N1-C6-O6   | 9.72  | 125.73      | 119.90   |
| 1   | AA    | 142  | G    | N1-C6-O6   | 9.71  | 125.73      | 119.90   |
| 27  | B8    | 285  | G    | N1-C6-O6   | 9.71  | 125.73      | 119.90   |
| 1   | AA    | 734  | G    | N1-C6-O6   | 9.71  | 125.73      | 119.90   |
| 27  | B8    | 1546 | G    | N1-C6-O6   | 9.71  | 125.73      | 119.90   |
| 27  | B8    | 1964 | G    | N1-C6-O6   | 9.71  | 125.73      | 119.90   |
| 1   | AA    | 318  | G    | N1-C6-O6   | 9.71  | 125.73      | 119.90   |
| 27  | B8    | 2718 | G    | N1-C6-O6   | 9.71  | 125.73      | 119.90   |
| 27  | B8    | 2557 | G    | N1-C6-O6   | 9.71  | 125.72      | 119.90   |
| 27  | B8    | 2801 | G    | N1-C6-O6   | 9.71  | 125.72      | 119.90   |
| 27  | B8    | 410  | G    | N1-C6-O6   | 9.71  | 125.72      | 119.90   |
| 1   | AA    | 449  | G    | C5-C6-O6   | -9.70 | 122.78      | 128.60   |
| 27  | B8    | 2556 | C    | O4'-C1'-N1 | 9.70  | 115.96      | 108.20   |
| 1   | AA    | 1349 | A    | N1-C6-N6   | 9.70  | 124.42      | 118.60   |
| 1   | AA    | 755  | G    | N1-C6-O6   | 9.69  | 125.72      | 119.90   |
| 1   | AA    | 1288 | A    | N1-C6-N6   | 9.70  | 124.42      | 118.60   |
| 27  | B8    | 287  | G    | N1-C6-O6   | 9.70  | 125.72      | 119.90   |
| 27  | B8    | 2630 | G    | N1-C6-O6   | 9.69  | 125.71      | 119.90   |
| 1   | AA    | 293  | G    | N1-C6-O6   | 9.69  | 125.71      | 119.90   |
| 1   | AA    | 416  | G    | N1-C6-O6   | 9.69  | 125.71      | 119.90   |
| 27  | B8    | 1560 | G    | N1-C6-O6   | 9.69  | 125.71      | 119.90   |
| 27  | B8    | 2640 | G    | N1-C6-O6   | 9.69  | 125.71      | 119.90   |
| 27  | B8    | 2685 | G    | N1-C6-O6   | 9.69  | 125.71      | 119.90   |
| 27  | B8    | 2592 | G    | N1-C6-O6   | 9.68  | 125.71      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1422 | G    | N1-C6-O6   | 9.68  | 125.71      | 119.90   |
| 27  | B8    | 760  | G    | N1-C6-O6   | 9.68  | 125.71      | 119.90   |
| 27  | B8    | 425  | G    | N1-C6-O6   | 9.68  | 125.70      | 119.90   |
| 1   | AA    | 1030 | U    | O4'-C1'-N1 | 9.67  | 115.94      | 108.20   |
| 1   | AA    | 9    | G    | N1-C6-O6   | 9.66  | 125.70      | 119.90   |
| 27  | B8    | 185  | G    | N1-C6-O6   | 9.66  | 125.70      | 119.90   |
| 27  | B8    | 1932 | A    | N1-C6-N6   | 9.66  | 124.40      | 118.60   |
| 27  | B8    | 939  | G    | N1-C6-O6   | 9.66  | 125.70      | 119.90   |
| 27  | B8    | 2508 | G    | N1-C6-O6   | 9.66  | 125.70      | 119.90   |
| 27  | B8    | 1190 | G    | N1-C6-O6   | 9.66  | 125.69      | 119.90   |
| 27  | B8    | 1206 | G    | N1-C6-O6   | 9.66  | 125.69      | 119.90   |
| 27  | B8    | 2115 | G    | N1-C6-O6   | 9.66  | 125.69      | 119.90   |
| 27  | B8    | 2484 | G    | N1-C6-O6   | 9.66  | 125.69      | 119.90   |
| 27  | B8    | 2498 | C    | O4'-C1'-N1 | 9.66  | 115.92      | 108.20   |
| 1   | AA    | 1343 | G    | N1-C6-O6   | 9.65  | 125.69      | 119.90   |
| 27  | B8    | 2040 | G    | N1-C6-O6   | 9.65  | 125.69      | 119.90   |
| 1   | AA    | 1050 | G    | N1-C6-O6   | 9.65  | 125.69      | 119.90   |
| 1   | AA    | 1373 | G    | N1-C6-O6   | 9.65  | 125.69      | 119.90   |
| 1   | AA    | 639  | G    | N1-C6-O6   | 9.65  | 125.69      | 119.90   |
| 27  | B8    | 220  | G    | N1-C6-O6   | 9.65  | 125.69      | 119.90   |
| 27  | B8    | 2208 | C    | O4'-C1'-N1 | 9.64  | 115.92      | 108.20   |
| 27  | B8    | 579  | G    | N1-C6-O6   | 9.64  | 125.68      | 119.90   |
| 27  | B8    | 1792 | G    | N1-C6-O6   | 9.64  | 125.68      | 119.90   |
| 26  | B7    | 66   | A    | P-O3'-C3'  | 9.63  | 131.26      | 119.70   |
| 27  | B8    | 1948 | G    | N1-C6-O6   | 9.63  | 125.68      | 119.90   |
| 1   | AA    | 319  | G    | N1-C6-O6   | 9.63  | 125.68      | 119.90   |
| 1   | AA    | 1154 | G    | N1-C6-O6   | 9.63  | 125.68      | 119.90   |
| 27  | B8    | 759  | G    | N1-C6-O6   | 9.63  | 125.68      | 119.90   |
| 1   | AA    | 1087 | G    | N1-C6-O6   | 9.63  | 125.68      | 119.90   |
| 27  | B8    | 377  | G    | N1-C6-O6   | 9.63  | 125.68      | 119.90   |
| 27  | B8    | 836  | G    | N1-C6-O6   | 9.63  | 125.68      | 119.90   |
| 1   | AA    | 802  | A    | N1-C6-N6   | 9.63  | 124.38      | 118.60   |
| 1   | AA    | 851  | G    | C5-C6-O6   | -9.63 | 122.83      | 128.60   |
| 27  | B8    | 2323 | G    | N1-C6-O6   | 9.62  | 125.67      | 119.90   |
| 27  | B8    | 2419 | U    | O4'-C1'-N1 | 9.62  | 115.90      | 108.20   |
| 1   | AA    | 1515 | G    | N1-C6-O6   | 9.61  | 125.67      | 119.90   |
| 1   | AA    | 714  | G    | N1-C6-O6   | 9.61  | 125.67      | 119.90   |
| 1   | AA    | 945  | G    | N1-C6-O6   | 9.61  | 125.67      | 119.90   |
| 27  | B8    | 1138 | G    | N1-C6-O6   | 9.61  | 125.67      | 119.90   |
| 1   | AA    | 861  | G    | N1-C6-O6   | 9.61  | 125.66      | 119.90   |
| 1   | AA    | 894  | G    | N1-C6-O6   | 9.61  | 125.66      | 119.90   |
| 1   | AA    | 1041 | G    | N1-C6-O6   | 9.61  | 125.66      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 107  | G    | N1-C6-O6   | 9.61  | 125.66      | 119.90   |
| 27  | B8    | 1482 | G    | N1-C6-O6   | 9.61  | 125.66      | 119.90   |
| 27  | B8    | 2209 | G    | N1-C6-O6   | 9.61  | 125.66      | 119.90   |
| 27  | B8    | 2235 | G    | N1-C6-O6   | 9.61  | 125.66      | 119.90   |
| 27  | B8    | 2570 | G    | N1-C6-O6   | 9.61  | 125.66      | 119.90   |
| 27  | B8    | 1037 | G    | N1-C6-O6   | 9.60  | 125.66      | 119.90   |
| 27  | B8    | 402  | A    | N1-C6-N6   | 9.60  | 124.36      | 118.60   |
| 27  | B8    | 1163 | G    | N1-C6-O6   | 9.60  | 125.66      | 119.90   |
| 27  | B8    | 1214 | A    | N1-C6-N6   | 9.60  | 124.36      | 118.60   |
| 1   | AA    | 1143 | G    | N1-C6-O6   | 9.60  | 125.66      | 119.90   |
| 27  | B8    | 2128 | G    | N1-C6-O6   | 9.60  | 125.66      | 119.90   |
| 1   | AA    | 227  | G    | N1-C6-O6   | 9.60  | 125.66      | 119.90   |
| 27  | B8    | 186  | G    | N1-C6-O6   | 9.59  | 125.66      | 119.90   |
| 27  | B8    | 797  | G    | N1-C6-O6   | 9.59  | 125.66      | 119.90   |
| 27  | B8    | 1698 | A    | N1-C6-N6   | 9.59  | 124.36      | 118.60   |
| 27  | B8    | 2330 | G    | N1-C6-O6   | 9.59  | 125.66      | 119.90   |
| 1   | AA    | 428  | G    | C5-C6-O6   | -9.59 | 122.85      | 128.60   |
| 26  | B7    | 23   | G    | N1-C6-O6   | 9.59  | 125.65      | 119.90   |
| 27  | B8    | 363  | G    | N1-C6-O6   | 9.59  | 125.65      | 119.90   |
| 1   | AA    | 939  | G    | N1-C6-O6   | 9.59  | 125.65      | 119.90   |
| 27  | B8    | 1296 | G    | N1-C6-O6   | 9.59  | 125.65      | 119.90   |
| 27  | B8    | 1511 | G    | N1-C6-O6   | 9.59  | 125.65      | 119.90   |
| 1   | AA    | 148  | G    | C5-C6-O6   | -9.58 | 122.85      | 128.60   |
| 1   | AA    | 877  | G    | N1-C6-O6   | 9.58  | 125.65      | 119.90   |
| 27  | B8    | 798  | G    | N1-C6-O6   | 9.58  | 125.65      | 119.90   |
| 27  | B8    | 1306 | C    | O4'-C1'-N1 | 9.58  | 115.86      | 108.20   |
| 27  | B8    | 2599 | G    | N1-C6-O6   | 9.58  | 125.65      | 119.90   |
| 27  | B8    | 2603 | G    | N1-C6-O6   | 9.58  | 125.65      | 119.90   |
| 1   | AA    | 763  | G    | N1-C6-O6   | 9.57  | 125.64      | 119.90   |
| 3   | AV    | 3    | G    | N1-C6-O6   | 9.57  | 125.64      | 119.90   |
| 27  | B8    | 924  | G    | N1-C6-O6   | 9.57  | 125.64      | 119.90   |
| 27  | B8    | 1660 | G    | N1-C6-O6   | 9.57  | 125.64      | 119.90   |
| 27  | B8    | 1162 | G    | N1-C6-O6   | 9.57  | 125.64      | 119.90   |
| 27  | B8    | 1124 | G    | N1-C6-O6   | 9.57  | 125.64      | 119.90   |
| 27  | B8    | 2487 | G    | N1-C6-O6   | 9.57  | 125.64      | 119.90   |
| 27  | B8    | 1845 | G    | N1-C6-O6   | 9.57  | 125.64      | 119.90   |
| 27  | B8    | 1238 | G    | N1-C6-O6   | 9.56  | 125.64      | 119.90   |
| 1   | AA    | 1221 | G    | N1-C6-O6   | 9.56  | 125.64      | 119.90   |
| 27  | B8    | 1309 | G    | N1-C6-O6   | 9.56  | 125.64      | 119.90   |
| 27  | B8    | 2399 | G    | N1-C6-O6   | 9.56  | 125.64      | 119.90   |
| 27  | B8    | 70   | G    | N1-C6-O6   | 9.56  | 125.64      | 119.90   |
| 27  | B8    | 396  | G    | N1-C6-O6   | 9.56  | 125.63      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1949 | G    | N1-C6-O6   | 9.56  | 125.64      | 119.90   |
| 1   | AA    | 377  | G    | N1-C6-O6   | 9.55  | 125.63      | 119.90   |
| 27  | B8    | 207  | A    | N1-C6-N6   | 9.55  | 124.33      | 118.60   |
| 27  | B8    | 605  | G    | N1-C6-O6   | 9.55  | 125.63      | 119.90   |
| 27  | B8    | 1545 | A    | N1-C6-N6   | 9.55  | 124.33      | 118.60   |
| 27  | B8    | 1642 | G    | N1-C6-O6   | 9.55  | 125.63      | 119.90   |
| 27  | B8    | 2664 | G    | C5-C6-O6   | -9.55 | 122.87      | 128.60   |
| 27  | B8    | 938  | G    | N1-C6-O6   | 9.55  | 125.63      | 119.90   |
| 27  | B8    | 2588 | G    | N1-C6-O6   | 9.55  | 125.63      | 119.90   |
| 1   | AA    | 1454 | G    | N1-C6-O6   | 9.54  | 125.63      | 119.90   |
| 1   | AA    | 1494 | G    | N1-C6-O6   | 9.55  | 125.63      | 119.90   |
| 27  | B8    | 122  | G    | N1-C6-O6   | 9.55  | 125.63      | 119.90   |
| 27  | B8    | 1799 | G    | N1-C6-O6   | 9.55  | 125.63      | 119.90   |
| 27  | B8    | 252  | G    | N1-C6-O6   | 9.54  | 125.63      | 119.90   |
| 27  | B8    | 536  | G    | N1-C6-O6   | 9.54  | 125.63      | 119.90   |
| 1   | AA    | 867  | G    | N1-C6-O6   | 9.54  | 125.62      | 119.90   |
| 27  | B8    | 1510 | G    | C5-C6-O6   | -9.54 | 122.88      | 128.60   |
| 1   | AA    | 113  | G    | N1-C6-O6   | 9.54  | 125.62      | 119.90   |
| 27  | B8    | 799  | G    | N1-C6-O6   | 9.54  | 125.62      | 119.90   |
| 27  | B8    | 1179 | G    | N1-C6-O6   | 9.54  | 125.62      | 119.90   |
| 27  | B8    | 1992 | G    | N1-C6-O6   | 9.54  | 125.62      | 119.90   |
| 27  | B8    | 2641 | G    | N1-C6-O6   | 9.54  | 125.62      | 119.90   |
| 27  | B8    | 550  | C    | O4'-C1'-N1 | 9.53  | 115.83      | 108.20   |
| 27  | B8    | 976  | G    | N1-C6-O6   | 9.53  | 125.62      | 119.90   |
| 27  | B8    | 1455 | G    | N1-C6-O6   | 9.53  | 125.62      | 119.90   |
| 27  | B8    | 1651 | G    | N1-C6-O6   | 9.53  | 125.62      | 119.90   |
| 27  | B8    | 2102 | G    | N1-C6-O6   | 9.53  | 125.62      | 119.90   |
| 27  | B8    | 1093 | G    | N1-C6-O6   | 9.53  | 125.62      | 119.90   |
| 27  | B8    | 1840 | G    | N1-C6-O6   | 9.53  | 125.62      | 119.90   |
| 27  | B8    | 2464 | G    | N1-C6-O6   | 9.53  | 125.62      | 119.90   |
| 27  | B8    | 2486 | C    | O4'-C1'-N1 | 9.53  | 115.82      | 108.20   |
| 27  | B8    | 989  | G    | N1-C6-O6   | 9.52  | 125.61      | 119.90   |
| 27  | B8    | 1137 | G    | N1-C6-O6   | 9.52  | 125.61      | 119.90   |
| 27  | B8    | 2545 | G    | N1-C6-O6   | 9.52  | 125.61      | 119.90   |
| 1   | AA    | 874  | G    | N1-C6-O6   | 9.52  | 125.61      | 119.90   |
| 27  | B8    | 2677 | G    | N1-C6-O6   | 9.52  | 125.61      | 119.90   |
| 27  | B8    | 1245 | G    | N1-C6-O6   | 9.51  | 125.61      | 119.90   |
| 1   | AA    | 592  | G    | N1-C6-O6   | 9.51  | 125.61      | 119.90   |
| 27  | B8    | 543  | G    | N1-C6-O6   | 9.51  | 125.61      | 119.90   |
| 27  | B8    | 2643 | G    | N1-C6-O6   | 9.51  | 125.61      | 119.90   |
| 1   | AA    | 892  | A    | N1-C6-N6   | 9.51  | 124.31      | 118.60   |
| 27  | B8    | 1259 | G    | N1-C6-O6   | 9.51  | 125.61      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1292 | G    | N1-C6-O6   | 9.51  | 125.60      | 119.90   |
| 27  | B8    | 2204 | G    | N1-C6-O6   | 9.51  | 125.60      | 119.90   |
| 27  | B8    | 1954 | G    | N1-C6-O6   | 9.50  | 125.60      | 119.90   |
| 27  | B8    | 212  | G    | N1-C6-O6   | 9.50  | 125.60      | 119.90   |
| 27  | B8    | 1891 | G    | N1-C6-O6   | 9.50  | 125.60      | 119.90   |
| 1   | AA    | 401  | C    | O4'-C1'-N1 | 9.50  | 115.80      | 108.20   |
| 1   | AA    | 577  | G    | N1-C6-O6   | 9.50  | 125.60      | 119.90   |
| 27  | B8    | 778  | G    | N1-C6-O6   | 9.50  | 125.60      | 119.90   |
| 27  | B8    | 1659 | G    | N1-C6-O6   | 9.50  | 125.60      | 119.90   |
| 1   | AA    | 725  | G    | N1-C6-O6   | 9.49  | 125.59      | 119.90   |
| 27  | B8    | 1351 | C    | O4'-C1'-N1 | 9.49  | 115.79      | 108.20   |
| 1   | AA    | 824  | G    | N1-C6-O6   | 9.49  | 125.59      | 119.90   |
| 1   | AA    | 1174 | G    | N1-C6-O6   | 9.49  | 125.59      | 119.90   |
| 27  | B8    | 2410 | G    | N1-C6-O6   | 9.49  | 125.59      | 119.90   |
| 27  | B8    | 2674 | G    | N1-C6-O6   | 9.49  | 125.59      | 119.90   |
| 1   | AA    | 779  | C    | O4'-C1'-N1 | 9.49  | 115.79      | 108.20   |
| 1   | AA    | 846  | G    | N1-C6-O6   | 9.49  | 125.59      | 119.90   |
| 27  | B8    | 121  | G    | N1-C6-O6   | 9.49  | 125.59      | 119.90   |
| 27  | B8    | 2029 | G    | C5-C6-O6   | -9.49 | 122.91      | 128.60   |
| 27  | B8    | 1310 | G    | N1-C6-O6   | 9.49  | 125.59      | 119.90   |
| 1   | AA    | 1310 | G    | N1-C6-O6   | 9.48  | 125.59      | 119.90   |
| 27  | B8    | 408  | G    | N1-C6-O6   | 9.48  | 125.59      | 119.90   |
| 27  | B8    | 1155 | A    | N1-C6-N6   | 9.48  | 124.29      | 118.60   |
| 27  | B8    | 1707 | G    | N1-C6-O6   | 9.48  | 125.59      | 119.90   |
| 27  | B8    | 245  | G    | N1-C6-O6   | 9.47  | 125.58      | 119.90   |
| 27  | B8    | 1661 | G    | N1-C6-O6   | 9.47  | 125.58      | 119.90   |
| 1   | AA    | 500  | G    | N1-C6-O6   | 9.47  | 125.58      | 119.90   |
| 27  | B8    | 821  | A    | N1-C6-N6   | 9.47  | 124.28      | 118.60   |
| 27  | B8    | 962  | G    | N1-C6-O6   | 9.47  | 125.58      | 119.90   |
| 27  | B8    | 1906 | G    | N1-C6-O6   | 9.47  | 125.58      | 119.90   |
| 27  | B8    | 2341 | G    | N1-C6-O6   | 9.47  | 125.58      | 119.90   |
| 1   | AA    | 1127 | G    | N1-C6-O6   | 9.47  | 125.58      | 119.90   |
| 1   | AA    | 198  | G    | N1-C6-O6   | 9.46  | 125.58      | 119.90   |
| 27  | B8    | 77   | G    | N1-C6-O6   | 9.46  | 125.58      | 119.90   |
| 27  | B8    | 2509 | G    | N1-C6-O6   | 9.46  | 125.58      | 119.90   |
| 27  | B8    | 2716 | C    | O4'-C1'-N1 | 9.46  | 115.77      | 108.20   |
| 1   | AA    | 615  | G    | N1-C6-O6   | 9.46  | 125.58      | 119.90   |
| 27  | B8    | 1041 | G    | N1-C6-O6   | 9.46  | 125.58      | 119.90   |
| 27  | B8    | 2078 | C    | O4'-C1'-N1 | 9.46  | 115.77      | 108.20   |
| 26  | B7    | 83   | G    | N1-C6-O6   | 9.46  | 125.57      | 119.90   |
| 27  | B8    | 2413 | G    | N1-C6-O6   | 9.46  | 125.57      | 119.90   |
| 1   | AA    | 1386 | G    | N1-C6-O6   | 9.45  | 125.57      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 27  | B8    | 187  | G    | N1-C6-O6   | 9.45 | 125.57      | 119.90   |
| 27  | B8    | 1256 | G    | N1-C6-O6   | 9.45 | 125.57      | 119.90   |
| 1   | AA    | 791  | G    | N1-C6-O6   | 9.45 | 125.57      | 119.90   |
| 27  | B8    | 2669 | G    | N1-C6-O6   | 9.45 | 125.57      | 119.90   |
| 27  | B8    | 2731 | G    | N1-C6-O6   | 9.45 | 125.57      | 119.90   |
| 1   | AA    | 347  | G    | N1-C6-O6   | 9.45 | 125.57      | 119.90   |
| 27  | B8    | 717  | C    | O4'-C1'-N1 | 9.45 | 115.76      | 108.20   |
| 27  | B8    | 1430 | G    | N1-C6-O6   | 9.45 | 125.57      | 119.90   |
| 27  | B8    | 2355 | G    | N1-C6-O6   | 9.45 | 125.57      | 119.90   |
| 27  | B8    | 2550 | G    | N1-C6-O6   | 9.45 | 125.57      | 119.90   |
| 27  | B8    | 2732 | G    | N1-C6-O6   | 9.45 | 125.57      | 119.90   |
| 27  | B8    | 998  | C    | O4'-C1'-N1 | 9.44 | 115.75      | 108.20   |
| 27  | B8    | 1414 | C    | O4'-C1'-N1 | 9.44 | 115.75      | 108.20   |
| 1   | AA    | 241  | G    | N1-C6-O6   | 9.44 | 125.56      | 119.90   |
| 27  | B8    | 132  | G    | N1-C6-O6   | 9.44 | 125.56      | 119.90   |
| 27  | B8    | 1601 | G    | N1-C6-O6   | 9.44 | 125.56      | 119.90   |
| 27  | B8    | 1988 | G    | N1-C6-O6   | 9.44 | 125.56      | 119.90   |
| 27  | B8    | 2782 | G    | N1-C6-O6   | 9.44 | 125.56      | 119.90   |
| 3   | AV    | 23   | G    | N1-C6-O6   | 9.44 | 125.56      | 119.90   |
| 27  | B8    | 585  | G    | N1-C6-O6   | 9.44 | 125.56      | 119.90   |
| 1   | AA    | 213  | G    | N1-C6-O6   | 9.43 | 125.56      | 119.90   |
| 27  | B8    | 258  | G    | N1-C6-O6   | 9.43 | 125.56      | 119.90   |
| 27  | B8    | 319  | G    | N1-C6-O6   | 9.43 | 125.56      | 119.90   |
| 27  | B8    | 966  | G    | N1-C6-O6   | 9.43 | 125.56      | 119.90   |
| 27  | B8    | 2523 | G    | N1-C6-O6   | 9.43 | 125.56      | 119.90   |
| 1   | AA    | 163  | C    | O4'-C1'-N1 | 9.43 | 115.74      | 108.20   |
| 27  | B8    | 2110 | G    | N1-C6-O6   | 9.43 | 125.56      | 119.90   |
| 27  | B8    | 1500 | G    | N1-C6-O6   | 9.43 | 125.56      | 119.90   |
| 27  | B8    | 1904 | G    | N1-C6-O6   | 9.43 | 125.56      | 119.90   |
| 27  | B8    | 914  | G    | N1-C6-O6   | 9.42 | 125.55      | 119.90   |
| 27  | B8    | 1216 | G    | N1-C6-O6   | 9.42 | 125.55      | 119.90   |
| 27  | B8    | 1429 | G    | N1-C6-O6   | 9.42 | 125.55      | 119.90   |
| 27  | B8    | 1519 | G    | N1-C6-O6   | 9.42 | 125.56      | 119.90   |
| 27  | B8    | 2276 | G    | N1-C6-O6   | 9.42 | 125.55      | 119.90   |
| 27  | B8    | 1120 | G    | N1-C6-O6   | 9.42 | 125.55      | 119.90   |
| 27  | B8    | 1731 | G    | N1-C6-O6   | 9.42 | 125.55      | 119.90   |
| 1   | AA    | 666  | G    | N1-C6-O6   | 9.42 | 125.55      | 119.90   |
| 27  | B8    | 1171 | G    | N1-C6-O6   | 9.41 | 125.55      | 119.90   |
| 27  | B8    | 1448 | G    | N1-C6-O6   | 9.41 | 125.55      | 119.90   |
| 27  | B8    | 1250 | G    | N1-C6-O6   | 9.41 | 125.55      | 119.90   |
| 27  | B8    | 2838 | G    | N1-C6-O6   | 9.41 | 125.55      | 119.90   |
| 27  | B8    | 792  | A    | P-O3'-C3'  | 9.41 | 130.99      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1011 | G    | N1-C6-O6   | 9.41  | 125.55      | 119.90   |
| 27  | B8    | 1862 | G    | N1-C6-O6   | 9.41  | 125.55      | 119.90   |
| 27  | B8    | 2242 | G    | N1-C6-O6   | 9.41  | 125.55      | 119.90   |
| 1   | AA    | 1026 | G    | N1-C6-O6   | 9.41  | 125.54      | 119.90   |
| 27  | B8    | 259  | G    | N1-C6-O6   | 9.41  | 125.54      | 119.90   |
| 1   | AA    | 141  | G    | N1-C6-O6   | 9.40  | 125.54      | 119.90   |
| 27  | B8    | 1530 | G    | N1-C6-O6   | 9.40  | 125.54      | 119.90   |
| 1   | AA    | 903  | G    | N1-C6-O6   | 9.40  | 125.54      | 119.90   |
| 27  | B8    | 700  | G    | N1-C6-O6   | 9.40  | 125.54      | 119.90   |
| 27  | B8    | 297  | G    | N1-C6-O6   | 9.40  | 125.54      | 119.90   |
| 27  | B8    | 261  | G    | N1-C6-O6   | 9.40  | 125.54      | 119.90   |
| 27  | B8    | 535  | G    | N1-C6-O6   | 9.40  | 125.54      | 119.90   |
| 27  | B8    | 723  | C    | O4'-C1'-N1 | 9.39  | 115.72      | 108.20   |
| 1   | AA    | 731  | G    | N1-C6-O6   | 9.39  | 125.53      | 119.90   |
| 27  | B8    | 1984 | G    | N1-C6-O6   | 9.39  | 125.53      | 119.90   |
| 1   | AA    | 111  | G    | N1-C6-O6   | 9.39  | 125.53      | 119.90   |
| 26  | B7    | 18   | G    | N1-C6-O6   | 9.39  | 125.53      | 119.90   |
| 1   | AA    | 1238 | A    | N1-C6-N6   | 9.39  | 124.23      | 118.60   |
| 27  | B8    | 214  | G    | N1-C6-O6   | 9.39  | 125.53      | 119.90   |
| 27  | B8    | 1031 | G    | N1-C6-O6   | 9.39  | 125.53      | 119.90   |
| 27  | B8    | 1    | G    | N1-C6-O6   | 9.39  | 125.53      | 119.90   |
| 1   | AA    | 1002 | G    | N1-C6-O6   | 9.38  | 125.53      | 119.90   |
| 26  | B7    | 6    | G    | N1-C6-O6   | 9.38  | 125.53      | 119.90   |
| 27  | B8    | 952  | G    | N1-C6-O6   | 9.38  | 125.53      | 119.90   |
| 1   | AA    | 491  | G    | N1-C6-O6   | 9.38  | 125.53      | 119.90   |
| 27  | B8    | 1192 | G    | N1-C6-O6   | 9.38  | 125.53      | 119.90   |
| 1   | AA    | 1032 | G    | N1-C6-O6   | 9.38  | 125.53      | 119.90   |
| 27  | B8    | 189  | G    | N1-C6-O6   | 9.38  | 125.53      | 119.90   |
| 27  | B8    | 1850 | G    | N1-C6-O6   | 9.38  | 125.53      | 119.90   |
| 1   | AA    | 1198 | G    | N1-C6-O6   | 9.38  | 125.53      | 119.90   |
| 1   | AA    | 1234 | C    | O4'-C1'-N1 | 9.38  | 115.70      | 108.20   |
| 1   | AA    | 585  | G    | N1-C6-O6   | 9.38  | 125.53      | 119.90   |
| 1   | AA    | 774  | G    | N1-C6-O6   | 9.37  | 125.52      | 119.90   |
| 27  | B8    | 956  | G    | N1-C6-O6   | 9.37  | 125.52      | 119.90   |
| 1   | AA    | 242  | G    | N1-C6-O6   | 9.37  | 125.52      | 119.90   |
| 27  | B8    | 1168 | G    | N1-C6-O6   | 9.37  | 125.52      | 119.90   |
| 27  | B8    | 2502 | G    | N1-C6-O6   | 9.37  | 125.52      | 119.90   |
| 27  | B8    | 2744 | G    | N1-C6-O6   | 9.37  | 125.52      | 119.90   |
| 1   | AA    | 1206 | G    | C5-C6-O6   | -9.37 | 122.98      | 128.60   |
| 27  | B8    | 468  | G    | N1-C6-O6   | 9.37  | 125.52      | 119.90   |
| 27  | B8    | 2828 | G    | N1-C6-O6   | 9.36  | 125.52      | 119.90   |
| 3   | AV    | 54   | G    | N1-C6-O6   | 9.36  | 125.52      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1388 | G    | N1-C6-O6   | 9.36  | 125.52      | 119.90   |
| 27  | B8    | 1922 | G    | N1-C6-O6   | 9.36  | 125.52      | 119.90   |
| 27  | B8    | 2846 | G    | N1-C6-O6   | 9.36  | 125.52      | 119.90   |
| 1   | AA    | 314  | C    | O4'-C1'-N1 | 9.36  | 115.69      | 108.20   |
| 1   | AA    | 929  | G    | N1-C6-O6   | 9.36  | 125.51      | 119.90   |
| 1   | AA    | 604  | G    | N1-C6-O6   | 9.35  | 125.51      | 119.90   |
| 1   | AA    | 671  | G    | N1-C6-O6   | 9.35  | 125.51      | 119.90   |
| 1   | AA    | 1039 | G    | N1-C6-O6   | 9.35  | 125.51      | 119.90   |
| 27  | B8    | 636  | G    | N1-C6-O6   | 9.35  | 125.51      | 119.90   |
| 27  | B8    | 993  | G    | N1-C6-O6   | 9.35  | 125.51      | 119.90   |
| 27  | B8    | 2107 | G    | N1-C6-O6   | 9.35  | 125.51      | 119.90   |
| 27  | B8    | 2729 | G    | N1-C6-O6   | 9.35  | 125.51      | 119.90   |
| 1   | AA    | 165  | G    | N1-C6-O6   | 9.35  | 125.51      | 119.90   |
| 27  | B8    | 2895 | G    | C5-C6-O6   | -9.35 | 122.99      | 128.60   |
| 27  | B8    | 2759 | G    | N1-C6-O6   | 9.35  | 125.51      | 119.90   |
| 27  | B8    | 424  | G    | C5-C6-O6   | -9.35 | 122.99      | 128.60   |
| 27  | B8    | 1358 | G    | N1-C6-O6   | 9.35  | 125.51      | 119.90   |
| 3   | AV    | 47   | G    | N1-C6-O6   | 9.34  | 125.51      | 119.90   |
| 26  | B7    | 7    | G    | N1-C6-O6   | 9.34  | 125.51      | 119.90   |
| 27  | B8    | 2173 | A    | N1-C6-N6   | 9.34  | 124.20      | 118.60   |
| 27  | B8    | 2325 | G    | N1-C6-O6   | 9.34  | 125.51      | 119.90   |
| 27  | B8    | 2876 | G    | N1-C6-O6   | 9.34  | 125.50      | 119.90   |
| 1   | AA    | 881  | G    | N1-C6-O6   | 9.34  | 125.50      | 119.90   |
| 26  | B7    | 20   | G    | N1-C6-O6   | 9.34  | 125.50      | 119.90   |
| 3   | AV    | 32   | C    | O4'-C1'-N1 | 9.34  | 115.67      | 108.20   |
| 27  | B8    | 438  | G    | N1-C6-O6   | 9.34  | 125.50      | 119.90   |
| 1   | AA    | 425  | G    | N1-C6-O6   | 9.33  | 125.50      | 119.90   |
| 27  | B8    | 738  | G    | N1-C6-O6   | 9.33  | 125.50      | 119.90   |
| 27  | B8    | 1724 | G    | N1-C6-O6   | 9.33  | 125.50      | 119.90   |
| 1   | AA    | 836  | G    | N1-C6-O6   | 9.33  | 125.50      | 119.90   |
| 1   | AA    | 902  | G    | N1-C6-O6   | 9.33  | 125.50      | 119.90   |
| 1   | AA    | 1215 | G    | N1-C6-O6   | 9.33  | 125.50      | 119.90   |
| 27  | B8    | 2490 | G    | N1-C6-O6   | 9.33  | 125.50      | 119.90   |
| 1   | AA    | 548  | G    | N1-C6-O6   | 9.33  | 125.50      | 119.90   |
| 1   | AA    | 1106 | G    | N1-C6-O6   | 9.32  | 125.49      | 119.90   |
| 26  | B7    | 85   | G    | N1-C6-O6   | 9.32  | 125.49      | 119.90   |
| 27  | B8    | 2582 | G    | N1-C6-O6   | 9.32  | 125.49      | 119.90   |
| 27  | B8    | 215  | G    | N1-C6-O6   | 9.32  | 125.49      | 119.90   |
| 27  | B8    | 1071 | G    | N1-C6-O6   | 9.32  | 125.49      | 119.90   |
| 27  | B8    | 1281 | G    | N1-C6-O6   | 9.32  | 125.49      | 119.90   |
| 1   | AA    | 203  | G    | N1-C6-O6   | 9.32  | 125.49      | 119.90   |
| 27  | B8    | 2339 | C    | O4'-C1'-N1 | 9.32  | 115.66      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2443 | C    | O4'-C1'-N1 | 9.32  | 115.66      | 108.20   |
| 27  | B8    | 2671 | G    | N1-C6-O6   | 9.32  | 125.49      | 119.90   |
| 27  | B8    | 638  | G    | N1-C6-O6   | 9.32  | 125.49      | 119.90   |
| 27  | B8    | 827  | U    | P-O3'-C3'  | 9.32  | 130.88      | 119.70   |
| 27  | B8    | 1813 | G    | N1-C6-O6   | 9.32  | 125.49      | 119.90   |
| 27  | B8    | 2686 | G    | N1-C6-O6   | 9.31  | 125.49      | 119.90   |
| 26  | B7    | 35   | C    | O4'-C1'-N1 | 9.31  | 115.65      | 108.20   |
| 27  | B8    | 276  | U    | O4'-C1'-N1 | 9.31  | 115.65      | 108.20   |
| 27  | B8    | 1921 | G    | N1-C6-O6   | 9.31  | 125.49      | 119.90   |
| 1   | AA    | 184  | G    | C5-C6-O6   | -9.31 | 123.01      | 128.60   |
| 26  | B7    | 44   | G    | N1-C6-O6   | 9.31  | 125.49      | 119.90   |
| 27  | B8    | 1221 | C    | O4'-C1'-N1 | 9.31  | 115.65      | 108.20   |
| 27  | B8    | 75   | G    | N1-C6-O6   | 9.31  | 125.48      | 119.90   |
| 1   | AA    | 925  | G    | N1-C6-O6   | 9.31  | 125.48      | 119.90   |
| 1   | AA    | 1469 | C    | O4'-C1'-N1 | 9.30  | 115.64      | 108.20   |
| 27  | B8    | 1610 | A    | N1-C6-N6   | 9.30  | 124.18      | 118.60   |
| 1   | AA    | 610  | U    | O4'-C1'-N1 | 9.30  | 115.64      | 108.20   |
| 1   | AA    | 821  | G    | N1-C6-O6   | 9.30  | 125.48      | 119.90   |
| 27  | B8    | 266  | G    | C5-C6-O6   | -9.30 | 123.02      | 128.60   |
| 27  | B8    | 893  | C    | O4'-C1'-N1 | 9.30  | 115.64      | 108.20   |
| 27  | B8    | 1444 | G    | N1-C6-O6   | 9.30  | 125.48      | 119.90   |
| 27  | B8    | 1910 | G    | C5-C6-O6   | -9.30 | 123.02      | 128.60   |
| 27  | B8    | 2889 | C    | O4'-C1'-N1 | 9.30  | 115.64      | 108.20   |
| 27  | B8    | 2316 | G    | N1-C6-O6   | 9.30  | 125.48      | 119.90   |
| 1   | AA    | 885  | G    | N1-C6-O6   | 9.30  | 125.48      | 119.90   |
| 27  | B8    | 856  | G    | N1-C6-O6   | 9.30  | 125.48      | 119.90   |
| 27  | B8    | 2228 | G    | N1-C6-O6   | 9.30  | 125.48      | 119.90   |
| 27  | B8    | 2567 | G    | N1-C6-O6   | 9.30  | 125.48      | 119.90   |
| 27  | B8    | 2633 | G    | N1-C6-O6   | 9.30  | 125.48      | 119.90   |
| 27  | B8    | 241  | A    | N1-C6-N6   | 9.29  | 124.18      | 118.60   |
| 27  | B8    | 578  | G    | N1-C6-O6   | 9.29  | 125.48      | 119.90   |
| 27  | B8    | 1625 | C    | O4'-C1'-N1 | 9.30  | 115.64      | 108.20   |
| 27  | B8    | 1202 | G    | N1-C6-O6   | 9.29  | 125.48      | 119.90   |
| 27  | B8    | 1357 | C    | O4'-C1'-N1 | 9.29  | 115.63      | 108.20   |
| 27  | B8    | 1860 | G    | N1-C6-O6   | 9.29  | 125.47      | 119.90   |
| 27  | B8    | 1766 | G    | N1-C6-O6   | 9.29  | 125.47      | 119.90   |
| 1   | AA    | 953  | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |
| 1   | AA    | 1138 | G    | N1-C6-O6   | 9.29  | 125.47      | 119.90   |
| 1   | AA    | 1242 | G    | N1-C6-O6   | 9.29  | 125.47      | 119.90   |
| 27  | B8    | 674  | G    | N1-C6-O6   | 9.29  | 125.47      | 119.90   |
| 26  | B7    | 75   | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |
| 1   | AA    | 1514 | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 301  | G    | C5-C6-O6   | -9.28 | 123.03      | 128.60   |
| 1   | AA    | 1435 | G    | C5-C6-O6   | -9.28 | 123.03      | 128.60   |
| 27  | B8    | 843  | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |
| 27  | B8    | 2495 | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |
| 27  | B8    | 2543 | G    | C5-C6-O6   | -9.28 | 123.03      | 128.60   |
| 27  | B8    | 2725 | A    | N1-C6-N6   | 9.28  | 124.17      | 118.60   |
| 27  | B8    | 2802 | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |
| 1   | AA    | 230  | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |
| 27  | B8    | 629  | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |
| 27  | B8    | 1645 | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |
| 27  | B8    | 2087 | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |
| 27  | B8    | 2403 | C    | O4'-C1'-N1 | 9.28  | 115.62      | 108.20   |
| 1   | AA    | 1458 | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |
| 27  | B8    | 313  | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |
| 27  | B8    | 1653 | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |
| 27  | B8    | 1666 | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |
| 27  | B8    | 1925 | C    | O4'-C1'-N1 | 9.28  | 115.62      | 108.20   |
| 27  | B8    | 2454 | G    | N1-C6-O6   | 9.28  | 125.47      | 119.90   |
| 1   | AA    | 102  | G    | N1-C6-O6   | 9.27  | 125.46      | 119.90   |
| 1   | AA    | 1438 | G    | N1-C6-O6   | 9.27  | 125.47      | 119.90   |
| 27  | B8    | 1723 | G    | N1-C6-O6   | 9.27  | 125.47      | 119.90   |
| 1   | AA    | 1144 | G    | N1-C6-O6   | 9.27  | 125.46      | 119.90   |
| 27  | B8    | 1185 | G    | N1-C6-O6   | 9.27  | 125.46      | 119.90   |
| 1   | AA    | 1462 | C    | O4'-C1'-N1 | 9.27  | 115.61      | 108.20   |
| 1   | AA    | 1529 | G    | N1-C6-O6   | 9.27  | 125.46      | 119.90   |
| 26  | B7    | 16   | G    | N1-C6-O6   | 9.27  | 125.46      | 119.90   |
| 27  | B8    | 681  | G    | N1-C6-O6   | 9.27  | 125.46      | 119.90   |
| 27  | B8    | 697  | G    | N1-C6-O6   | 9.27  | 125.46      | 119.90   |
| 27  | B8    | 1835 | G    | N1-C6-O6   | 9.27  | 125.46      | 119.90   |
| 27  | B8    | 974  | G    | N1-C6-O6   | 9.27  | 125.46      | 119.90   |
| 1   | AA    | 462  | G    | N1-C6-O6   | 9.26  | 125.46      | 119.90   |
| 27  | B8    | 2666 | C    | O4'-C1'-N1 | 9.26  | 115.61      | 108.20   |
| 1   | AA    | 332  | G    | N1-C6-O6   | 9.26  | 125.46      | 119.90   |
| 27  | B8    | 380  | G    | N1-C6-O6   | 9.26  | 125.46      | 119.90   |
| 27  | B8    | 2290 | G    | N1-C6-O6   | 9.26  | 125.46      | 119.90   |
| 27  | B8    | 1441 | G    | N1-C6-O6   | 9.26  | 125.46      | 119.90   |
| 27  | B8    | 2251 | G    | N1-C6-O6   | 9.26  | 125.45      | 119.90   |
| 1   | AA    | 337  | G    | N1-C6-O6   | 9.26  | 125.45      | 119.90   |
| 1   | AA    | 1043 | G    | N1-C6-O6   | 9.26  | 125.45      | 119.90   |
| 27  | B8    | 604  | G    | N1-C6-O6   | 9.25  | 125.45      | 119.90   |
| 27  | B8    | 1136 | G    | N1-C6-O6   | 9.25  | 125.45      | 119.90   |
| 27  | B8    | 1628 | G    | N1-C6-O6   | 9.25  | 125.45      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 46   | G    | N1-C6-O6   | 9.25  | 125.45      | 119.90   |
| 27  | B8    | 695  | G    | N1-C6-O6   | 9.25  | 125.45      | 119.90   |
| 27  | B8    | 770  | G    | N1-C6-O6   | 9.25  | 125.45      | 119.90   |
| 1   | AA    | 978  | A    | N1-C6-N6   | 9.24  | 124.14      | 118.60   |
| 27  | B8    | 1416 | G    | N1-C6-O6   | 9.24  | 125.44      | 119.90   |
| 27  | B8    | 1622 | G    | N1-C6-O6   | 9.24  | 125.44      | 119.90   |
| 27  | B8    | 289  | G    | N1-C6-O6   | 9.24  | 125.44      | 119.90   |
| 27  | B8    | 1343 | G    | N1-C6-O6   | 9.24  | 125.44      | 119.90   |
| 27  | B8    | 2852 | G    | N1-C6-O6   | 9.24  | 125.44      | 119.90   |
| 1   | AA    | 1356 | G    | N1-C6-O6   | 9.23  | 125.44      | 119.90   |
| 27  | B8    | 796  | C    | O4'-C1'-N1 | 9.23  | 115.59      | 108.20   |
| 27  | B8    | 2428 | G    | N1-C6-O6   | 9.23  | 125.44      | 119.90   |
| 1   | AA    | 299  | G    | N1-C6-O6   | 9.23  | 125.44      | 119.90   |
| 26  | B7    | 61   | G    | N1-C6-O6   | 9.23  | 125.44      | 119.90   |
| 27  | B8    | 151  | C    | O4'-C1'-N1 | 9.23  | 115.59      | 108.20   |
| 1   | AA    | 1294 | G    | N1-C6-O6   | 9.23  | 125.44      | 119.90   |
| 1   | AA    | 1526 | G    | N1-C6-O6   | 9.23  | 125.44      | 119.90   |
| 27  | B8    | 1878 | G    | N1-C6-O6   | 9.23  | 125.44      | 119.90   |
| 27  | B8    | 774  | G    | N1-C6-O6   | 9.23  | 125.44      | 119.90   |
| 27  | B8    | 2642 | G    | N1-C6-O6   | 9.23  | 125.44      | 119.90   |
| 27  | B8    | 35   | G    | N1-C6-O6   | 9.23  | 125.44      | 119.90   |
| 1   | AA    | 988  | G    | N1-C6-O6   | 9.22  | 125.44      | 119.90   |
| 1   | AA    | 404  | G    | N1-C6-O6   | 9.22  | 125.43      | 119.90   |
| 27  | B8    | 647  | G    | N1-C6-O6   | 9.22  | 125.43      | 119.90   |
| 1   | AA    | 1088 | G    | N1-C6-O6   | 9.22  | 125.43      | 119.90   |
| 27  | B8    | 134  | G    | N1-C6-O6   | 9.22  | 125.43      | 119.90   |
| 27  | B8    | 907  | G    | N1-C6-O6   | 9.22  | 125.43      | 119.90   |
| 27  | B8    | 1116 | G    | N1-C6-O6   | 9.22  | 125.43      | 119.90   |
| 1   | AA    | 670  | G    | N1-C6-O6   | 9.21  | 125.43      | 119.90   |
| 27  | B8    | 271  | G    | N1-C6-O6   | 9.21  | 125.43      | 119.90   |
| 27  | B8    | 656  | G    | N1-C6-O6   | 9.21  | 125.43      | 119.90   |
| 27  | B8    | 1106 | G    | C5-C6-O6   | -9.21 | 123.07      | 128.60   |
| 1   | AA    | 962  | C    | O4'-C1'-N1 | 9.21  | 115.57      | 108.20   |
| 27  | B8    | 469  | G    | N1-C6-O6   | 9.21  | 125.43      | 119.90   |
| 27  | B8    | 2752 | C    | O4'-C1'-N1 | 9.21  | 115.57      | 108.20   |
| 27  | B8    | 1491 | G    | N1-C6-O6   | 9.21  | 125.43      | 119.90   |
| 27  | B8    | 2256 | G    | N1-C6-O6   | 9.21  | 125.43      | 119.90   |
| 27  | B8    | 2415 | G    | N1-C6-O6   | 9.21  | 125.43      | 119.90   |
| 26  | B7    | 84   | G    | N1-C6-O6   | 9.20  | 125.42      | 119.90   |
| 27  | B8    | 2002 | G    | N1-C6-O6   | 9.20  | 125.42      | 119.90   |
| 27  | B8    | 2693 | G    | N1-C6-O6   | 9.20  | 125.42      | 119.90   |
| 27  | B8    | 2854 | G    | N1-C6-O6   | 9.20  | 125.42      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1087 | G    | N1-C6-O6   | 9.20  | 125.42      | 119.90   |
| 1   | AA    | 1389 | C    | O4'-C1'-N1 | 9.20  | 115.56      | 108.20   |
| 27  | B8    | 99   | U    | O4'-C1'-N1 | 9.20  | 115.56      | 108.20   |
| 27  | B8    | 1361 | G    | N1-C6-O6   | 9.20  | 125.42      | 119.90   |
| 27  | B8    | 1674 | G    | N1-C6-O6   | 9.19  | 125.42      | 119.90   |
| 1   | AA    | 1415 | G    | N1-C6-O6   | 9.19  | 125.42      | 119.90   |
| 27  | B8    | 2625 | G    | N1-C6-O6   | 9.19  | 125.41      | 119.90   |
| 1   | AA    | 191  | G    | N1-C6-O6   | 9.19  | 125.41      | 119.90   |
| 27  | B8    | 2777 | G    | N1-C6-O6   | 9.19  | 125.41      | 119.90   |
| 1   | AA    | 538  | G    | N1-C6-O6   | 9.19  | 125.41      | 119.90   |
| 27  | B8    | 1377 | G    | N1-C6-O6   | 9.19  | 125.41      | 119.90   |
| 27  | B8    | 1450 | G    | N1-C6-O6   | 9.19  | 125.41      | 119.90   |
| 1   | AA    | 529  | G    | N1-C6-O6   | 9.18  | 125.41      | 119.90   |
| 1   | AA    | 1312 | G    | N1-C6-O6   | 9.18  | 125.41      | 119.90   |
| 27  | B8    | 356  | G    | N1-C6-O6   | 9.18  | 125.41      | 119.90   |
| 27  | B8    | 1842 | G    | N1-C6-O6   | 9.18  | 125.41      | 119.90   |
| 27  | B8    | 1861 | G    | N1-C6-O6   | 9.18  | 125.41      | 119.90   |
| 1   | AA    | 1124 | G    | N1-C6-O6   | 9.18  | 125.41      | 119.90   |
| 1   | AA    | 1337 | G    | N1-C6-O6   | 9.18  | 125.41      | 119.90   |
| 27  | B8    | 1261 | C    | O4'-C1'-N1 | 9.18  | 115.54      | 108.20   |
| 27  | B8    | 2337 | G    | N1-C6-O6   | 9.18  | 125.41      | 119.90   |
| 27  | B8    | 2763 | G    | N1-C6-O6   | 9.18  | 125.41      | 119.90   |
| 27  | B8    | 325  | G    | N1-C6-O6   | 9.17  | 125.40      | 119.90   |
| 27  | B8    | 733  | G    | N1-C6-O6   | 9.17  | 125.40      | 119.90   |
| 1   | AA    | 31   | G    | N1-C6-O6   | 9.17  | 125.40      | 119.90   |
| 27  | B8    | 1062 | G    | N1-C6-O6   | 9.17  | 125.40      | 119.90   |
| 27  | B8    | 1730 | C    | P-O3'-C3'  | 9.17  | 130.70      | 119.70   |
| 27  | B8    | 2246 | G    | N1-C6-O6   | 9.17  | 125.40      | 119.90   |
| 27  | B8    | 2318 | G    | N1-C6-O6   | 9.17  | 125.40      | 119.90   |
| 26  | B7    | 98   | G    | N1-C6-O6   | 9.16  | 125.40      | 119.90   |
| 27  | B8    | 361  | G    | N1-C6-O6   | 9.16  | 125.40      | 119.90   |
| 27  | B8    | 1410 | G    | N1-C6-O6   | 9.16  | 125.40      | 119.90   |
| 1   | AA    | 688  | G    | N1-C6-O6   | 9.16  | 125.40      | 119.90   |
| 27  | B8    | 1280 | G    | N1-C6-O6   | 9.16  | 125.40      | 119.90   |
| 1   | AA    | 550  | G    | N1-C6-O6   | 9.16  | 125.39      | 119.90   |
| 1   | AA    | 1255 | G    | N1-C6-O6   | 9.16  | 125.39      | 119.90   |
| 27  | B8    | 768  | G    | C5-C6-O6   | -9.16 | 123.11      | 128.60   |
| 27  | B8    | 2405 | G    | N1-C6-O6   | 9.16  | 125.39      | 119.90   |
| 27  | B8    | 205  | G    | N1-C6-O6   | 9.15  | 125.39      | 119.90   |
| 27  | B8    | 1210 | G    | N1-C6-O6   | 9.15  | 125.39      | 119.90   |
| 27  | B8    | 178  | G    | N1-C6-O6   | 9.15  | 125.39      | 119.90   |
| 27  | B8    | 204  | A    | N1-C6-N6   | 9.15  | 124.09      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2230 | G    | N1-C6-O6   | 9.15  | 125.39      | 119.90   |
| 27  | B8    | 2367 | G    | N1-C6-O6   | 9.15  | 125.39      | 119.90   |
| 3   | AV    | 10   | G    | N1-C6-O6   | 9.15  | 125.39      | 119.90   |
| 26  | B7    | 64   | G    | N1-C6-O6   | 9.15  | 125.39      | 119.90   |
| 27  | B8    | 175  | G    | N1-C6-O6   | 9.15  | 125.39      | 119.90   |
| 27  | B8    | 179  | C    | O4'-C1'-N1 | 9.15  | 115.52      | 108.20   |
| 27  | B8    | 874  | G    | N1-C6-O6   | 9.15  | 125.39      | 119.90   |
| 27  | B8    | 1371 | G    | N1-C6-O6   | 9.15  | 125.39      | 119.90   |
| 27  | B8    | 2373 | G    | N1-C6-O6   | 9.15  | 125.39      | 119.90   |
| 1   | AA    | 348  | G    | N1-C6-O6   | 9.14  | 125.39      | 119.90   |
| 27  | B8    | 909  | A    | N1-C6-N6   | 9.14  | 124.09      | 118.60   |
| 27  | B8    | 2389 | G    | N1-C6-O6   | 9.14  | 125.39      | 119.90   |
| 27  | B8    | 940  | G    | N1-C6-O6   | 9.14  | 125.39      | 119.90   |
| 1   | AA    | 1272 | G    | N1-C6-O6   | 9.14  | 125.38      | 119.90   |
| 1   | AA    | 1459 | G    | N1-C6-O6   | 9.14  | 125.38      | 119.90   |
| 27  | B8    | 375  | G    | N1-C6-O6   | 9.14  | 125.38      | 119.90   |
| 1   | AA    | 42   | G    | N1-C6-O6   | 9.13  | 125.38      | 119.90   |
| 1   | AA    | 289  | G    | N1-C6-O6   | 9.13  | 125.38      | 119.90   |
| 3   | AV    | 70   | G    | C5-C6-O6   | -9.14 | 123.12      | 128.60   |
| 1   | AA    | 11   | G    | N1-C6-O6   | 9.13  | 125.38      | 119.90   |
| 27  | B8    | 2132 | U    | O4'-C1'-N1 | 9.13  | 115.51      | 108.20   |
| 27  | B8    | 2526 | G    | N1-C6-O6   | 9.13  | 125.38      | 119.90   |
| 27  | B8    | 2869 | G    | N1-C6-O6   | 9.13  | 125.38      | 119.90   |
| 27  | B8    | 847  | U    | O4'-C1'-N1 | 9.13  | 115.50      | 108.20   |
| 1   | AA    | 400  | C    | O4'-C1'-N1 | 9.13  | 115.50      | 108.20   |
| 27  | B8    | 17   | G    | N1-C6-O6   | 9.13  | 125.38      | 119.90   |
| 27  | B8    | 971  | G    | N1-C6-O6   | 9.13  | 125.38      | 119.90   |
| 27  | B8    | 1997 | C    | O4'-C1'-N1 | 9.13  | 115.50      | 108.20   |
| 1   | AA    | 126  | G    | N1-C6-O6   | 9.13  | 125.38      | 119.90   |
| 1   | AA    | 567  | G    | N1-C6-O6   | 9.12  | 125.38      | 119.90   |
| 3   | AV    | 51   | G    | N1-C6-O6   | 9.13  | 125.38      | 119.90   |
| 1   | AA    | 927  | G    | N1-C6-O6   | 9.12  | 125.37      | 119.90   |
| 27  | B8    | 1846 | G    | N1-C6-O6   | 9.12  | 125.37      | 119.90   |
| 1   | AA    | 1187 | G    | N1-C6-O6   | 9.12  | 125.37      | 119.90   |
| 1   | AA    | 588  | G    | N1-C6-O6   | 9.12  | 125.37      | 119.90   |
| 1   | AA    | 1047 | G    | N1-C6-O6   | 9.12  | 125.37      | 119.90   |
| 1   | AA    | 276  | G    | N1-C6-O6   | 9.12  | 125.37      | 119.90   |
| 1   | AA    | 158  | G    | N1-C6-O6   | 9.11  | 125.37      | 119.90   |
| 1   | AA    | 388  | G    | N1-C6-O6   | 9.11  | 125.37      | 119.90   |
| 1   | AA    | 444  | G    | N1-C6-O6   | 9.12  | 125.37      | 119.90   |
| 1   | AA    | 730  | G    | N1-C6-O6   | 9.11  | 125.37      | 119.90   |
| 27  | B8    | 1036 | G    | N1-C6-O6   | 9.11  | 125.37      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1220 | G    | N1-C6-O6   | 9.11  | 125.37      | 119.90   |
| 27  | B8    | 1337 | G    | N1-C6-O6   | 9.11  | 125.37      | 119.90   |
| 1   | AA    | 1033 | G    | C5-C6-O6   | -9.11 | 123.14      | 128.60   |
| 1   | AA    | 1153 | G    | N1-C6-O6   | 9.11  | 125.36      | 119.90   |
| 27  | B8    | 785  | G    | N1-C6-O6   | 9.11  | 125.36      | 119.90   |
| 1   | AA    | 542  | G    | N1-C6-O6   | 9.11  | 125.36      | 119.90   |
| 1   | AA    | 1177 | G    | N1-C6-O6   | 9.11  | 125.36      | 119.90   |
| 26  | B7    | 26   | C    | O4'-C1'-N1 | 9.11  | 115.48      | 108.20   |
| 27  | B8    | 2396 | G    | N1-C6-O6   | 9.11  | 125.36      | 119.90   |
| 1   | AA    | 196  | A    | N1-C6-N6   | 9.10  | 124.06      | 118.60   |
| 27  | B8    | 930  | G    | N1-C6-O6   | 9.10  | 125.36      | 119.90   |
| 27  | B8    | 2277 | G    | N1-C6-O6   | 9.10  | 125.36      | 119.90   |
| 1   | AA    | 146  | G    | N1-C6-O6   | 9.10  | 125.36      | 119.90   |
| 1   | AA    | 570  | G    | C5-C6-O6   | -9.10 | 123.14      | 128.60   |
| 27  | B8    | 283  | G    | N1-C6-O6   | 9.10  | 125.36      | 119.90   |
| 1   | AA    | 1054 | C    | O4'-C1'-N1 | 9.10  | 115.48      | 108.20   |
| 27  | B8    | 1177 | G    | N1-C6-O6   | 9.10  | 125.36      | 119.90   |
| 27  | B8    | 1303 | G    | N1-C6-O6   | 9.10  | 125.36      | 119.90   |
| 27  | B8    | 1751 | U    | O4'-C1'-N1 | 9.10  | 115.48      | 108.20   |
| 1   | AA    | 887  | G    | N1-C6-O6   | 9.09  | 125.36      | 119.90   |
| 1   | AA    | 1186 | G    | N1-C6-O6   | 9.09  | 125.36      | 119.90   |
| 1   | AA    | 1309 | G    | N1-C6-O6   | 9.09  | 125.36      | 119.90   |
| 27  | B8    | 584  | C    | O4'-C1'-N1 | 9.09  | 115.47      | 108.20   |
| 27  | B8    | 841  | G    | N1-C6-O6   | 9.09  | 125.35      | 119.90   |
| 27  | B8    | 2480 | C    | O4'-C1'-N1 | 9.09  | 115.47      | 108.20   |
| 27  | B8    | 2862 | G    | N1-C6-O6   | 9.09  | 125.35      | 119.90   |
| 1   | AA    | 361  | G    | N1-C6-O6   | 9.09  | 125.35      | 119.90   |
| 1   | AA    | 872  | A    | N1-C6-N6   | 9.08  | 124.05      | 118.60   |
| 27  | B8    | 712  | G    | N1-C6-O6   | 9.08  | 125.35      | 119.90   |
| 1   | AA    | 776  | G    | N1-C6-O6   | 9.08  | 125.35      | 119.90   |
| 27  | B8    | 1623 | G    | N1-C6-O6   | 9.08  | 125.35      | 119.90   |
| 27  | B8    | 2488 | G    | N1-C6-O6   | 9.08  | 125.35      | 119.90   |
| 27  | B8    | 1620 | G    | N1-C6-O6   | 9.07  | 125.34      | 119.90   |
| 1   | AA    | 104  | G    | C5-C6-O6   | -9.07 | 123.16      | 128.60   |
| 27  | B8    | 1968 | G    | N1-C6-O6   | 9.07  | 125.34      | 119.90   |
| 1   | AA    | 76   | G    | C5-C6-O6   | -9.07 | 123.16      | 128.60   |
| 27  | B8    | 406  | G    | N1-C6-O6   | 9.07  | 125.34      | 119.90   |
| 27  | B8    | 1139 | G    | N1-C6-O6   | 9.07  | 125.34      | 119.90   |
| 27  | B8    | 1369 | G    | N1-C6-O6   | 9.07  | 125.34      | 119.90   |
| 27  | B8    | 1382 | G    | O4'-C1'-N9 | 9.07  | 115.45      | 108.20   |
| 27  | B8    | 1719 | G    | N1-C6-O6   | 9.07  | 125.34      | 119.90   |
| 27  | B8    | 992  | C    | O4'-C1'-N1 | 9.07  | 115.45      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2569 | G    | N1-C6-O6   | 9.07  | 125.34      | 119.90   |
| 27  | B8    | 2708 | G    | N1-C6-O6   | 9.07  | 125.34      | 119.90   |
| 1   | AA    | 544  | G    | N1-C6-O6   | 9.07  | 125.34      | 119.90   |
| 27  | B8    | 85   | G    | N1-C6-O6   | 9.07  | 125.34      | 119.90   |
| 27  | B8    | 1480 | C    | O4'-C1'-N1 | 9.07  | 115.45      | 108.20   |
| 1   | AA    | 597  | G    | N1-C6-O6   | 9.06  | 125.34      | 119.90   |
| 1   | AA    | 1299 | A    | N1-C6-N6   | 9.06  | 124.04      | 118.60   |
| 27  | B8    | 2100 | G    | N1-C6-O6   | 9.06  | 125.34      | 119.90   |
| 1   | AA    | 442  | G    | N1-C6-O6   | 9.06  | 125.34      | 119.90   |
| 1   | AA    | 540  | G    | N1-C6-O6   | 9.06  | 125.34      | 119.90   |
| 1   | AA    | 987  | G    | N1-C6-O6   | 9.06  | 125.34      | 119.90   |
| 27  | B8    | 2190 | G    | N1-C6-O6   | 9.06  | 125.34      | 119.90   |
| 27  | B8    | 2691 | C    | O4'-C1'-N1 | 9.06  | 115.45      | 108.20   |
| 27  | B8    | 771  | G    | N1-C6-O6   | 9.06  | 125.34      | 119.90   |
| 27  | B8    | 1696 | G    | N1-C6-O6   | 9.06  | 125.34      | 119.90   |
| 1   | AA    | 100  | G    | N1-C6-O6   | 9.06  | 125.34      | 119.90   |
| 27  | B8    | 2474 | U    | O4'-C1'-N1 | 9.06  | 115.45      | 108.20   |
| 27  | B8    | 2864 | G    | N1-C6-O6   | 9.06  | 125.34      | 119.90   |
| 1   | AA    | 1185 | G    | N1-C6-O6   | 9.06  | 125.33      | 119.90   |
| 1   | AA    | 1401 | G    | N1-C6-O6   | 9.06  | 125.33      | 119.90   |
| 1   | AA    | 1486 | G    | C5-C6-O6   | -9.06 | 123.17      | 128.60   |
| 27  | B8    | 110  | G    | N1-C6-O6   | 9.06  | 125.33      | 119.90   |
| 27  | B8    | 2004 | G    | N1-C6-O6   | 9.06  | 125.33      | 119.90   |
| 1   | AA    | 1258 | G    | N1-C6-O6   | 9.06  | 125.33      | 119.90   |
| 1   | AA    | 830  | G    | N1-C6-O6   | 9.05  | 125.33      | 119.90   |
| 27  | B8    | 327  | G    | N1-C6-O6   | 9.05  | 125.33      | 119.90   |
| 27  | B8    | 1128 | G    | N1-C6-O6   | 9.05  | 125.33      | 119.90   |
| 27  | B8    | 1407 | G    | N1-C6-O6   | 9.05  | 125.33      | 119.90   |
| 27  | B8    | 1740 | G    | N1-C6-O6   | 9.05  | 125.33      | 119.90   |
| 1   | AA    | 46   | G    | N1-C6-O6   | 9.05  | 125.33      | 119.90   |
| 1   | AA    | 1104 | G    | N1-C6-O6   | 9.05  | 125.33      | 119.90   |
| 27  | B8    | 1849 | G    | N1-C6-O6   | 9.05  | 125.33      | 119.90   |
| 27  | B8    | 692  | C    | O4'-C1'-N1 | 9.05  | 115.44      | 108.20   |
| 27  | B8    | 1449 | G    | N1-C6-O6   | 9.05  | 125.33      | 119.90   |
| 1   | AA    | 848  | C    | O4'-C1'-N1 | 9.05  | 115.44      | 108.20   |
| 1   | AA    | 1270 | G    | N1-C6-O6   | 9.05  | 125.33      | 119.90   |
| 27  | B8    | 2382 | G    | N1-C6-O6   | 9.05  | 125.33      | 119.90   |
| 27  | B8    | 124  | G    | N1-C6-O6   | 9.04  | 125.33      | 119.90   |
| 27  | B8    | 763  | G    | N1-C6-O6   | 9.04  | 125.33      | 119.90   |
| 27  | B8    | 1149 | G    | N1-C6-O6   | 9.04  | 125.33      | 119.90   |
| 1   | AA    | 41   | G    | N1-C6-O6   | 9.04  | 125.33      | 119.90   |
| 27  | B8    | 1663 | G    | N1-C6-O6   | 9.04  | 125.33      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 1   | AA    | 474  | G    | N1-C6-O6   | 9.04 | 125.32      | 119.90   |
| 1   | AA    | 799  | G    | N1-C6-O6   | 9.04 | 125.32      | 119.90   |
| 27  | B8    | 301  | G    | N1-C6-O6   | 9.04 | 125.32      | 119.90   |
| 27  | B8    | 728  | G    | N1-C6-O6   | 9.04 | 125.32      | 119.90   |
| 27  | B8    | 1633 | G    | N1-C6-O6   | 9.04 | 125.32      | 119.90   |
| 1   | AA    | 721  | G    | N1-C6-O6   | 9.04 | 125.32      | 119.90   |
| 27  | B8    | 776  | G    | N1-C6-O6   | 9.04 | 125.32      | 119.90   |
| 27  | B8    | 1266 | G    | N1-C6-O6   | 9.04 | 125.32      | 119.90   |
| 27  | B8    | 1863 | G    | N1-C6-O6   | 9.04 | 125.32      | 119.90   |
| 27  | B8    | 1972 | G    | N1-C6-O6   | 9.04 | 125.32      | 119.90   |
| 27  | B8    | 708  | G    | N1-C6-O6   | 9.03 | 125.32      | 119.90   |
| 27  | B8    | 1380 | G    | N1-C6-O6   | 9.03 | 125.32      | 119.90   |
| 27  | B8    | 1125 | G    | N1-C6-O6   | 9.03 | 125.32      | 119.90   |
| 27  | B8    | 1225 | G    | N1-C6-O6   | 9.03 | 125.32      | 119.90   |
| 27  | B8    | 27   | G    | N1-C6-O6   | 9.03 | 125.32      | 119.90   |
| 27  | B8    | 1750 | G    | N1-C6-O6   | 9.03 | 125.32      | 119.90   |
| 1   | AA    | 1370 | G    | N1-C6-O6   | 9.03 | 125.32      | 119.90   |
| 27  | B8    | 2216 | G    | N1-C6-O6   | 9.03 | 125.32      | 119.90   |
| 1   | AA    | 1241 | G    | N1-C6-O6   | 9.03 | 125.32      | 119.90   |
| 27  | B8    | 119  | A    | N1-C6-N6   | 9.03 | 124.02      | 118.60   |
| 1   | AA    | 251  | G    | N1-C6-O6   | 9.02 | 125.31      | 119.90   |
| 1   | AA    | 1244 | G    | N1-C6-O6   | 9.02 | 125.31      | 119.90   |
| 1   | AA    | 391  | G    | N1-C6-O6   | 9.02 | 125.31      | 119.90   |
| 1   | AA    | 748  | G    | N1-C6-O6   | 9.02 | 125.31      | 119.90   |
| 1   | AA    | 1141 | C    | O4'-C1'-N1 | 9.02 | 115.42      | 108.20   |
| 27  | B8    | 302  | C    | O4'-C1'-N1 | 9.02 | 115.42      | 108.20   |
| 27  | B8    | 498  | G    | N1-C6-O6   | 9.02 | 125.31      | 119.90   |
| 27  | B8    | 2770 | G    | N1-C6-O6   | 9.02 | 125.31      | 119.90   |
| 27  | B8    | 1592 | C    | O4'-C1'-N1 | 9.02 | 115.42      | 108.20   |
| 27  | B8    | 780  | G    | N1-C6-O6   | 9.02 | 125.31      | 119.90   |
| 1   | AA    | 64   | G    | N1-C6-O6   | 9.02 | 125.31      | 119.90   |
| 27  | B8    | 1332 | G    | N1-C6-O6   | 9.02 | 125.31      | 119.90   |
| 27  | B8    | 1516 | G    | N1-C6-O6   | 9.01 | 125.31      | 119.90   |
| 27  | B8    | 2223 | G    | N1-C6-O6   | 9.01 | 125.31      | 119.90   |
| 27  | B8    | 2280 | G    | N1-C6-O6   | 9.01 | 125.31      | 119.90   |
| 27  | B8    | 612  | G    | N1-C6-O6   | 9.01 | 125.31      | 119.90   |
| 27  | B8    | 1291 | C    | O4'-C1'-N1 | 9.01 | 115.41      | 108.20   |
| 27  | B8    | 1684 | G    | N1-C6-O6   | 9.01 | 125.31      | 119.90   |
| 27  | B8    | 2525 | G    | N1-C6-O6   | 9.01 | 125.31      | 119.90   |
| 27  | B8    | 92   | U    | O4'-C1'-N1 | 9.01 | 115.41      | 108.20   |
| 27  | B8    | 822  | G    | N1-C6-O6   | 9.01 | 125.31      | 119.90   |
| 27  | B8    | 1164 | C    | O4'-C1'-N1 | 9.01 | 115.41      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 247  | G    | N1-C6-O6   | 9.01  | 125.31      | 119.90   |
| 27  | B8    | 834  | G    | N1-C6-O6   | 9.01  | 125.31      | 119.90   |
| 1   | AA    | 292  | G    | N1-C6-O6   | 9.01  | 125.31      | 119.90   |
| 1   | AA    | 144  | G    | N1-C6-O6   | 9.01  | 125.30      | 119.90   |
| 1   | AA    | 362  | G    | N1-C6-O6   | 9.00  | 125.30      | 119.90   |
| 1   | AA    | 212  | G    | N1-C6-O6   | 9.00  | 125.30      | 119.90   |
| 1   | AA    | 421  | U    | O4'-C1'-N1 | 9.00  | 115.40      | 108.20   |
| 1   | AA    | 445  | G    | N1-C6-O6   | 9.00  | 125.30      | 119.90   |
| 1   | AA    | 993  | G    | N1-C6-O6   | 9.00  | 125.30      | 119.90   |
| 27  | B8    | 1404 | C    | O4'-C1'-N1 | 9.00  | 115.40      | 108.20   |
| 27  | B8    | 2458 | G    | N1-C6-O6   | 9.00  | 125.30      | 119.90   |
| 27  | B8    | 2890 | G    | N1-C6-O6   | 9.00  | 125.30      | 119.90   |
| 27  | B8    | 1606 | C    | O4'-C1'-N1 | 9.00  | 115.40      | 108.20   |
| 27  | B8    | 2485 | G    | C5-C6-O6   | -9.00 | 123.20      | 128.60   |
| 27  | B8    | 2061 | G    | N1-C6-O6   | 9.00  | 125.30      | 119.90   |
| 27  | B8    | 2747 | G    | C5-C6-O6   | -9.00 | 123.20      | 128.60   |
| 27  | B8    | 23   | G    | N1-C6-O6   | 9.00  | 125.30      | 119.90   |
| 1   | AA    | 859  | G    | N1-C6-O6   | 8.99  | 125.30      | 119.90   |
| 1   | AA    | 1253 | G    | N1-C6-O6   | 8.99  | 125.30      | 119.90   |
| 1   | AA    | 1460 | C    | O4'-C1'-N1 | 8.99  | 115.39      | 108.20   |
| 27  | B8    | 298  | G    | N1-C6-O6   | 8.99  | 125.30      | 119.90   |
| 27  | B8    | 551  | G    | N1-C6-O6   | 8.99  | 125.30      | 119.90   |
| 27  | B8    | 775  | G    | N1-C6-O6   | 8.99  | 125.30      | 119.90   |
| 27  | B8    | 1588 | G    | N1-C6-O6   | 8.99  | 125.30      | 119.90   |
| 27  | B8    | 2218 | G    | N1-C6-O6   | 8.99  | 125.30      | 119.90   |
| 27  | B8    | 307  | G    | N1-C6-O6   | 8.99  | 125.30      | 119.90   |
| 1   | AA    | 324  | G    | N1-C6-O6   | 8.99  | 125.29      | 119.90   |
| 27  | B8    | 411  | G    | N1-C6-O6   | 8.99  | 125.29      | 119.90   |
| 27  | B8    | 1452 | G    | N1-C6-O6   | 8.99  | 125.30      | 119.90   |
| 27  | B8    | 2831 | G    | N1-C6-O6   | 8.99  | 125.29      | 119.90   |
| 27  | B8    | 1828 | G    | N1-C6-O6   | 8.99  | 125.29      | 119.90   |
| 27  | B8    | 2293 | G    | N1-C6-O6   | 8.99  | 125.29      | 119.90   |
| 1   | AA    | 1146 | A    | N1-C6-N6   | 8.99  | 123.99      | 118.60   |
| 1   | AA    | 82   | G    | N1-C6-O6   | 8.99  | 125.29      | 119.90   |
| 1   | AA    | 1296 | C    | O4'-C1'-N1 | 8.99  | 115.39      | 108.20   |
| 27  | B8    | 303  | G    | N1-C6-O6   | 8.99  | 125.29      | 119.90   |
| 27  | B8    | 630  | G    | N1-C6-O6   | 8.99  | 125.29      | 119.90   |
| 27  | B8    | 1195 | G    | N1-C6-O6   | 8.99  | 125.29      | 119.90   |
| 27  | B8    | 2038 | G    | N1-C6-O6   | 8.99  | 125.29      | 119.90   |
| 27  | B8    | 1212 | G    | N1-C6-O6   | 8.98  | 125.29      | 119.90   |
| 1   | AA    | 928  | G    | N1-C6-O6   | 8.98  | 125.29      | 119.90   |
| 1   | AA    | 226  | G    | N1-C6-O6   | 8.98  | 125.29      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 682  | G    | N1-C6-O6   | 8.98  | 125.29      | 119.90   |
| 1   | AA    | 971  | G    | N1-C6-O6   | 8.98  | 125.29      | 119.90   |
| 1   | AA    | 1084 | G    | N1-C6-O6   | 8.98  | 125.29      | 119.90   |
| 27  | B8    | 277  | G    | N1-C6-O6   | 8.98  | 125.29      | 119.90   |
| 27  | B8    | 2303 | G    | N1-C6-O6   | 8.98  | 125.29      | 119.90   |
| 1   | AA    | 220  | G    | N1-C6-O6   | 8.98  | 125.29      | 119.90   |
| 1   | AA    | 527  | G    | N1-C6-O6   | 8.98  | 125.29      | 119.90   |
| 27  | B8    | 188  | G    | N1-C6-O6   | 8.98  | 125.29      | 119.90   |
| 3   | AV    | 15   | G    | N1-C6-O6   | 8.98  | 125.29      | 119.90   |
| 1   | AA    | 1304 | G    | N1-C6-O6   | 8.97  | 125.28      | 119.90   |
| 27  | B8    | 537  | G    | N1-C6-O6   | 8.97  | 125.28      | 119.90   |
| 27  | B8    | 2661 | G    | N1-C6-O6   | 8.97  | 125.28      | 119.90   |
| 27  | B8    | 862  | G    | N1-C6-O6   | 8.97  | 125.28      | 119.90   |
| 27  | B8    | 1150 | C    | O4'-C1'-N1 | 8.97  | 115.38      | 108.20   |
| 1   | AA    | 1530 | G    | N1-C6-O6   | 8.97  | 125.28      | 119.90   |
| 27  | B8    | 1897 | G    | N1-C6-O6   | 8.97  | 125.28      | 119.90   |
| 27  | B8    | 359  | G    | N1-C6-O6   | 8.97  | 125.28      | 119.90   |
| 27  | B8    | 2121 | G    | N1-C6-O6   | 8.97  | 125.28      | 119.90   |
| 27  | B8    | 2732 | G    | C5-C6-O6   | -8.97 | 123.22      | 128.60   |
| 27  | B8    | 7    | G    | N1-C6-O6   | 8.97  | 125.28      | 119.90   |
| 27  | B8    | 942  | G    | N1-C6-O6   | 8.96  | 125.28      | 119.90   |
| 27  | B8    | 1324 | G    | N1-C6-O6   | 8.96  | 125.28      | 119.90   |
| 27  | B8    | 1436 | G    | N1-C6-O6   | 8.96  | 125.28      | 119.90   |
| 27  | B8    | 2578 | G    | N1-C6-O6   | 8.96  | 125.28      | 119.90   |
| 1   | AA    | 1276 | G    | N1-C6-O6   | 8.96  | 125.28      | 119.90   |
| 1   | AA    | 803  | G    | N1-C6-O6   | 8.96  | 125.27      | 119.90   |
| 27  | B8    | 57   | C    | O4'-C1'-N1 | 8.96  | 115.37      | 108.20   |
| 27  | B8    | 923  | G    | N1-C6-O6   | 8.96  | 125.28      | 119.90   |
| 27  | B8    | 463  | G    | N1-C6-O6   | 8.96  | 125.27      | 119.90   |
| 27  | B8    | 997  | G    | N1-C6-O6   | 8.96  | 125.27      | 119.90   |
| 27  | B8    | 1333 | G    | P-O3'-C3'  | 8.96  | 130.45      | 119.70   |
| 27  | B8    | 1381 | G    | C5-C6-O6   | -8.96 | 123.22      | 128.60   |
| 1   | AA    | 505  | G    | N1-C6-O6   | 8.96  | 125.27      | 119.90   |
| 27  | B8    | 1537 | G    | N1-C6-O6   | 8.96  | 125.27      | 119.90   |
| 27  | B8    | 31   | C    | O4'-C1'-N1 | 8.95  | 115.36      | 108.20   |
| 27  | B8    | 1475 | G    | N1-C6-O6   | 8.95  | 125.27      | 119.90   |
| 27  | B8    | 1514 | G    | N1-C6-O6   | 8.95  | 125.27      | 119.90   |
| 27  | B8    | 2844 | G    | N1-C6-O6   | 8.95  | 125.27      | 119.90   |
| 1   | AA    | 147  | G    | C5-C6-O6   | -8.95 | 123.23      | 128.60   |
| 1   | AA    | 773  | G    | N1-C6-O6   | 8.95  | 125.27      | 119.90   |
| 27  | B8    | 1445 | G    | C5-C6-O6   | -8.95 | 123.23      | 128.60   |
| 27  | B8    | 1767 | G    | N1-C6-O6   | 8.95  | 125.27      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1697 | G    | N1-C6-O6   | 8.95  | 125.27      | 119.90   |
| 27  | B8    | 1063 | G    | N1-C6-O6   | 8.95  | 125.27      | 119.90   |
| 1   | AA    | 1473 | G    | N1-C6-O6   | 8.95  | 125.27      | 119.90   |
| 27  | B8    | 2857 | G    | N1-C6-O6   | 8.94  | 125.27      | 119.90   |
| 27  | B8    | 2877 | G    | N1-C6-O6   | 8.95  | 125.27      | 119.90   |
| 1   | AA    | 833  | G    | N1-C6-O6   | 8.94  | 125.27      | 119.90   |
| 27  | B8    | 549  | G    | N1-C6-O6   | 8.94  | 125.27      | 119.90   |
| 1   | AA    | 498  | A    | N1-C6-N6   | 8.94  | 123.96      | 118.60   |
| 27  | B8    | 2697 | G    | N1-C6-O6   | 8.94  | 125.26      | 119.90   |
| 27  | B8    | 916  | G    | C5-C6-O6   | -8.94 | 123.24      | 128.60   |
| 27  | B8    | 2867 | G    | N1-C6-O6   | 8.94  | 125.26      | 119.90   |
| 1   | AA    | 1207 | G    | N1-C6-O6   | 8.94  | 125.26      | 119.90   |
| 27  | B8    | 618  | G    | N1-C6-O6   | 8.94  | 125.26      | 119.90   |
| 27  | B8    | 2717 | C    | O4'-C1'-N1 | 8.94  | 115.35      | 108.20   |
| 27  | B8    | 736  | C    | O4'-C1'-N1 | 8.94  | 115.35      | 108.20   |
| 27  | B8    | 1166 | G    | N1-C6-O6   | 8.94  | 125.26      | 119.90   |
| 1   | AA    | 237  | G    | N1-C6-O6   | 8.93  | 125.26      | 119.90   |
| 1   | AA    | 354  | G    | N1-C6-O6   | 8.93  | 125.26      | 119.90   |
| 1   | AA    | 447  | G    | N1-C6-O6   | 8.93  | 125.26      | 119.90   |
| 27  | B8    | 1811 | G    | N1-C6-O6   | 8.93  | 125.26      | 119.90   |
| 1   | AA    | 944  | G    | N1-C6-O6   | 8.93  | 125.26      | 119.90   |
| 1   | AA    | 1504 | G    | N1-C6-O6   | 8.93  | 125.26      | 119.90   |
| 3   | AV    | 73   | G    | N1-C6-O6   | 8.93  | 125.26      | 119.90   |
| 27  | B8    | 2645 | G    | N1-C6-O6   | 8.93  | 125.26      | 119.90   |
| 1   | AA    | 710  | G    | N1-C6-O6   | 8.93  | 125.26      | 119.90   |
| 27  | B8    | 518  | G    | N1-C6-O6   | 8.93  | 125.26      | 119.90   |
| 27  | B8    | 1002 | G    | N1-C6-O6   | 8.93  | 125.26      | 119.90   |
| 27  | B8    | 1160 | G    | N1-C6-O6   | 8.93  | 125.26      | 119.90   |
| 27  | B8    | 2201 | G    | C5-C6-O6   | -8.93 | 123.24      | 128.60   |
| 27  | B8    | 24   | G    | N1-C6-O6   | 8.93  | 125.26      | 119.90   |
| 27  | B8    | 1959 | G    | N1-C6-O6   | 8.93  | 125.26      | 119.90   |
| 27  | B8    | 2773 | C    | O4'-C1'-N1 | 8.93  | 115.34      | 108.20   |
| 27  | B8    | 2168 | G    | N1-C6-O6   | 8.92  | 125.25      | 119.90   |
| 27  | B8    | 2730 | C    | O4'-C1'-N1 | 8.92  | 115.34      | 108.20   |
| 27  | B8    | 2806 | C    | O4'-C1'-N1 | 8.92  | 115.34      | 108.20   |
| 1   | AA    | 703  | G    | N1-C6-O6   | 8.92  | 125.25      | 119.90   |
| 27  | B8    | 565  | C    | O4'-C1'-N1 | 8.92  | 115.34      | 108.20   |
| 27  | B8    | 831  | G    | N1-C6-O6   | 8.92  | 125.25      | 119.90   |
| 27  | B8    | 1442 | U    | O4'-C1'-N1 | 8.92  | 115.33      | 108.20   |
| 27  | B8    | 2436 | G    | N1-C6-O6   | 8.92  | 125.25      | 119.90   |
| 27  | B8    | 433  | C    | O4'-C1'-N1 | 8.92  | 115.33      | 108.20   |
| 27  | B8    | 1334 | G    | N1-C6-O6   | 8.92  | 125.25      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1568 | G    | N1-C6-O6   | 8.92  | 125.25      | 119.90   |
| 27  | B8    | 1733 | G    | N1-C6-O6   | 8.92  | 125.25      | 119.90   |
| 27  | B8    | 2892 | G    | N1-C6-O6   | 8.92  | 125.25      | 119.90   |
| 27  | B8    | 1157 | G    | C5-C6-O6   | -8.91 | 123.25      | 128.60   |
| 27  | B8    | 1248 | G    | N1-C6-O6   | 8.91  | 125.25      | 119.90   |
| 27  | B8    | 1567 | G    | N1-C6-O6   | 8.91  | 125.25      | 119.90   |
| 27  | B8    | 1604 | C    | O4'-C1'-N1 | 8.91  | 115.33      | 108.20   |
| 26  | B7    | 51   | G    | N1-C6-O6   | 8.91  | 125.25      | 119.90   |
| 27  | B8    | 969  | G    | N1-C6-O6   | 8.91  | 125.24      | 119.90   |
| 1   | AA    | 490  | C    | O4'-C1'-N1 | 8.90  | 115.32      | 108.20   |
| 1   | AA    | 1442 | G    | N1-C6-O6   | 8.90  | 125.24      | 119.90   |
| 3   | AV    | 25   | G    | N1-C6-O6   | 8.90  | 125.24      | 119.90   |
| 1   | AA    | 115  | G    | C5-C6-O6   | -8.90 | 123.26      | 128.60   |
| 27  | B8    | 295  | G    | N1-C6-O6   | 8.90  | 125.24      | 119.90   |
| 27  | B8    | 2409 | G    | C5-C6-O6   | -8.90 | 123.26      | 128.60   |
| 1   | AA    | 558  | G    | N1-C6-O6   | 8.90  | 125.24      | 119.90   |
| 27  | B8    | 136  | G    | N1-C6-O6   | 8.90  | 125.24      | 119.90   |
| 27  | B8    | 1577 | C    | O4'-C1'-N1 | 8.90  | 115.32      | 108.20   |
| 1   | AA    | 1392 | G    | C5-C6-O6   | -8.90 | 123.26      | 128.60   |
| 27  | B8    | 1555 | G    | N1-C6-O6   | 8.90  | 125.24      | 119.90   |
| 26  | B7    | 79   | G    | N1-C6-O6   | 8.90  | 125.24      | 119.90   |
| 27  | B8    | 1425 | G    | N1-C6-O6   | 8.90  | 125.24      | 119.90   |
| 1   | AA    | 127  | G    | N1-C6-O6   | 8.89  | 125.24      | 119.90   |
| 3   | AV    | 2    | G    | N1-C6-O6   | 8.89  | 125.24      | 119.90   |
| 27  | B8    | 60   | G    | N1-C6-O6   | 8.89  | 125.24      | 119.90   |
| 27  | B8    | 1299 | G    | N1-C6-O6   | 8.89  | 125.24      | 119.90   |
| 1   | AA    | 331  | G    | N1-C6-O6   | 8.89  | 125.23      | 119.90   |
| 27  | B8    | 232  | G    | N1-C6-O6   | 8.89  | 125.23      | 119.90   |
| 27  | B8    | 864  | G    | C5-C6-O6   | -8.89 | 123.27      | 128.60   |
| 27  | B8    | 2494 | G    | N1-C6-O6   | 8.89  | 125.23      | 119.90   |
| 1   | AA    | 1139 | G    | N1-C6-O6   | 8.89  | 125.23      | 119.90   |
| 1   | AA    | 433  | G    | N1-C6-O6   | 8.89  | 125.23      | 119.90   |
| 27  | B8    | 926  | G    | N1-C6-O6   | 8.89  | 125.23      | 119.90   |
| 1   | AA    | 742  | G    | N1-C6-O6   | 8.88  | 125.23      | 119.90   |
| 26  | B7    | 27   | C    | O4'-C1'-N1 | 8.88  | 115.31      | 108.20   |
| 27  | B8    | 2894 | G    | C5-C6-O6   | -8.89 | 123.27      | 128.60   |
| 1   | AA    | 94   | G    | N1-C6-O6   | 8.88  | 125.23      | 119.90   |
| 27  | B8    | 389  | G    | N1-C6-O6   | 8.88  | 125.23      | 119.90   |
| 27  | B8    | 648  | G    | N1-C6-O6   | 8.88  | 125.23      | 119.90   |
| 27  | B8    | 1047 | G    | N1-C6-O6   | 8.88  | 125.23      | 119.90   |
| 27  | B8    | 2186 | G    | N1-C6-O6   | 8.88  | 125.23      | 119.90   |
| 27  | B8    | 553  | G    | N1-C6-O6   | 8.88  | 125.23      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1368 | G    | N1-C6-O6   | 8.88  | 125.23      | 119.90   |
| 1   | AA    | 1120 | C    | O4'-C1'-N1 | 8.88  | 115.30      | 108.20   |
| 27  | B8    | 1814 | G    | N1-C6-O6   | 8.88  | 125.23      | 119.90   |
| 1   | AA    | 69   | G    | N1-C6-O6   | 8.88  | 125.23      | 119.90   |
| 1   | AA    | 399  | G    | N1-C6-O6   | 8.88  | 125.22      | 119.90   |
| 1   | AA    | 1190 | G    | N1-C6-O6   | 8.88  | 125.22      | 119.90   |
| 26  | B7    | 100  | G    | N1-C6-O6   | 8.87  | 125.22      | 119.90   |
| 27  | B8    | 1223 | G    | N1-C6-O6   | 8.87  | 125.22      | 119.90   |
| 27  | B8    | 2116 | G    | N1-C6-O6   | 8.88  | 125.22      | 119.90   |
| 1   | AA    | 1290 | G    | C5-C6-O6   | -8.87 | 123.28      | 128.60   |
| 26  | B7    | 96   | G    | N1-C6-O6   | 8.87  | 125.22      | 119.90   |
| 27  | B8    | 401  | A    | O4'-C1'-N9 | 8.87  | 115.30      | 108.20   |
| 27  | B8    | 653  | U    | O4'-C1'-N1 | 8.87  | 115.30      | 108.20   |
| 27  | B8    | 1681 | G    | N1-C6-O6   | 8.87  | 125.22      | 119.90   |
| 27  | B8    | 1421 | G    | C5-C6-O6   | -8.87 | 123.28      | 128.60   |
| 1   | AA    | 973  | G    | C5-C6-O6   | -8.87 | 123.28      | 128.60   |
| 1   | AA    | 1439 | G    | N1-C6-O6   | 8.87  | 125.22      | 119.90   |
| 27  | B8    | 1228 | G    | N1-C6-O6   | 8.87  | 125.22      | 119.90   |
| 27  | B8    | 2724 | U    | O4'-C1'-N1 | 8.87  | 115.30      | 108.20   |
| 27  | B8    | 1776 | G    | N1-C6-O6   | 8.87  | 125.22      | 119.90   |
| 27  | B8    | 1824 | G    | N1-C6-O6   | 8.87  | 125.22      | 119.90   |
| 27  | B8    | 2901 | C    | O4'-C1'-N1 | 8.87  | 115.29      | 108.20   |
| 1   | AA    | 446  | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |
| 1   | AA    | 809  | G    | N1-C6-O6   | 8.87  | 125.22      | 119.90   |
| 1   | AA    | 1426 | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |
| 27  | B8    | 254  | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |
| 27  | B8    | 885  | C    | O4'-C1'-N1 | 8.86  | 115.29      | 108.20   |
| 27  | B8    | 1631 | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |
| 27  | B8    | 2028 | U    | O4'-C1'-N1 | 8.86  | 115.29      | 108.20   |
| 27  | B8    | 2538 | C    | O4'-C1'-N1 | 8.87  | 115.29      | 108.20   |
| 1   | AA    | 771  | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |
| 1   | AA    | 775  | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |
| 1   | AA    | 1305 | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |
| 1   | AA    | 1365 | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |
| 27  | B8    | 1945 | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |
| 26  | B7    | 107  | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |
| 27  | B8    | 15   | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |
| 27  | B8    | 2282 | G    | P-O3'-C3'  | 8.86  | 130.33      | 119.70   |
| 1   | AA    | 369  | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |
| 27  | B8    | 458  | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |
| 27  | B8    | 467  | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |
| 27  | B8    | 622  | G    | N1-C6-O6   | 8.86  | 125.22      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 530  | G    | N1-C6-O6   | 8.86  | 125.21      | 119.90   |
| 1   | AA    | 285  | C    | O4'-C1'-N1 | 8.86  | 115.28      | 108.20   |
| 1   | AA    | 976  | G    | N1-C6-O6   | 8.86  | 125.21      | 119.90   |
| 3   | AV    | 30   | G    | N1-C6-O6   | 8.86  | 125.21      | 119.90   |
| 27  | B8    | 1524 | G    | N1-C6-O6   | 8.86  | 125.21      | 119.90   |
| 27  | B8    | 1527 | G    | N1-C6-O6   | 8.86  | 125.21      | 119.90   |
| 1   | AA    | 847  | G    | N1-C6-O6   | 8.85  | 125.21      | 119.90   |
| 27  | B8    | 169  | G    | N1-C6-O6   | 8.85  | 125.21      | 119.90   |
| 27  | B8    | 1152 | C    | O4'-C1'-N1 | 8.85  | 115.28      | 108.20   |
| 27  | B8    | 1721 | G    | N1-C6-O6   | 8.85  | 125.21      | 119.90   |
| 1   | AA    | 1064 | G    | N1-C6-O6   | 8.85  | 125.21      | 119.90   |
| 27  | B8    | 859  | G    | N1-C6-O6   | 8.85  | 125.21      | 119.90   |
| 27  | B8    | 1405 | U    | O4'-C1'-N1 | 8.85  | 115.28      | 108.20   |
| 27  | B8    | 1581 | G    | N1-C6-O6   | 8.85  | 125.21      | 119.90   |
| 27  | B8    | 1795 | C    | O4'-C1'-N1 | 8.85  | 115.28      | 108.20   |
| 27  | B8    | 1933 | G    | N1-C6-O6   | 8.85  | 125.21      | 119.90   |
| 1   | AA    | 79   | G    | N1-C6-O6   | 8.85  | 125.21      | 119.90   |
| 27  | B8    | 45   | G    | N1-C6-O6   | 8.85  | 125.21      | 119.90   |
| 1   | AA    | 880  | C    | O4'-C1'-N1 | 8.84  | 115.28      | 108.20   |
| 27  | B8    | 2286 | G    | N1-C6-O6   | 8.84  | 125.21      | 119.90   |
| 27  | B8    | 2371 | G    | N1-C6-O6   | 8.84  | 125.21      | 119.90   |
| 1   | AA    | 424  | G    | C5-C6-O6   | -8.84 | 123.30      | 128.60   |
| 1   | AA    | 1108 | G    | N1-C6-O6   | 8.84  | 125.20      | 119.90   |
| 27  | B8    | 263  | G    | N1-C6-O6   | 8.84  | 125.20      | 119.90   |
| 27  | B8    | 524  | G    | C5-C6-O6   | -8.84 | 123.30      | 128.60   |
| 27  | B8    | 620  | G    | N1-C6-O6   | 8.84  | 125.20      | 119.90   |
| 27  | B8    | 1994 | C    | O4'-C1'-N1 | 8.84  | 115.27      | 108.20   |
| 1   | AA    | 423  | G    | N1-C6-O6   | 8.84  | 125.20      | 119.90   |
| 27  | B8    | 1875 | G    | N1-C6-O6   | 8.84  | 125.20      | 119.90   |
| 27  | B8    | 2529 | G    | N1-C6-O6   | 8.84  | 125.20      | 119.90   |
| 27  | B8    | 2795 | C    | O4'-C1'-N1 | 8.84  | 115.27      | 108.20   |
| 1   | AA    | 646  | G    | N1-C6-O6   | 8.83  | 125.20      | 119.90   |
| 1   | AA    | 750  | C    | O4'-C1'-N1 | 8.83  | 115.27      | 108.20   |
| 27  | B8    | 1753 | G    | N1-C6-O6   | 8.83  | 125.20      | 119.90   |
| 27  | B8    | 2536 | G    | N1-C6-O6   | 8.83  | 125.20      | 119.90   |
| 27  | B8    | 1283 | G    | N1-C6-O6   | 8.83  | 125.20      | 119.90   |
| 27  | B8    | 2120 | G    | N1-C6-O6   | 8.83  | 125.20      | 119.90   |
| 27  | B8    | 2843 | G    | N1-C6-O6   | 8.83  | 125.20      | 119.90   |
| 1   | AA    | 674  | G    | C5-C6-O6   | -8.83 | 123.30      | 128.60   |
| 27  | B8    | 1903 | G    | N1-C6-O6   | 8.83  | 125.20      | 119.90   |
| 27  | B8    | 2549 | G    | N1-C6-O6   | 8.83  | 125.20      | 119.90   |
| 27  | B8    | 1374 | G    | N1-C6-O6   | 8.83  | 125.20      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1884 | G    | N1-C6-O6   | 8.83  | 125.19      | 119.90   |
| 1   | AA    | 1057 | G    | N1-C6-O6   | 8.82  | 125.19      | 119.90   |
| 27  | B8    | 86   | G    | C5-C6-O6   | -8.82 | 123.31      | 128.60   |
| 27  | B8    | 2853 | C    | O4'-C1'-N1 | 8.82  | 115.26      | 108.20   |
| 1   | AA    | 963  | G    | N1-C6-O6   | 8.82  | 125.19      | 119.90   |
| 26  | B7    | 113  | C    | O4'-C1'-N1 | 8.82  | 115.26      | 108.20   |
| 27  | B8    | 48   | G    | N1-C6-O6   | 8.82  | 125.19      | 119.90   |
| 27  | B8    | 51   | G    | N1-C6-O6   | 8.82  | 125.19      | 119.90   |
| 27  | B8    | 473  | G    | N1-C6-O6   | 8.82  | 125.19      | 119.90   |
| 27  | B8    | 2357 | G    | N1-C6-O6   | 8.82  | 125.19      | 119.90   |
| 27  | B8    | 2360 | G    | N1-C6-O6   | 8.82  | 125.19      | 119.90   |
| 1   | AA    | 378  | G    | N1-C6-O6   | 8.82  | 125.19      | 119.90   |
| 1   | AA    | 869  | G    | N1-C6-O6   | 8.82  | 125.19      | 119.90   |
| 26  | B7    | 116  | G    | N1-C6-O6   | 8.82  | 125.19      | 119.90   |
| 27  | B8    | 1277 | G    | N1-C6-O6   | 8.82  | 125.19      | 119.90   |
| 27  | B8    | 1873 | G    | N1-C6-O6   | 8.82  | 125.19      | 119.90   |
| 27  | B8    | 664  | G    | N1-C6-O6   | 8.82  | 125.19      | 119.90   |
| 27  | B8    | 2239 | G    | N1-C6-O6   | 8.82  | 125.19      | 119.90   |
| 27  | B8    | 2870 | C    | O4'-C1'-N1 | 8.82  | 115.25      | 108.20   |
| 1   | AA    | 406  | G    | N1-C6-O6   | 8.81  | 125.19      | 119.90   |
| 1   | AA    | 1209 | C    | O4'-C1'-N1 | 8.81  | 115.25      | 108.20   |
| 27  | B8    | 1186 | G    | N1-C6-O6   | 8.81  | 125.19      | 119.90   |
| 1   | AA    | 255  | G    | N1-C6-O6   | 8.81  | 125.19      | 119.90   |
| 27  | B8    | 1888 | G    | N1-C6-O6   | 8.81  | 125.19      | 119.90   |
| 1   | AA    | 469  | C    | O4'-C1'-N1 | 8.81  | 115.25      | 108.20   |
| 27  | B8    | 338  | G    | N1-C6-O6   | 8.81  | 125.19      | 119.90   |
| 27  | B8    | 1649 | G    | C5-C6-O6   | -8.81 | 123.31      | 128.60   |
| 27  | B8    | 1763 | G    | N1-C6-O6   | 8.81  | 125.19      | 119.90   |
| 27  | B8    | 1869 | G    | N1-C6-O6   | 8.81  | 125.19      | 119.90   |
| 27  | B8    | 80   | G    | N1-C6-O6   | 8.81  | 125.19      | 119.90   |
| 1   | AA    | 278  | G    | N1-C6-O6   | 8.81  | 125.18      | 119.90   |
| 1   | AA    | 1488 | G    | N1-C6-O6   | 8.81  | 125.18      | 119.90   |
| 3   | AV    | 72   | C    | O4'-C1'-N1 | 8.80  | 115.24      | 108.20   |
| 27  | B8    | 58   | G    | N1-C6-O6   | 8.80  | 125.18      | 119.90   |
| 27  | B8    | 372  | G    | N1-C6-O6   | 8.80  | 125.18      | 119.90   |
| 27  | B8    | 855  | G    | N1-C6-O6   | 8.80  | 125.18      | 119.90   |
| 1   | AA    | 1013 | G    | N1-C6-O6   | 8.80  | 125.18      | 119.90   |
| 27  | B8    | 2465 | C    | O4'-C1'-N1 | 8.80  | 115.24      | 108.20   |
| 3   | AV    | 43   | G    | N1-C6-O6   | 8.80  | 125.18      | 119.90   |
| 26  | B7    | 17   | C    | O4'-C1'-N1 | 8.80  | 115.24      | 108.20   |
| 27  | B8    | 950  | G    | N1-C6-O6   | 8.80  | 125.18      | 119.90   |
| 27  | B8    | 818  | G    | N1-C6-O6   | 8.80  | 125.18      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1975 | G    | C5-C6-O6   | -8.80 | 123.32      | 128.60   |
| 27  | B8    | 2157 | G    | N1-C6-O6   | 8.80  | 125.18      | 119.90   |
| 27  | B8    | 583  | G    | N1-C6-O6   | 8.79  | 125.18      | 119.90   |
| 27  | B8    | 2455 | G    | N1-C6-O6   | 8.79  | 125.18      | 119.90   |
| 1   | AA    | 584  | G    | C5-C6-O6   | -8.79 | 123.32      | 128.60   |
| 26  | B7    | 24   | G    | N1-C6-O6   | 8.79  | 125.18      | 119.90   |
| 27  | B8    | 577  | G    | N1-C6-O6   | 8.79  | 125.18      | 119.90   |
| 1   | AA    | 470  | C    | O4'-C1'-N1 | 8.79  | 115.23      | 108.20   |
| 27  | B8    | 1243 | C    | O4'-C1'-N1 | 8.79  | 115.23      | 108.20   |
| 27  | B8    | 2668 | G    | N1-C6-O6   | 8.79  | 125.17      | 119.90   |
| 3   | AV    | 35   | G    | N1-C6-O6   | 8.79  | 125.17      | 119.90   |
| 26  | B7    | 117  | G    | N1-C6-O6   | 8.79  | 125.17      | 119.90   |
| 27  | B8    | 1288 | G    | N1-C6-O6   | 8.79  | 125.17      | 119.90   |
| 27  | B8    | 1687 | G    | N1-C6-O6   | 8.79  | 125.17      | 119.90   |
| 27  | B8    | 2049 | G    | N1-C6-O6   | 8.79  | 125.17      | 119.90   |
| 27  | B8    | 418  | C    | O4'-C1'-N1 | 8.79  | 115.23      | 108.20   |
| 27  | B8    | 2027 | G    | C5-C6-O6   | -8.79 | 123.33      | 128.60   |
| 1   | AA    | 1048 | G    | C5-C6-O6   | -8.79 | 123.33      | 128.60   |
| 1   | AA    | 581  | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 27  | B8    | 157  | C    | O4'-C1'-N1 | 8.78  | 115.23      | 108.20   |
| 27  | B8    | 2253 | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 27  | B8    | 2446 | G    | N1-C6-O6   | 8.79  | 125.17      | 119.90   |
| 1   | AA    | 350  | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 27  | B8    | 248  | G    | C5-C6-O6   | -8.78 | 123.33      | 128.60   |
| 27  | B8    | 1074 | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 27  | B8    | 1003 | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 27  | B8    | 1110 | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 27  | B8    | 1271 | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 27  | B8    | 2524 | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 1   | AA    | 481  | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 1   | AA    | 966  | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 27  | B8    | 1710 | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 27  | B8    | 2592 | G    | C5-C6-O6   | -8.78 | 123.33      | 128.60   |
| 1   | AA    | 108  | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 1   | AA    | 1387 | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 27  | B8    | 2825 | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 27  | B8    | 2834 | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 1   | AA    | 394  | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 1   | AA    | 1255 | G    | C5-C6-O6   | -8.78 | 123.33      | 128.60   |
| 27  | B8    | 2162 | G    | N1-C6-O6   | 8.78  | 125.17      | 119.90   |
| 1   | AA    | 275  | G    | C5-C6-O6   | -8.77 | 123.34      | 128.60   |
| 1   | AA    | 656  | G    | N1-C6-O6   | 8.77  | 125.16      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1466 | C    | O4'-C1'-N1 | 8.77  | 115.22      | 108.20   |
| 27  | B8    | 1839 | G    | N1-C6-O6   | 8.77  | 125.16      | 119.90   |
| 27  | B8    | 2065 | C    | O4'-C1'-N1 | 8.77  | 115.22      | 108.20   |
| 27  | B8    | 2623 | G    | C5-C6-O6   | -8.77 | 123.34      | 128.60   |
| 1   | AA    | 947  | G    | N1-C6-O6   | 8.77  | 125.16      | 119.90   |
| 27  | B8    | 808  | G    | N1-C6-O6   | 8.77  | 125.16      | 119.90   |
| 27  | B8    | 1619 | G    | N1-C6-O6   | 8.77  | 125.16      | 119.90   |
| 27  | B8    | 1024 | G    | N1-C6-O6   | 8.77  | 125.16      | 119.90   |
| 27  | B8    | 1356 | G    | N1-C6-O6   | 8.77  | 125.16      | 119.90   |
| 27  | B8    | 1408 | G    | N1-C6-O6   | 8.77  | 125.16      | 119.90   |
| 27  | B8    | 1986 | C    | O4'-C1'-N1 | 8.77  | 115.21      | 108.20   |
| 1   | AA    | 713  | G    | N1-C6-O6   | 8.77  | 125.16      | 119.90   |
| 27  | B8    | 69   | C    | O4'-C1'-N1 | 8.77  | 115.21      | 108.20   |
| 27  | B8    | 257  | C    | O4'-C1'-N1 | 8.77  | 115.21      | 108.20   |
| 27  | B8    | 857  | G    | N1-C6-O6   | 8.77  | 125.16      | 119.90   |
| 27  | B8    | 1831 | G    | N1-C6-O6   | 8.77  | 125.16      | 119.90   |
| 1   | AA    | 700  | G    | N1-C6-O6   | 8.76  | 125.16      | 119.90   |
| 1   | AA    | 745  | G    | N1-C6-O6   | 8.76  | 125.16      | 119.90   |
| 27  | B8    | 1051 | G    | N1-C6-O6   | 8.76  | 125.16      | 119.90   |
| 27  | B8    | 2811 | G    | N1-C6-O6   | 8.76  | 125.16      | 119.90   |
| 27  | B8    | 68   | G    | N1-C6-O6   | 8.76  | 125.16      | 119.90   |
| 27  | B8    | 672  | C    | O4'-C1'-N1 | 8.76  | 115.21      | 108.20   |
| 27  | B8    | 1049 | C    | O4'-C1'-N1 | 8.76  | 115.21      | 108.20   |
| 27  | B8    | 2271 | G    | N1-C6-O6   | 8.76  | 125.16      | 119.90   |
| 27  | B8    | 1823 | G    | N1-C6-O6   | 8.76  | 125.16      | 119.90   |
| 1   | AA    | 281  | G    | N1-C6-O6   | 8.76  | 125.15      | 119.90   |
| 27  | B8    | 117  | G    | N1-C6-O6   | 8.76  | 125.16      | 119.90   |
| 27  | B8    | 1471 | G    | N1-C6-O6   | 8.76  | 125.15      | 119.90   |
| 1   | AA    | 202  | G    | N1-C6-O6   | 8.75  | 125.15      | 119.90   |
| 1   | AA    | 726  | C    | O4'-C1'-N1 | 8.75  | 115.20      | 108.20   |
| 27  | B8    | 1346 | G    | N1-C6-O6   | 8.75  | 125.15      | 119.90   |
| 27  | B8    | 1971 | U    | O4'-C1'-N1 | 8.75  | 115.20      | 108.20   |
| 27  | B8    | 39   | G    | N1-C6-O6   | 8.75  | 125.15      | 119.90   |
| 27  | B8    | 1702 | G    | N1-C6-O6   | 8.75  | 125.15      | 119.90   |
| 27  | B8    | 555  | G    | N1-C6-O6   | 8.75  | 125.15      | 119.90   |
| 27  | B8    | 663  | G    | C5-C6-O6   | -8.75 | 123.35      | 128.60   |
| 27  | B8    | 1292 | G    | N1-C6-O6   | 8.75  | 125.15      | 119.90   |
| 27  | B8    | 2447 | G    | C5-C6-O6   | -8.75 | 123.35      | 128.60   |
| 3   | AV    | 45   | G    | N1-C6-O6   | 8.75  | 125.15      | 119.90   |
| 1   | AA    | 661  | G    | N1-C6-O6   | 8.75  | 125.15      | 119.90   |
| 1   | AA    | 852  | G    | N1-C6-O6   | 8.75  | 125.15      | 119.90   |
| 27  | B8    | 130  | C    | O4'-C1'-N1 | 8.75  | 115.20      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 904  | G    | N1-C6-O6   | 8.75  | 125.15      | 119.90   |
| 27  | B8    | 2780 | G    | N1-C6-O6   | 8.75  | 125.15      | 119.90   |
| 27  | B8    | 334  | C    | O4'-C1'-N1 | 8.74  | 115.20      | 108.20   |
| 1   | AA    | 858  | G    | N1-C6-O6   | 8.74  | 125.15      | 119.90   |
| 1   | AA    | 1317 | C    | O4'-C1'-N1 | 8.74  | 115.19      | 108.20   |
| 26  | B7    | 72   | G    | N1-C6-O6   | 8.74  | 125.15      | 119.90   |
| 27  | B8    | 30   | G    | N1-C6-O6   | 8.74  | 125.15      | 119.90   |
| 27  | B8    | 2237 | G    | N1-C6-O6   | 8.74  | 125.15      | 119.90   |
| 27  | B8    | 2805 | C    | O4'-C1'-N1 | 8.74  | 115.20      | 108.20   |
| 27  | B8    | 1025 | G    | N1-C6-O6   | 8.74  | 125.14      | 119.90   |
| 27  | B8    | 1934 | C    | O4'-C1'-N1 | 8.74  | 115.19      | 108.20   |
| 27  | B8    | 1699 | G    | N1-C6-O6   | 8.74  | 125.14      | 119.90   |
| 27  | B8    | 1989 | G    | N1-C6-O6   | 8.74  | 125.14      | 119.90   |
| 27  | B8    | 376  | G    | N1-C6-O6   | 8.74  | 125.14      | 119.90   |
| 1   | AA    | 360  | G    | N1-C6-O6   | 8.73  | 125.14      | 119.90   |
| 1   | AA    | 1024 | G    | N1-C6-O6   | 8.73  | 125.14      | 119.90   |
| 27  | B8    | 379  | G    | N1-C6-O6   | 8.73  | 125.14      | 119.90   |
| 1   | AA    | 844  | G    | N1-C6-O6   | 8.73  | 125.14      | 119.90   |
| 1   | AA    | 1231 | G    | N1-C6-O6   | 8.73  | 125.14      | 119.90   |
| 27  | B8    | 370  | G    | N1-C6-O6   | 8.73  | 125.14      | 119.90   |
| 27  | B8    | 2553 | G    | N1-C6-O6   | 8.73  | 125.14      | 119.90   |
| 1   | AA    | 575  | G    | N1-C6-O6   | 8.73  | 125.14      | 119.90   |
| 1   | AA    | 1297 | G    | N1-C6-O6   | 8.73  | 125.14      | 119.90   |
| 1   | AA    | 169  | C    | O4'-C1'-N1 | 8.73  | 115.18      | 108.20   |
| 27  | B8    | 1627 | G    | C5-C6-O6   | -8.73 | 123.36      | 128.60   |
| 27  | B8    | 2368 | C    | O4'-C1'-N1 | 8.73  | 115.18      | 108.20   |
| 27  | B8    | 2723 | C    | O4'-C1'-N1 | 8.73  | 115.18      | 108.20   |
| 1   | AA    | 752  | G    | N1-C6-O6   | 8.72  | 125.14      | 119.90   |
| 1   | AA    | 1003 | G    | N1-C6-O6   | 8.72  | 125.14      | 119.90   |
| 1   | AA    | 193  | C    | O4'-C1'-N1 | 8.72  | 115.18      | 108.20   |
| 1   | AA    | 616  | G    | C5-C6-O6   | -8.72 | 123.37      | 128.60   |
| 1   | AA    | 888  | G    | N1-C6-O6   | 8.72  | 125.13      | 119.90   |
| 27  | B8    | 1311 | G    | N1-C6-O6   | 8.72  | 125.13      | 119.90   |
| 27  | B8    | 489  | G    | N1-C6-O6   | 8.72  | 125.13      | 119.90   |
| 1   | AA    | 346  | G    | N1-C6-O6   | 8.72  | 125.13      | 119.90   |
| 1   | AA    | 606  | G    | N1-C6-O6   | 8.72  | 125.13      | 119.90   |
| 26  | B7    | 102  | G    | N1-C6-O6   | 8.72  | 125.13      | 119.90   |
| 27  | B8    | 517  | C    | O4'-C1'-N1 | 8.72  | 115.17      | 108.20   |
| 27  | B8    | 891  | G    | O4'-C1'-N9 | 8.72  | 115.17      | 108.20   |
| 27  | B8    | 98   | G    | N1-C6-O6   | 8.72  | 125.13      | 119.90   |
| 1   | AA    | 769  | G    | N1-C6-O6   | 8.71  | 125.13      | 119.90   |
| 27  | B8    | 1426 | G    | N1-C6-O6   | 8.71  | 125.13      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 1   | AA    | 517  | G    | N1-C6-O6   | 8.71 | 125.13      | 119.90   |
| 27  | B8    | 2    | G    | N1-C6-O6   | 8.71 | 125.13      | 119.90   |
| 27  | B8    | 1473 | G    | N1-C6-O6   | 8.71 | 125.13      | 119.90   |
| 27  | B8    | 1756 | G    | N1-C6-O6   | 8.71 | 125.13      | 119.90   |
| 27  | B8    | 2076 | U    | O4'-C1'-N1 | 8.71 | 115.17      | 108.20   |
| 27  | B8    | 2532 | G    | N1-C6-O6   | 8.71 | 125.13      | 119.90   |
| 1   | AA    | 112  | G    | N1-C6-O6   | 8.71 | 125.13      | 119.90   |
| 1   | AA    | 398  | U    | O4'-C1'-N1 | 8.71 | 115.17      | 108.20   |
| 1   | AA    | 419  | C    | O4'-C1'-N1 | 8.70 | 115.16      | 108.20   |
| 1   | AA    | 1277 | C    | O4'-C1'-N1 | 8.71 | 115.16      | 108.20   |
| 27  | B8    | 1827 | U    | O4'-C1'-N1 | 8.71 | 115.16      | 108.20   |
| 27  | B8    | 2319 | G    | N1-C6-O6   | 8.71 | 125.12      | 119.90   |
| 27  | B8    | 2379 | G    | N1-C6-O6   | 8.70 | 125.12      | 119.90   |
| 1   | AA    | 357  | G    | N1-C6-O6   | 8.70 | 125.12      | 119.90   |
| 1   | AA    | 524  | G    | N1-C6-O6   | 8.70 | 125.12      | 119.90   |
| 1   | AA    | 1166 | G    | N1-C6-O6   | 8.70 | 125.12      | 119.90   |
| 27  | B8    | 393  | C    | O4'-C1'-N1 | 8.70 | 115.16      | 108.20   |
| 27  | B8    | 1703 | G    | N1-C6-O6   | 8.70 | 125.12      | 119.90   |
| 1   | AA    | 1409 | C    | O4'-C1'-N1 | 8.70 | 115.16      | 108.20   |
| 27  | B8    | 247  | G    | N1-C6-O6   | 8.70 | 125.12      | 119.90   |
| 27  | B8    | 711  | G    | N1-C6-O6   | 8.70 | 125.12      | 119.90   |
| 1   | AA    | 503  | C    | O4'-C1'-N1 | 8.69 | 115.16      | 108.20   |
| 1   | AA    | 1316 | G    | N1-C6-O6   | 8.70 | 125.12      | 119.90   |
| 1   | AA    | 1326 | U    | O4'-C1'-N1 | 8.69 | 115.16      | 108.20   |
| 27  | B8    | 1432 | G    | N1-C6-O6   | 8.69 | 125.12      | 119.90   |
| 27  | B8    | 2735 | G    | N1-C6-O6   | 8.69 | 125.12      | 119.90   |
| 1   | AA    | 690  | G    | N1-C6-O6   | 8.69 | 125.11      | 119.90   |
| 1   | AA    | 698  | G    | N1-C6-O6   | 8.69 | 125.11      | 119.90   |
| 1   | AA    | 1099 | G    | N1-C6-O6   | 8.69 | 125.11      | 119.90   |
| 3   | AV    | 44   | G    | N1-C6-O6   | 8.69 | 125.11      | 119.90   |
| 27  | B8    | 725  | G    | N1-C6-O6   | 8.69 | 125.11      | 119.90   |
| 27  | B8    | 1950 | G    | N1-C6-O6   | 8.69 | 125.11      | 119.90   |
| 27  | B8    | 600  | G    | N1-C6-O6   | 8.69 | 125.11      | 119.90   |
| 27  | B8    | 1542 | U    | O4'-C1'-N1 | 8.69 | 115.15      | 108.20   |
| 1   | AA    | 172  | A    | N1-C6-N6   | 8.69 | 123.81      | 118.60   |
| 27  | B8    | 704  | G    | N1-C6-O6   | 8.69 | 125.11      | 119.90   |
| 27  | B8    | 805  | G    | N1-C6-O6   | 8.69 | 125.11      | 119.90   |
| 27  | B8    | 2791 | G    | N1-C6-O6   | 8.69 | 125.11      | 119.90   |
| 1   | AA    | 886  | G    | N1-C6-O6   | 8.69 | 125.11      | 119.90   |
| 1   | AA    | 940  | C    | O4'-C1'-N1 | 8.69 | 115.15      | 108.20   |
| 27  | B8    | 328  | U    | O4'-C1'-N1 | 8.69 | 115.15      | 108.20   |
| 27  | B8    | 2144 | G    | N1-C6-O6   | 8.69 | 125.11      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2676 | C    | O4'-C1'-N1 | 8.69  | 115.15      | 108.20   |
| 27  | B8    | 548  | G    | N1-C6-O6   | 8.69  | 125.11      | 119.90   |
| 27  | B8    | 671  | C    | O4'-C1'-N1 | 8.69  | 115.15      | 108.20   |
| 27  | B8    | 2462 | C    | O4'-C1'-N1 | 8.69  | 115.15      | 108.20   |
| 1   | AA    | 1087 | G    | C5-C6-O6   | -8.68 | 123.39      | 128.60   |
| 26  | B7    | 112  | G    | C5-C6-O6   | -8.68 | 123.39      | 128.60   |
| 27  | B8    | 1279 | G    | N1-C6-O6   | 8.68  | 125.11      | 119.90   |
| 27  | B8    | 1667 | G    | N1-C6-O6   | 8.68  | 125.11      | 119.90   |
| 1   | AA    | 637  | C    | O4'-C1'-N1 | 8.68  | 115.14      | 108.20   |
| 1   | AA    | 1182 | G    | N1-C6-O6   | 8.68  | 125.11      | 119.90   |
| 1   | AA    | 506  | G    | N1-C6-O6   | 8.68  | 125.11      | 119.90   |
| 1   | AA    | 1475 | G    | N1-C6-O6   | 8.68  | 125.11      | 119.90   |
| 27  | B8    | 273  | G    | C5-C6-O6   | -8.68 | 123.39      | 128.60   |
| 27  | B8    | 1237 | A    | O4'-C1'-N9 | 8.68  | 115.14      | 108.20   |
| 2   | AX    | 14   | G    | N1-C6-O6   | 8.68  | 125.11      | 119.90   |
| 26  | B7    | 62   | C    | O4'-C1'-N1 | 8.68  | 115.14      | 108.20   |
| 27  | B8    | 1930 | G    | N1-C6-O6   | 8.67  | 125.10      | 119.90   |
| 27  | B8    | 2193 | G    | N1-C6-O6   | 8.67  | 125.10      | 119.90   |
| 27  | B8    | 2638 | G    | N1-C6-O6   | 8.67  | 125.10      | 119.90   |
| 1   | AA    | 761  | G    | N1-C6-O6   | 8.67  | 125.10      | 119.90   |
| 27  | B8    | 159  | G    | N1-C6-O6   | 8.67  | 125.10      | 119.90   |
| 27  | B8    | 1770 | G    | N1-C6-O6   | 8.67  | 125.10      | 119.90   |
| 1   | AA    | 568  | G    | N1-C6-O6   | 8.67  | 125.10      | 119.90   |
| 1   | AA    | 1432 | G    | N1-C6-O6   | 8.67  | 125.10      | 119.90   |
| 26  | B7    | 71   | C    | O4'-C1'-N1 | 8.67  | 115.13      | 108.20   |
| 27  | B8    | 1437 | C    | O4'-C1'-N1 | 8.67  | 115.13      | 108.20   |
| 27  | B8    | 2138 | G    | N1-C6-O6   | 8.67  | 125.10      | 119.90   |
| 27  | B8    | 43   | G    | N1-C6-O6   | 8.66  | 125.10      | 119.90   |
| 1   | AA    | 1074 | G    | N1-C6-O6   | 8.66  | 125.10      | 119.90   |
| 27  | B8    | 488  | G    | N1-C6-O6   | 8.66  | 125.10      | 119.90   |
| 1   | AA    | 515  | G    | N1-C6-O6   | 8.66  | 125.10      | 119.90   |
| 27  | B8    | 2737 | G    | N1-C6-O6   | 8.66  | 125.10      | 119.90   |
| 27  | B8    | 533  | G    | C5-C6-O6   | -8.66 | 123.41      | 128.60   |
| 27  | B8    | 1099 | G    | C5-C6-O6   | -8.66 | 123.41      | 128.60   |
| 27  | B8    | 2353 | G    | N1-C6-O6   | 8.66  | 125.09      | 119.90   |
| 27  | B8    | 2429 | G    | N1-C6-O6   | 8.66  | 125.09      | 119.90   |
| 1   | AA    | 113  | G    | C5-C6-O6   | -8.65 | 123.41      | 128.60   |
| 1   | AA    | 628  | G    | N1-C6-O6   | 8.65  | 125.09      | 119.90   |
| 1   | AA    | 856  | C    | O4'-C1'-N1 | 8.65  | 115.12      | 108.20   |
| 27  | B8    | 495  | G    | N1-C6-O6   | 8.65  | 125.09      | 119.90   |
| 3   | AV    | 37   | G    | N1-C6-O6   | 8.65  | 125.09      | 119.90   |
| 27  | B8    | 579  | G    | C5-C6-O6   | -8.65 | 123.41      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 336  | C    | O4'-C1'-N1 | 8.65  | 115.12      | 108.20   |
| 27  | B8    | 506  | G    | N1-C6-O6   | 8.65  | 125.09      | 119.90   |
| 27  | B8    | 707  | G    | N1-C6-O6   | 8.65  | 125.09      | 119.90   |
| 27  | B8    | 651  | G    | N1-C6-O6   | 8.65  | 125.09      | 119.90   |
| 27  | B8    | 2535 | G    | C5-C6-O6   | -8.65 | 123.41      | 128.60   |
| 27  | B8    | 2775 | G    | N1-C6-O6   | 8.65  | 125.09      | 119.90   |
| 27  | B8    | 876  | C    | O4'-C1'-N1 | 8.65  | 115.12      | 108.20   |
| 27  | B8    | 2659 | G    | N1-C6-O6   | 8.65  | 125.09      | 119.90   |
| 1   | AA    | 1134 | G    | N1-C6-O6   | 8.65  | 125.09      | 119.90   |
| 27  | B8    | 601  | C    | O4'-C1'-N1 | 8.65  | 115.12      | 108.20   |
| 1   | AA    | 1222 | G    | N1-C6-O6   | 8.64  | 125.09      | 119.90   |
| 1   | AA    | 1489 | G    | N1-C6-O6   | 8.64  | 125.09      | 119.90   |
| 27  | B8    | 2364 | C    | O4'-C1'-N1 | 8.64  | 115.12      | 108.20   |
| 3   | AV    | 20   | G    | N1-C6-O6   | 8.64  | 125.09      | 119.90   |
| 27  | B8    | 2673 | G    | C5-C6-O6   | -8.64 | 123.41      | 128.60   |
| 1   | AA    | 1113 | C    | O4'-C1'-N1 | 8.64  | 115.11      | 108.20   |
| 27  | B8    | 1115 | G    | N1-C6-O6   | 8.64  | 125.08      | 119.90   |
| 27  | B8    | 2699 | C    | O4'-C1'-N1 | 8.64  | 115.11      | 108.20   |
| 27  | B8    | 2751 | G    | N1-C6-O6   | 8.64  | 125.08      | 119.90   |
| 1   | AA    | 1455 | G    | C5-C6-O6   | -8.64 | 123.42      | 128.60   |
| 27  | B8    | 625  | G    | N1-C6-O6   | 8.64  | 125.08      | 119.90   |
| 27  | B8    | 2255 | G    | N1-C6-O6   | 8.64  | 125.08      | 119.90   |
| 27  | B8    | 2544 | G    | C5-C6-O6   | -8.64 | 123.42      | 128.60   |
| 1   | AA    | 187  | G    | N1-C6-O6   | 8.64  | 125.08      | 119.90   |
| 27  | B8    | 713  | G    | N1-C6-O6   | 8.64  | 125.08      | 119.90   |
| 27  | B8    | 882  | G    | N1-C6-O6   | 8.63  | 125.08      | 119.90   |
| 27  | B8    | 2365 | G    | N1-C6-O6   | 8.63  | 125.08      | 119.90   |
| 27  | B8    | 2808 | G    | N1-C6-O6   | 8.63  | 125.08      | 119.90   |
| 27  | B8    | 2822 | G    | N1-C6-O6   | 8.63  | 125.08      | 119.90   |
| 1   | AA    | 75   | G    | C5-C6-O6   | -8.63 | 123.42      | 128.60   |
| 27  | B8    | 2885 | G    | N1-C6-O6   | 8.63  | 125.08      | 119.90   |
| 1   | AA    | 733  | G    | N1-C6-O6   | 8.63  | 125.08      | 119.90   |
| 1   | AA    | 1417 | G    | N1-C6-O6   | 8.63  | 125.08      | 119.90   |
| 27  | B8    | 426  | C    | O4'-C1'-N1 | 8.63  | 115.11      | 108.20   |
| 27  | B8    | 2045 | C    | O4'-C1'-N1 | 8.63  | 115.11      | 108.20   |
| 27  | B8    | 2663 | G    | N1-C6-O6   | 8.63  | 125.08      | 119.90   |
| 1   | AA    | 1172 | C    | O4'-C1'-N1 | 8.63  | 115.10      | 108.20   |
| 1   | AA    | 1398 | A    | O4'-C1'-N9 | 8.63  | 115.10      | 108.20   |
| 26  | B7    | 4    | C    | O4'-C1'-N1 | 8.63  | 115.10      | 108.20   |
| 27  | B8    | 474  | G    | N1-C6-O6   | 8.63  | 125.08      | 119.90   |
| 27  | B8    | 2338 | C    | O4'-C1'-N1 | 8.63  | 115.10      | 108.20   |
| 1   | AA    | 1347 | G    | N1-C6-O6   | 8.62  | 125.08      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | AV    | 12   | G    | N1-C6-O6   | 8.62  | 125.08      | 119.90   |
| 27  | B8    | 493  | G    | N1-C6-O6   | 8.62  | 125.08      | 119.90   |
| 27  | B8    | 1551 | A    | P-O3'-C3'  | 8.62  | 130.05      | 119.70   |
| 27  | B8    | 2342 | C    | O4'-C1'-N1 | 8.63  | 115.10      | 108.20   |
| 27  | B8    | 2289 | G    | N1-C6-O6   | 8.62  | 125.07      | 119.90   |
| 27  | B8    | 2608 | G    | N1-C6-O6   | 8.62  | 125.08      | 119.90   |
| 1   | AA    | 145  | G    | C5-C6-O6   | -8.62 | 123.43      | 128.60   |
| 1   | AA    | 310  | G    | N1-C6-O6   | 8.62  | 125.07      | 119.90   |
| 27  | B8    | 757  | G    | C5-C6-O6   | -8.62 | 123.43      | 128.60   |
| 1   | AA    | 35   | G    | N1-C6-O6   | 8.62  | 125.07      | 119.90   |
| 1   | AA    | 305  | G    | N1-C6-O6   | 8.62  | 125.07      | 119.90   |
| 1   | AA    | 1331 | G    | N1-C6-O6   | 8.62  | 125.07      | 119.90   |
| 27  | B8    | 1929 | G    | N1-C6-O6   | 8.62  | 125.07      | 119.90   |
| 27  | B8    | 2127 | G    | N1-C6-O6   | 8.62  | 125.07      | 119.90   |
| 1   | AA    | 297  | G    | N1-C6-O6   | 8.62  | 125.07      | 119.90   |
| 27  | B8    | 1034 | G    | C5-C6-O6   | -8.62 | 123.43      | 128.60   |
| 27  | B8    | 143  | C    | O4'-C1'-N1 | 8.62  | 115.09      | 108.20   |
| 27  | B8    | 1646 | C    | O4'-C1'-N1 | 8.62  | 115.09      | 108.20   |
| 27  | B8    | 318  | C    | O4'-C1'-N1 | 8.62  | 115.09      | 108.20   |
| 27  | B8    | 253  | C    | O4'-C1'-N1 | 8.62  | 115.09      | 108.20   |
| 27  | B8    | 726  | G    | N1-C6-O6   | 8.62  | 125.07      | 119.90   |
| 27  | B8    | 570  | G    | N1-C6-O6   | 8.61  | 125.07      | 119.90   |
| 27  | B8    | 1092 | C    | O4'-C1'-N1 | 8.62  | 115.09      | 108.20   |
| 27  | B8    | 1493 | C    | O4'-C1'-N1 | 8.62  | 115.09      | 108.20   |
| 27  | B8    | 1538 | G    | C5-C6-O6   | -8.62 | 123.43      | 128.60   |
| 1   | AA    | 311  | C    | O4'-C1'-N1 | 8.61  | 115.09      | 108.20   |
| 1   | AA    | 537  | G    | N1-C6-O6   | 8.61  | 125.07      | 119.90   |
| 27  | B8    | 1333 | G    | N1-C6-O6   | 8.61  | 125.07      | 119.90   |
| 27  | B8    | 1456 | G    | N1-C6-O6   | 8.61  | 125.07      | 119.90   |
| 1   | AA    | 677  | U    | O4'-C1'-N1 | 8.61  | 115.09      | 108.20   |
| 1   | AA    | 829  | G    | N1-C6-O6   | 8.61  | 125.07      | 119.90   |
| 1   | AA    | 857  | C    | O4'-C1'-N1 | 8.61  | 115.09      | 108.20   |
| 1   | AA    | 691  | G    | N1-C6-O6   | 8.61  | 125.06      | 119.90   |
| 27  | B8    | 869  | G    | N1-C6-O6   | 8.61  | 125.07      | 119.90   |
| 27  | B8    | 1364 | G    | N1-C6-O6   | 8.61  | 125.07      | 119.90   |
| 27  | B8    | 2860 | A    | C4-C5-C6   | 8.61  | 121.31      | 117.00   |
| 27  | B8    | 2863 | C    | O4'-C1'-N1 | 8.61  | 115.09      | 108.20   |
| 27  | B8    | 623  | C    | O4'-C1'-N1 | 8.61  | 115.09      | 108.20   |
| 27  | B8    | 891  | G    | N1-C6-O6   | 8.61  | 125.06      | 119.90   |
| 27  | B8    | 1235 | G    | N1-C6-O6   | 8.61  | 125.06      | 119.90   |
| 27  | B8    | 2331 | G    | N1-C6-O6   | 8.61  | 125.06      | 119.90   |
| 1   | AA    | 370  | C    | O4'-C1'-N1 | 8.60  | 115.08      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1718 | G    | N1-C6-O6   | 8.60  | 125.06      | 119.90   |
| 27  | B8    | 1857 | G    | N1-C6-O6   | 8.60  | 125.06      | 119.90   |
| 1   | AA    | 626  | G    | C5-C6-O6   | -8.60 | 123.44      | 128.60   |
| 1   | AA    | 351  | G    | N1-C6-O6   | 8.60  | 125.06      | 119.90   |
| 3   | AV    | 40   | G    | N1-C6-O6   | 8.60  | 125.06      | 119.90   |
| 27  | B8    | 1907 | G    | C5-C6-O6   | -8.60 | 123.44      | 128.60   |
| 1   | AA    | 1521 | C    | O4'-C1'-N1 | 8.60  | 115.08      | 108.20   |
| 27  | B8    | 2159 | G    | N1-C6-O6   | 8.60  | 125.06      | 119.90   |
| 1   | AA    | 107  | G    | N1-C6-O6   | 8.60  | 125.06      | 119.90   |
| 1   | AA    | 1094 | G    | N1-C6-O6   | 8.60  | 125.06      | 119.90   |
| 27  | B8    | 2607 | G    | N1-C6-O6   | 8.59  | 125.06      | 119.90   |
| 27  | B8    | 1459 | G    | N1-C6-O6   | 8.59  | 125.05      | 119.90   |
| 27  | B8    | 1956 | U    | O4'-C1'-N1 | 8.59  | 115.07      | 108.20   |
| 1   | AA    | 83   | C    | O4'-C1'-N1 | 8.59  | 115.07      | 108.20   |
| 1   | AA    | 647  | C    | O4'-C1'-N1 | 8.59  | 115.07      | 108.20   |
| 1   | AA    | 1278 | G    | N1-C6-O6   | 8.59  | 125.05      | 119.90   |
| 2   | AX    | 20   | G    | N1-C6-O6   | 8.59  | 125.05      | 119.90   |
| 27  | B8    | 481  | G    | N1-C6-O6   | 8.59  | 125.05      | 119.90   |
| 27  | B8    | 1807 | G    | N1-C6-O6   | 8.59  | 125.05      | 119.90   |
| 27  | B8    | 341  | C    | O4'-C1'-N1 | 8.58  | 115.07      | 108.20   |
| 27  | B8    | 669  | G    | N1-C6-O6   | 8.58  | 125.05      | 119.90   |
| 27  | B8    | 2470 | G    | N1-C6-O6   | 8.58  | 125.05      | 119.90   |
| 27  | B8    | 446  | G    | N1-C6-O6   | 8.58  | 125.05      | 119.90   |
| 27  | B8    | 634  | C    | O4'-C1'-N1 | 8.58  | 115.06      | 108.20   |
| 27  | B8    | 1726 | C    | O4'-C1'-N1 | 8.58  | 115.06      | 108.20   |
| 27  | B8    | 1068 | G    | N1-C6-O6   | 8.58  | 125.05      | 119.90   |
| 1   | AA    | 134  | G    | N1-C6-O6   | 8.58  | 125.05      | 119.90   |
| 1   | AA    | 1193 | G    | C5-C6-O6   | -8.58 | 123.45      | 128.60   |
| 27  | B8    | 22   | C    | O4'-C1'-N1 | 8.58  | 115.06      | 108.20   |
| 1   | AA    | 159  | G    | N1-C6-O6   | 8.57  | 125.05      | 119.90   |
| 3   | AV    | 7    | G    | N1-C6-O6   | 8.57  | 125.05      | 119.90   |
| 26  | B7    | 105  | G    | N1-C6-O6   | 8.57  | 125.05      | 119.90   |
| 27  | B8    | 500  | G    | N1-C6-O6   | 8.57  | 125.05      | 119.90   |
| 27  | B8    | 561  | G    | N1-C6-O6   | 8.57  | 125.05      | 119.90   |
| 27  | B8    | 1005 | C    | O4'-C1'-N1 | 8.57  | 115.06      | 108.20   |
| 27  | B8    | 1501 | G    | N1-C6-O6   | 8.57  | 125.04      | 119.90   |
| 27  | B8    | 1879 | C    | O4'-C1'-N1 | 8.57  | 115.06      | 108.20   |
| 27  | B8    | 2658 | C    | O4'-C1'-N1 | 8.57  | 115.06      | 108.20   |
| 1   | AA    | 708  | C    | O4'-C1'-N1 | 8.57  | 115.06      | 108.20   |
| 1   | AA    | 1178 | G    | N1-C6-O6   | 8.57  | 125.04      | 119.90   |
| 27  | B8    | 1006 | C    | O4'-C1'-N1 | 8.57  | 115.06      | 108.20   |
| 27  | B8    | 2018 | G    | N1-C6-O6   | 8.57  | 125.04      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2206 | C    | O4'-C1'-N1 | 8.57  | 115.06      | 108.20   |
| 27  | B8    | 2351 | G    | N1-C6-O6   | 8.57  | 125.04      | 119.90   |
| 27  | B8    | 308  | G    | N1-C6-O6   | 8.57  | 125.04      | 119.90   |
| 27  | B8    | 718  | A    | O4'-C1'-N9 | 8.57  | 115.06      | 108.20   |
| 27  | B8    | 858  | G    | N1-C6-O6   | 8.57  | 125.04      | 119.90   |
| 27  | B8    | 1339 | G    | N1-C6-O6   | 8.57  | 125.04      | 119.90   |
| 1   | AA    | 290  | C    | O4'-C1'-N1 | 8.57  | 115.05      | 108.20   |
| 1   | AA    | 501  | C    | O4'-C1'-N1 | 8.57  | 115.05      | 108.20   |
| 1   | AA    | 1156 | G    | N1-C6-O6   | 8.57  | 125.04      | 119.90   |
| 3   | AV    | 53   | G    | N1-C6-O6   | 8.57  | 125.04      | 119.90   |
| 27  | B8    | 47   | C    | O4'-C1'-N1 | 8.57  | 115.05      | 108.20   |
| 27  | B8    | 1844 | C    | O4'-C1'-N1 | 8.57  | 115.05      | 108.20   |
| 27  | B8    | 2363 | G    | C5-C6-O6   | -8.57 | 123.46      | 128.60   |
| 27  | B8    | 1760 | C    | O4'-C1'-N1 | 8.57  | 115.05      | 108.20   |
| 27  | B8    | 2787 | C    | O4'-C1'-N1 | 8.56  | 115.05      | 108.20   |
| 1   | AA    | 359  | G    | C5-C6-O6   | -8.56 | 123.46      | 128.60   |
| 3   | AV    | 7    | G    | P-O3'-C3'  | 8.56  | 129.98      | 119.70   |
| 27  | B8    | 381  | G    | N1-C6-O6   | 8.56  | 125.04      | 119.90   |
| 27  | B8    | 417  | C    | O4'-C1'-N1 | 8.56  | 115.05      | 108.20   |
| 1   | AA    | 1020 | G    | C5-C6-O6   | -8.56 | 123.46      | 128.60   |
| 27  | B8    | 367  | G    | N1-C6-O6   | 8.56  | 125.04      | 119.90   |
| 26  | B7    | 114  | C    | O4'-C1'-N1 | 8.56  | 115.05      | 108.20   |
| 27  | B8    | 1521 | G    | N1-C6-O6   | 8.56  | 125.04      | 119.90   |
| 27  | B8    | 1550 | C    | O4'-C1'-N1 | 8.56  | 115.05      | 108.20   |
| 1   | AA    | 128  | G    | N1-C6-O6   | 8.56  | 125.03      | 119.90   |
| 27  | B8    | 2072 | C    | O4'-C1'-N1 | 8.56  | 115.05      | 108.20   |
| 27  | B8    | 2156 | G    | N1-C6-O6   | 8.56  | 125.03      | 119.90   |
| 26  | B7    | 91   | C    | O4'-C1'-N1 | 8.56  | 115.05      | 108.20   |
| 1   | AA    | 667  | G    | C5-C6-O6   | -8.55 | 123.47      | 128.60   |
| 26  | B7    | 13   | G    | N1-C6-O6   | 8.55  | 125.03      | 119.90   |
| 27  | B8    | 1715 | G    | N1-C6-O6   | 8.55  | 125.03      | 119.90   |
| 27  | B8    | 2678 | C    | O4'-C1'-N1 | 8.55  | 115.04      | 108.20   |
| 27  | B8    | 444  | C    | O4'-C1'-N1 | 8.55  | 115.04      | 108.20   |
| 27  | B8    | 703  | U    | O4'-C1'-N1 | 8.55  | 115.04      | 108.20   |
| 27  | B8    | 1812 | U    | O4'-C1'-N1 | 8.55  | 115.04      | 108.20   |
| 27  | B8    | 2141 | G    | C5-C6-O6   | -8.55 | 123.47      | 128.60   |
| 27  | B8    | 2370 | G    | N1-C6-O6   | 8.55  | 125.03      | 119.90   |
| 27  | B8    | 1    | G    | C5-C6-O6   | -8.55 | 123.47      | 128.60   |
| 27  | B8    | 2719 | G    | N1-C6-O6   | 8.55  | 125.03      | 119.90   |
| 1   | AA    | 926  | G    | N1-C6-O6   | 8.54  | 125.03      | 119.90   |
| 27  | B8    | 1483 | G    | N1-C6-O6   | 8.54  | 125.03      | 119.90   |
| 1   | AA    | 272  | C    | O4'-C1'-N1 | 8.54  | 115.03      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 664  | G    | N1-C6-O6   | 8.54  | 125.03      | 119.90   |
| 27  | B8    | 1298 | C    | O4'-C1'-N1 | 8.54  | 115.03      | 108.20   |
| 27  | B8    | 2207 | C    | O4'-C1'-N1 | 8.54  | 115.03      | 108.20   |
| 27  | B8    | 2688 | G    | N1-C6-O6   | 8.54  | 125.03      | 119.90   |
| 27  | B8    | 1738 | G    | N1-C6-O6   | 8.54  | 125.02      | 119.90   |
| 1   | AA    | 683  | G    | N1-C6-O6   | 8.54  | 125.02      | 119.90   |
| 26  | B7    | 2    | G    | N1-C6-O6   | 8.54  | 125.02      | 119.90   |
| 27  | B8    | 440  | C    | O4'-C1'-N1 | 8.54  | 115.03      | 108.20   |
| 27  | B8    | 1227 | G    | N1-C6-O6   | 8.54  | 125.02      | 119.90   |
| 27  | B8    | 2066 | C    | O4'-C1'-N1 | 8.54  | 115.03      | 108.20   |
| 27  | B8    | 2749 | A    | N1-C6-N6   | 8.54  | 123.72      | 118.60   |
| 27  | B8    | 2902 | C    | O4'-C1'-N1 | 8.54  | 115.03      | 108.20   |
| 1   | AA    | 890  | G    | N1-C6-O6   | 8.54  | 125.02      | 119.90   |
| 1   | AA    | 1079 | G    | N1-C6-O6   | 8.54  | 125.02      | 119.90   |
| 27  | B8    | 619  | G    | N1-C6-O6   | 8.54  | 125.02      | 119.90   |
| 27  | B8    | 817  | C    | O4'-C1'-N1 | 8.54  | 115.03      | 108.20   |
| 3   | AV    | 46   | G    | N1-C6-O6   | 8.53  | 125.02      | 119.90   |
| 1   | AA    | 417  | G    | C5-C6-O6   | -8.53 | 123.48      | 128.60   |
| 1   | AA    | 1089 | G    | N1-C6-O6   | 8.53  | 125.02      | 119.90   |
| 27  | B8    | 1793 | C    | O4'-C1'-N1 | 8.53  | 115.03      | 108.20   |
| 27  | B8    | 2252 | G    | N1-C6-O6   | 8.53  | 125.02      | 119.90   |
| 1   | AA    | 1184 | G    | C5-C6-O6   | -8.53 | 123.48      | 128.60   |
| 27  | B8    | 1460 | U    | O4'-C1'-N1 | 8.53  | 115.03      | 108.20   |
| 1   | AA    | 1068 | G    | N1-C6-O6   | 8.53  | 125.02      | 119.90   |
| 1   | AA    | 1487 | G    | N1-C6-O6   | 8.53  | 125.02      | 119.90   |
| 1   | AA    | 489  | C    | O4'-C1'-N1 | 8.53  | 115.02      | 108.20   |
| 27  | B8    | 809  | G    | C5-C6-O6   | -8.53 | 123.48      | 128.60   |
| 1   | AA    | 972  | C    | O4'-C1'-N1 | 8.53  | 115.02      | 108.20   |
| 27  | B8    | 168  | G    | N1-C6-O6   | 8.53  | 125.02      | 119.90   |
| 27  | B8    | 512  | G    | N1-C6-O6   | 8.53  | 125.02      | 119.90   |
| 27  | B8    | 180  | G    | N1-C6-O6   | 8.53  | 125.02      | 119.90   |
| 27  | B8    | 559  | G    | C5-C6-O6   | -8.53 | 123.48      | 128.60   |
| 27  | B8    | 597  | G    | N1-C6-O6   | 8.53  | 125.02      | 119.90   |
| 27  | B8    | 2848 | G    | N1-C6-O6   | 8.53  | 125.02      | 119.90   |
| 1   | AA    | 124  | C    | O4'-C1'-N1 | 8.52  | 115.02      | 108.20   |
| 27  | B8    | 557  | C    | O4'-C1'-N1 | 8.52  | 115.02      | 108.20   |
| 1   | AA    | 639  | G    | C5-C6-O6   | -8.52 | 123.49      | 128.60   |
| 1   | AA    | 727  | G    | N1-C6-O6   | 8.52  | 125.01      | 119.90   |
| 27  | B8    | 494  | G    | N1-C6-O6   | 8.52  | 125.01      | 119.90   |
| 27  | B8    | 2816 | G    | N1-C6-O6   | 8.52  | 125.01      | 119.90   |
| 1   | AA    | 122  | G    | C5-C6-O6   | -8.52 | 123.49      | 128.60   |
| 1   | AA    | 376  | G    | N1-C6-O6   | 8.52  | 125.01      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 657  | U    | O4'-C1'-N1 | 8.52  | 115.01      | 108.20   |
| 1   | AA    | 1416 | G    | N1-C6-O6   | 8.52  | 125.01      | 119.90   |
| 27  | B8    | 530  | G    | N1-C6-O6   | 8.52  | 125.01      | 119.90   |
| 26  | B7    | 23   | G    | C5-C6-O6   | -8.51 | 123.49      | 128.60   |
| 27  | B8    | 881  | G    | N1-C6-O6   | 8.51  | 125.01      | 119.90   |
| 27  | B8    | 1252 | G    | N1-C6-O6   | 8.51  | 125.01      | 119.90   |
| 1   | AA    | 15   | G    | C5-C6-O6   | -8.51 | 123.49      | 128.60   |
| 1   | AA    | 741  | G    | N1-C6-O6   | 8.51  | 125.01      | 119.90   |
| 1   | AA    | 1516 | G    | N1-C6-O6   | 8.51  | 125.01      | 119.90   |
| 26  | B7    | 76   | G    | N1-C6-O6   | 8.51  | 125.01      | 119.90   |
| 27  | B8    | 1741 | C    | O4'-C1'-N1 | 8.51  | 115.01      | 108.20   |
| 27  | B8    | 1985 | C    | O4'-C1'-N1 | 8.51  | 115.01      | 108.20   |
| 27  | B8    | 2324 | U    | O4'-C1'-N1 | 8.51  | 115.01      | 108.20   |
| 3   | AV    | 1    | C    | O4'-C1'-N1 | 8.51  | 115.01      | 108.20   |
| 26  | B7    | 41   | G    | N1-C6-O6   | 8.51  | 125.01      | 119.90   |
| 27  | B8    | 2742 | G    | N1-C6-O6   | 8.51  | 125.01      | 119.90   |
| 27  | B8    | 1146 | C    | O4'-C1'-N1 | 8.51  | 115.01      | 108.20   |
| 27  | B8    | 2089 | C    | O4'-C1'-N1 | 8.51  | 115.00      | 108.20   |
| 27  | B8    | 93   | G    | N1-C6-O6   | 8.51  | 125.00      | 119.90   |
| 1   | AA    | 1279 | G    | N1-C6-O6   | 8.50  | 125.00      | 119.90   |
| 27  | B8    | 242  | G    | N1-C6-O6   | 8.50  | 125.00      | 119.90   |
| 27  | B8    | 366  | C    | O4'-C1'-N1 | 8.50  | 115.00      | 108.20   |
| 27  | B8    | 1315 | C    | O4'-C1'-N1 | 8.50  | 115.00      | 108.20   |
| 1   | AA    | 651  | C    | O4'-C1'-N1 | 8.50  | 115.00      | 108.20   |
| 27  | B8    | 55   | G    | N1-C6-O6   | 8.50  | 125.00      | 119.90   |
| 27  | B8    | 317  | G    | N1-C6-O6   | 8.50  | 125.00      | 119.90   |
| 27  | B8    | 1038 | G    | C5-C6-O6   | -8.50 | 123.50      | 128.60   |
| 1   | AA    | 810  | C    | O4'-C1'-N1 | 8.50  | 115.00      | 108.20   |
| 27  | B8    | 745  | G    | N1-C6-O6   | 8.50  | 125.00      | 119.90   |
| 1   | AA    | 1260 | G    | N1-C6-O6   | 8.50  | 125.00      | 119.90   |
| 27  | B8    | 413  | C    | O4'-C1'-N1 | 8.50  | 115.00      | 108.20   |
| 27  | B8    | 1585 | C    | O4'-C1'-N1 | 8.50  | 115.00      | 108.20   |
| 27  | B8    | 2032 | G    | N1-C6-O6   | 8.50  | 125.00      | 119.90   |
| 27  | B8    | 2056 | G    | C5-C6-O6   | -8.50 | 123.50      | 128.60   |
| 27  | B8    | 2083 | G    | N1-C6-O6   | 8.50  | 125.00      | 119.90   |
| 27  | B8    | 2466 | C    | O4'-C1'-N1 | 8.50  | 115.00      | 108.20   |
| 26  | B7    | 54   | G    | C5-C6-O6   | -8.49 | 123.50      | 128.60   |
| 27  | B8    | 1892 | C    | O4'-C1'-N1 | 8.49  | 115.00      | 108.20   |
| 27  | B8    | 2637 | U    | O4'-C1'-N1 | 8.49  | 115.00      | 108.20   |
| 27  | B8    | 442  | G    | C5-C6-O6   | -8.49 | 123.51      | 128.60   |
| 27  | B8    | 1355 | G    | N1-C6-O6   | 8.49  | 124.99      | 119.90   |
| 1   | AA    | 403  | C    | O4'-C1'-N1 | 8.49  | 114.99      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 388  | G    | N1-C6-O6   | 8.49  | 124.99      | 119.90   |
| 27  | B8    | 737  | C    | O4'-C1'-N1 | 8.49  | 114.99      | 108.20   |
| 27  | B8    | 2481 | G    | N1-C6-O6   | 8.49  | 124.99      | 119.90   |
| 1   | AA    | 457  | G    | C5-C6-O6   | -8.48 | 123.51      | 128.60   |
| 1   | AA    | 879  | C    | O4'-C1'-N1 | 8.48  | 114.99      | 108.20   |
| 27  | B8    | 1440 | U    | O4'-C1'-N1 | 8.48  | 114.99      | 108.20   |
| 1   | AA    | 260  | G    | N1-C6-O6   | 8.48  | 124.99      | 119.90   |
| 27  | B8    | 1197 | G    | N1-C6-O6   | 8.48  | 124.99      | 119.90   |
| 27  | B8    | 1529 | G    | N1-C6-O6   | 8.48  | 124.99      | 119.90   |
| 1   | AA    | 658  | C    | O4'-C1'-N1 | 8.48  | 114.98      | 108.20   |
| 1   | AA    | 1524 | C    | O4'-C1'-N1 | 8.48  | 114.98      | 108.20   |
| 26  | B7    | 33   | G    | C5-C6-O6   | -8.48 | 123.51      | 128.60   |
| 1   | AA    | 322  | C    | O4'-C1'-N1 | 8.48  | 114.98      | 108.20   |
| 1   | AA    | 1405 | G    | C5-C6-O6   | -8.48 | 123.51      | 128.60   |
| 27  | B8    | 398  | C    | O4'-C1'-N1 | 8.48  | 114.98      | 108.20   |
| 1   | AA    | 302  | G    | C5-C6-O6   | -8.47 | 123.52      | 128.60   |
| 27  | B8    | 1817 | G    | N1-C6-O6   | 8.47  | 124.98      | 119.90   |
| 1   | AA    | 1421 | G    | N1-C6-O6   | 8.47  | 124.98      | 119.90   |
| 26  | B7    | 56   | G    | N1-C6-O6   | 8.47  | 124.98      | 119.90   |
| 27  | B8    | 2444 | G    | N1-C6-O6   | 8.47  | 124.98      | 119.90   |
| 1   | AA    | 832  | G    | N1-C6-O6   | 8.47  | 124.98      | 119.90   |
| 1   | AA    | 1077 | G    | N1-C6-O6   | 8.47  | 124.98      | 119.90   |
| 27  | B8    | 1233 | C    | O4'-C1'-N1 | 8.47  | 114.98      | 108.20   |
| 27  | B8    | 1867 | G    | N1-C6-O6   | 8.47  | 124.98      | 119.90   |
| 1   | AA    | 22   | G    | C5-C6-O6   | -8.47 | 123.52      | 128.60   |
| 27  | B8    | 1447 | C    | O4'-C1'-N1 | 8.47  | 114.97      | 108.20   |
| 27  | B8    | 333  | G    | N1-C6-O6   | 8.47  | 124.98      | 119.90   |
| 27  | B8    | 1492 | G    | C5-C6-O6   | -8.47 | 123.52      | 128.60   |
| 27  | B8    | 1543 | G    | N1-C6-O6   | 8.47  | 124.98      | 119.90   |
| 27  | B8    | 1686 | C    | O4'-C1'-N1 | 8.47  | 114.97      | 108.20   |
| 27  | B8    | 2627 | G    | N1-C6-O6   | 8.47  | 124.98      | 119.90   |
| 1   | AA    | 258  | G    | C5-C6-O6   | -8.47 | 123.52      | 128.60   |
| 1   | AA    | 942  | G    | N1-C6-O6   | 8.46  | 124.98      | 119.90   |
| 27  | B8    | 2035 | G    | N1-C6-O6   | 8.46  | 124.98      | 119.90   |
| 1   | AA    | 380  | G    | N1-C6-O6   | 8.46  | 124.98      | 119.90   |
| 27  | B8    | 1515 | A    | N1-C6-N6   | 8.46  | 123.68      | 118.60   |
| 1   | AA    | 1369 | C    | O4'-C1'-N1 | 8.46  | 114.97      | 108.20   |
| 27  | B8    | 696  | G    | N1-C6-O6   | 8.46  | 124.97      | 119.90   |
| 27  | B8    | 1236 | G    | N1-C6-O6   | 8.46  | 124.97      | 119.90   |
| 27  | B8    | 1983 | G    | N1-C6-O6   | 8.46  | 124.97      | 119.90   |
| 1   | AA    | 248  | C    | O4'-C1'-N1 | 8.46  | 114.96      | 108.20   |
| 27  | B8    | 2694 | G    | C5-C6-O6   | -8.46 | 123.53      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 450  | G    | N1-C6-O6   | 8.45  | 124.97      | 119.90   |
| 27  | B8    | 777  | G    | C5-C6-O6   | -8.46 | 123.53      | 128.60   |
| 1   | AA    | 785  | G    | C5-C6-O6   | -8.45 | 123.53      | 128.60   |
| 1   | AA    | 1453 | G    | N1-C6-O6   | 8.45  | 124.97      | 119.90   |
| 27  | B8    | 1973 | G    | C5-C6-O6   | -8.45 | 123.53      | 128.60   |
| 27  | B8    | 2133 | G    | N1-C6-O6   | 8.45  | 124.97      | 119.90   |
| 27  | B8    | 2378 | A    | C4-C5-C6   | 8.45  | 121.23      | 117.00   |
| 1   | AA    | 488  | C    | O4'-C1'-N1 | 8.45  | 114.96      | 108.20   |
| 27  | B8    | 814  | C    | O4'-C1'-N1 | 8.45  | 114.96      | 108.20   |
| 27  | B8    | 1896 | G    | C5-C6-O6   | -8.45 | 123.53      | 128.60   |
| 27  | B8    | 396  | G    | C5-C6-O6   | -8.44 | 123.53      | 128.60   |
| 27  | B8    | 1964 | G    | C5-C6-O6   | -8.44 | 123.53      | 128.60   |
| 27  | B8    | 1423 | G    | N1-C6-O6   | 8.44  | 124.97      | 119.90   |
| 27  | B8    | 1401 | G    | N1-C6-O6   | 8.44  | 124.97      | 119.90   |
| 27  | B8    | 1541 | C    | O4'-C1'-N1 | 8.44  | 114.95      | 108.20   |
| 27  | B8    | 2624 | G    | C5-C6-O6   | -8.44 | 123.53      | 128.60   |
| 1   | AA    | 4    | U    | O4'-C1'-N1 | 8.44  | 114.95      | 108.20   |
| 27  | B8    | 2269 | G    | N1-C6-O6   | 8.44  | 124.96      | 119.90   |
| 27  | B8    | 2437 | G    | C5-C6-O6   | -8.44 | 123.54      | 128.60   |
| 27  | B8    | 2594 | C    | O4'-C1'-N1 | 8.44  | 114.95      | 108.20   |
| 27  | B8    | 2597 | G    | N1-C6-O6   | 8.44  | 124.96      | 119.90   |
| 1   | AA    | 235  | C    | O4'-C1'-N1 | 8.44  | 114.95      | 108.20   |
| 1   | AA    | 486  | U    | O4'-C1'-N1 | 8.44  | 114.95      | 108.20   |
| 27  | B8    | 1843 | C    | O4'-C1'-N1 | 8.44  | 114.95      | 108.20   |
| 27  | B8    | 2512 | C    | O4'-C1'-N1 | 8.44  | 114.95      | 108.20   |
| 1   | AA    | 1384 | C    | O4'-C1'-N1 | 8.44  | 114.95      | 108.20   |
| 3   | AV    | 68   | G    | N1-C6-O6   | 8.44  | 124.96      | 119.90   |
| 27  | B8    | 1682 | G    | C5-C6-O6   | -8.44 | 123.54      | 128.60   |
| 27  | B8    | 192  | C    | O4'-C1'-N1 | 8.43  | 114.94      | 108.20   |
| 27  | B8    | 2214 | C    | O4'-C1'-N1 | 8.43  | 114.95      | 108.20   |
| 1   | AA    | 168  | G    | C5-C6-O6   | -8.43 | 123.54      | 128.60   |
| 1   | AA    | 1505 | G    | N1-C6-O6   | 8.43  | 124.96      | 119.90   |
| 1   | AA    | 1018 | G    | N1-C6-O6   | 8.43  | 124.96      | 119.90   |
| 1   | AA    | 1265 | C    | O4'-C1'-N1 | 8.43  | 114.94      | 108.20   |
| 1   | AA    | 259  | G    | C5-C6-O6   | -8.43 | 123.55      | 128.60   |
| 1   | AA    | 941  | G    | N1-C6-O6   | 8.43  | 124.95      | 119.90   |
| 1   | AA    | 257  | G    | N1-C6-O6   | 8.42  | 124.95      | 119.90   |
| 1   | AA    | 650  | G    | N1-C6-O6   | 8.42  | 124.95      | 119.90   |
| 1   | AA    | 1175 | G    | N1-C6-O6   | 8.42  | 124.95      | 119.90   |
| 27  | B8    | 16   | C    | O4'-C1'-N1 | 8.42  | 114.94      | 108.20   |
| 27  | B8    | 679  | C    | O4'-C1'-N1 | 8.42  | 114.94      | 108.20   |
| 27  | B8    | 1947 | C    | O4'-C1'-N1 | 8.42  | 114.94      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 38   | G    | N1-C6-O6   | 8.42  | 124.95      | 119.90   |
| 27  | B8    | 2858 | C    | O4'-C1'-N1 | 8.42  | 114.94      | 108.20   |
| 1   | AA    | 440  | C    | O4'-C1'-N1 | 8.42  | 114.94      | 108.20   |
| 1   | AA    | 931  | C    | O4'-C1'-N1 | 8.42  | 114.94      | 108.20   |
| 1   | AA    | 326  | G    | N1-C6-O6   | 8.41  | 124.95      | 119.90   |
| 1   | AA    | 800  | G    | N1-C6-O6   | 8.41  | 124.95      | 119.90   |
| 27  | B8    | 880  | G    | N1-C6-O6   | 8.41  | 124.95      | 119.90   |
| 27  | B8    | 1180 | U    | O4'-C1'-N1 | 8.41  | 114.93      | 108.20   |
| 27  | B8    | 935  | C    | O4'-C1'-N1 | 8.41  | 114.93      | 108.20   |
| 27  | B8    | 2576 | G    | N1-C6-O6   | 8.41  | 124.95      | 119.90   |
| 1   | AA    | 215  | C    | O4'-C1'-N1 | 8.41  | 114.93      | 108.20   |
| 1   | AA    | 614  | C    | O4'-C1'-N1 | 8.41  | 114.93      | 108.20   |
| 26  | B7    | 97   | C    | O4'-C1'-N1 | 8.41  | 114.93      | 108.20   |
| 27  | B8    | 1239 | G    | C5-C6-O6   | -8.41 | 123.55      | 128.60   |
| 27  | B8    | 316  | C    | O4'-C1'-N1 | 8.41  | 114.93      | 108.20   |
| 27  | B8    | 1017 | G    | N1-C6-O6   | 8.41  | 124.94      | 119.90   |
| 27  | B8    | 1061 | U    | C2-N1-C1'  | 8.41  | 127.79      | 117.70   |
| 27  | B8    | 1183 | U    | O4'-C1'-N1 | 8.41  | 114.93      | 108.20   |
| 1   | AA    | 1058 | G    | C5-C6-O6   | -8.41 | 123.56      | 128.60   |
| 27  | B8    | 2361 | G    | N1-C6-O6   | 8.41  | 124.94      | 119.90   |
| 1   | AA    | 86   | G    | N1-C6-O6   | 8.40  | 124.94      | 119.90   |
| 27  | B8    | 1695 | G    | N1-C6-O6   | 8.40  | 124.94      | 119.90   |
| 27  | B8    | 2874 | C    | O4'-C1'-N1 | 8.40  | 114.92      | 108.20   |
| 1   | AA    | 812  | G    | C5-C6-O6   | -8.40 | 123.56      | 128.60   |
| 1   | AA    | 1338 | G    | N1-C6-O6   | 8.40  | 124.94      | 119.90   |
| 27  | B8    | 315  | G    | N1-C6-O6   | 8.40  | 124.94      | 119.90   |
| 27  | B8    | 486  | C    | O4'-C1'-N1 | 8.40  | 114.92      | 108.20   |
| 27  | B8    | 2294 | G    | N1-C6-O6   | 8.40  | 124.94      | 119.90   |
| 27  | B8    | 2414 | G    | C5-C6-O6   | -8.40 | 123.56      | 128.60   |
| 27  | B8    | 564  | C    | O4'-C1'-N1 | 8.40  | 114.92      | 108.20   |
| 27  | B8    | 765  | C    | O4'-C1'-N1 | 8.40  | 114.92      | 108.20   |
| 27  | B8    | 1957 | C    | O4'-C1'-N1 | 8.40  | 114.92      | 108.20   |
| 27  | B8    | 491  | G    | N1-C6-O6   | 8.40  | 124.94      | 119.90   |
| 27  | B8    | 948  | C    | O4'-C1'-N1 | 8.40  | 114.92      | 108.20   |
| 27  | B8    | 2055 | C    | O4'-C1'-N1 | 8.40  | 114.92      | 108.20   |
| 27  | B8    | 2332 | C    | O4'-C1'-N1 | 8.40  | 114.92      | 108.20   |
| 27  | B8    | 2591 | C    | O4'-C1'-N1 | 8.39  | 114.92      | 108.20   |
| 27  | B8    | 2644 | G    | N1-C6-O6   | 8.39  | 124.94      | 119.90   |
| 1   | AA    | 201  | G    | N1-C6-O6   | 8.39  | 124.94      | 119.90   |
| 27  | B8    | 2842 | G    | N1-C6-O6   | 8.39  | 124.94      | 119.90   |
| 1   | AA    | 1154 | G    | C5-C6-O6   | -8.39 | 123.56      | 128.60   |
| 27  | B8    | 2421 | G    | C5-C6-O6   | -8.39 | 123.56      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1217 | C    | O4'-C1'-N1 | 8.39  | 114.91      | 108.20   |
| 27  | B8    | 2124 | G    | C5-C6-O6   | -8.39 | 123.57      | 128.60   |
| 27  | B8    | 2215 | C    | O4'-C1'-N1 | 8.39  | 114.91      | 108.20   |
| 26  | B7    | 118  | C    | O4'-C1'-N1 | 8.39  | 114.91      | 108.20   |
| 27  | B8    | 1587 | G    | N1-C6-O6   | 8.39  | 124.93      | 119.90   |
| 27  | B8    | 1908 | C    | O4'-C1'-N1 | 8.39  | 114.91      | 108.20   |
| 27  | B8    | 2177 | C    | O4'-C1'-N1 | 8.38  | 114.91      | 108.20   |
| 27  | B8    | 2264 | C    | O4'-C1'-N1 | 8.38  | 114.91      | 108.20   |
| 1   | AA    | 818  | G    | N1-C6-O6   | 8.38  | 124.93      | 119.90   |
| 3   | AV    | 19   | G    | N1-C6-O6   | 8.38  | 124.93      | 119.90   |
| 27  | B8    | 830  | G    | N1-C6-O6   | 8.38  | 124.93      | 119.90   |
| 27  | B8    | 922  | C    | O4'-C1'-N1 | 8.38  | 114.91      | 108.20   |
| 27  | B8    | 1187 | G    | N1-C6-O6   | 8.38  | 124.93      | 119.90   |
| 27  | B8    | 1788 | C    | O4'-C1'-N1 | 8.38  | 114.91      | 108.20   |
| 27  | B8    | 2618 | G    | N1-C6-O6   | 8.38  | 124.93      | 119.90   |
| 27  | B8    | 2655 | G    | N1-C6-O6   | 8.38  | 124.93      | 119.90   |
| 1   | AA    | 1273 | C    | O4'-C1'-N1 | 8.38  | 114.90      | 108.20   |
| 1   | AA    | 693  | G    | N1-C6-O6   | 8.38  | 124.93      | 119.90   |
| 1   | AA    | 90   | C    | O4'-C1'-N1 | 8.38  | 114.90      | 108.20   |
| 1   | AA    | 1203 | C    | O4'-C1'-N1 | 8.38  | 114.90      | 108.20   |
| 27  | B8    | 951  | C    | O4'-C1'-N1 | 8.37  | 114.90      | 108.20   |
| 27  | B8    | 1743 | G    | C5-C6-O6   | -8.37 | 123.58      | 128.60   |
| 27  | B8    | 2774 | C    | O4'-C1'-N1 | 8.38  | 114.90      | 108.20   |
| 27  | B8    | 836  | G    | C5-C6-O6   | -8.37 | 123.58      | 128.60   |
| 27  | B8    | 662  | G    | C5-C6-O6   | -8.37 | 123.58      | 128.60   |
| 27  | B8    | 1704 | C    | O4'-C1'-N1 | 8.37  | 114.90      | 108.20   |
| 27  | B8    | 2048 | G    | N1-C6-O6   | 8.37  | 124.92      | 119.90   |
| 27  | B8    | 2397 | G    | N1-C6-O6   | 8.37  | 124.92      | 119.90   |
| 1   | AA    | 1382 | C    | O4'-C1'-N1 | 8.37  | 114.90      | 108.20   |
| 27  | B8    | 1935 | G    | N1-C6-O6   | 8.37  | 124.92      | 119.90   |
| 27  | B8    | 452  | G    | N1-C6-O6   | 8.37  | 124.92      | 119.90   |
| 27  | B8    | 1685 | C    | O4'-C1'-N1 | 8.37  | 114.89      | 108.20   |
| 27  | B8    | 1931 | U    | O4'-C1'-N1 | 8.36  | 114.89      | 108.20   |
| 1   | AA    | 211  | G    | N1-C6-O6   | 8.36  | 124.92      | 119.90   |
| 27  | B8    | 2683 | C    | O4'-C1'-N1 | 8.36  | 114.89      | 108.20   |
| 27  | B8    | 329  | G    | N1-C6-O6   | 8.36  | 124.92      | 119.90   |
| 27  | B8    | 1331 | G    | N1-C6-O6   | 8.36  | 124.92      | 119.90   |
| 27  | B8    | 2507 | C    | O4'-C1'-N1 | 8.36  | 114.89      | 108.20   |
| 3   | AV    | 36   | G    | N1-C6-O6   | 8.36  | 124.91      | 119.90   |
| 1   | AA    | 895  | G    | N1-C6-O6   | 8.35  | 124.91      | 119.90   |
| 1   | AA    | 1259 | C    | O4'-C1'-N1 | 8.35  | 114.88      | 108.20   |
| 26  | B7    | 81   | G    | C5-C6-O6   | -8.35 | 123.59      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1464 | G    | N1-C6-O6   | 8.35  | 124.91      | 119.90   |
| 1   | AA    | 97   | G    | N1-C6-O6   | 8.35  | 124.91      | 119.90   |
| 1   | AA    | 1361 | G    | N1-C6-O6   | 8.35  | 124.91      | 119.90   |
| 27  | B8    | 1967 | C    | O4'-C1'-N1 | 8.35  | 114.88      | 108.20   |
| 1   | AA    | 1049 | U    | P-O3'-C3'  | 8.35  | 129.72      | 119.70   |
| 1   | AA    | 1325 | C    | O4'-C1'-N1 | 8.35  | 114.88      | 108.20   |
| 27  | B8    | 20   | C    | O4'-C1'-N1 | 8.34  | 114.87      | 108.20   |
| 27  | B8    | 194  | G    | C5-C6-O6   | -8.34 | 123.59      | 128.60   |
| 27  | B8    | 795  | C    | O4'-C1'-N1 | 8.34  | 114.87      | 108.20   |
| 27  | B8    | 1465 | G    | C5-C6-O6   | -8.34 | 123.59      | 128.60   |
| 27  | B8    | 2257 | U    | O4'-C1'-N1 | 8.34  | 114.87      | 108.20   |
| 27  | B8    | 929  | U    | O4'-C1'-N1 | 8.34  | 114.87      | 108.20   |
| 27  | B8    | 903  | C    | O4'-C1'-N1 | 8.34  | 114.87      | 108.20   |
| 27  | B8    | 1140 | C    | O4'-C1'-N1 | 8.34  | 114.87      | 108.20   |
| 27  | B8    | 1739 | A    | N1-C6-N6   | 8.34  | 123.60      | 118.60   |
| 1   | AA    | 582  | C    | O4'-C1'-N1 | 8.34  | 114.87      | 108.20   |
| 1   | AA    | 613  | C    | O4'-C1'-N1 | 8.34  | 114.87      | 108.20   |
| 1   | AA    | 1016 | A    | C4-C5-C6   | 8.34  | 121.17      | 117.00   |
| 27  | B8    | 2282 | G    | N1-C6-O6   | 8.34  | 124.90      | 119.90   |
| 27  | B8    | 1184 | U    | O4'-C1'-N1 | 8.34  | 114.87      | 108.20   |
| 27  | B8    | 846  | U    | O4'-C1'-N1 | 8.33  | 114.87      | 108.20   |
| 27  | B8    | 1122 | G    | N1-C6-O6   | 8.33  | 124.90      | 119.90   |
| 27  | B8    | 1026 | G    | N1-C6-O6   | 8.33  | 124.90      | 119.90   |
| 3   | AV    | 65   | C    | O4'-C1'-N1 | 8.33  | 114.86      | 108.20   |
| 27  | B8    | 1370 | C    | O4'-C1'-N1 | 8.33  | 114.86      | 108.20   |
| 27  | B8    | 690  | G    | N1-C6-O6   | 8.33  | 124.90      | 119.90   |
| 1   | AA    | 1461 | G    | N1-C6-O6   | 8.33  | 124.90      | 119.90   |
| 27  | B8    | 260  | G    | C5-C6-O6   | -8.33 | 123.60      | 128.60   |
| 27  | B8    | 897  | C    | O4'-C1'-N1 | 8.33  | 114.86      | 108.20   |
| 26  | B7    | 38   | C    | O4'-C1'-N1 | 8.32  | 114.86      | 108.20   |
| 27  | B8    | 700  | G    | C5-C6-O6   | -8.32 | 123.61      | 128.60   |
| 27  | B8    | 748  | G    | N1-C6-O6   | 8.32  | 124.89      | 119.90   |
| 27  | B8    | 1114 | C    | O4'-C1'-N1 | 8.32  | 114.86      | 108.20   |
| 1   | AA    | 1164 | G    | C5-C6-O6   | -8.32 | 123.61      | 128.60   |
| 27  | B8    | 558  | U    | O4'-C1'-N1 | 8.32  | 114.86      | 108.20   |
| 27  | B8    | 2410 | G    | C5-C6-O6   | -8.32 | 123.61      | 128.60   |
| 27  | B8    | 684  | G    | N1-C6-O6   | 8.32  | 124.89      | 119.90   |
| 3   | AV    | 50   | G    | N1-C6-O6   | 8.32  | 124.89      | 119.90   |
| 27  | B8    | 2140 | G    | C5-C6-O6   | -8.32 | 123.61      | 128.60   |
| 1   | AA    | 304  | U    | O4'-C1'-N1 | 8.31  | 114.85      | 108.20   |
| 1   | AA    | 1148 | U    | O4'-C1'-N1 | 8.31  | 114.85      | 108.20   |
| 1   | AA    | 1344 | C    | O4'-C1'-N1 | 8.31  | 114.85      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1362 | C    | O4'-C1'-N1 | 8.31  | 114.85      | 108.20   |
| 1   | AA    | 1268 | G    | N1-C6-O6   | 8.31  | 124.89      | 119.90   |
| 1   | AA    | 842  | U    | O4'-C1'-N1 | 8.31  | 114.85      | 108.20   |
| 1   | AA    | 1515 | G    | C5-C6-O6   | -8.31 | 123.61      | 128.60   |
| 27  | B8    | 2224 | G    | N1-C6-O6   | 8.31  | 124.89      | 119.90   |
| 27  | B8    | 1769 | U    | O4'-C1'-N1 | 8.31  | 114.85      | 108.20   |
| 27  | B8    | 2595 | G    | N1-C6-O6   | 8.31  | 124.89      | 119.90   |
| 1   | AA    | 21   | G    | N1-C6-O6   | 8.30  | 124.88      | 119.90   |
| 1   | AA    | 936  | C    | O4'-C1'-N1 | 8.30  | 114.84      | 108.20   |
| 27  | B8    | 1153 | C    | O4'-C1'-N1 | 8.31  | 114.84      | 108.20   |
| 1   | AA    | 1038 | C    | O4'-C1'-N1 | 8.30  | 114.84      | 108.20   |
| 1   | AA    | 1355 | G    | N1-C6-O6   | 8.30  | 124.88      | 119.90   |
| 27  | B8    | 97   | C    | O4'-C1'-N1 | 8.30  | 114.84      | 108.20   |
| 27  | B8    | 112  | U    | O4'-C1'-N1 | 8.30  | 114.84      | 108.20   |
| 27  | B8    | 210  | C    | O4'-C1'-N1 | 8.30  | 114.84      | 108.20   |
| 27  | B8    | 350  | G    | C5-C6-O6   | -8.30 | 123.62      | 128.60   |
| 27  | B8    | 784  | G    | O4'-C1'-N9 | 8.30  | 114.84      | 108.20   |
| 27  | B8    | 977  | G    | C5-C6-O6   | -8.30 | 123.62      | 128.60   |
| 27  | B8    | 1575 | C    | O4'-C1'-N1 | 8.30  | 114.84      | 108.20   |
| 27  | B8    | 2010 | G    | N1-C6-O6   | 8.30  | 124.88      | 119.90   |
| 1   | AA    | 6    | G    | N1-C6-O6   | 8.30  | 124.88      | 119.90   |
| 26  | B7    | 10   | G    | C5-C6-O6   | -8.30 | 123.62      | 128.60   |
| 27  | B8    | 186  | G    | C5-C6-O6   | -8.30 | 123.62      | 128.60   |
| 27  | B8    | 1605 | C    | O4'-C1'-N1 | 8.30  | 114.84      | 108.20   |
| 27  | B8    | 2839 | G    | C5-C6-O6   | -8.30 | 123.62      | 128.60   |
| 27  | B8    | 854  | C    | O4'-C1'-N1 | 8.30  | 114.84      | 108.20   |
| 27  | B8    | 870  | U    | O4'-C1'-N1 | 8.30  | 114.84      | 108.20   |
| 27  | B8    | 1874 | C    | O4'-C1'-N1 | 8.30  | 114.84      | 108.20   |
| 26  | B7    | 60   | C    | O4'-C1'-N1 | 8.30  | 114.84      | 108.20   |
| 27  | B8    | 1300 | G    | N1-C6-O6   | 8.30  | 124.88      | 119.90   |
| 27  | B8    | 2067 | G    | N1-C6-O6   | 8.30  | 124.88      | 119.90   |
| 1   | AA    | 268  | U    | O4'-C1'-N1 | 8.29  | 114.83      | 108.20   |
| 1   | AA    | 45   | G    | C5-C6-O6   | -8.29 | 123.62      | 128.60   |
| 1   | AA    | 633  | G    | N1-C6-O6   | 8.29  | 124.88      | 119.90   |
| 1   | AA    | 882  | C    | O4'-C1'-N1 | 8.29  | 114.83      | 108.20   |
| 1   | AA    | 910  | C    | O4'-C1'-N1 | 8.29  | 114.83      | 108.20   |
| 1   | AA    | 985  | C    | O4'-C1'-N1 | 8.29  | 114.83      | 108.20   |
| 27  | B8    | 2350 | C    | O4'-C1'-N1 | 8.29  | 114.83      | 108.20   |
| 1   | AA    | 379  | C    | O4'-C1'-N1 | 8.29  | 114.83      | 108.20   |
| 27  | B8    | 1056 | G    | N1-C6-O6   | 8.29  | 124.87      | 119.90   |
| 27  | B8    | 1737 | G    | N1-C6-O6   | 8.29  | 124.87      | 119.90   |
| 27  | B8    | 2417 | C    | O4'-C1'-N1 | 8.29  | 114.83      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2803 | G    | C5-C6-O6   | -8.29 | 123.63      | 128.60   |
| 1   | AA    | 594  | U    | O4'-C1'-N1 | 8.28  | 114.83      | 108.20   |
| 1   | AA    | 216  | U    | O4'-C1'-N1 | 8.28  | 114.83      | 108.20   |
| 1   | AA    | 519  | C    | O4'-C1'-N1 | 8.28  | 114.83      | 108.20   |
| 27  | B8    | 1613 | G    | N1-C6-O6   | 8.28  | 124.87      | 119.90   |
| 1   | AA    | 57   | G    | C5-C6-O6   | -8.28 | 123.63      | 128.60   |
| 1   | AA    | 1026 | G    | C5-C6-O6   | -8.28 | 123.63      | 128.60   |
| 27  | B8    | 1391 | U    | O4'-C1'-N1 | 8.28  | 114.82      | 108.20   |
| 27  | B8    | 2222 | C    | O4'-C1'-N1 | 8.28  | 114.82      | 108.20   |
| 1   | AA    | 838  | G    | C5-C6-O6   | -8.28 | 123.64      | 128.60   |
| 27  | B8    | 312  | G    | C5-C6-O6   | -8.28 | 123.64      | 128.60   |
| 27  | B8    | 875  | G    | C5-C6-O6   | -8.28 | 123.64      | 128.60   |
| 27  | B8    | 2023 | C    | O4'-C1'-N1 | 8.28  | 114.82      | 108.20   |
| 27  | B8    | 2304 | G    | C5-C6-O6   | -8.28 | 123.63      | 128.60   |
| 27  | B8    | 2640 | G    | C5-C6-O6   | -8.28 | 123.64      | 128.60   |
| 27  | B8    | 2855 | C    | O4'-C1'-N1 | 8.28  | 114.82      | 108.20   |
| 1   | AA    | 627  | G    | C5-C6-O6   | -8.27 | 123.64      | 128.60   |
| 27  | B8    | 185  | G    | C5-C6-O6   | -8.27 | 123.64      | 128.60   |
| 27  | B8    | 326  | G    | C5-C6-O6   | -8.27 | 123.64      | 128.60   |
| 27  | B8    | 2391 | G    | N1-C6-O6   | 8.27  | 124.86      | 119.90   |
| 1   | AA    | 254  | G    | N1-C6-O6   | 8.27  | 124.86      | 119.90   |
| 27  | B8    | 2400 | G    | C5-C6-O6   | -8.27 | 123.64      | 128.60   |
| 27  | B8    | 2649 | C    | O4'-C1'-N1 | 8.27  | 114.82      | 108.20   |
| 1   | AA    | 557  | G    | N1-C6-O6   | 8.27  | 124.86      | 119.90   |
| 1   | AA    | 1239 | A    | N1-C6-N6   | 8.27  | 123.56      | 118.60   |
| 27  | B8    | 853  | C    | O4'-C1'-N1 | 8.27  | 114.82      | 108.20   |
| 27  | B8    | 985  | C    | O4'-C1'-N1 | 8.27  | 114.82      | 108.20   |
| 27  | B8    | 1167 | C    | O4'-C1'-N1 | 8.27  | 114.82      | 108.20   |
| 1   | AA    | 689  | C    | O4'-C1'-N1 | 8.27  | 114.81      | 108.20   |
| 27  | B8    | 816  | C    | O4'-C1'-N1 | 8.27  | 114.82      | 108.20   |
| 1   | AA    | 1517 | G    | N1-C6-O6   | 8.27  | 124.86      | 119.90   |
| 1   | AA    | 1520 | C    | O4'-C1'-N1 | 8.27  | 114.81      | 108.20   |
| 3   | AV    | 75   | C    | O4'-C1'-N1 | 8.27  | 114.82      | 108.20   |
| 27  | B8    | 208  | C    | O4'-C1'-N1 | 8.27  | 114.81      | 108.20   |
| 27  | B8    | 2285 | C    | O4'-C1'-N1 | 8.27  | 114.81      | 108.20   |
| 27  | B8    | 26   | G    | N1-C6-O6   | 8.27  | 124.86      | 119.90   |
| 27  | B8    | 2620 | C    | O4'-C1'-N1 | 8.27  | 114.81      | 108.20   |
| 27  | B8    | 987  | C    | O4'-C1'-N1 | 8.26  | 114.81      | 108.20   |
| 27  | B8    | 2574 | G    | C5-C6-O6   | -8.26 | 123.64      | 128.60   |
| 27  | B8    | 137  | U    | O4'-C1'-N1 | 8.26  | 114.81      | 108.20   |
| 1   | AA    | 385  | C    | O4'-C1'-N1 | 8.26  | 114.81      | 108.20   |
| 1   | AA    | 1495 | U    | O4'-C1'-N1 | 8.26  | 114.81      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 409  | U    | O4'-C1'-N1 | 8.26  | 114.81      | 108.20   |
| 1   | AA    | 1071 | C    | O4'-C1'-N1 | 8.26  | 114.81      | 108.20   |
| 27  | B8    | 36   | G    | N1-C6-O6   | 8.26  | 124.86      | 119.90   |
| 27  | B8    | 1826 | G    | C5-C6-O6   | -8.26 | 123.64      | 128.60   |
| 1   | AA    | 755  | G    | C5-C6-O6   | -8.26 | 123.64      | 128.60   |
| 1   | AA    | 1371 | G    | N1-C6-O6   | 8.26  | 124.85      | 119.90   |
| 26  | B7    | 92   | C    | O4'-C1'-N1 | 8.26  | 114.81      | 108.20   |
| 1   | AA    | 823  | C    | O4'-C1'-N1 | 8.25  | 114.80      | 108.20   |
| 27  | B8    | 129  | C    | O4'-C1'-N1 | 8.25  | 114.80      | 108.20   |
| 27  | B8    | 1573 | G    | N1-C6-O6   | 8.25  | 124.85      | 119.90   |
| 1   | AA    | 756  | C    | O4'-C1'-N1 | 8.25  | 114.80      | 108.20   |
| 1   | AA    | 898  | G    | N1-C6-O6   | 8.25  | 124.85      | 119.90   |
| 26  | B7    | 63   | C    | O4'-C1'-N1 | 8.25  | 114.80      | 108.20   |
| 27  | B8    | 1980 | G    | N1-C6-O6   | 8.25  | 124.85      | 119.90   |
| 1   | AA    | 319  | G    | C5-C6-O6   | -8.24 | 123.65      | 128.60   |
| 1   | AA    | 455  | G    | C5-C6-O6   | -8.24 | 123.65      | 128.60   |
| 1   | AA    | 580  | C    | O4'-C1'-N1 | 8.24  | 114.80      | 108.20   |
| 27  | B8    | 201  | C    | O4'-C1'-N1 | 8.24  | 114.80      | 108.20   |
| 1   | AA    | 732  | C    | O4'-C1'-N1 | 8.24  | 114.79      | 108.20   |
| 27  | B8    | 687  | C    | O4'-C1'-N1 | 8.24  | 114.79      | 108.20   |
| 27  | B8    | 1547 | C    | O4'-C1'-N1 | 8.24  | 114.79      | 108.20   |
| 1   | AA    | 999  | C    | O4'-C1'-N1 | 8.24  | 114.79      | 108.20   |
| 27  | B8    | 121  | G    | C5-C6-O6   | -8.24 | 123.66      | 128.60   |
| 27  | B8    | 409  | G    | C5-C6-O6   | -8.24 | 123.66      | 128.60   |
| 27  | B8    | 1270 | C    | O4'-C1'-N1 | 8.24  | 114.79      | 108.20   |
| 27  | B8    | 2217 | G    | C5-C6-O6   | -8.24 | 123.66      | 128.60   |
| 26  | B7    | 9    | G    | C5-C6-O6   | -8.24 | 123.66      | 128.60   |
| 27  | B8    | 539  | G    | N1-C6-O6   | 8.24  | 124.84      | 119.90   |
| 27  | B8    | 2362 | C    | O4'-C1'-N1 | 8.24  | 114.79      | 108.20   |
| 27  | B8    | 2704 | C    | O4'-C1'-N1 | 8.24  | 114.79      | 108.20   |
| 1   | AA    | 778  | G    | C5-C6-O6   | -8.23 | 123.66      | 128.60   |
| 3   | AV    | 67   | C    | O4'-C1'-N1 | 8.23  | 114.79      | 108.20   |
| 27  | B8    | 2559 | C    | O4'-C1'-N1 | 8.23  | 114.79      | 108.20   |
| 1   | AA    | 105  | G    | C5-C6-O6   | -8.23 | 123.66      | 128.60   |
| 27  | B8    | 1191 | G    | C5-C6-O6   | -8.23 | 123.66      | 128.60   |
| 1   | AA    | 764  | C    | O4'-C1'-N1 | 8.23  | 114.78      | 108.20   |
| 27  | B8    | 1540 | G    | C5-C6-O6   | -8.23 | 123.66      | 128.60   |
| 1   | AA    | 1266 | G    | N1-C6-O6   | 8.23  | 124.84      | 119.90   |
| 27  | B8    | 109  | C    | O4'-C1'-N1 | 8.23  | 114.78      | 108.20   |
| 27  | B8    | 968  | C    | O4'-C1'-N1 | 8.23  | 114.78      | 108.20   |
| 1   | AA    | 899  | C    | O4'-C1'-N1 | 8.23  | 114.78      | 108.20   |
| 27  | B8    | 954  | G    | C5-C6-O6   | -8.23 | 123.66      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2648 | G    | C5-C6-O6   | -8.23 | 123.66      | 128.60   |
| 27  | B8    | 2896 | C    | O4'-C1'-N1 | 8.23  | 114.78      | 108.20   |
| 27  | B8    | 2715 | C    | O4'-C1'-N1 | 8.23  | 114.78      | 108.20   |
| 1   | AA    | 269  | C    | O4'-C1'-N1 | 8.22  | 114.78      | 108.20   |
| 27  | B8    | 355  | U    | O4'-C1'-N1 | 8.22  | 114.78      | 108.20   |
| 27  | B8    | 1961 | C    | O4'-C1'-N1 | 8.22  | 114.78      | 108.20   |
| 1   | AA    | 668  | G    | C5-C6-O6   | -8.22 | 123.67      | 128.60   |
| 27  | B8    | 2641 | G    | C5-C6-O6   | -8.22 | 123.67      | 128.60   |
| 27  | B8    | 465  | G    | N1-C6-O6   | 8.22  | 124.83      | 119.90   |
| 27  | B8    | 673  | C    | O4'-C1'-N1 | 8.21  | 114.77      | 108.20   |
| 27  | B8    | 2380 | C    | O4'-C1'-N1 | 8.21  | 114.77      | 108.20   |
| 1   | AA    | 291  | U    | O4'-C1'-N1 | 8.21  | 114.77      | 108.20   |
| 1   | AA    | 392  | C    | O4'-C1'-N1 | 8.21  | 114.77      | 108.20   |
| 27  | B8    | 879  | G    | N1-C6-O6   | 8.21  | 124.83      | 119.90   |
| 26  | B7    | 110  | C    | O4'-C1'-N1 | 8.21  | 114.77      | 108.20   |
| 1   | AA    | 1002 | G    | C5-C6-O6   | -8.21 | 123.67      | 128.60   |
| 26  | B7    | 90   | C    | O4'-C1'-N1 | 8.21  | 114.77      | 108.20   |
| 27  | B8    | 54   | G    | N1-C6-O6   | 8.21  | 124.83      | 119.90   |
| 27  | B8    | 245  | G    | C5-C6-O6   | -8.21 | 123.67      | 128.60   |
| 27  | B8    | 1837 | C    | O4'-C1'-N1 | 8.21  | 114.77      | 108.20   |
| 1   | AA    | 85   | U    | O4'-C1'-N1 | 8.20  | 114.76      | 108.20   |
| 1   | AA    | 286  | C    | O4'-C1'-N1 | 8.20  | 114.76      | 108.20   |
| 1   | AA    | 232  | G    | N1-C6-O6   | 8.20  | 124.82      | 119.90   |
| 1   | AA    | 731  | G    | C5-C6-O6   | -8.20 | 123.68      | 128.60   |
| 1   | AA    | 1352 | C    | O4'-C1'-N1 | 8.20  | 114.76      | 108.20   |
| 27  | B8    | 81   | G    | C5-C6-O6   | -8.20 | 123.68      | 128.60   |
| 27  | B8    | 2819 | G    | C5-C6-O6   | -8.20 | 123.68      | 128.60   |
| 1   | AA    | 138  | G    | C5-C6-O6   | -8.20 | 123.68      | 128.60   |
| 1   | AA    | 853  | C    | O4'-C1'-N1 | 8.20  | 114.76      | 108.20   |
| 27  | B8    | 331  | C    | O4'-C1'-N1 | 8.20  | 114.76      | 108.20   |
| 27  | B8    | 476  | G    | N1-C6-O6   | 8.20  | 124.82      | 119.90   |
| 27  | B8    | 2057 | G    | C5-C6-O6   | -8.19 | 123.68      | 128.60   |
| 27  | B8    | 2185 | U    | O4'-C1'-N1 | 8.19  | 114.76      | 108.20   |
| 27  | B8    | 2424 | C    | O4'-C1'-N1 | 8.19  | 114.75      | 108.20   |
| 27  | B8    | 2801 | G    | C5-C6-O6   | -8.20 | 123.68      | 128.60   |
| 27  | B8    | 2588 | G    | C5-C6-O6   | -8.19 | 123.68      | 128.60   |
| 1   | AA    | 1328 | C    | O4'-C1'-N1 | 8.19  | 114.75      | 108.20   |
| 27  | B8    | 1293 | C    | O4'-C1'-N1 | 8.19  | 114.75      | 108.20   |
| 27  | B8    | 2557 | G    | C5-C6-O6   | -8.19 | 123.69      | 128.60   |
| 27  | B8    | 2722 | G    | C5-C6-O6   | -8.19 | 123.69      | 128.60   |
| 1   | AA    | 454  | G    | C5-C6-O6   | -8.19 | 123.69      | 128.60   |
| 27  | B8    | 611  | C    | O4'-C1'-N1 | 8.19  | 114.75      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1341 | G    | N1-C6-O6   | 8.19  | 124.81      | 119.90   |
| 27  | B8    | 2283 | C    | O4'-C1'-N1 | 8.19  | 114.75      | 108.20   |
| 1   | AA    | 1132 | C    | O4'-C1'-N1 | 8.19  | 114.75      | 108.20   |
| 27  | B8    | 2375 | G    | N1-C6-O6   | 8.19  | 124.81      | 119.90   |
| 1   | AA    | 998  | C    | O4'-C1'-N1 | 8.18  | 114.75      | 108.20   |
| 1   | AA    | 1320 | C    | O4'-C1'-N1 | 8.18  | 114.75      | 108.20   |
| 1   | AA    | 1414 | U    | O4'-C1'-N1 | 8.18  | 114.75      | 108.20   |
| 1   | AA    | 242  | G    | C5-C6-O6   | -8.18 | 123.69      | 128.60   |
| 1   | AA    | 786  | G    | C5-C6-O6   | -8.18 | 123.69      | 128.60   |
| 3   | AV    | 6    | C    | O4'-C1'-N1 | 8.18  | 114.75      | 108.20   |
| 27  | B8    | 1435 | G    | C5-C6-O6   | -8.18 | 123.69      | 128.60   |
| 1   | AA    | 1454 | G    | C5-C6-O6   | -8.18 | 123.69      | 128.60   |
| 27  | B8    | 425  | G    | C5-C6-O6   | -8.18 | 123.69      | 128.60   |
| 27  | B8    | 2581 | G    | N1-C6-O6   | 8.18  | 124.81      | 119.90   |
| 27  | B8    | 2631 | G    | C5-C6-O6   | -8.18 | 123.69      | 128.60   |
| 1   | AA    | 264  | C    | O4'-C1'-N1 | 8.18  | 114.74      | 108.20   |
| 1   | AA    | 1136 | C    | O4'-C1'-N1 | 8.18  | 114.74      | 108.20   |
| 27  | B8    | 496  | G    | C5-C6-O6   | -8.18 | 123.69      | 128.60   |
| 27  | B8    | 1858 | A    | N1-C6-N6   | 8.18  | 123.51      | 118.60   |
| 27  | B8    | 1463 | C    | O4'-C1'-N1 | 8.18  | 114.74      | 108.20   |
| 27  | B8    | 1734 | G    | C5-C6-O6   | -8.17 | 123.70      | 128.60   |
| 1   | AA    | 587  | G    | N1-C6-O6   | 8.17  | 124.80      | 119.90   |
| 1   | AA    | 654  | G    | N1-C6-O6   | 8.17  | 124.80      | 119.90   |
| 27  | B8    | 617  | G    | C5-C6-O6   | -8.17 | 123.70      | 128.60   |
| 27  | B8    | 754  | U    | O4'-C1'-N1 | 8.17  | 114.73      | 108.20   |
| 1   | AA    | 475  | C    | O4'-C1'-N1 | 8.17  | 114.73      | 108.20   |
| 1   | AA    | 1323 | G    | C5-C6-O6   | -8.17 | 123.70      | 128.60   |
| 27  | B8    | 784  | G    | C5-C6-O6   | -8.17 | 123.70      | 128.60   |
| 1   | AA    | 384  | G    | N1-C6-O6   | 8.16  | 124.80      | 119.90   |
| 1   | AA    | 484  | G    | C5-C6-O6   | -8.16 | 123.70      | 128.60   |
| 1   | AA    | 426  | U    | O4'-C1'-N1 | 8.16  | 114.73      | 108.20   |
| 1   | AA    | 578  | C    | O4'-C1'-N1 | 8.16  | 114.73      | 108.20   |
| 1   | AA    | 722  | G    | N1-C6-O6   | 8.16  | 124.80      | 119.90   |
| 1   | AA    | 1263 | C    | O4'-C1'-N1 | 8.16  | 114.73      | 108.20   |
| 1   | AA    | 1283 | U    | O4'-C1'-N1 | 8.16  | 114.73      | 108.20   |
| 27  | B8    | 88   | G    | N1-C6-O6   | 8.16  | 124.80      | 119.90   |
| 27  | B8    | 105  | C    | O4'-C1'-N1 | 8.16  | 114.73      | 108.20   |
| 27  | B8    | 236  | C    | O4'-C1'-N1 | 8.16  | 114.73      | 108.20   |
| 27  | B8    | 386  | G    | N1-C6-O6   | 8.16  | 124.80      | 119.90   |
| 27  | B8    | 2515 | C    | O4'-C1'-N1 | 8.16  | 114.73      | 108.20   |
| 1   | AA    | 1484 | C    | O4'-C1'-N1 | 8.16  | 114.73      | 108.20   |
| 27  | B8    | 1917 | U    | O4'-C1'-N1 | 8.16  | 114.72      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1200 | C    | O4'-C1'-N1 | 8.15  | 114.72      | 108.20   |
| 1   | AA    | 765  | G    | N1-C6-O6   | 8.15  | 124.79      | 119.90   |
| 1   | AA    | 1343 | G    | C5-C6-O6   | -8.15 | 123.71      | 128.60   |
| 27  | B8    | 731  | C    | O4'-C1'-N1 | 8.15  | 114.72      | 108.20   |
| 27  | B8    | 986  | C    | O4'-C1'-N1 | 8.15  | 114.72      | 108.20   |
| 27  | B8    | 1561 | C    | O4'-C1'-N1 | 8.15  | 114.72      | 108.20   |
| 27  | B8    | 2714 | G    | C5-C6-O6   | -8.15 | 123.71      | 128.60   |
| 27  | B8    | 2859 | G    | N1-C6-O6   | 8.15  | 124.79      | 119.90   |
| 1   | AA    | 1525 | G    | N1-C6-O6   | 8.15  | 124.79      | 119.90   |
| 27  | B8    | 2520 | C    | O4'-C1'-N1 | 8.15  | 114.72      | 108.20   |
| 1   | AA    | 162  | A    | C4-C5-C6   | 8.15  | 121.07      | 117.00   |
| 27  | B8    | 1949 | G    | C5-C6-O6   | -8.15 | 123.71      | 128.60   |
| 27  | B8    | 2483 | C    | O4'-C1'-N1 | 8.15  | 114.72      | 108.20   |
| 1   | AA    | 948  | C    | O4'-C1'-N1 | 8.14  | 114.72      | 108.20   |
| 1   | AA    | 1096 | C    | O4'-C1'-N1 | 8.14  | 114.71      | 108.20   |
| 27  | B8    | 1488 | C    | O4'-C1'-N1 | 8.14  | 114.71      | 108.20   |
| 27  | B8    | 2200 | C    | O4'-C1'-N1 | 8.14  | 114.71      | 108.20   |
| 1   | AA    | 84   | U    | O4'-C1'-N1 | 8.13  | 114.71      | 108.20   |
| 27  | B8    | 633  | A    | C4-C5-C6   | 8.13  | 121.07      | 117.00   |
| 27  | B8    | 991  | C    | O4'-C1'-N1 | 8.13  | 114.71      | 108.20   |
| 27  | B8    | 1171 | G    | C5-C6-O6   | -8.13 | 123.72      | 128.60   |
| 27  | B8    | 1424 | G    | C5-C6-O6   | -8.13 | 123.72      | 128.60   |
| 27  | B8    | 520  | G    | C5-C6-O6   | -8.13 | 123.72      | 128.60   |
| 27  | B8    | 724  | U    | O4'-C1'-N1 | 8.13  | 114.70      | 108.20   |
| 27  | B8    | 1595 | C    | O4'-C1'-N1 | 8.13  | 114.71      | 108.20   |
| 27  | B8    | 2248 | C    | O4'-C1'-N1 | 8.13  | 114.71      | 108.20   |
| 27  | B8    | 628  | G    | C5-C6-O6   | -8.13 | 123.72      | 128.60   |
| 1   | AA    | 188  | C    | O4'-C1'-N1 | 8.13  | 114.70      | 108.20   |
| 27  | B8    | 1213 | A    | C4-C5-C6   | 8.13  | 121.06      | 117.00   |
| 27  | B8    | 2628 | C    | O4'-C1'-N1 | 8.13  | 114.70      | 108.20   |
| 27  | B8    | 212  | G    | C5-C6-O6   | -8.12 | 123.72      | 128.60   |
| 27  | B8    | 1319 | C    | O4'-C1'-N1 | 8.12  | 114.70      | 108.20   |
| 27  | B8    | 970  | U    | O4'-C1'-N1 | 8.12  | 114.70      | 108.20   |
| 1   | AA    | 1037 | C    | O4'-C1'-N1 | 8.12  | 114.70      | 108.20   |
| 1   | AA    | 1510 | C    | O4'-C1'-N1 | 8.12  | 114.70      | 108.20   |
| 27  | B8    | 445  | C    | O4'-C1'-N1 | 8.12  | 114.70      | 108.20   |
| 1   | AA    | 222  | C    | O4'-C1'-N1 | 8.12  | 114.69      | 108.20   |
| 1   | AA    | 1109 | C    | O4'-C1'-N1 | 8.12  | 114.69      | 108.20   |
| 27  | B8    | 801  | G    | N1-C6-O6   | 8.12  | 124.77      | 119.90   |
| 27  | B8    | 1493 | C    | C2-N1-C1'  | 8.12  | 127.73      | 118.80   |
| 1   | AA    | 1069 | C    | O4'-C1'-N1 | 8.12  | 114.69      | 108.20   |
| 27  | B8    | 337  | C    | O4'-C1'-N1 | 8.12  | 114.69      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 556  | C    | O4'-C1'-N1 | 8.11  | 114.69      | 108.20   |
| 1   | AA    | 883  | C    | O4'-C1'-N1 | 8.11  | 114.69      | 108.20   |
| 3   | AV    | 26   | C    | O4'-C1'-N1 | 8.11  | 114.69      | 108.20   |
| 1   | AA    | 51   | A    | P-O3'-C3'  | 8.11  | 129.43      | 119.70   |
| 1   | AA    | 458  | U    | O4'-C1'-N1 | 8.11  | 114.69      | 108.20   |
| 1   | AA    | 660  | C    | O4'-C1'-N1 | 8.11  | 114.69      | 108.20   |
| 26  | B7    | 28   | C    | O4'-C1'-N1 | 8.11  | 114.69      | 108.20   |
| 27  | B8    | 894  | U    | O4'-C1'-N1 | 8.11  | 114.69      | 108.20   |
| 27  | B8    | 1102 | C    | O4'-C1'-N1 | 8.11  | 114.69      | 108.20   |
| 27  | B8    | 1112 | G    | N1-C6-O6   | 8.11  | 124.77      | 119.90   |
| 27  | B8    | 1990 | C    | O4'-C1'-N1 | 8.11  | 114.69      | 108.20   |
| 27  | B8    | 2299 | U    | O4'-C1'-N1 | 8.11  | 114.69      | 108.20   |
| 1   | AA    | 106  | C    | O4'-C1'-N1 | 8.11  | 114.69      | 108.20   |
| 1   | AA    | 1143 | G    | C5-C6-O6   | -8.11 | 123.74      | 128.60   |
| 27  | B8    | 1108 | U    | O4'-C1'-N1 | 8.11  | 114.68      | 108.20   |
| 27  | B8    | 1338 | G    | C5-C6-O6   | -8.11 | 123.74      | 128.60   |
| 27  | B8    | 1728 | C    | O4'-C1'-N1 | 8.11  | 114.69      | 108.20   |
| 1   | AA    | 995  | C    | O4'-C1'-N1 | 8.10  | 114.68      | 108.20   |
| 1   | AA    | 1449 | C    | O4'-C1'-N1 | 8.10  | 114.68      | 108.20   |
| 27  | B8    | 163  | C    | O4'-C1'-N1 | 8.10  | 114.68      | 108.20   |
| 27  | B8    | 2420 | C    | O4'-C1'-N1 | 8.10  | 114.68      | 108.20   |
| 1   | AA    | 1523 | G    | C5-C6-O6   | -8.10 | 123.74      | 128.60   |
| 27  | B8    | 147  | C    | O4'-C1'-N1 | 8.10  | 114.68      | 108.20   |
| 27  | B8    | 1075 | C    | O4'-C1'-N1 | 8.10  | 114.68      | 108.20   |
| 1   | AA    | 27   | G    | C5-C6-O6   | -8.10 | 123.74      | 128.60   |
| 27  | B8    | 1100 | C    | O4'-C1'-N1 | 8.10  | 114.68      | 108.20   |
| 27  | B8    | 1546 | G    | C5-C6-O6   | -8.10 | 123.74      | 128.60   |
| 27  | B8    | 2539 | C    | O4'-C1'-N1 | 8.10  | 114.68      | 108.20   |
| 1   | AA    | 34   | C    | O4'-C1'-N1 | 8.10  | 114.68      | 108.20   |
| 1   | AA    | 61   | G    | C5-C6-O6   | -8.10 | 123.74      | 128.60   |
| 1   | AA    | 190  | A    | C4-C5-C6   | 8.10  | 121.05      | 117.00   |
| 3   | AV    | 21   | U    | O4'-C1'-N1 | 8.10  | 114.68      | 108.20   |
| 27  | B8    | 598  | U    | O4'-C1'-N1 | 8.10  | 114.68      | 108.20   |
| 27  | B8    | 2300 | C    | O4'-C1'-N1 | 8.10  | 114.68      | 108.20   |
| 27  | B8    | 2794 | C    | O4'-C1'-N1 | 8.10  | 114.68      | 108.20   |
| 1   | AA    | 1098 | C    | O4'-C1'-N1 | 8.09  | 114.67      | 108.20   |
| 27  | B8    | 1835 | G    | C5-C6-O6   | -8.09 | 123.75      | 128.60   |
| 1   | AA    | 1051 | C    | O4'-C1'-N1 | 8.09  | 114.67      | 108.20   |
| 1   | AA    | 1391 | U    | O4'-C1'-N1 | 8.09  | 114.67      | 108.20   |
| 27  | B8    | 2046 | G    | C5-C6-O6   | -8.09 | 123.75      | 128.60   |
| 27  | B8    | 2226 | C    | O4'-C1'-N1 | 8.09  | 114.67      | 108.20   |
| 1   | AA    | 1482 | G    | N1-C6-O6   | 8.09  | 124.75      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1042 | G    | N1-C6-O6   | 8.09  | 124.75      | 119.90   |
| 27  | B8    | 1658 | C    | O4'-C1'-N1 | 8.09  | 114.67      | 108.20   |
| 27  | B8    | 1893 | C    | O4'-C1'-N1 | 8.09  | 114.67      | 108.20   |
| 27  | B8    | 2523 | G    | C5-C6-O6   | -8.09 | 123.75      | 128.60   |
| 27  | B8    | 237  | C    | O4'-C1'-N1 | 8.09  | 114.67      | 108.20   |
| 27  | B8    | 949  | G    | C5-C6-O6   | -8.09 | 123.75      | 128.60   |
| 27  | B8    | 283  | G    | O4'-C1'-N9 | 8.08  | 114.67      | 108.20   |
| 27  | B8    | 1022 | G    | N1-C6-O6   | 8.08  | 124.75      | 119.90   |
| 1   | AA    | 507  | C    | O4'-C1'-N1 | 8.08  | 114.66      | 108.20   |
| 1   | AA    | 1379 | G    | N1-C6-O6   | 8.08  | 124.75      | 119.90   |
| 26  | B7    | 8    | C    | O4'-C1'-N1 | 8.08  | 114.67      | 108.20   |
| 27  | B8    | 2772 | C    | O4'-C1'-N1 | 8.08  | 114.66      | 108.20   |
| 27  | B8    | 2812 | G    | C5-C6-O6   | -8.08 | 123.75      | 128.60   |
| 27  | B8    | 1059 | G    | C5-C6-O6   | -8.08 | 123.75      | 128.60   |
| 27  | B8    | 116  | C    | O4'-C1'-N1 | 8.07  | 114.66      | 108.20   |
| 27  | B8    | 953  | G    | C5-C6-O6   | -8.07 | 123.75      | 128.60   |
| 27  | B8    | 2383 | G    | C5-C6-O6   | -8.07 | 123.75      | 128.60   |
| 27  | B8    | 6    | A    | C5-C6-N6   | -8.07 | 117.24      | 123.70   |
| 27  | B8    | 2345 | G    | N1-C6-O6   | 8.07  | 124.74      | 119.90   |
| 27  | B8    | 2540 | C    | O4'-C1'-N1 | 8.07  | 114.66      | 108.20   |
| 1   | AA    | 178  | C    | O4'-C1'-N1 | 8.07  | 114.65      | 108.20   |
| 27  | B8    | 1822 | C    | O4'-C1'-N1 | 8.07  | 114.65      | 108.20   |
| 1   | AA    | 525  | C    | O4'-C1'-N1 | 8.07  | 114.65      | 108.20   |
| 1   | AA    | 1027 | C    | N3-C4-N4   | 8.07  | 123.65      | 118.00   |
| 27  | B8    | 1386 | C    | O4'-C1'-N1 | 8.07  | 114.65      | 108.20   |
| 1   | AA    | 150  | U    | O4'-C1'-N1 | 8.06  | 114.65      | 108.20   |
| 1   | AA    | 1491 | G    | N1-C6-O6   | 8.06  | 124.74      | 119.90   |
| 27  | B8    | 198  | C    | O4'-C1'-N1 | 8.06  | 114.65      | 108.20   |
| 27  | B8    | 523  | C    | O4'-C1'-N1 | 8.06  | 114.65      | 108.20   |
| 27  | B8    | 2148 | G    | N1-C6-O6   | 8.06  | 124.74      | 119.90   |
| 27  | B8    | 973  | A    | N1-C6-N6   | 8.06  | 123.44      | 118.60   |
| 27  | B8    | 2039 | U    | O4'-C1'-N1 | 8.06  | 114.65      | 108.20   |
| 1   | AA    | 724  | G    | C5-C6-O6   | -8.06 | 123.76      | 128.60   |
| 1   | AA    | 868  | C    | O4'-C1'-N1 | 8.06  | 114.65      | 108.20   |
| 27  | B8    | 1107 | G    | C5-C6-O6   | -8.06 | 123.76      | 128.60   |
| 27  | B8    | 1121 | C    | O4'-C1'-N1 | 8.06  | 114.65      | 108.20   |
| 27  | B8    | 1259 | G    | C5-C6-O6   | -8.06 | 123.76      | 128.60   |
| 27  | B8    | 1642 | G    | C5-C6-O6   | -8.06 | 123.76      | 128.60   |
| 26  | B7    | 6    | G    | C5-C6-O6   | -8.06 | 123.77      | 128.60   |
| 26  | B7    | 85   | G    | C5-C6-O6   | -8.06 | 123.77      | 128.60   |
| 27  | B8    | 407  | G    | C5-C6-O6   | -8.06 | 123.76      | 128.60   |
| 27  | B8    | 1723 | G    | C5-C6-O6   | -8.06 | 123.77      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2301 | C    | O4'-C1'-N1 | 8.06  | 114.65      | 108.20   |
| 27  | B8    | 9    | G    | C5-C6-O6   | -8.06 | 123.77      | 128.60   |
| 1   | AA    | 1388 | C    | O4'-C1'-N1 | 8.05  | 114.64      | 108.20   |
| 27  | B8    | 719  | C    | O4'-C1'-N1 | 8.05  | 114.64      | 108.20   |
| 27  | B8    | 1422 | G    | C5-C6-O6   | -8.05 | 123.77      | 128.60   |
| 27  | B8    | 2234 | G    | C5-C6-O6   | -8.05 | 123.77      | 128.60   |
| 27  | B8    | 2359 | C    | O4'-C1'-N1 | 8.05  | 114.64      | 108.20   |
| 1   | AA    | 1385 | G    | C5-C6-O6   | -8.05 | 123.77      | 128.60   |
| 27  | B8    | 2450 | A    | N1-C6-N6   | 8.05  | 123.43      | 118.60   |
| 1   | AA    | 504  | C    | O4'-C1'-N1 | 8.05  | 114.64      | 108.20   |
| 1   | AA    | 1386 | G    | C5-C6-O6   | -8.05 | 123.77      | 128.60   |
| 27  | B8    | 183  | C    | O4'-C1'-N1 | 8.05  | 114.64      | 108.20   |
| 27  | B8    | 540  | C    | O4'-C1'-N1 | 8.05  | 114.64      | 108.20   |
| 27  | B8    | 1920 | C    | O4'-C1'-N1 | 8.05  | 114.64      | 108.20   |
| 1   | AA    | 1090 | U    | O4'-C1'-N1 | 8.04  | 114.64      | 108.20   |
| 1   | AA    | 1218 | C    | O4'-C1'-N1 | 8.04  | 114.64      | 108.20   |
| 1   | AA    | 111  | G    | C5-C6-O6   | -8.04 | 123.78      | 128.60   |
| 1   | AA    | 522  | C    | O4'-C1'-N1 | 8.04  | 114.63      | 108.20   |
| 27  | B8    | 729  | G    | C5-C6-O6   | -8.04 | 123.77      | 128.60   |
| 27  | B8    | 963  | U    | O4'-C1'-N1 | 8.04  | 114.63      | 108.20   |
| 27  | B8    | 1123 | C    | O4'-C1'-N1 | 8.04  | 114.63      | 108.20   |
| 1   | AA    | 1001 | C    | O4'-C1'-N1 | 8.04  | 114.63      | 108.20   |
| 27  | B8    | 1345 | C    | O4'-C1'-N1 | 8.04  | 114.63      | 108.20   |
| 27  | B8    | 1736 | U    | O4'-C1'-N1 | 8.04  | 114.63      | 108.20   |
| 27  | B8    | 2666 | C    | C2-N1-C1'  | 8.04  | 127.64      | 118.80   |
| 27  | B8    | 758  | C    | O4'-C1'-N1 | 8.04  | 114.63      | 108.20   |
| 27  | B8    | 798  | G    | C5-C6-O6   | -8.04 | 123.78      | 128.60   |
| 27  | B8    | 2527 | C    | O4'-C1'-N1 | 8.04  | 114.63      | 108.20   |
| 27  | B8    | 2667 | C    | O4'-C1'-N1 | 8.04  | 114.63      | 108.20   |
| 1   | AA    | 861  | G    | C5-C6-O6   | -8.04 | 123.78      | 128.60   |
| 27  | B8    | 1415 | U    | O4'-C1'-N1 | 8.04  | 114.63      | 108.20   |
| 1   | AA    | 468  | A    | O4'-C1'-N9 | 8.03  | 114.63      | 108.20   |
| 1   | AA    | 808  | C    | O4'-C1'-N1 | 8.03  | 114.63      | 108.20   |
| 27  | B8    | 1193 | G    | C5-C6-O6   | -8.03 | 123.78      | 128.60   |
| 27  | B8    | 2053 | G    | C5-C6-O6   | -8.04 | 123.78      | 128.60   |
| 1   | AA    | 601  | G    | C5-C6-O6   | -8.03 | 123.78      | 128.60   |
| 1   | AA    | 632  | U    | O4'-C1'-N1 | 8.03  | 114.63      | 108.20   |
| 1   | AA    | 1337 | G    | C5-C6-O6   | -8.03 | 123.78      | 128.60   |
| 27  | B8    | 2295 | C    | O4'-C1'-N1 | 8.03  | 114.63      | 108.20   |
| 27  | B8    | 66   | C    | O4'-C1'-N1 | 8.03  | 114.62      | 108.20   |
| 27  | B8    | 2463 | C    | O4'-C1'-N1 | 8.03  | 114.62      | 108.20   |
| 1   | AA    | 1509 | C    | O4'-C1'-N1 | 8.03  | 114.62      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2276 | G    | C5-C6-O6   | -8.03 | 123.78      | 128.60   |
| 27  | B8    | 77   | G    | C5-C6-O6   | -8.03 | 123.78      | 128.60   |
| 27  | B8    | 2175 | C    | O4'-C1'-N1 | 8.03  | 114.62      | 108.20   |
| 1   | AA    | 1262 | C    | O4'-C1'-N1 | 8.03  | 114.62      | 108.20   |
| 27  | B8    | 1072 | C    | O4'-C1'-N1 | 8.03  | 114.62      | 108.20   |
| 27  | B8    | 2260 | C    | O4'-C1'-N1 | 8.03  | 114.62      | 108.20   |
| 27  | B8    | 732  | C    | O4'-C1'-N1 | 8.03  | 114.62      | 108.20   |
| 27  | B8    | 1594 | U    | O4'-C1'-N1 | 8.03  | 114.62      | 108.20   |
| 1   | AA    | 1045 | C    | O4'-C1'-N1 | 8.02  | 114.62      | 108.20   |
| 27  | B8    | 976  | G    | C5-C6-O6   | -8.02 | 123.79      | 128.60   |
| 27  | B8    | 2261 | C    | O4'-C1'-N1 | 8.02  | 114.62      | 108.20   |
| 27  | B8    | 2521 | C    | O4'-C1'-N1 | 8.02  | 114.62      | 108.20   |
| 1   | AA    | 922  | G    | N1-C6-O6   | 8.02  | 124.71      | 119.90   |
| 27  | B8    | 2830 | C    | O4'-C1'-N1 | 8.02  | 114.62      | 108.20   |
| 27  | B8    | 2432 | A    | O4'-C1'-N9 | 8.02  | 114.61      | 108.20   |
| 27  | B8    | 2625 | G    | C5-C6-O6   | -8.02 | 123.79      | 128.60   |
| 1   | AA    | 585  | G    | C5-C6-O6   | -8.02 | 123.79      | 128.60   |
| 1   | AA    | 636  | U    | O4'-C1'-N1 | 8.02  | 114.61      | 108.20   |
| 1   | AA    | 1485 | U    | O4'-C1'-N1 | 8.02  | 114.61      | 108.20   |
| 26  | B7    | 68   | C    | O4'-C1'-N1 | 8.02  | 114.61      | 108.20   |
| 27  | B8    | 832  | U    | O4'-C1'-N1 | 8.02  | 114.61      | 108.20   |
| 27  | B8    | 2841 | C    | O4'-C1'-N1 | 8.02  | 114.61      | 108.20   |
| 1   | AA    | 623  | C    | O4'-C1'-N1 | 8.01  | 114.61      | 108.20   |
| 27  | B8    | 1182 | G    | C5-C6-O6   | -8.01 | 123.79      | 128.60   |
| 27  | B8    | 2128 | G    | C5-C6-O6   | -8.01 | 123.79      | 128.60   |
| 27  | B8    | 2254 | C    | O4'-C1'-N1 | 8.01  | 114.61      | 108.20   |
| 1   | AA    | 39   | G    | C5-C6-O6   | -8.01 | 123.80      | 128.60   |
| 27  | B8    | 682  | G    | C5-C6-O6   | -8.01 | 123.79      | 128.60   |
| 27  | B8    | 1905 | C    | O4'-C1'-N1 | 8.01  | 114.61      | 108.20   |
| 27  | B8    | 2505 | G    | N1-C6-O6   | 8.01  | 124.71      | 119.90   |
| 27  | B8    | 2744 | G    | C5-C6-O6   | -8.01 | 123.79      | 128.60   |
| 1   | AA    | 43   | C    | O4'-C1'-N1 | 8.01  | 114.61      | 108.20   |
| 1   | AA    | 402  | G    | C5-C6-O6   | -8.01 | 123.80      | 128.60   |
| 1   | AA    | 1293 | C    | O4'-C1'-N1 | 8.01  | 114.61      | 108.20   |
| 27  | B8    | 1571 | A    | C4-C5-C6   | 8.01  | 121.00      | 117.00   |
| 27  | B8    | 978  | G    | C5-C6-O6   | -8.01 | 123.80      | 128.60   |
| 27  | B8    | 2347 | C    | O4'-C1'-N1 | 8.01  | 114.60      | 108.20   |
| 27  | B8    | 457  | A    | N1-C6-N6   | 8.00  | 123.40      | 118.60   |
| 27  | B8    | 2279 | G    | C5-C6-O6   | -8.00 | 123.80      | 128.60   |
| 27  | B8    | 2603 | G    | C5-C6-O6   | -8.00 | 123.80      | 128.60   |
| 27  | B8    | 2238 | G    | N1-C6-O6   | 8.00  | 124.70      | 119.90   |
| 1   | AA    | 1245 | C    | O4'-C1'-N1 | 8.00  | 114.60      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | AV    | 31   | U    | O4'-C1'-N1 | 8.00  | 114.60      | 108.20   |
| 27  | B8    | 1656 | C    | O4'-C1'-N1 | 8.00  | 114.60      | 108.20   |
| 1   | AA    | 1300 | G    | P-O3'-C3'  | 8.00  | 129.30      | 119.70   |
| 1   | AA    | 23   | C    | O4'-C1'-N1 | 8.00  | 114.60      | 108.20   |
| 1   | AA    | 317  | U    | O4'-C1'-N1 | 8.00  | 114.60      | 108.20   |
| 1   | AA    | 1086 | U    | O4'-C1'-N1 | 8.00  | 114.60      | 108.20   |
| 27  | B8    | 1305 | C    | O4'-C1'-N1 | 8.00  | 114.60      | 108.20   |
| 27  | B8    | 305  | C    | O4'-C1'-N1 | 8.00  | 114.60      | 108.20   |
| 1   | AA    | 624  | C    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 1   | AA    | 1411 | C    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 27  | B8    | 153  | U    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 27  | B8    | 238  | C    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 27  | B8    | 566  | U    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 27  | B8    | 1030 | C    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 27  | B8    | 1651 | G    | C5-C6-O6   | -7.99 | 123.80      | 128.60   |
| 27  | B8    | 1924 | C    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 1   | AA    | 551  | U    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 27  | B8    | 1023 | U    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 27  | B8    | 2081 | U    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 27  | B8    | 106  | C    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 27  | B8    | 1105 | U    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 27  | B8    | 2508 | G    | C5-C6-O6   | -7.99 | 123.81      | 128.60   |
| 1   | AA    | 89   | U    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 3   | AV    | 47   | G    | C5-C6-O6   | -7.99 | 123.81      | 128.60   |
| 27  | B8    | 1109 | C    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 27  | B8    | 1124 | G    | C5-C6-O6   | -7.99 | 123.81      | 128.60   |
| 1   | AA    | 413  | G    | C5-C6-O6   | -7.99 | 123.81      | 128.60   |
| 27  | B8    | 938  | G    | C5-C6-O6   | -7.99 | 123.81      | 128.60   |
| 27  | B8    | 1135 | C    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 27  | B8    | 1948 | G    | C5-C6-O6   | -7.99 | 123.81      | 128.60   |
| 1   | AA    | 876  | C    | O4'-C1'-N1 | 7.98  | 114.59      | 108.20   |
| 27  | B8    | 1417 | C    | O4'-C1'-N1 | 7.98  | 114.59      | 108.20   |
| 27  | B8    | 2024 | G    | C5-C6-O6   | -7.98 | 123.81      | 128.60   |
| 3   | AV    | 3    | G    | C5-C6-O6   | -7.98 | 123.81      | 128.60   |
| 27  | B8    | 351  | C    | O4'-C1'-N1 | 7.98  | 114.59      | 108.20   |
| 27  | B8    | 1245 | G    | C5-C6-O6   | -7.98 | 123.81      | 128.60   |
| 1   | AA    | 300  | A    | O4'-C1'-N9 | 7.98  | 114.58      | 108.20   |
| 1   | AA    | 1470 | U    | O4'-C1'-N1 | 7.98  | 114.58      | 108.20   |
| 27  | B8    | 287  | G    | C5-C6-O6   | -7.98 | 123.81      | 128.60   |
| 1   | AA    | 740  | U    | O4'-C1'-N1 | 7.98  | 114.58      | 108.20   |
| 27  | B8    | 170  | U    | O4'-C1'-N1 | 7.98  | 114.58      | 108.20   |
| 27  | B8    | 1101 | U    | O4'-C1'-N1 | 7.98  | 114.58      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 701  | G    | C5-C6-O6   | -7.98 | 123.81      | 128.60   |
| 27  | B8    | 2596 | U    | O4'-C1'-N1 | 7.98  | 114.58      | 108.20   |
| 1   | AA    | 867  | G    | C5-C6-O6   | -7.97 | 123.81      | 128.60   |
| 1   | AA    | 1050 | G    | C5-C6-O6   | -7.97 | 123.81      | 128.60   |
| 1   | AA    | 152  | A    | N1-C6-N6   | 7.97  | 123.38      | 118.60   |
| 27  | B8    | 1232 | G    | C5-C6-O6   | -7.97 | 123.82      | 128.60   |
| 27  | B8    | 823  | C    | O4'-C1'-N1 | 7.97  | 114.58      | 108.20   |
| 1   | AA    | 17   | U    | O4'-C1'-N1 | 7.97  | 114.58      | 108.20   |
| 27  | B8    | 265  | A    | O4'-C1'-N9 | 7.97  | 114.58      | 108.20   |
| 27  | B8    | 649  | G    | C5-C6-O6   | -7.97 | 123.82      | 128.60   |
| 27  | B8    | 1520 | U    | O4'-C1'-N1 | 7.97  | 114.58      | 108.20   |
| 27  | B8    | 1562 | U    | O4'-C1'-N1 | 7.97  | 114.58      | 108.20   |
| 27  | B8    | 2558 | C    | O4'-C1'-N1 | 7.97  | 114.58      | 108.20   |
| 1   | AA    | 153  | C    | O4'-C1'-N1 | 7.97  | 114.57      | 108.20   |
| 1   | AA    | 267  | C    | O4'-C1'-N1 | 7.97  | 114.57      | 108.20   |
| 27  | B8    | 787  | C    | O4'-C1'-N1 | 7.97  | 114.57      | 108.20   |
| 27  | B8    | 2157 | G    | O4'-C1'-N9 | 7.97  | 114.57      | 108.20   |
| 27  | B8    | 2315 | G    | C5-C6-O6   | -7.97 | 123.82      | 128.60   |
| 1   | AA    | 1029 | U    | O4'-C1'-N1 | 7.96  | 114.57      | 108.20   |
| 26  | B7    | 7    | G    | C5-C6-O6   | -7.96 | 123.82      | 128.60   |
| 27  | B8    | 177  | G    | N1-C6-O6   | 7.96  | 124.68      | 119.90   |
| 27  | B8    | 919  | U    | O4'-C1'-N1 | 7.96  | 114.57      | 108.20   |
| 27  | B8    | 2651 | C    | O4'-C1'-N1 | 7.96  | 114.57      | 108.20   |
| 27  | B8    | 385  | C    | O4'-C1'-N1 | 7.96  | 114.57      | 108.20   |
| 1   | AA    | 114  | U    | O4'-C1'-N1 | 7.96  | 114.56      | 108.20   |
| 1   | AA    | 1133 | G    | C5-C6-O6   | -7.96 | 123.83      | 128.60   |
| 27  | B8    | 581  | C    | O4'-C1'-N1 | 7.96  | 114.57      | 108.20   |
| 27  | B8    | 2195 | U    | O4'-C1'-N1 | 7.96  | 114.56      | 108.20   |
| 27  | B8    | 1016 | G    | C5-C6-O6   | -7.96 | 123.83      | 128.60   |
| 27  | B8    | 1207 | C    | O4'-C1'-N1 | 7.96  | 114.56      | 108.20   |
| 27  | B8    | 1661 | G    | C5-C6-O6   | -7.96 | 123.83      | 128.60   |
| 27  | B8    | 1162 | G    | C5-C6-O6   | -7.95 | 123.83      | 128.60   |
| 27  | B8    | 1278 | C    | O4'-C1'-N1 | 7.95  | 114.56      | 108.20   |
| 27  | B8    | 2599 | G    | C5-C6-O6   | -7.95 | 123.83      | 128.60   |
| 26  | B7    | 22   | U    | O4'-C1'-N1 | 7.95  | 114.56      | 108.20   |
| 1   | AA    | 142  | G    | C5-C6-O6   | -7.95 | 123.83      | 128.60   |
| 27  | B8    | 1518 | C    | O4'-C1'-N1 | 7.95  | 114.56      | 108.20   |
| 1   | AA    | 1075 | U    | O4'-C1'-N1 | 7.95  | 114.56      | 108.20   |
| 27  | B8    | 383  | C    | O4'-C1'-N1 | 7.95  | 114.56      | 108.20   |
| 27  | B8    | 759  | G    | C5-C6-O6   | -7.95 | 123.83      | 128.60   |
| 27  | B8    | 1429 | G    | C5-C6-O6   | -7.95 | 123.83      | 128.60   |
| 1   | AA    | 52   | C    | O4'-C1'-N1 | 7.95  | 114.56      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1479 | G    | C5-C6-O6   | -7.95 | 123.83      | 128.60   |
| 1   | AA    | 214  | C    | O4'-C1'-N1 | 7.95  | 114.56      | 108.20   |
| 1   | AA    | 739  | C    | O4'-C1'-N1 | 7.95  | 114.56      | 108.20   |
| 27  | B8    | 1816 | C    | O4'-C1'-N1 | 7.95  | 114.56      | 108.20   |
| 27  | B8    | 1890 | A    | N1-C6-N6   | 7.94  | 123.37      | 118.60   |
| 27  | B8    | 2250 | G    | N1-C6-O6   | 7.94  | 124.67      | 119.90   |
| 1   | AA    | 1401 | G    | C5-C6-O6   | -7.94 | 123.83      | 128.60   |
| 27  | B8    | 1258 | U    | O4'-C1'-N1 | 7.94  | 114.55      | 108.20   |
| 27  | B8    | 2484 | G    | C5-C6-O6   | -7.94 | 123.83      | 128.60   |
| 27  | B8    | 2804 | U    | O4'-C1'-N1 | 7.94  | 114.55      | 108.20   |
| 1   | AA    | 1041 | G    | C5-C6-O6   | -7.94 | 123.84      | 128.60   |
| 27  | B8    | 1181 | U    | O4'-C1'-N1 | 7.94  | 114.55      | 108.20   |
| 27  | B8    | 2096 | C    | O4'-C1'-N1 | 7.94  | 114.55      | 108.20   |
| 1   | AA    | 798  | U    | O4'-C1'-N1 | 7.94  | 114.55      | 108.20   |
| 27  | B8    | 680  | C    | O4'-C1'-N1 | 7.94  | 114.55      | 108.20   |
| 27  | B8    | 1031 | G    | C5-C6-O6   | -7.94 | 123.84      | 128.60   |
| 27  | B8    | 2021 | C    | O4'-C1'-N1 | 7.94  | 114.55      | 108.20   |
| 1   | AA    | 1061 | G    | C5-C6-O6   | -7.94 | 123.84      | 128.60   |
| 1   | AA    | 951  | G    | C5-C6-O6   | -7.93 | 123.84      | 128.60   |
| 3   | AV    | 39   | U    | O4'-C1'-N1 | 7.93  | 114.55      | 108.20   |
| 27  | B8    | 164  | C    | O4'-C1'-N1 | 7.93  | 114.55      | 108.20   |
| 27  | B8    | 1145 | C    | O4'-C1'-N1 | 7.93  | 114.55      | 108.20   |
| 27  | B8    | 1206 | G    | C5-C6-O6   | -7.93 | 123.84      | 128.60   |
| 27  | B8    | 1389 | G    | C5-C6-O6   | -7.93 | 123.84      | 128.60   |
| 27  | B8    | 46   | G    | C5-C6-O6   | -7.93 | 123.84      | 128.60   |
| 27  | B8    | 131  | A    | O4'-C1'-N9 | 7.93  | 114.55      | 108.20   |
| 1   | AA    | 1210 | C    | O4'-C1'-N1 | 7.93  | 114.54      | 108.20   |
| 27  | B8    | 2643 | G    | C5-C6-O6   | -7.93 | 123.84      | 128.60   |
| 27  | B8    | 1131 | G    | N1-C6-O6   | 7.93  | 124.66      | 119.90   |
| 27  | B8    | 1154 | G    | C5-C6-O6   | -7.93 | 123.84      | 128.60   |
| 27  | B8    | 2329 | U    | O4'-C1'-N1 | 7.93  | 114.54      | 108.20   |
| 26  | B7    | 3    | C    | O4'-C1'-N1 | 7.93  | 114.54      | 108.20   |
| 1   | AA    | 1039 | G    | C5-C6-O6   | -7.92 | 123.84      | 128.60   |
| 27  | B8    | 898  | C    | O4'-C1'-N1 | 7.92  | 114.54      | 108.20   |
| 27  | B8    | 2390 | U    | O4'-C1'-N1 | 7.92  | 114.54      | 108.20   |
| 27  | B8    | 2579 | C    | O4'-C1'-N1 | 7.92  | 114.54      | 108.20   |
| 27  | B8    | 815  | C    | O4'-C1'-N1 | 7.92  | 114.54      | 108.20   |
| 27  | B8    | 230  | G    | C5-C6-O6   | -7.92 | 123.85      | 128.60   |
| 27  | B8    | 363  | G    | C5-C6-O6   | -7.92 | 123.85      | 128.60   |
| 1   | AA    | 186  | C    | O4'-C1'-N1 | 7.92  | 114.53      | 108.20   |
| 1   | AA    | 271  | C    | O4'-C1'-N1 | 7.92  | 114.53      | 108.20   |
| 1   | AA    | 617  | G    | C5-C6-O6   | -7.92 | 123.85      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 824  | G    | C5-C6-O6   | -7.92 | 123.85      | 128.60   |
| 27  | B8    | 799  | G    | C5-C6-O6   | -7.92 | 123.85      | 128.60   |
| 27  | B8    | 2458 | G    | O4'-C1'-N9 | 7.92  | 114.53      | 108.20   |
| 1   | AA    | 518  | C    | O4'-C1'-N1 | 7.92  | 114.53      | 108.20   |
| 27  | B8    | 288  | U    | O4'-C1'-N1 | 7.92  | 114.53      | 108.20   |
| 1   | AA    | 1497 | G    | C5-C6-O6   | -7.91 | 123.85      | 128.60   |
| 27  | B8    | 414  | C    | O4'-C1'-N1 | 7.91  | 114.53      | 108.20   |
| 27  | B8    | 1643 | G    | C5-C6-O6   | -7.91 | 123.85      | 128.60   |
| 27  | B8    | 2069 | G    | C5-C6-O6   | -7.91 | 123.85      | 128.60   |
| 1   | AA    | 538  | G    | C5-C6-O6   | -7.91 | 123.85      | 128.60   |
| 27  | B8    | 202  | U    | O4'-C1'-N1 | 7.91  | 114.53      | 108.20   |
| 27  | B8    | 487  | C    | O4'-C1'-N1 | 7.91  | 114.53      | 108.20   |
| 1   | AA    | 1010 | U    | O4'-C1'-N1 | 7.91  | 114.53      | 108.20   |
| 27  | B8    | 1418 | G    | C5-C6-O6   | -7.91 | 123.85      | 128.60   |
| 27  | B8    | 2802 | G    | C5-C6-O6   | -7.91 | 123.86      | 128.60   |
| 27  | B8    | 1768 | C    | O4'-C1'-N1 | 7.91  | 114.53      | 108.20   |
| 27  | B8    | 2785 | C    | O4'-C1'-N1 | 7.91  | 114.53      | 108.20   |
| 26  | B7    | 111  | U    | O4'-C1'-N1 | 7.91  | 114.52      | 108.20   |
| 27  | B8    | 1531 | C    | O4'-C1'-N1 | 7.91  | 114.52      | 108.20   |
| 1   | AA    | 1366 | C    | O4'-C1'-N1 | 7.90  | 114.52      | 108.20   |
| 26  | B7    | 88   | C    | O4'-C1'-N1 | 7.90  | 114.52      | 108.20   |
| 1   | AA    | 135  | C    | O4'-C1'-N1 | 7.90  | 114.52      | 108.20   |
| 1   | AA    | 821  | G    | C5-C6-O6   | -7.90 | 123.86      | 128.60   |
| 1   | AA    | 1478 | U    | O4'-C1'-N1 | 7.90  | 114.52      | 108.20   |
| 27  | B8    | 2441 | U    | O4'-C1'-N1 | 7.90  | 114.52      | 108.20   |
| 27  | B8    | 2464 | G    | C5-C6-O6   | -7.90 | 123.86      | 128.60   |
| 27  | B8    | 1914 | C    | O4'-C1'-N1 | 7.90  | 114.52      | 108.20   |
| 27  | B8    | 2396 | G    | C5-C6-O6   | -7.90 | 123.86      | 128.60   |
| 1   | AA    | 234  | C    | O4'-C1'-N1 | 7.90  | 114.52      | 108.20   |
| 27  | B8    | 946  | C    | O4'-C1'-N1 | 7.90  | 114.52      | 108.20   |
| 1   | AA    | 450  | G    | C5-C6-O6   | -7.90 | 123.86      | 128.60   |
| 27  | B8    | 1706 | C    | O4'-C1'-N1 | 7.90  | 114.52      | 108.20   |
| 1   | AA    | 241  | G    | C5-C6-O6   | -7.89 | 123.86      | 128.60   |
| 26  | B7    | 36   | C    | O4'-C1'-N1 | 7.89  | 114.51      | 108.20   |
| 27  | B8    | 224  | U    | O4'-C1'-N1 | 7.89  | 114.51      | 108.20   |
| 27  | B8    | 867  | C    | O4'-C1'-N1 | 7.89  | 114.51      | 108.20   |
| 27  | B8    | 1462 | C    | O4'-C1'-N1 | 7.89  | 114.51      | 108.20   |
| 27  | B8    | 2416 | C    | O4'-C1'-N1 | 7.89  | 114.51      | 108.20   |
| 27  | B8    | 914  | G    | C5-C6-O6   | -7.89 | 123.86      | 128.60   |
| 27  | B8    | 1170 | C    | O4'-C1'-N1 | 7.89  | 114.51      | 108.20   |
| 1   | AA    | 634  | C    | O4'-C1'-N1 | 7.89  | 114.51      | 108.20   |
| 27  | B8    | 807  | U    | O4'-C1'-N1 | 7.89  | 114.51      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1563 | U    | O4'-C1'-N1 | 7.89  | 114.51      | 108.20   |
| 1   | AA    | 117  | G    | C5-C6-O6   | -7.89 | 123.87      | 128.60   |
| 1   | AA    | 146  | G    | C5-C6-O6   | -7.89 | 123.87      | 128.60   |
| 1   | AA    | 583  | A    | N1-C6-N6   | 7.89  | 123.33      | 118.60   |
| 1   | AA    | 744  | C    | O4'-C1'-N1 | 7.89  | 114.51      | 108.20   |
| 1   | AA    | 862  | C    | O4'-C1'-N1 | 7.89  | 114.51      | 108.20   |
| 1   | AA    | 513  | C    | O4'-C1'-N1 | 7.88  | 114.51      | 108.20   |
| 27  | B8    | 2063 | C    | O4'-C1'-N1 | 7.88  | 114.51      | 108.20   |
| 27  | B8    | 797  | G    | C5-C6-O6   | -7.88 | 123.87      | 128.60   |
| 27  | B8    | 1093 | G    | C5-C6-O6   | -7.88 | 123.87      | 128.60   |
| 27  | B8    | 2867 | G    | O4'-C1'-N9 | 7.88  | 114.51      | 108.20   |
| 1   | AA    | 849  | G    | C5-C6-O6   | -7.88 | 123.87      | 128.60   |
| 3   | AV    | 11   | C    | O4'-C1'-N1 | 7.88  | 114.50      | 108.20   |
| 27  | B8    | 812  | C    | O4'-C1'-N1 | 7.88  | 114.50      | 108.20   |
| 27  | B8    | 1343 | G    | C5-C6-O6   | -7.88 | 123.87      | 128.60   |
| 27  | B8    | 2146 | C    | O4'-C1'-N1 | 7.88  | 114.50      | 108.20   |
| 27  | B8    | 2093 | G    | C5-C6-O6   | -7.88 | 123.87      | 128.60   |
| 1   | AA    | 986  | U    | O4'-C1'-N1 | 7.88  | 114.50      | 108.20   |
| 27  | B8    | 924  | G    | C5-C6-O6   | -7.88 | 123.87      | 128.60   |
| 27  | B8    | 2630 | G    | C5-C6-O6   | -7.88 | 123.87      | 128.60   |
| 1   | AA    | 835  | U    | O4'-C1'-N1 | 7.87  | 114.50      | 108.20   |
| 1   | AA    | 1006 | G    | C5-C6-O6   | -7.87 | 123.88      | 128.60   |
| 27  | B8    | 115  | C    | O4'-C1'-N1 | 7.87  | 114.50      | 108.20   |
| 27  | B8    | 2824 | C    | O4'-C1'-N1 | 7.87  | 114.50      | 108.20   |
| 1   | AA    | 500  | G    | C5-C6-O6   | -7.87 | 123.88      | 128.60   |
| 1   | AA    | 592  | G    | C5-C6-O6   | -7.87 | 123.88      | 128.60   |
| 1   | AA    | 1282 | C    | O4'-C1'-N1 | 7.87  | 114.50      | 108.20   |
| 27  | B8    | 123  | G    | C5-C6-O6   | -7.87 | 123.88      | 128.60   |
| 27  | B8    | 1909 | C    | O4'-C1'-N1 | 7.87  | 114.50      | 108.20   |
| 27  | B8    | 2880 | C    | O4'-C1'-N1 | 7.87  | 114.50      | 108.20   |
| 27  | B8    | 1289 | C    | O4'-C1'-N1 | 7.87  | 114.50      | 108.20   |
| 27  | B8    | 593  | U    | O4'-C1'-N1 | 7.87  | 114.50      | 108.20   |
| 27  | B8    | 650  | C    | O4'-C1'-N1 | 7.87  | 114.49      | 108.20   |
| 27  | B8    | 1530 | G    | C5-C6-O6   | -7.87 | 123.88      | 128.60   |
| 27  | B8    | 2189 | U    | O4'-C1'-N1 | 7.87  | 114.50      | 108.20   |
| 1   | AA    | 334  | C    | O4'-C1'-N1 | 7.86  | 114.49      | 108.20   |
| 27  | B8    | 509  | C    | O4'-C1'-N1 | 7.86  | 114.49      | 108.20   |
| 27  | B8    | 534  | U    | O4'-C1'-N1 | 7.86  | 114.49      | 108.20   |
| 27  | B8    | 1083 | U    | O4'-C1'-N1 | 7.86  | 114.49      | 108.20   |
| 27  | B8    | 1238 | G    | C5-C6-O6   | -7.86 | 123.88      | 128.60   |
| 27  | B8    | 1691 | C    | O4'-C1'-N1 | 7.86  | 114.49      | 108.20   |
| 1   | AA    | 9    | G    | C5-C6-O6   | -7.86 | 123.88      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 599  | C    | O4'-C1'-N1 | 7.86  | 114.49      | 108.20   |
| 27  | B8    | 234  | U    | O4'-C1'-N1 | 7.86  | 114.49      | 108.20   |
| 27  | B8    | 252  | G    | C5-C6-O6   | -7.86 | 123.88      | 128.60   |
| 27  | B8    | 902  | C    | O4'-C1'-N1 | 7.86  | 114.49      | 108.20   |
| 27  | B8    | 1297 | C    | O4'-C1'-N1 | 7.86  | 114.49      | 108.20   |
| 27  | B8    | 2041 | U    | O4'-C1'-N1 | 7.86  | 114.49      | 108.20   |
| 1   | AA    | 487  | A    | C4-C5-C6   | 7.86  | 120.93      | 117.00   |
| 27  | B8    | 1752 | C    | O4'-C1'-N1 | 7.86  | 114.49      | 108.20   |
| 27  | B8    | 2698 | U    | O4'-C1'-N1 | 7.86  | 114.49      | 108.20   |
| 27  | B8    | 325  | G    | C5-C6-O6   | -7.86 | 123.89      | 128.60   |
| 27  | B8    | 2782 | G    | C5-C6-O6   | -7.85 | 123.89      | 128.60   |
| 1   | AA    | 1425 | U    | O4'-C1'-N1 | 7.85  | 114.48      | 108.20   |
| 3   | AV    | 62   | C    | O4'-C1'-N1 | 7.85  | 114.48      | 108.20   |
| 27  | B8    | 1888 | G    | O4'-C1'-N9 | 7.85  | 114.48      | 108.20   |
| 1   | AA    | 191  | G    | C5-C6-O6   | -7.85 | 123.89      | 128.60   |
| 1   | AA    | 225  | C    | O4'-C1'-N1 | 7.85  | 114.48      | 108.20   |
| 1   | AA    | 970  | C    | O4'-C1'-N1 | 7.85  | 114.48      | 108.20   |
| 3   | AV    | 23   | G    | C5-C6-O6   | -7.85 | 123.89      | 128.60   |
| 27  | B8    | 209  | C    | O4'-C1'-N1 | 7.85  | 114.48      | 108.20   |
| 1   | AA    | 308  | C    | O4'-C1'-N1 | 7.85  | 114.48      | 108.20   |
| 1   | AA    | 1220 | G    | C5-C6-O6   | -7.85 | 123.89      | 128.60   |
| 1   | AA    | 176  | C    | O4'-C1'-N1 | 7.84  | 114.48      | 108.20   |
| 1   | AA    | 207  | C    | O4'-C1'-N1 | 7.84  | 114.48      | 108.20   |
| 27  | B8    | 2221 | G    | C5-C6-O6   | -7.84 | 123.89      | 128.60   |
| 27  | B8    | 2467 | C    | O4'-C1'-N1 | 7.84  | 114.48      | 108.20   |
| 1   | AA    | 1540 | U    | O4'-C1'-N1 | 7.84  | 114.47      | 108.20   |
| 1   | AA    | 25   | C    | O4'-C1'-N1 | 7.84  | 114.47      | 108.20   |
| 1   | AA    | 917  | G    | C5-C6-O6   | -7.84 | 123.90      | 128.60   |
| 26  | B7    | 117  | G    | P-O3'-C3'  | 7.84  | 129.11      | 119.70   |
| 27  | B8    | 605  | G    | C5-C6-O6   | -7.84 | 123.89      | 128.60   |
| 27  | B8    | 822  | G    | C5-C6-O6   | -7.84 | 123.89      | 128.60   |
| 27  | B8    | 2232 | C    | O4'-C1'-N1 | 7.84  | 114.47      | 108.20   |
| 26  | B7    | 106  | G    | C5-C6-O6   | -7.84 | 123.90      | 128.60   |
| 27  | B8    | 141  | G    | C5-C6-O6   | -7.84 | 123.90      | 128.60   |
| 27  | B8    | 1455 | G    | C5-C6-O6   | -7.84 | 123.90      | 128.60   |
| 27  | B8    | 1727 | C    | O4'-C1'-N1 | 7.84  | 114.47      | 108.20   |
| 27  | B8    | 1850 | G    | C5-C6-O6   | -7.84 | 123.90      | 128.60   |
| 1   | AA    | 1230 | C    | O4'-C1'-N1 | 7.84  | 114.47      | 108.20   |
| 27  | B8    | 552  | U    | O4'-C1'-N1 | 7.84  | 114.47      | 108.20   |
| 27  | B8    | 2104 | C    | O4'-C1'-N1 | 7.84  | 114.47      | 108.20   |
| 1   | AA    | 543  | U    | O4'-C1'-N1 | 7.84  | 114.47      | 108.20   |
| 1   | AA    | 748  | G    | C5-C6-O6   | -7.84 | 123.90      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1149 | C    | O4'-C1'-N1 | 7.84  | 114.47      | 108.20   |
| 26  | B7    | 86   | G    | C5-C6-O6   | -7.84 | 123.90      | 128.60   |
| 27  | B8    | 1673 | G    | N1-C6-O6   | 7.84  | 124.60      | 119.90   |
| 27  | B8    | 2209 | G    | C5-C6-O6   | -7.84 | 123.90      | 128.60   |
| 1   | AA    | 266  | G    | N1-C6-O6   | 7.83  | 124.60      | 119.90   |
| 27  | B8    | 485  | C    | O4'-C1'-N1 | 7.83  | 114.47      | 108.20   |
| 27  | B8    | 2530 | A    | O4'-C1'-N9 | 7.83  | 114.47      | 108.20   |
| 1   | AA    | 1072 | G    | C5-C6-O6   | -7.83 | 123.90      | 128.60   |
| 1   | AA    | 1147 | C    | O4'-C1'-N1 | 7.83  | 114.47      | 108.20   |
| 26  | B7    | 84   | G    | C5-C6-O6   | -7.83 | 123.90      | 128.60   |
| 27  | B8    | 1427 | A    | N1-C6-N6   | 7.83  | 123.30      | 118.60   |
| 27  | B8    | 1816 | C    | C2-N1-C1'  | 7.83  | 127.42      | 118.80   |
| 27  | B8    | 2355 | G    | C5-C6-O6   | -7.83 | 123.90      | 128.60   |
| 27  | B8    | 1806 | C    | O4'-C1'-N1 | 7.83  | 114.47      | 108.20   |
| 27  | B8    | 2323 | G    | C5-C6-O6   | -7.83 | 123.90      | 128.60   |
| 27  | B8    | 2325 | G    | C5-C6-O6   | -7.83 | 123.90      | 128.60   |
| 1   | AA    | 361  | G    | C5-C6-O6   | -7.83 | 123.90      | 128.60   |
| 27  | B8    | 767  | U    | O4'-C1'-N1 | 7.83  | 114.46      | 108.20   |
| 27  | B8    | 834  | G    | C5-C6-O6   | -7.83 | 123.90      | 128.60   |
| 27  | B8    | 1448 | G    | C5-C6-O6   | -7.83 | 123.90      | 128.60   |
| 27  | B8    | 1196 | C    | O4'-C1'-N1 | 7.83  | 114.46      | 108.20   |
| 27  | B8    | 1902 | C    | O4'-C1'-N1 | 7.83  | 114.46      | 108.20   |
| 1   | AA    | 335  | C    | O4'-C1'-N1 | 7.83  | 114.46      | 108.20   |
| 27  | B8    | 267  | C    | O4'-C1'-N1 | 7.83  | 114.46      | 108.20   |
| 27  | B8    | 1517 | G    | C5-C6-O6   | -7.83 | 123.91      | 128.60   |
| 27  | B8    | 2548 | U    | O4'-C1'-N1 | 7.83  | 114.46      | 108.20   |
| 27  | B8    | 1832 | C    | O4'-C1'-N1 | 7.82  | 114.46      | 108.20   |
| 27  | B8    | 1188 | U    | O4'-C1'-N1 | 7.82  | 114.46      | 108.20   |
| 27  | B8    | 1472 | C    | O4'-C1'-N1 | 7.82  | 114.46      | 108.20   |
| 27  | B8    | 1612 | C    | O4'-C1'-N1 | 7.82  | 114.46      | 108.20   |
| 27  | B8    | 1636 | U    | O4'-C1'-N1 | 7.82  | 114.46      | 108.20   |
| 27  | B8    | 1766 | G    | C5-C6-O6   | -7.82 | 123.91      | 128.60   |
| 27  | B8    | 1999 | C    | O4'-C1'-N1 | 7.82  | 114.46      | 108.20   |
| 27  | B8    | 2861 | U    | O4'-C1'-N1 | 7.82  | 114.46      | 108.20   |
| 27  | B8    | 274  | C    | O4'-C1'-N1 | 7.82  | 114.45      | 108.20   |
| 27  | B8    | 467  | G    | C5-C6-O6   | -7.82 | 123.91      | 128.60   |
| 27  | B8    | 995  | C    | O4'-C1'-N1 | 7.82  | 114.45      | 108.20   |
| 27  | B8    | 1372 | U    | O4'-C1'-N1 | 7.82  | 114.45      | 108.20   |
| 27  | B8    | 2677 | G    | C5-C6-O6   | -7.82 | 123.91      | 128.60   |
| 1   | AA    | 36   | C    | O4'-C1'-N1 | 7.82  | 114.45      | 108.20   |
| 27  | B8    | 1256 | G    | C5-C6-O6   | -7.82 | 123.91      | 128.60   |
| 27  | B8    | 2382 | G    | C5-C6-O6   | -7.81 | 123.91      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 140  | C    | O4'-C1'-N1 | 7.81  | 114.45      | 108.20   |
| 27  | B8    | 778  | G    | C5-C6-O6   | -7.81 | 123.91      | 128.60   |
| 27  | B8    | 61   | C    | O4'-C1'-N1 | 7.81  | 114.45      | 108.20   |
| 27  | B8    | 1323 | C    | O4'-C1'-N1 | 7.81  | 114.45      | 108.20   |
| 27  | B8    | 2718 | G    | C5-C6-O6   | -7.81 | 123.91      | 128.60   |
| 1   | AA    | 492  | C    | O4'-C1'-N1 | 7.81  | 114.45      | 108.20   |
| 1   | AA    | 645  | G    | C5-C6-O6   | -7.81 | 123.92      | 128.60   |
| 1   | AA    | 1531 | A    | O4'-C1'-N9 | 7.81  | 114.45      | 108.20   |
| 1   | AA    | 428  | G    | P-O3'-C3'  | 7.81  | 129.07      | 119.70   |
| 27  | B8    | 214  | G    | C5-C6-O6   | -7.81 | 123.92      | 128.60   |
| 27  | B8    | 850  | U    | O4'-C1'-N1 | 7.81  | 114.45      | 108.20   |
| 27  | B8    | 1601 | G    | C5-C6-O6   | -7.81 | 123.92      | 128.60   |
| 27  | B8    | 2827 | C    | O4'-C1'-N1 | 7.81  | 114.45      | 108.20   |
| 1   | AA    | 425  | G    | C5-C6-O6   | -7.80 | 123.92      | 128.60   |
| 1   | AA    | 1272 | G    | C5-C6-O6   | -7.80 | 123.92      | 128.60   |
| 3   | AV    | 71   | C    | O4'-C1'-N1 | 7.80  | 114.44      | 108.20   |
| 27  | B8    | 246  | C    | O4'-C1'-N1 | 7.80  | 114.44      | 108.20   |
| 27  | B8    | 1058 | U    | O4'-C1'-N1 | 7.80  | 114.44      | 108.20   |
| 27  | B8    | 1904 | G    | C5-C6-O6   | -7.80 | 123.92      | 128.60   |
| 1   | AA    | 725  | G    | C5-C6-O6   | -7.80 | 123.92      | 128.60   |
| 1   | AA    | 738  | C    | O4'-C1'-N1 | 7.80  | 114.44      | 108.20   |
| 27  | B8    | 108  | G    | C5-C6-O6   | -7.80 | 123.92      | 128.60   |
| 1   | AA    | 933  | G    | C5-C6-O6   | -7.80 | 123.92      | 128.60   |
| 27  | B8    | 851  | C    | O4'-C1'-N1 | 7.80  | 114.44      | 108.20   |
| 27  | B8    | 1119 | U    | O4'-C1'-N1 | 7.80  | 114.44      | 108.20   |
| 1   | AA    | 165  | G    | C5-C6-O6   | -7.79 | 123.92      | 128.60   |
| 1   | AA    | 439  | U    | O4'-C1'-N1 | 7.79  | 114.44      | 108.20   |
| 27  | B8    | 1192 | G    | C5-C6-O6   | -7.79 | 123.92      | 128.60   |
| 27  | B8    | 239  | C    | O4'-C1'-N1 | 7.79  | 114.43      | 108.20   |
| 27  | B8    | 1796 | U    | O4'-C1'-N1 | 7.79  | 114.44      | 108.20   |
| 1   | AA    | 341  | C    | O4'-C1'-N1 | 7.79  | 114.43      | 108.20   |
| 1   | AA    | 620  | C    | O4'-C1'-N1 | 7.79  | 114.43      | 108.20   |
| 27  | B8    | 2228 | G    | C5-C6-O6   | -7.79 | 123.92      | 128.60   |
| 27  | B8    | 2703 | C    | O4'-C1'-N1 | 7.79  | 114.43      | 108.20   |
| 27  | B8    | 1457 | U    | O4'-C1'-N1 | 7.79  | 114.43      | 108.20   |
| 1   | AA    | 1494 | G    | C5-C6-O6   | -7.79 | 123.93      | 128.60   |
| 27  | B8    | 468  | G    | C5-C6-O6   | -7.79 | 123.93      | 128.60   |
| 27  | B8    | 2120 | G    | P-O3'-C3'  | 7.79  | 129.04      | 119.70   |
| 1   | AA    | 1190 | G    | P-O3'-C3'  | 7.79  | 129.04      | 119.70   |
| 27  | B8    | 2652 | C    | O4'-C1'-N1 | 7.79  | 114.43      | 108.20   |
| 1   | AA    | 1276 | G    | C5-C6-O6   | -7.79 | 123.93      | 128.60   |
| 27  | B8    | 2509 | G    | C5-C6-O6   | -7.79 | 123.93      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 894  | G    | C5-C6-O6   | -7.78 | 123.93      | 128.60   |
| 1   | AA    | 1310 | G    | C5-C6-O6   | -7.78 | 123.93      | 128.60   |
| 27  | B8    | 2153 | C    | O4'-C1'-N1 | 7.78  | 114.43      | 108.20   |
| 1   | AA    | 164  | G    | C5-C6-O6   | -7.78 | 123.93      | 128.60   |
| 1   | AA    | 567  | G    | C5-C6-O6   | -7.78 | 123.93      | 128.60   |
| 26  | B7    | 73   | A    | C4-C5-C6   | 7.78  | 120.89      | 117.00   |
| 27  | B8    | 1094 | U    | O4'-C1'-N1 | 7.78  | 114.42      | 108.20   |
| 27  | B8    | 806  | C    | O4'-C1'-N1 | 7.78  | 114.42      | 108.20   |
| 27  | B8    | 1954 | G    | C5-C6-O6   | -7.78 | 123.93      | 128.60   |
| 1   | AA    | 1334 | G    | C5-C6-O6   | -7.78 | 123.93      | 128.60   |
| 1   | AA    | 1471 | U    | O4'-C1'-N1 | 7.78  | 114.42      | 108.20   |
| 27  | B8    | 1534 | U    | O4'-C1'-N1 | 7.78  | 114.42      | 108.20   |
| 27  | B8    | 2731 | G    | C5-C6-O6   | -7.78 | 123.93      | 128.60   |
| 1   | AA    | 87   | C    | O4'-C1'-N1 | 7.78  | 114.42      | 108.20   |
| 1   | AA    | 377  | G    | C5-C6-O6   | -7.78 | 123.93      | 128.60   |
| 27  | B8    | 678  | C    | O4'-C1'-N1 | 7.78  | 114.42      | 108.20   |
| 27  | B8    | 2502 | G    | C5-C6-O6   | -7.77 | 123.94      | 128.60   |
| 1   | AA    | 289  | G    | C5-C6-O6   | -7.77 | 123.94      | 128.60   |
| 1   | AA    | 669  | G    | C5-C6-O6   | -7.77 | 123.94      | 128.60   |
| 1   | AA    | 763  | G    | C5-C6-O6   | -7.77 | 123.94      | 128.60   |
| 27  | B8    | 1784 | A    | C5-C6-N6   | -7.77 | 117.48      | 123.70   |
| 1   | AA    | 797  | C    | O4'-C1'-N1 | 7.77  | 114.42      | 108.20   |
| 1   | AA    | 1018 | G    | O4'-C1'-N9 | 7.77  | 114.42      | 108.20   |
| 1   | AA    | 1407 | C    | O4'-C1'-N1 | 7.77  | 114.41      | 108.20   |
| 27  | B8    | 394  | C    | O4'-C1'-N1 | 7.77  | 114.42      | 108.20   |
| 27  | B8    | 2134 | A    | O4'-C1'-N9 | 7.77  | 114.41      | 108.20   |
| 27  | B8    | 2550 | G    | C5-C6-O6   | -7.77 | 123.94      | 128.60   |
| 1   | AA    | 1162 | C    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |
| 27  | B8    | 416  | U    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |
| 27  | B8    | 2854 | G    | C5-C6-O6   | -7.76 | 123.94      | 128.60   |
| 1   | AA    | 527  | G    | C5-C6-O6   | -7.76 | 123.94      | 128.60   |
| 1   | AA    | 586  | C    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |
| 1   | AA    | 685  | G    | C5-C6-O6   | -7.76 | 123.94      | 128.60   |
| 1   | AA    | 1336 | C    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |
| 27  | B8    | 1044 | C    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |
| 27  | B8    | 1348 | C    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |
| 27  | B8    | 2263 | C    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |
| 1   | AA    | 284  | C    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |
| 27  | B8    | 2838 | G    | C5-C6-O6   | -7.76 | 123.94      | 128.60   |
| 27  | B8    | 2011 | U    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |
| 1   | AA    | 477  | C    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |
| 1   | AA    | 1205 | U    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1443 | C    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |
| 27  | B8    | 2084 | C    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |
| 27  | B8    | 843  | G    | C5-C6-O6   | -7.75 | 123.95      | 128.60   |
| 27  | B8    | 1731 | G    | C5-C6-O6   | -7.75 | 123.95      | 128.60   |
| 27  | B8    | 1790 | C    | O4'-C1'-N1 | 7.75  | 114.40      | 108.20   |
| 1   | AA    | 156  | C    | O4'-C1'-N1 | 7.75  | 114.40      | 108.20   |
| 1   | AA    | 1181 | G    | N1-C6-O6   | 7.75  | 124.55      | 119.90   |
| 3   | AV    | 54   | G    | C5-C6-O6   | -7.75 | 123.95      | 128.60   |
| 27  | B8    | 1804 | C    | O4'-C1'-N1 | 7.75  | 114.40      | 108.20   |
| 1   | AA    | 312  | C    | O4'-C1'-N1 | 7.75  | 114.40      | 108.20   |
| 1   | AA    | 347  | G    | C5-C6-O6   | -7.75 | 123.95      | 128.60   |
| 27  | B8    | 964  | C    | O4'-C1'-N1 | 7.75  | 114.40      | 108.20   |
| 27  | B8    | 2040 | G    | C5-C6-O6   | -7.75 | 123.95      | 128.60   |
| 1   | AA    | 544  | G    | C5-C6-O6   | -7.75 | 123.95      | 128.60   |
| 27  | B8    | 883  | G    | N1-C6-O6   | 7.75  | 124.55      | 119.90   |
| 1   | AA    | 707  | U    | O4'-C1'-N1 | 7.75  | 114.40      | 108.20   |
| 27  | B8    | 32   | C    | O4'-C1'-N1 | 7.75  | 114.40      | 108.20   |
| 27  | B8    | 128  | C    | O4'-C1'-N1 | 7.75  | 114.40      | 108.20   |
| 1   | AA    | 897  | C    | O4'-C1'-N1 | 7.75  | 114.40      | 108.20   |
| 1   | AA    | 924  | C    | O4'-C1'-N1 | 7.75  | 114.40      | 108.20   |
| 1   | AA    | 1040 | U    | O4'-C1'-N1 | 7.75  | 114.40      | 108.20   |
| 1   | AA    | 939  | G    | C5-C6-O6   | -7.74 | 123.95      | 128.60   |
| 1   | AA    | 541  | G    | C5-C6-O6   | -7.74 | 123.95      | 128.60   |
| 1   | AA    | 1121 | U    | O4'-C1'-N1 | 7.74  | 114.39      | 108.20   |
| 27  | B8    | 2582 | G    | C5-C6-O6   | -7.74 | 123.96      | 128.60   |
| 27  | B8    | 2692 | G    | C5-C6-O6   | -7.74 | 123.96      | 128.60   |
| 1   | AA    | 1195 | C    | O4'-C1'-N1 | 7.74  | 114.39      | 108.20   |
| 27  | B8    | 2472 | G    | C5-C6-O6   | -7.74 | 123.96      | 128.60   |
| 27  | B8    | 2510 | C    | O4'-C1'-N1 | 7.74  | 114.39      | 108.20   |
| 27  | B8    | 1670 | C    | O4'-C1'-N1 | 7.73  | 114.39      | 108.20   |
| 27  | B8    | 2136 | G    | C5-C6-O6   | -7.73 | 123.96      | 128.60   |
| 27  | B8    | 1375 | U    | O4'-C1'-N1 | 7.73  | 114.39      | 108.20   |
| 1   | AA    | 404  | G    | C5-C6-O6   | -7.73 | 123.96      | 128.60   |
| 1   | AA    | 1031 | C    | O4'-C1'-N1 | 7.73  | 114.38      | 108.20   |
| 1   | AA    | 1427 | C    | O4'-C1'-N1 | 7.73  | 114.38      | 108.20   |
| 27  | B8    | 2155 | U    | O4'-C1'-N1 | 7.73  | 114.38      | 108.20   |
| 27  | B8    | 811  | U    | O4'-C1'-N1 | 7.73  | 114.38      | 108.20   |
| 27  | B8    | 2098 | U    | O4'-C1'-N1 | 7.73  | 114.38      | 108.20   |
| 1   | AA    | 58   | C    | O4'-C1'-N1 | 7.72  | 114.38      | 108.20   |
| 27  | B8    | 7    | G    | C5-C6-O6   | -7.72 | 123.97      | 128.60   |
| 27  | B8    | 921  | C    | O4'-C1'-N1 | 7.72  | 114.38      | 108.20   |
| 27  | B8    | 2233 | U    | O4'-C1'-N1 | 7.72  | 114.38      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1519 | G    | C5-C6-O6   | -7.72 | 123.97      | 128.60   |
| 27  | B8    | 2851 | A    | N1-C6-N6   | 7.72  | 123.23      | 118.60   |
| 27  | B8    | 1056 | G    | O4'-C1'-N9 | 7.72  | 114.38      | 108.20   |
| 27  | B8    | 1792 | G    | C5-C6-O6   | -7.72 | 123.97      | 128.60   |
| 27  | B8    | 2125 | G    | N1-C6-O6   | 7.72  | 124.53      | 119.90   |
| 27  | B8    | 2739 | U    | O4'-C1'-N1 | 7.72  | 114.38      | 108.20   |
| 1   | AA    | 175  | C    | O4'-C1'-N1 | 7.72  | 114.37      | 108.20   |
| 1   | AA    | 1059 | C    | O4'-C1'-N1 | 7.72  | 114.38      | 108.20   |
| 1   | AA    | 1053 | G    | N1-C6-O6   | 7.72  | 124.53      | 119.90   |
| 27  | B8    | 813  | U    | O4'-C1'-N1 | 7.72  | 114.37      | 108.20   |
| 27  | B8    | 1478 | G    | C5-C6-O6   | -7.72 | 123.97      | 128.60   |
| 27  | B8    | 2404 | U    | O4'-C1'-N1 | 7.71  | 114.37      | 108.20   |
| 26  | B7    | 1    | U    | O4'-C1'-N1 | 7.71  | 114.37      | 108.20   |
| 27  | B8    | 2091 | C    | O4'-C1'-N1 | 7.71  | 114.37      | 108.20   |
| 1   | AA    | 240  | G    | C5-C6-O6   | -7.71 | 123.97      | 128.60   |
| 1   | AA    | 806  | C    | O4'-C1'-N1 | 7.71  | 114.37      | 108.20   |
| 1   | AA    | 1383 | C    | O4'-C1'-N1 | 7.71  | 114.37      | 108.20   |
| 27  | B8    | 1296 | G    | C5-C6-O6   | -7.71 | 123.97      | 128.60   |
| 27  | B8    | 41   | C    | O4'-C1'-N1 | 7.71  | 114.37      | 108.20   |
| 27  | B8    | 1988 | G    | C5-C6-O6   | -7.71 | 123.97      | 128.60   |
| 1   | AA    | 217  | C    | O4'-C1'-N1 | 7.71  | 114.37      | 108.20   |
| 1   | AA    | 997  | U    | O4'-C1'-N1 | 7.71  | 114.37      | 108.20   |
| 3   | AV    | 10   | G    | C5-C6-O6   | -7.71 | 123.97      | 128.60   |
| 27  | B8    | 1799 | G    | C5-C6-O6   | -7.71 | 123.97      | 128.60   |
| 27  | B8    | 2230 | G    | C5-C6-O6   | -7.71 | 123.97      | 128.60   |
| 27  | B8    | 2729 | G    | C5-C6-O6   | -7.71 | 123.97      | 128.60   |
| 27  | B8    | 1215 | G    | C5-C6-O6   | -7.71 | 123.98      | 128.60   |
| 27  | B8    | 2573 | C    | O4'-C1'-N1 | 7.71  | 114.36      | 108.20   |
| 27  | B8    | 291  | G    | C5-C6-O6   | -7.71 | 123.98      | 128.60   |
| 27  | B8    | 2343 | U    | O4'-C1'-N1 | 7.71  | 114.36      | 108.20   |
| 27  | B8    | 2240 | U    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 27  | B8    | 2766 | A    | C5-C6-N6   | -7.70 | 117.54      | 123.70   |
| 26  | B7    | 49   | C    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 27  | B8    | 211  | C    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 27  | B8    | 240  | C    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 27  | B8    | 2777 | G    | C5-C6-O6   | -7.70 | 123.98      | 128.60   |
| 1   | AA    | 497  | G    | C5-C6-O6   | -7.70 | 123.98      | 128.60   |
| 1   | AA    | 604  | G    | C5-C6-O6   | -7.70 | 123.98      | 128.60   |
| 1   | AA    | 788  | U    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 1   | AA    | 1128 | C    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 27  | B8    | 835  | C    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 27  | B8    | 1281 | G    | C5-C6-O6   | -7.70 | 123.98      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2789 | C    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 1   | AA    | 1097 | C    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 1   | AA    | 930  | C    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 27  | B8    | 2554 | U    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 27  | B8    | 1118 | C    | O4'-C1'-N1 | 7.69  | 114.36      | 108.20   |
| 27  | B8    | 436  | C    | O4'-C1'-N1 | 7.69  | 114.36      | 108.20   |
| 27  | B8    | 1218 | G    | C5-C6-O6   | -7.69 | 123.98      | 128.60   |
| 1   | AA    | 443  | C    | O4'-C1'-N1 | 7.69  | 114.35      | 108.20   |
| 27  | B8    | 319  | G    | C5-C6-O6   | -7.69 | 123.99      | 128.60   |
| 27  | B8    | 659  | G    | C5-C6-O6   | -7.69 | 123.99      | 128.60   |
| 27  | B8    | 1906 | G    | C5-C6-O6   | -7.69 | 123.98      | 128.60   |
| 27  | B8    | 2161 | C    | P-O3'-C3'  | 7.69  | 128.93      | 119.70   |
| 27  | B8    | 292  | U    | O4'-C1'-N1 | 7.69  | 114.35      | 108.20   |
| 27  | B8    | 635  | C    | O4'-C1'-N1 | 7.69  | 114.35      | 108.20   |
| 1   | AA    | 136  | C    | O4'-C1'-N1 | 7.69  | 114.35      | 108.20   |
| 1   | AA    | 1253 | G    | C5-C6-O6   | -7.69 | 123.99      | 128.60   |
| 26  | B7    | 67   | G    | N1-C6-O6   | 7.69  | 124.51      | 119.90   |
| 1   | AA    | 1174 | G    | C5-C6-O6   | -7.69 | 123.99      | 128.60   |
| 27  | B8    | 18   | U    | O4'-C1'-N1 | 7.69  | 114.35      | 108.20   |
| 1   | AA    | 1292 | G    | C5-C6-O6   | -7.68 | 123.99      | 128.60   |
| 27  | B8    | 2202 | U    | O4'-C1'-N1 | 7.68  | 114.35      | 108.20   |
| 1   | AA    | 18   | C    | O4'-C1'-N1 | 7.68  | 114.35      | 108.20   |
| 1   | AA    | 680  | C    | O4'-C1'-N1 | 7.68  | 114.35      | 108.20   |
| 27  | B8    | 85   | G    | C5-C6-O6   | -7.68 | 123.99      | 128.60   |
| 27  | B8    | 1830 | C    | O4'-C1'-N1 | 7.68  | 114.35      | 108.20   |
| 27  | B8    | 2899 | A    | C5-C6-N6   | -7.68 | 117.55      | 123.70   |
| 27  | B8    | 1511 | G    | C5-C6-O6   | -7.68 | 123.99      | 128.60   |
| 27  | B8    | 1684 | G    | C5-C6-O6   | -7.68 | 123.99      | 128.60   |
| 26  | B7    | 93   | C    | O4'-C1'-N1 | 7.68  | 114.34      | 108.20   |
| 1   | AA    | 552  | U    | O4'-C1'-N1 | 7.68  | 114.34      | 108.20   |
| 1   | AA    | 1309 | G    | C5-C6-O6   | -7.68 | 123.99      | 128.60   |
| 1   | AA    | 1511 | G    | C5-C6-O6   | -7.68 | 123.99      | 128.60   |
| 27  | B8    | 1277 | G    | O4'-C1'-N9 | 7.68  | 114.34      | 108.20   |
| 27  | B8    | 1657 | U    | O4'-C1'-N1 | 7.68  | 114.34      | 108.20   |
| 27  | B8    | 2506 | U    | O4'-C1'-N1 | 7.68  | 114.34      | 108.20   |
| 1   | AA    | 859  | G    | C5-C6-O6   | -7.67 | 124.00      | 128.60   |
| 1   | AA    | 1215 | G    | C5-C6-O6   | -7.67 | 124.00      | 128.60   |
| 3   | AV    | 42   | C    | O4'-C1'-N1 | 7.67  | 114.34      | 108.20   |
| 27  | B8    | 17   | G    | C5-C6-O6   | -7.67 | 124.00      | 128.60   |
| 27  | B8    | 1979 | U    | O4'-C1'-N1 | 7.67  | 114.34      | 108.20   |
| 27  | B8    | 2743 | U    | O4'-C1'-N1 | 7.67  | 114.34      | 108.20   |
| 1   | AA    | 41   | G    | C5-C6-O6   | -7.67 | 124.00      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 184  | C    | O4'-C1'-N1 | 7.67  | 114.34      | 108.20   |
| 1   | AA    | 774  | G    | C5-C6-O6   | -7.67 | 124.00      | 128.60   |
| 27  | B8    | 1104 | C    | O4'-C1'-N1 | 7.67  | 114.33      | 108.20   |
| 27  | B8    | 1113 | U    | O4'-C1'-N1 | 7.67  | 114.33      | 108.20   |
| 27  | B8    | 2277 | G    | C5-C6-O6   | -7.67 | 124.00      | 128.60   |
| 1   | AA    | 1514 | G    | C5-C6-O6   | -7.67 | 124.00      | 128.60   |
| 27  | B8    | 285  | G    | C5-C6-O6   | -7.67 | 124.00      | 128.60   |
| 27  | B8    | 1432 | G    | O4'-C1'-N9 | 7.67  | 114.33      | 108.20   |
| 27  | B8    | 1526 | C    | O4'-C1'-N1 | 7.67  | 114.33      | 108.20   |
| 1   | AA    | 62   | U    | O4'-C1'-N1 | 7.66  | 114.33      | 108.20   |
| 1   | AA    | 494  | G    | N1-C6-O6   | 7.66  | 124.50      | 119.90   |
| 1   | AA    | 1364 | U    | O4'-C1'-N1 | 7.66  | 114.33      | 108.20   |
| 27  | B8    | 2229 | U    | O4'-C1'-N1 | 7.66  | 114.33      | 108.20   |
| 27  | B8    | 2308 | G    | N1-C6-O6   | 7.66  | 124.50      | 119.90   |
| 1   | AA    | 418  | C    | O4'-C1'-N1 | 7.66  | 114.33      | 108.20   |
| 1   | AA    | 203  | G    | O4'-C1'-N9 | 7.66  | 114.33      | 108.20   |
| 27  | B8    | 2636 | C    | O4'-C1'-N1 | 7.66  | 114.33      | 108.20   |
| 2   | AX    | 17   | C    | O4'-C1'-N1 | 7.66  | 114.33      | 108.20   |
| 3   | AV    | 57   | C    | O4'-C1'-N1 | 7.66  | 114.33      | 108.20   |
| 27  | B8    | 1317 | G    | N1-C6-O6   | 7.66  | 124.50      | 119.90   |
| 27  | B8    | 2460 | U    | O4'-C1'-N1 | 7.66  | 114.33      | 108.20   |
| 27  | B8    | 400  | G    | C5-C6-O6   | -7.66 | 124.01      | 128.60   |
| 27  | B8    | 937  | C    | O4'-C1'-N1 | 7.66  | 114.33      | 108.20   |
| 27  | B8    | 2043 | C    | O4'-C1'-N1 | 7.66  | 114.33      | 108.20   |
| 27  | B8    | 258  | G    | C5-C6-O6   | -7.66 | 124.01      | 128.60   |
| 27  | B8    | 1250 | G    | C5-C6-O6   | -7.66 | 124.01      | 128.60   |
| 27  | B8    | 838  | C    | O4'-C1'-N1 | 7.65  | 114.32      | 108.20   |
| 27  | B8    | 1581 | G    | C5-C6-O6   | -7.65 | 124.01      | 128.60   |
| 1   | AA    | 734  | G    | C5-C6-O6   | -7.65 | 124.01      | 128.60   |
| 1   | AA    | 758  | C    | O4'-C1'-N1 | 7.65  | 114.32      | 108.20   |
| 1   | AA    | 1107 | C    | O4'-C1'-N1 | 7.65  | 114.32      | 108.20   |
| 27  | B8    | 40   | U    | O4'-C1'-N1 | 7.65  | 114.32      | 108.20   |
| 27  | B8    | 966  | G    | C5-C6-O6   | -7.65 | 124.01      | 128.60   |
| 27  | B8    | 1921 | G    | C5-C6-O6   | -7.65 | 124.01      | 128.60   |
| 27  | B8    | 2671 | G    | C5-C6-O6   | -7.65 | 124.01      | 128.60   |
| 1   | AA    | 170  | U    | O4'-C1'-N1 | 7.65  | 114.32      | 108.20   |
| 1   | AA    | 954  | G    | C5-C6-O6   | -7.65 | 124.01      | 128.60   |
| 1   | AA    | 1424 | U    | O4'-C1'-N1 | 7.65  | 114.32      | 108.20   |
| 27  | B8    | 290  | U    | O4'-C1'-N1 | 7.65  | 114.32      | 108.20   |
| 1   | AA    | 337  | G    | C5-C6-O6   | -7.65 | 124.01      | 128.60   |
| 1   | AA    | 1448 | C    | O4'-C1'-N1 | 7.65  | 114.32      | 108.20   |
| 26  | B7    | 47   | C    | O4'-C1'-N1 | 7.65  | 114.32      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1930 | G    | O4'-C1'-N9 | 7.65  | 114.32      | 108.20   |
| 1   | AA    | 1237 | C    | O4'-C1'-N1 | 7.65  | 114.32      | 108.20   |
| 1   | AA    | 1161 | C    | O4'-C1'-N1 | 7.64  | 114.31      | 108.20   |
| 1   | AA    | 476  | U    | O4'-C1'-N1 | 7.64  | 114.31      | 108.20   |
| 27  | B8    | 2626 | C    | O4'-C1'-N1 | 7.64  | 114.31      | 108.20   |
| 1   | AA    | 679  | C    | O4'-C1'-N1 | 7.64  | 114.31      | 108.20   |
| 27  | B8    | 624  | C    | O4'-C1'-N1 | 7.64  | 114.31      | 108.20   |
| 27  | B8    | 763  | G    | C5-C6-O6   | -7.64 | 124.02      | 128.60   |
| 27  | B8    | 901  | C    | O4'-C1'-N1 | 7.64  | 114.31      | 108.20   |
| 27  | B8    | 940  | G    | C5-C6-O6   | -7.64 | 124.02      | 128.60   |
| 1   | AA    | 902  | G    | C5-C6-O6   | -7.64 | 124.02      | 128.60   |
| 1   | AA    | 1252 | A    | C5-C6-N6   | -7.64 | 117.59      | 123.70   |
| 27  | B8    | 779  | U    | O4'-C1'-N1 | 7.64  | 114.31      | 108.20   |
| 27  | B8    | 2430 | A    | C4-C5-C6   | 7.64  | 120.82      | 117.00   |
| 1   | AA    | 1247 | U    | O4'-C1'-N1 | 7.63  | 114.31      | 108.20   |
| 27  | B8    | 27   | G    | O4'-C1'-N9 | 7.63  | 114.31      | 108.20   |
| 27  | B8    | 250  | G    | N1-C6-O6   | 7.63  | 124.48      | 119.90   |
| 27  | B8    | 2783 | U    | O4'-C1'-N1 | 7.63  | 114.31      | 108.20   |
| 1   | AA    | 540  | G    | C5-C6-O6   | -7.63 | 124.02      | 128.60   |
| 27  | B8    | 2306 | C    | O4'-C1'-N1 | 7.63  | 114.31      | 108.20   |
| 3   | AV    | 66   | U    | O4'-C1'-N1 | 7.63  | 114.30      | 108.20   |
| 27  | B8    | 110  | G    | C5-C6-O6   | -7.63 | 124.02      | 128.60   |
| 27  | B8    | 1201 | U    | O4'-C1'-N1 | 7.63  | 114.30      | 108.20   |
| 1   | AA    | 688  | G    | C5-C6-O6   | -7.63 | 124.02      | 128.60   |
| 27  | B8    | 2798 | U    | O4'-C1'-N1 | 7.63  | 114.30      | 108.20   |
| 27  | B8    | 2876 | G    | C5-C6-O6   | -7.63 | 124.02      | 128.60   |
| 27  | B8    | 261  | G    | C5-C6-O6   | -7.62 | 124.03      | 128.60   |
| 27  | B8    | 1179 | G    | C5-C6-O6   | -7.62 | 124.03      | 128.60   |
| 1   | AA    | 854  | U    | O4'-C1'-N1 | 7.62  | 114.30      | 108.20   |
| 27  | B8    | 1290 | C    | O4'-C1'-N1 | 7.62  | 114.30      | 108.20   |
| 1   | AA    | 846  | G    | C5-C6-O6   | -7.62 | 124.03      | 128.60   |
| 1   | AA    | 1390 | U    | O4'-C1'-N1 | 7.62  | 114.30      | 108.20   |
| 27  | B8    | 275  | C    | O4'-C1'-N1 | 7.62  | 114.30      | 108.20   |
| 27  | B8    | 1399 | C    | O4'-C1'-N1 | 7.62  | 114.30      | 108.20   |
| 27  | B8    | 1482 | G    | C5-C6-O6   | -7.62 | 124.03      | 128.60   |
| 1   | AA    | 206  | C    | O4'-C1'-N1 | 7.62  | 114.30      | 108.20   |
| 27  | B8    | 1977 | A    | C5-C6-N6   | -7.62 | 117.60      | 123.70   |
| 1   | AA    | 141  | G    | C5-C6-O6   | -7.62 | 124.03      | 128.60   |
| 1   | AA    | 1140 | C    | O4'-C1'-N1 | 7.62  | 114.29      | 108.20   |
| 27  | B8    | 677  | A    | C5-C6-N6   | -7.62 | 117.61      | 123.70   |
| 27  | B8    | 863  | A    | C5-C6-N6   | -7.62 | 117.61      | 123.70   |
| 27  | B8    | 2686 | G    | C5-C6-O6   | -7.62 | 124.03      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 35  | BG    | 93   | TYR  | CB-CG-CD1  | -7.62 | 116.43      | 121.00   |
| 27  | B8    | 1499 | C    | O4'-C1'-N1 | 7.61  | 114.29      | 108.20   |
| 27  | B8    | 2394 | C    | O4'-C1'-N1 | 7.61  | 114.29      | 108.20   |
| 27  | B8    | 2165 | C    | P-O3'-C3'  | 7.61  | 128.83      | 119.70   |
| 27  | B8    | 2442 | C    | O4'-C1'-N1 | 7.61  | 114.29      | 108.20   |
| 27  | B8    | 2844 | G    | O4'-C1'-N9 | 7.61  | 114.29      | 108.20   |
| 1   | AA    | 348  | G    | C5-C6-O6   | -7.61 | 124.03      | 128.60   |
| 27  | B8    | 1416 | G    | C5-C6-O6   | -7.61 | 124.03      | 128.60   |
| 27  | B8    | 1992 | G    | C5-C6-O6   | -7.61 | 124.04      | 128.60   |
| 1   | AA    | 1070 | U    | O4'-C1'-N1 | 7.61  | 114.28      | 108.20   |
| 27  | B8    | 698  | C    | O4'-C1'-N1 | 7.61  | 114.28      | 108.20   |
| 27  | B8    | 1411 | U    | O4'-C1'-N1 | 7.61  | 114.28      | 108.20   |
| 27  | B8    | 79   | C    | O4'-C1'-N1 | 7.60  | 114.28      | 108.20   |
| 27  | B8    | 1096 | A    | O4'-C1'-N9 | 7.60  | 114.28      | 108.20   |
| 27  | B8    | 2330 | G    | C5-C6-O6   | -7.60 | 124.04      | 128.60   |
| 1   | AA    | 929  | G    | C5-C6-O6   | -7.60 | 124.04      | 128.60   |
| 1   | AA    | 1356 | G    | C5-C6-O6   | -7.60 | 124.04      | 128.60   |
| 1   | AA    | 1481 | U    | O4'-C1'-N1 | 7.60  | 114.28      | 108.20   |
| 27  | B8    | 959  | A    | C5-C6-N6   | -7.60 | 117.62      | 123.70   |
| 27  | B8    | 1062 | G    | C5-C6-O6   | -7.60 | 124.04      | 128.60   |
| 27  | B8    | 1007 | C    | O4'-C1'-N1 | 7.60  | 114.28      | 108.20   |
| 27  | B8    | 1708 | C    | O4'-C1'-N1 | 7.60  | 114.28      | 108.20   |
| 27  | B8    | 2123 | G    | C5-C6-O6   | -7.60 | 124.04      | 128.60   |
| 1   | AA    | 277  | C    | O4'-C1'-N1 | 7.60  | 114.28      | 108.20   |
| 27  | B8    | 122  | G    | C5-C6-O6   | -7.60 | 124.04      | 128.60   |
| 1   | AA    | 1183 | U    | O4'-C1'-N1 | 7.59  | 114.28      | 108.20   |
| 27  | B8    | 810  | U    | O4'-C1'-N1 | 7.59  | 114.28      | 108.20   |
| 27  | B8    | 1641 | A    | C4-C5-C6   | 7.59  | 120.80      | 117.00   |
| 27  | B8    | 2514 | U    | O4'-C1'-N1 | 7.59  | 114.28      | 108.20   |
| 1   | AA    | 659  | U    | O4'-C1'-N1 | 7.59  | 114.27      | 108.20   |
| 27  | B8    | 2427 | C    | O4'-C1'-N1 | 7.59  | 114.27      | 108.20   |
| 1   | AA    | 1353 | G    | C5-C6-O6   | -7.59 | 124.05      | 128.60   |
| 1   | AA    | 1536 | C    | O4'-C1'-N1 | 7.59  | 114.27      | 108.20   |
| 27  | B8    | 674  | G    | C5-C6-O6   | -7.59 | 124.05      | 128.60   |
| 27  | B8    | 1064 | C    | O4'-C1'-N1 | 7.59  | 114.27      | 108.20   |
| 27  | B8    | 1974 | C    | O4'-C1'-N1 | 7.59  | 114.27      | 108.20   |
| 27  | B8    | 2875 | C    | O4'-C1'-N1 | 7.59  | 114.27      | 108.20   |
| 1   | AA    | 474  | G    | C5-C6-O6   | -7.59 | 124.05      | 128.60   |
| 1   | AA    | 1373 | G    | C5-C6-O6   | -7.59 | 124.05      | 128.60   |
| 27  | B8    | 1052 | C    | O4'-C1'-N1 | 7.59  | 114.27      | 108.20   |
| 27  | B8    | 1933 | G    | C5-C6-O6   | -7.59 | 124.05      | 128.60   |
| 1   | AA    | 29   | U    | O4'-C1'-N1 | 7.59  | 114.27      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 123  | U    | O4'-C1'-N1 | 7.59  | 114.27      | 108.20   |
| 26  | B7    | 19   | C    | O4'-C1'-N1 | 7.59  | 114.27      | 108.20   |
| 27  | B8    | 2621 | G    | C5-C6-O6   | -7.59 | 124.05      | 128.60   |
| 1   | AA    | 1341 | U    | O4'-C1'-N1 | 7.59  | 114.27      | 108.20   |
| 1   | AA    | 1367 | C    | O4'-C1'-N1 | 7.59  | 114.27      | 108.20   |
| 27  | B8    | 441  | U    | O4'-C1'-N1 | 7.59  | 114.27      | 108.20   |
| 1   | AA    | 1100 | C    | O4'-C1'-N1 | 7.58  | 114.27      | 108.20   |
| 27  | B8    | 1833 | C    | O4'-C1'-N1 | 7.58  | 114.27      | 108.20   |
| 27  | B8    | 1861 | G    | C5-C6-O6   | -7.58 | 124.05      | 128.60   |
| 27  | B8    | 314  | C    | O4'-C1'-N1 | 7.58  | 114.27      | 108.20   |
| 27  | B8    | 1019 | U    | O4'-C1'-N1 | 7.58  | 114.27      | 108.20   |
| 27  | B8    | 1190 | G    | C5-C6-O6   | -7.58 | 124.05      | 128.60   |
| 1   | AA    | 671  | G    | C5-C6-O6   | -7.58 | 124.05      | 128.60   |
| 27  | B8    | 1675 | C    | O4'-C1'-N1 | 7.58  | 114.26      | 108.20   |
| 27  | B8    | 2047 | C    | O4'-C1'-N1 | 7.58  | 114.26      | 108.20   |
| 1   | AA    | 342  | C    | O4'-C1'-N1 | 7.58  | 114.26      | 108.20   |
| 1   | AA    | 1027 | C    | O4'-C1'-N1 | 7.58  | 114.26      | 108.20   |
| 1   | AA    | 1114 | C    | O4'-C1'-N1 | 7.58  | 114.26      | 108.20   |
| 27  | B8    | 1771 | C    | O4'-C1'-N1 | 7.58  | 114.26      | 108.20   |
| 1   | AA    | 615  | G    | O4'-C1'-N9 | 7.58  | 114.26      | 108.20   |
| 27  | B8    | 1097 | U    | O4'-C1'-N1 | 7.58  | 114.26      | 108.20   |
| 27  | B8    | 2840 | C    | O4'-C1'-N1 | 7.58  | 114.26      | 108.20   |
| 1   | AA    | 233  | C    | O4'-C1'-N1 | 7.58  | 114.26      | 108.20   |
| 27  | B8    | 1707 | G    | C5-C6-O6   | -7.58 | 124.06      | 128.60   |
| 27  | B8    | 2672 | U    | O4'-C1'-N1 | 7.58  | 114.26      | 108.20   |
| 1   | AA    | 811  | C    | O4'-C1'-N1 | 7.57  | 114.26      | 108.20   |
| 27  | B8    | 1537 | G    | C5-C6-O6   | -7.57 | 124.06      | 128.60   |
| 27  | B8    | 1941 | C    | O4'-C1'-N1 | 7.57  | 114.26      | 108.20   |
| 1   | AA    | 1457 | G    | C5-C6-O6   | -7.57 | 124.06      | 128.60   |
| 27  | B8    | 2012 | G    | C5-C6-O6   | -7.57 | 124.06      | 128.60   |
| 27  | B8    | 406  | G    | C5-C6-O6   | -7.57 | 124.06      | 128.60   |
| 27  | B8    | 994  | C    | O4'-C1'-N1 | 7.57  | 114.26      | 108.20   |
| 27  | B8    | 2702 | G    | C5-C6-O6   | -7.57 | 124.06      | 128.60   |
| 1   | AA    | 396  | C    | O4'-C1'-N1 | 7.57  | 114.25      | 108.20   |
| 1   | AA    | 1119 | C    | O4'-C1'-N1 | 7.57  | 114.25      | 108.20   |
| 1   | AA    | 436  | C    | O4'-C1'-N1 | 7.57  | 114.25      | 108.20   |
| 26  | B7    | 64   | G    | C5-C6-O6   | -7.57 | 124.06      | 128.60   |
| 27  | B8    | 560  | C    | O4'-C1'-N1 | 7.57  | 114.25      | 108.20   |
| 27  | B8    | 2878 | U    | O4'-C1'-N1 | 7.57  | 114.25      | 108.20   |
| 27  | B8    | 760  | G    | C5-C6-O6   | -7.57 | 124.06      | 128.60   |
| 27  | B8    | 1241 | A    | O4'-C1'-N9 | 7.57  | 114.25      | 108.20   |
| 27  | B8    | 1533 | C    | O4'-C1'-N1 | 7.57  | 114.25      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1984 | G    | C5-C6-O6   | -7.57 | 124.06      | 128.60   |
| 27  | B8    | 2456 | C    | O4'-C1'-N1 | 7.57  | 114.25      | 108.20   |
| 27  | B8    | 420  | C    | O4'-C1'-N1 | 7.56  | 114.25      | 108.20   |
| 27  | B8    | 2313 | C    | O4'-C1'-N1 | 7.56  | 114.25      | 108.20   |
| 27  | B8    | 2440 | C    | O4'-C1'-N1 | 7.56  | 114.25      | 108.20   |
| 1   | AA    | 545  | C    | O4'-C1'-N1 | 7.56  | 114.25      | 108.20   |
| 27  | B8    | 2888 | C    | O4'-C1'-N1 | 7.56  | 114.25      | 108.20   |
| 1   | AA    | 1412 | C    | O4'-C1'-N1 | 7.56  | 114.25      | 108.20   |
| 27  | B8    | 1624 | U    | O4'-C1'-N1 | 7.56  | 114.25      | 108.20   |
| 27  | B8    | 2150 | C    | O4'-C1'-N1 | 7.56  | 114.25      | 108.20   |
| 27  | B8    | 2235 | G    | C5-C6-O6   | -7.56 | 124.06      | 128.60   |
| 1   | AA    | 221  | C    | O4'-C1'-N1 | 7.56  | 114.25      | 108.20   |
| 3   | AV    | 41   | U    | O4'-C1'-N1 | 7.56  | 114.25      | 108.20   |
| 27  | B8    | 1081 | U    | O4'-C1'-N1 | 7.56  | 114.25      | 108.20   |
| 27  | B8    | 2247 | A    | O4'-C1'-N9 | 7.56  | 114.25      | 108.20   |
| 27  | B8    | 2293 | G    | C5-C6-O6   | -7.56 | 124.06      | 128.60   |
| 27  | B8    | 1158 | C    | O4'-C1'-N1 | 7.56  | 114.25      | 108.20   |
| 1   | AA    | 249  | U    | O4'-C1'-N1 | 7.55  | 114.24      | 108.20   |
| 27  | B8    | 873  | C    | O4'-C1'-N1 | 7.55  | 114.24      | 108.20   |
| 27  | B8    | 2004 | G    | C5-C6-O6   | -7.55 | 124.07      | 128.60   |
| 1   | AA    | 786  | G    | O4'-C1'-N9 | 7.55  | 114.24      | 108.20   |
| 27  | B8    | 1808 | A    | O4'-C1'-N9 | 7.55  | 114.24      | 108.20   |
| 27  | B8    | 1976 | U    | O4'-C1'-N1 | 7.55  | 114.24      | 108.20   |
| 1   | AA    | 395  | C    | O4'-C1'-N1 | 7.55  | 114.24      | 108.20   |
| 3   | AV    | 24   | C    | O4'-C1'-N1 | 7.55  | 114.24      | 108.20   |
| 26  | B7    | 16   | G    | O4'-C1'-N9 | 7.55  | 114.24      | 108.20   |
| 26  | B7    | 83   | G    | C5-C6-O6   | -7.55 | 124.07      | 128.60   |
| 27  | B8    | 786  | C    | O4'-C1'-N1 | 7.55  | 114.24      | 108.20   |
| 1   | AA    | 737  | C    | O4'-C1'-N1 | 7.55  | 114.24      | 108.20   |
| 1   | AA    | 766  | A    | O4'-C1'-N9 | 7.55  | 114.24      | 108.20   |
| 1   | AA    | 805  | C    | O4'-C1'-N1 | 7.55  | 114.24      | 108.20   |
| 26  | B7    | 108  | A    | C5-C6-N6   | -7.55 | 117.66      | 123.70   |
| 27  | B8    | 738  | G    | C5-C6-O6   | -7.55 | 124.07      | 128.60   |
| 27  | B8    | 2026 | U    | O4'-C1'-N1 | 7.55  | 114.24      | 108.20   |
| 27  | B8    | 2650 | U    | O4'-C1'-N1 | 7.55  | 114.24      | 108.20   |
| 1   | AA    | 656  | G    | O4'-C1'-N9 | 7.54  | 114.23      | 108.20   |
| 1   | AA    | 1468 | A    | C4-C5-C6   | 7.54  | 120.77      | 117.00   |
| 27  | B8    | 1220 | G    | O4'-C1'-N9 | 7.54  | 114.23      | 108.20   |
| 27  | B8    | 1438 | U    | O4'-C1'-N1 | 7.54  | 114.23      | 108.20   |
| 27  | B8    | 1560 | G    | C5-C6-O6   | -7.54 | 124.07      | 128.60   |
| 27  | B8    | 1564 | C    | O4'-C1'-N1 | 7.54  | 114.24      | 108.20   |
| 27  | B8    | 1881 | C    | O4'-C1'-N1 | 7.54  | 114.23      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2322 | A    | O4'-C1'-N9 | 7.54  | 114.23      | 108.20   |
| 27  | B8    | 1430 | G    | C5-C6-O6   | -7.54 | 124.08      | 128.60   |
| 35  | BG    | 93   | TYR  | CB-CG-CD2  | 7.54  | 125.52      | 121.00   |
| 1   | AA    | 1444 | U    | O4'-C1'-N1 | 7.54  | 114.23      | 108.20   |
| 27  | B8    | 1535 | A    | O4'-C1'-N9 | 7.54  | 114.23      | 108.20   |
| 27  | B8    | 2567 | G    | C5-C6-O6   | -7.54 | 124.08      | 128.60   |
| 1   | AA    | 795  | C    | O4'-C1'-N1 | 7.54  | 114.23      | 108.20   |
| 1   | AA    | 984  | C    | O4'-C1'-N1 | 7.54  | 114.23      | 108.20   |
| 1   | AA    | 1078 | U    | O4'-C1'-N1 | 7.54  | 114.23      | 108.20   |
| 27  | B8    | 2903 | U    | C2-N1-C1'  | 7.54  | 126.74      | 117.70   |
| 1   | AA    | 1232 | U    | O4'-C1'-N1 | 7.53  | 114.23      | 108.20   |
| 27  | B8    | 1195 | G    | C5-C6-O6   | -7.53 | 124.08      | 128.60   |
| 27  | B8    | 1330 | C    | O4'-C1'-N1 | 7.53  | 114.23      | 108.20   |
| 1   | AA    | 916  | U    | O4'-C1'-N1 | 7.53  | 114.22      | 108.20   |
| 27  | B8    | 1653 | G    | C5-C6-O6   | -7.53 | 124.08      | 128.60   |
| 27  | B8    | 2569 | G    | C5-C6-O6   | -7.53 | 124.08      | 128.60   |
| 27  | B8    | 2583 | G    | C5-C6-O6   | -7.53 | 124.08      | 128.60   |
| 27  | B8    | 2303 | G    | C5-C6-O6   | -7.53 | 124.08      | 128.60   |
| 1   | AA    | 110  | C    | O4'-C1'-N1 | 7.53  | 114.22      | 108.20   |
| 1   | AA    | 709  | U    | O4'-C1'-N1 | 7.53  | 114.22      | 108.20   |
| 1   | AA    | 1351 | U    | O4'-C1'-N1 | 7.53  | 114.22      | 108.20   |
| 27  | B8    | 358  | U    | O4'-C1'-N1 | 7.53  | 114.22      | 108.20   |
| 27  | B8    | 380  | G    | C5-C6-O6   | -7.53 | 124.08      | 128.60   |
| 27  | B8    | 681  | G    | C5-C6-O6   | -7.53 | 124.08      | 128.60   |
| 27  | B8    | 865  | C    | O4'-C1'-N1 | 7.53  | 114.22      | 108.20   |
| 27  | B8    | 908  | C    | O4'-C1'-N1 | 7.53  | 114.22      | 108.20   |
| 1   | AA    | 1056 | U    | O4'-C1'-N1 | 7.53  | 114.22      | 108.20   |
| 27  | B8    | 1764 | C    | O4'-C1'-N1 | 7.53  | 114.22      | 108.20   |
| 27  | B8    | 45   | G    | C5-C6-O6   | -7.52 | 124.09      | 128.60   |
| 27  | B8    | 281  | C    | O4'-C1'-N1 | 7.52  | 114.22      | 108.20   |
| 27  | B8    | 554  | U    | O4'-C1'-N1 | 7.52  | 114.22      | 108.20   |
| 27  | B8    | 1486 | U    | O4'-C1'-N1 | 7.52  | 114.22      | 108.20   |
| 1   | AA    | 1348 | U    | O4'-C1'-N1 | 7.52  | 114.22      | 108.20   |
| 27  | B8    | 2087 | G    | C5-C6-O6   | -7.52 | 124.09      | 128.60   |
| 1   | AA    | 1472 | U    | O4'-C1'-N1 | 7.52  | 114.22      | 108.20   |
| 27  | B8    | 2006 | C    | O4'-C1'-N1 | 7.52  | 114.22      | 108.20   |
| 27  | B8    | 2316 | G    | C5-C6-O6   | -7.52 | 124.09      | 128.60   |
| 1   | AA    | 521  | G    | C5-C6-O6   | -7.52 | 124.09      | 128.60   |
| 27  | B8    | 906  | U    | O4'-C1'-N1 | 7.52  | 114.21      | 108.20   |
| 27  | B8    | 1043 | C    | O4'-C1'-N1 | 7.52  | 114.21      | 108.20   |
| 1   | AA    | 953  | G    | C5-C6-O6   | -7.52 | 124.09      | 128.60   |
| 27  | B8    | 145  | C    | O4'-C1'-N1 | 7.52  | 114.21      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1441 | G    | C5-C6-O6   | -7.52 | 124.09      | 128.60   |
| 1   | AA    | 720  | C    | O4'-C1'-N1 | 7.51  | 114.21      | 108.20   |
| 1   | AA    | 1207 | G    | C5-C6-O6   | -7.51 | 124.09      | 128.60   |
| 27  | B8    | 271  | G    | C5-C6-O6   | -7.51 | 124.09      | 128.60   |
| 27  | B8    | 2413 | G    | C5-C6-O6   | -7.51 | 124.09      | 128.60   |
| 1   | AA    | 200  | G    | C5-C6-O6   | -7.51 | 124.09      | 128.60   |
| 3   | AV    | 28   | C    | O4'-C1'-N1 | 7.51  | 114.21      | 108.20   |
| 1   | AA    | 276  | G    | C5-C6-O6   | -7.51 | 124.09      | 128.60   |
| 27  | B8    | 691  | C    | O4'-C1'-N1 | 7.51  | 114.21      | 108.20   |
| 27  | B8    | 1500 | G    | C5-C6-O6   | -7.51 | 124.09      | 128.60   |
| 27  | B8    | 2428 | G    | C5-C6-O6   | -7.51 | 124.09      | 128.60   |
| 27  | B8    | 141  | G    | O4'-C1'-N9 | 7.51  | 114.21      | 108.20   |
| 27  | B8    | 1216 | G    | C5-C6-O6   | -7.51 | 124.10      | 128.60   |
| 27  | B8    | 2606 | C    | O4'-C1'-N1 | 7.51  | 114.20      | 108.20   |
| 27  | B8    | 498  | G    | C5-C6-O6   | -7.50 | 124.10      | 128.60   |
| 27  | B8    | 588  | U    | O4'-C1'-N1 | 7.50  | 114.20      | 108.20   |
| 27  | B8    | 1175 | A    | O4'-C1'-N9 | 7.50  | 114.20      | 108.20   |
| 27  | B8    | 1208 | C    | O4'-C1'-N1 | 7.50  | 114.20      | 108.20   |
| 1   | AA    | 1043 | G    | C5-C6-O6   | -7.50 | 124.10      | 128.60   |
| 1   | AA    | 1187 | G    | C5-C6-O6   | -7.50 | 124.10      | 128.60   |
| 1   | AA    | 1370 | G    | C5-C6-O6   | -7.50 | 124.10      | 128.60   |
| 27  | B8    | 60   | G    | C5-C6-O6   | -7.50 | 124.10      | 128.60   |
| 27  | B8    | 2341 | G    | C5-C6-O6   | -7.50 | 124.10      | 128.60   |
| 27  | B8    | 2389 | G    | C5-C6-O6   | -7.50 | 124.10      | 128.60   |
| 27  | B8    | 335  | C    | O4'-C1'-N1 | 7.50  | 114.20      | 108.20   |
| 27  | B8    | 2788 | C    | O4'-C1'-N1 | 7.50  | 114.20      | 108.20   |
| 27  | B8    | 1337 | G    | C5-C6-O6   | -7.50 | 124.10      | 128.60   |
| 27  | B8    | 1368 | G    | C5-C6-O6   | -7.50 | 124.10      | 128.60   |
| 27  | B8    | 1382 | G    | N1-C6-O6   | 7.50  | 124.40      | 119.90   |
| 27  | B8    | 2246 | G    | C5-C6-O6   | -7.50 | 124.10      | 128.60   |
| 1   | AA    | 1423 | G    | C5-C6-O6   | -7.50 | 124.10      | 128.60   |
| 27  | B8    | 2619 | C    | O4'-C1'-N1 | 7.50  | 114.20      | 108.20   |
| 27  | B8    | 2126 | A    | O4'-C1'-N9 | 7.50  | 114.20      | 108.20   |
| 1   | AA    | 804  | U    | O4'-C1'-N1 | 7.49  | 114.19      | 108.20   |
| 1   | AA    | 885  | G    | C5-C6-O6   | -7.49 | 124.11      | 128.60   |
| 27  | B8    | 2633 | G    | C5-C6-O6   | -7.49 | 124.11      | 128.60   |
| 1   | AA    | 548  | G    | C5-C6-O6   | -7.49 | 124.11      | 128.60   |
| 1   | AA    | 643  | C    | O4'-C1'-N1 | 7.49  | 114.19      | 108.20   |
| 27  | B8    | 229  | C    | O4'-C1'-N1 | 7.49  | 114.19      | 108.20   |
| 27  | B8    | 839  | U    | O4'-C1'-N1 | 7.49  | 114.19      | 108.20   |
| 27  | B8    | 1017 | G    | O4'-C1'-N9 | 7.49  | 114.19      | 108.20   |
| 27  | B8    | 1185 | G    | C5-C6-O6   | -7.49 | 124.11      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1663 | G    | C5-C6-O6   | -7.49 | 124.11      | 128.60   |
| 1   | AA    | 293  | G    | C5-C6-O6   | -7.49 | 124.11      | 128.60   |
| 1   | AA    | 937  | A    | C5-C6-N6   | -7.49 | 117.71      | 123.70   |
| 27  | B8    | 944  | C    | O4'-C1'-N1 | 7.49  | 114.19      | 108.20   |
| 27  | B8    | 1390 | U    | O4'-C1'-N1 | 7.49  | 114.19      | 108.20   |
| 27  | B8    | 2709 | G    | C5-C6-O6   | -7.49 | 124.11      | 128.60   |
| 27  | B8    | 1303 | G    | C5-C6-O6   | -7.49 | 124.11      | 128.60   |
| 27  | B8    | 1555 | G    | C5-C6-O6   | -7.49 | 124.11      | 128.60   |
| 27  | B8    | 2661 | G    | C5-C6-O6   | -7.49 | 124.11      | 128.60   |
| 26  | B7    | 65   | U    | O4'-C1'-N1 | 7.49  | 114.19      | 108.20   |
| 27  | B8    | 1491 | G    | C5-C6-O6   | -7.49 | 124.11      | 128.60   |
| 27  | B8    | 2337 | G    | C5-C6-O6   | -7.49 | 124.11      | 128.60   |
| 1   | AA    | 611  | C    | O4'-C1'-N1 | 7.48  | 114.19      | 108.20   |
| 1   | AA    | 943  | U    | O4'-C1'-N1 | 7.48  | 114.19      | 108.20   |
| 27  | B8    | 82   | U    | O4'-C1'-N1 | 7.48  | 114.19      | 108.20   |
| 27  | B8    | 2064 | C    | O4'-C1'-N1 | 7.48  | 114.19      | 108.20   |
| 27  | B8    | 2167 | U    | O4'-C1'-N1 | 7.48  | 114.19      | 108.20   |
| 1   | AA    | 493  | A    | O4'-C1'-N9 | 7.48  | 114.18      | 108.20   |
| 3   | AV    | 17   | C    | O4'-C1'-N1 | 7.48  | 114.19      | 108.20   |
| 27  | B8    | 1873 | G    | C5-C6-O6   | -7.48 | 124.11      | 128.60   |
| 27  | B8    | 640  | C    | O4'-C1'-N1 | 7.48  | 114.18      | 108.20   |
| 1   | AA    | 227  | G    | C5-C6-O6   | -7.48 | 124.11      | 128.60   |
| 27  | B8    | 132  | G    | C5-C6-O6   | -7.48 | 124.11      | 128.60   |
| 27  | B8    | 2454 | G    | C5-C6-O6   | -7.47 | 124.12      | 128.60   |
| 1   | AA    | 911  | U    | O4'-C1'-N1 | 7.47  | 114.18      | 108.20   |
| 1   | AA    | 1327 | C    | O4'-C1'-N1 | 7.47  | 114.18      | 108.20   |
| 27  | B8    | 2272 | U    | O4'-C1'-N1 | 7.47  | 114.18      | 108.20   |
| 27  | B8    | 2642 | G    | C5-C6-O6   | -7.47 | 124.12      | 128.60   |
| 27  | B8    | 76   | C    | O4'-C1'-N1 | 7.47  | 114.17      | 108.20   |
| 27  | B8    | 553  | G    | C5-C6-O6   | -7.47 | 124.12      | 128.60   |
| 27  | B8    | 2152 | G    | N1-C6-O6   | 7.47  | 124.38      | 119.90   |
| 27  | B8    | 2334 | U    | O4'-C1'-N1 | 7.47  | 114.18      | 108.20   |
| 1   | AA    | 37   | U    | O4'-C1'-N1 | 7.47  | 114.17      | 108.20   |
| 1   | AA    | 68   | G    | N1-C6-O6   | 7.47  | 124.38      | 119.90   |
| 27  | B8    | 410  | G    | C5-C6-O6   | -7.47 | 124.12      | 128.60   |
| 1   | AA    | 697  | U    | O4'-C1'-N1 | 7.47  | 114.17      | 108.20   |
| 1   | AA    | 1442 | G    | C5-C6-O6   | -7.47 | 124.12      | 128.60   |
| 26  | B7    | 89   | U    | O4'-C1'-N1 | 7.47  | 114.17      | 108.20   |
| 27  | B8    | 848  | C    | O4'-C1'-N1 | 7.47  | 114.17      | 108.20   |
| 27  | B8    | 697  | G    | C5-C6-O6   | -7.46 | 124.12      | 128.60   |
| 27  | B8    | 1202 | G    | C5-C6-O6   | -7.46 | 124.12      | 128.60   |
| 27  | B8    | 2669 | G    | C5-C6-O6   | -7.46 | 124.12      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2710 | C    | O4'-C1'-N1 | 7.46  | 114.17      | 108.20   |
| 1   | AA    | 590  | U    | O4'-C1'-N1 | 7.46  | 114.17      | 108.20   |
| 26  | B7    | 117  | G    | C5-C6-O6   | -7.46 | 124.12      | 128.60   |
| 27  | B8    | 1443 | U    | O4'-C1'-N1 | 7.46  | 114.17      | 108.20   |
| 27  | B8    | 1474 | U    | O4'-C1'-N1 | 7.46  | 114.17      | 108.20   |
| 27  | B8    | 2818 | U    | O4'-C1'-N1 | 7.46  | 114.17      | 108.20   |
| 1   | AA    | 903  | G    | C5-C6-O6   | -7.46 | 124.12      | 128.60   |
| 1   | AA    | 955  | U    | O4'-C1'-N1 | 7.46  | 114.17      | 108.20   |
| 1   | AA    | 1339 | A    | C4-C5-C6   | 7.46  | 120.73      | 117.00   |
| 27  | B8    | 1868 | C    | O4'-C1'-N1 | 7.46  | 114.17      | 108.20   |
| 27  | B8    | 484  | C    | O4'-C1'-N1 | 7.46  | 114.17      | 108.20   |
| 27  | B8    | 1894 | C    | O4'-C1'-N1 | 7.46  | 114.17      | 108.20   |
| 27  | B8    | 536  | G    | C5-C6-O6   | -7.46 | 124.12      | 128.60   |
| 1   | AA    | 485  | U    | O4'-C1'-N1 | 7.46  | 114.17      | 108.20   |
| 27  | B8    | 1295 | C    | O4'-C1'-N1 | 7.46  | 114.17      | 108.20   |
| 27  | B8    | 1112 | G    | O4'-C1'-N9 | 7.46  | 114.16      | 108.20   |
| 26  | B7    | 48   | U    | O4'-C1'-N1 | 7.45  | 114.16      | 108.20   |
| 27  | B8    | 1740 | G    | C5-C6-O6   | -7.45 | 124.13      | 128.60   |
| 1   | AA    | 678  | U    | O4'-C1'-N1 | 7.45  | 114.16      | 108.20   |
| 1   | AA    | 1186 | G    | C5-C6-O6   | -7.45 | 124.13      | 128.60   |
| 1   | AA    | 1208 | C    | O4'-C1'-N1 | 7.45  | 114.16      | 108.20   |
| 1   | AA    | 1376 | U    | O4'-C1'-N1 | 7.45  | 114.16      | 108.20   |
| 26  | B7    | 116  | G    | C5-C6-O6   | -7.45 | 124.13      | 128.60   |
| 27  | B8    | 134  | G    | C5-C6-O6   | -7.45 | 124.13      | 128.60   |
| 27  | B8    | 2180 | U    | O4'-C1'-N1 | 7.45  | 114.16      | 108.20   |
| 27  | B8    | 2495 | G    | C5-C6-O6   | -7.45 | 124.13      | 128.60   |
| 27  | B8    | 2528 | U    | O4'-C1'-N1 | 7.45  | 114.16      | 108.20   |
| 27  | B8    | 80   | G    | C5-C6-O6   | -7.45 | 124.13      | 128.60   |
| 27  | B8    | 2762 | C    | O4'-C1'-N1 | 7.45  | 114.16      | 108.20   |
| 1   | AA    | 73   | C    | O4'-C1'-N1 | 7.45  | 114.16      | 108.20   |
| 27  | B8    | 1761 | C    | O4'-C1'-N1 | 7.45  | 114.16      | 108.20   |
| 1   | AA    | 372  | C    | O4'-C1'-N1 | 7.44  | 114.16      | 108.20   |
| 27  | B8    | 1576 | U    | O4'-C1'-N1 | 7.44  | 114.16      | 108.20   |
| 27  | B8    | 2241 | A    | O4'-C1'-N9 | 7.44  | 114.16      | 108.20   |
| 27  | B8    | 856  | G    | C5-C6-O6   | -7.44 | 124.13      | 128.60   |
| 27  | B8    | 1409 | U    | O4'-C1'-N1 | 7.44  | 114.15      | 108.20   |
| 1   | AA    | 1131 | G    | N1-C6-O6   | 7.44  | 124.36      | 119.90   |
| 27  | B8    | 852  | U    | O4'-C1'-N1 | 7.44  | 114.15      | 108.20   |
| 27  | B8    | 2395 | C    | O4'-C1'-N1 | 7.44  | 114.15      | 108.20   |
| 27  | B8    | 2525 | G    | C5-C6-O6   | -7.44 | 124.14      | 128.60   |
| 1   | AA    | 877  | G    | C5-C6-O6   | -7.44 | 124.14      | 128.60   |
| 1   | AA    | 1354 | U    | O4'-C1'-N1 | 7.44  | 114.15      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1335 | C    | O4'-C1'-N1 | 7.44  | 114.15      | 108.20   |
| 27  | B8    | 510  | C    | O4'-C1'-N1 | 7.44  | 114.15      | 108.20   |
| 27  | B8    | 1660 | G    | C5-C6-O6   | -7.44 | 124.14      | 128.60   |
| 1   | AA    | 391  | G    | C5-C6-O6   | -7.43 | 124.14      | 128.60   |
| 1   | AA    | 847  | G    | O4'-C1'-N9 | 7.43  | 114.15      | 108.20   |
| 27  | B8    | 774  | G    | C5-C6-O6   | -7.43 | 124.14      | 128.60   |
| 1   | AA    | 920  | U    | O4'-C1'-N1 | 7.43  | 114.15      | 108.20   |
| 26  | B7    | 21   | G    | C5-C6-O6   | -7.43 | 124.14      | 128.60   |
| 27  | B8    | 70   | G    | C5-C6-O6   | -7.43 | 124.14      | 128.60   |
| 27  | B8    | 1813 | G    | C5-C6-O6   | -7.43 | 124.14      | 128.60   |
| 27  | B8    | 2367 | G    | C5-C6-O6   | -7.43 | 124.14      | 128.60   |
| 1   | AA    | 1264 | U    | O4'-C1'-N1 | 7.43  | 114.14      | 108.20   |
| 27  | B8    | 37   | C    | O4'-C1'-N1 | 7.43  | 114.14      | 108.20   |
| 27  | B8    | 702  | U    | O4'-C1'-N1 | 7.43  | 114.14      | 108.20   |
| 27  | B8    | 1923 | U    | O4'-C1'-N1 | 7.43  | 114.14      | 108.20   |
| 27  | B8    | 993  | G    | C5-C6-O6   | -7.43 | 124.14      | 128.60   |
| 27  | B8    | 1055 | G    | C5-C6-O6   | -7.43 | 124.14      | 128.60   |
| 1   | AA    | 577  | G    | C5-C6-O6   | -7.42 | 124.14      | 128.60   |
| 26  | B7    | 98   | G    | C5-C6-O6   | -7.42 | 124.14      | 128.60   |
| 1   | AA    | 1342 | C    | O4'-C1'-N1 | 7.42  | 114.14      | 108.20   |
| 26  | B7    | 32   | U    | O4'-C1'-N1 | 7.42  | 114.14      | 108.20   |
| 27  | B8    | 304  | U    | O4'-C1'-N1 | 7.42  | 114.14      | 108.20   |
| 27  | B8    | 1722 | A    | C4-C5-C6   | 7.42  | 120.71      | 117.00   |
| 27  | B8    | 35   | G    | C5-C6-O6   | -7.42 | 124.15      | 128.60   |
| 27  | B8    | 2212 | A    | O4'-C1'-N9 | 7.42  | 114.14      | 108.20   |
| 27  | B8    | 2219 | U    | O4'-C1'-N1 | 7.42  | 114.14      | 108.20   |
| 1   | AA    | 453  | G    | N1-C6-O6   | 7.42  | 124.35      | 119.90   |
| 1   | AA    | 1300 | G    | C5-C6-O6   | -7.42 | 124.15      | 128.60   |
| 27  | B8    | 1282 | U    | O4'-C1'-N1 | 7.42  | 114.13      | 108.20   |
| 27  | B8    | 2290 | G    | C5-C6-O6   | -7.42 | 124.15      | 128.60   |
| 1   | AA    | 144  | G    | C5-C6-O6   | -7.41 | 124.15      | 128.60   |
| 1   | AA    | 40   | C    | O4'-C1'-N1 | 7.41  | 114.13      | 108.20   |
| 1   | AA    | 837  | U    | O4'-C1'-N1 | 7.41  | 114.13      | 108.20   |
| 1   | AA    | 1198 | G    | C5-C6-O6   | -7.41 | 124.15      | 128.60   |
| 27  | B8    | 1449 | G    | C5-C6-O6   | -7.41 | 124.15      | 128.60   |
| 1   | AA    | 1233 | G    | C5-C6-O6   | -7.41 | 124.16      | 128.60   |
| 27  | B8    | 178  | G    | C5-C6-O6   | -7.41 | 124.16      | 128.60   |
| 27  | B8    | 683  | U    | O4'-C1'-N1 | 7.41  | 114.13      | 108.20   |
| 27  | B8    | 1887 | C    | O4'-C1'-N1 | 7.41  | 114.12      | 108.20   |
| 1   | AA    | 1314 | C    | O4'-C1'-N1 | 7.41  | 114.12      | 108.20   |
| 27  | B8    | 877  | A    | C4-C5-C6   | 7.41  | 120.70      | 117.00   |
| 27  | B8    | 1011 | G    | C5-C6-O6   | -7.41 | 124.16      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1574 | C    | O4'-C1'-N1 | 7.41  | 114.12      | 108.20   |
| 27  | B8    | 2487 | G    | C5-C6-O6   | -7.41 | 124.16      | 128.60   |
| 1   | AA    | 491  | G    | C5-C6-O6   | -7.40 | 124.16      | 128.60   |
| 1   | AA    | 791  | G    | C5-C6-O6   | -7.40 | 124.16      | 128.60   |
| 1   | AA    | 1243 | C    | O4'-C1'-N1 | 7.40  | 114.12      | 108.20   |
| 27  | B8    | 296  | U    | O4'-C1'-N1 | 7.40  | 114.12      | 108.20   |
| 27  | B8    | 708  | G    | C5-C6-O6   | -7.40 | 124.16      | 128.60   |
| 27  | B8    | 1846 | G    | C5-C6-O6   | -7.40 | 124.16      | 128.60   |
| 27  | B8    | 1867 | G    | C5-C6-O6   | -7.40 | 124.16      | 128.60   |
| 1   | AA    | 550  | G    | C5-C6-O6   | -7.40 | 124.16      | 128.60   |
| 1   | AA    | 1538 | C    | O4'-C1'-N1 | 7.40  | 114.12      | 108.20   |
| 27  | B8    | 884  | U    | O4'-C1'-N1 | 7.40  | 114.12      | 108.20   |
| 1   | AA    | 1307 | U    | O4'-C1'-N1 | 7.40  | 114.12      | 108.20   |
| 27  | B8    | 934  | U    | O4'-C1'-N1 | 7.40  | 114.12      | 108.20   |
| 27  | B8    | 1053 | C    | O4'-C1'-N1 | 7.40  | 114.12      | 108.20   |
| 27  | B8    | 1628 | G    | C5-C6-O6   | -7.40 | 124.16      | 128.60   |
| 1   | AA    | 896  | C    | O4'-C1'-N1 | 7.39  | 114.11      | 108.20   |
| 1   | AA    | 1159 | U    | O4'-C1'-N1 | 7.39  | 114.11      | 108.20   |
| 26  | B7    | 70   | C    | O4'-C1'-N1 | 7.39  | 114.11      | 108.20   |
| 27  | B8    | 378  | C    | O4'-C1'-N1 | 7.39  | 114.12      | 108.20   |
| 27  | B8    | 449  | A    | C5-C6-N6   | -7.39 | 117.79      | 123.70   |
| 27  | B8    | 2251 | G    | C5-C6-O6   | -7.39 | 124.17      | 128.60   |
| 1   | AA    | 967  | C    | O4'-C1'-N1 | 7.39  | 114.11      | 108.20   |
| 27  | B8    | 301  | G    | C5-C6-O6   | -7.39 | 124.17      | 128.60   |
| 1   | AA    | 119  | A    | C4-C5-C6   | 7.39  | 120.69      | 117.00   |
| 27  | B8    | 1897 | G    | C5-C6-O6   | -7.39 | 124.17      | 128.60   |
| 1   | AA    | 212  | G    | C5-C6-O6   | -7.39 | 124.17      | 128.60   |
| 27  | B8    | 464  | U    | O4'-C1'-N1 | 7.39  | 114.11      | 108.20   |
| 27  | B8    | 773  | U    | O4'-C1'-N1 | 7.39  | 114.11      | 108.20   |
| 26  | B7    | 30   | C    | O4'-C1'-N1 | 7.39  | 114.11      | 108.20   |
| 27  | B8    | 805  | G    | C5-C6-O6   | -7.39 | 124.17      | 128.60   |
| 27  | B8    | 1136 | G    | C5-C6-O6   | -7.39 | 124.17      | 128.60   |
| 27  | B8    | 1388 | G    | C5-C6-O6   | -7.39 | 124.17      | 128.60   |
| 27  | B8    | 1747 | U    | O4'-C1'-N1 | 7.39  | 114.11      | 108.20   |
| 1   | AA    | 410  | G    | N1-C6-O6   | 7.38  | 124.33      | 119.90   |
| 27  | B8    | 1013 | C    | O4'-C1'-N1 | 7.38  | 114.11      | 108.20   |
| 27  | B8    | 2187 | U    | O4'-C1'-N1 | 7.38  | 114.11      | 108.20   |
| 27  | B8    | 585  | G    | C5-C6-O6   | -7.38 | 124.17      | 128.60   |
| 1   | AA    | 316  | C    | O4'-C1'-N1 | 7.38  | 114.11      | 108.20   |
| 1   | AA    | 1535 | C    | O4'-C1'-N1 | 7.38  | 114.11      | 108.20   |
| 27  | B8    | 1161 | C    | O4'-C1'-N1 | 7.38  | 114.10      | 108.20   |
| 27  | B8    | 1659 | G    | C5-C6-O6   | -7.38 | 124.17      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1725 | U    | O4'-C1'-N1 | 7.38  | 114.10      | 108.20   |
| 27  | B8    | 2555 | U    | O4'-C1'-N1 | 7.38  | 114.10      | 108.20   |
| 1   | AA    | 783  | C    | O4'-C1'-N1 | 7.37  | 114.10      | 108.20   |
| 1   | AA    | 836  | G    | C5-C6-O6   | -7.37 | 124.18      | 128.60   |
| 27  | B8    | 392  | U    | O4'-C1'-N1 | 7.37  | 114.10      | 108.20   |
| 1   | AA    | 1270 | G    | C5-C6-O6   | -7.37 | 124.18      | 128.60   |
| 27  | B8    | 1037 | G    | C5-C6-O6   | -7.37 | 124.18      | 128.60   |
| 27  | B8    | 2036 | C    | O4'-C1'-N1 | 7.37  | 114.10      | 108.20   |
| 1   | AA    | 154  | U    | O4'-C1'-N1 | 7.37  | 114.10      | 108.20   |
| 1   | AA    | 1142 | G    | P-O3'-C3'  | 7.37  | 128.54      | 119.70   |
| 27  | B8    | 1666 | G    | C5-C6-O6   | -7.37 | 124.18      | 128.60   |
| 1   | AA    | 406  | G    | C5-C6-O6   | -7.37 | 124.18      | 128.60   |
| 1   | AA    | 723  | U    | O4'-C1'-N1 | 7.37  | 114.09      | 108.20   |
| 1   | AA    | 893  | C    | O4'-C1'-N1 | 7.37  | 114.09      | 108.20   |
| 1   | AA    | 765  | G    | O4'-C1'-N9 | 7.37  | 114.09      | 108.20   |
| 27  | B8    | 2445 | G    | C5-C6-O6   | -7.37 | 124.18      | 128.60   |
| 1   | AA    | 515  | G    | C5-C6-O6   | -7.37 | 124.18      | 128.60   |
| 1   | AA    | 1316 | G    | N3-C2-N2   | 7.37  | 125.06      | 119.90   |
| 27  | B8    | 656  | G    | C5-C6-O6   | -7.37 | 124.18      | 128.60   |
| 27  | B8    | 1608 | A    | C4-C5-C6   | 7.37  | 120.68      | 117.00   |
| 1   | AA    | 839  | C    | O4'-C1'-N1 | 7.36  | 114.09      | 108.20   |
| 1   | AA    | 1312 | G    | C5-C6-O6   | -7.36 | 124.18      | 128.60   |
| 27  | B8    | 1360 | G    | N1-C6-O6   | 7.36  | 124.32      | 119.90   |
| 27  | B8    | 1444 | G    | C5-C6-O6   | -7.36 | 124.18      | 128.60   |
| 27  | B8    | 1450 | G    | C5-C6-O6   | -7.36 | 124.18      | 128.60   |
| 1   | AA    | 1228 | C    | O4'-C1'-N1 | 7.36  | 114.09      | 108.20   |
| 27  | B8    | 1228 | G    | C5-C6-O6   | -7.36 | 124.18      | 128.60   |
| 27  | B8    | 1446 | C    | O4'-C1'-N1 | 7.36  | 114.09      | 108.20   |
| 27  | B8    | 1748 | C    | O4'-C1'-N1 | 7.36  | 114.09      | 108.20   |
| 1   | AA    | 665  | A    | O4'-C1'-N9 | 7.36  | 114.09      | 108.20   |
| 1   | AA    | 612  | C    | O4'-C1'-N1 | 7.36  | 114.09      | 108.20   |
| 27  | B8    | 1050 | A    | O4'-C1'-N9 | 7.36  | 114.09      | 108.20   |
| 27  | B8    | 1645 | G    | C5-C6-O6   | -7.36 | 124.19      | 128.60   |
| 27  | B8    | 2815 | C    | O4'-C1'-N1 | 7.36  | 114.09      | 108.20   |
| 1   | AA    | 388  | G    | C5-C6-O6   | -7.36 | 124.19      | 128.60   |
| 1   | AA    | 529  | G    | C5-C6-O6   | -7.36 | 124.19      | 128.60   |
| 1   | AA    | 813  | U    | O4'-C1'-N1 | 7.36  | 114.08      | 108.20   |
| 1   | AA    | 1329 | A    | O4'-C1'-N9 | 7.36  | 114.08      | 108.20   |
| 27  | B8    | 2687 | U    | O4'-C1'-N1 | 7.36  | 114.08      | 108.20   |
| 27  | B8    | 2760 | C    | O4'-C1'-N1 | 7.36  | 114.08      | 108.20   |
| 27  | B8    | 2862 | G    | C5-C6-O6   | -7.36 | 124.19      | 128.60   |
| 27  | B8    | 1139 | G    | C5-C6-O6   | -7.35 | 124.19      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 444  | G    | C5-C6-O6   | -7.35 | 124.19      | 128.60   |
| 1   | AA    | 863  | U    | O4'-C1'-N1 | 7.35  | 114.08      | 108.20   |
| 1   | AA    | 925  | G    | C5-C6-O6   | -7.35 | 124.19      | 128.60   |
| 26  | B7    | 16   | G    | C5-C6-O6   | -7.35 | 124.19      | 128.60   |
| 27  | B8    | 890  | C    | O4'-C1'-N1 | 7.35  | 114.08      | 108.20   |
| 27  | B8    | 2373 | G    | C5-C6-O6   | -7.35 | 124.19      | 128.60   |
| 1   | AA    | 69   | G    | C5-C6-O6   | -7.35 | 124.19      | 128.60   |
| 27  | B8    | 840  | C    | O4'-C1'-N1 | 7.35  | 114.08      | 108.20   |
| 27  | B8    | 862  | G    | C5-C6-O6   | -7.35 | 124.19      | 128.60   |
| 27  | B8    | 2401 | U    | O4'-C1'-N1 | 7.35  | 114.08      | 108.20   |
| 27  | B8    | 2892 | G    | C5-C6-O6   | -7.35 | 124.19      | 128.60   |
| 1   | AA    | 254  | G    | O4'-C1'-N9 | 7.35  | 114.08      | 108.20   |
| 1   | AA    | 698  | G    | C5-C6-O6   | -7.35 | 124.19      | 128.60   |
| 1   | AA    | 987  | G    | C5-C6-O6   | -7.35 | 124.19      | 128.60   |
| 27  | B8    | 967  | U    | O4'-C1'-N1 | 7.35  | 114.08      | 108.20   |
| 27  | B8    | 1003 | G    | C5-C6-O6   | -7.35 | 124.19      | 128.60   |
| 1   | AA    | 355  | C    | O4'-C1'-N1 | 7.35  | 114.08      | 108.20   |
| 27  | B8    | 1995 | U    | O4'-C1'-N1 | 7.34  | 114.08      | 108.20   |
| 27  | B8    | 2178 | C    | O4'-C1'-N1 | 7.34  | 114.08      | 108.20   |
| 27  | B8    | 2585 | U    | P-O3'-C3'  | 7.34  | 128.51      | 119.70   |
| 1   | AA    | 776  | G    | C5-C6-O6   | -7.34 | 124.19      | 128.60   |
| 27  | B8    | 657  | U    | O4'-C1'-N1 | 7.34  | 114.07      | 108.20   |
| 27  | B8    | 1172 | C    | O4'-C1'-N1 | 7.34  | 114.07      | 108.20   |
| 27  | B8    | 171  | U    | O4'-C1'-N1 | 7.34  | 114.07      | 108.20   |
| 1   | AA    | 423  | G    | O4'-C1'-N9 | 7.34  | 114.07      | 108.20   |
| 1   | AA    | 631  | C    | O4'-C1'-N1 | 7.34  | 114.07      | 108.20   |
| 1   | AA    | 1522 | U    | O4'-C1'-N1 | 7.34  | 114.07      | 108.20   |
| 3   | AV    | 13   | C    | O4'-C1'-N1 | 7.34  | 114.07      | 108.20   |
| 2   | AX    | 16   | C    | O4'-C1'-N1 | 7.34  | 114.07      | 108.20   |
| 27  | B8    | 364  | C    | O4'-C1'-N1 | 7.34  | 114.07      | 108.20   |
| 27  | B8    | 2008 | C    | O4'-C1'-N1 | 7.34  | 114.07      | 108.20   |
| 27  | B8    | 2845 | U    | O4'-C1'-N1 | 7.33  | 114.07      | 108.20   |
| 26  | B7    | 43   | C    | O4'-C1'-N1 | 7.33  | 114.07      | 108.20   |
| 27  | B8    | 516  | C    | O4'-C1'-N1 | 7.33  | 114.07      | 108.20   |
| 3   | AV    | 48   | U    | O4'-C1'-N1 | 7.33  | 114.06      | 108.20   |
| 27  | B8    | 187  | G    | C5-C6-O6   | -7.33 | 124.20      | 128.60   |
| 27  | B8    | 694  | U    | O4'-C1'-N1 | 7.33  | 114.06      | 108.20   |
| 27  | B8    | 1638 | C    | O4'-C1'-N1 | 7.33  | 114.06      | 108.20   |
| 1   | AA    | 1073 | U    | O4'-C1'-N1 | 7.33  | 114.06      | 108.20   |
| 27  | B8    | 2001 | C    | O4'-C1'-N1 | 7.33  | 114.06      | 108.20   |
| 1   | AA    | 1315 | U    | O4'-C1'-N1 | 7.33  | 114.06      | 108.20   |
| 27  | B8    | 1688 | U    | O4'-C1'-N1 | 7.33  | 114.06      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1479 | C    | O4'-C1'-N1 | 7.33  | 114.06      | 108.20   |
| 1   | AA    | 213  | G    | C5-C6-O6   | -7.32 | 124.21      | 128.60   |
| 1   | AA    | 549  | C    | O4'-C1'-N1 | 7.32  | 114.06      | 108.20   |
| 27  | B8    | 408  | G    | C5-C6-O6   | -7.32 | 124.21      | 128.60   |
| 27  | B8    | 2755 | C    | O4'-C1'-N1 | 7.32  | 114.06      | 108.20   |
| 1   | AA    | 56   | U    | O4'-C1'-N1 | 7.32  | 114.06      | 108.20   |
| 1   | AA    | 140  | U    | O4'-C1'-N1 | 7.32  | 114.06      | 108.20   |
| 1   | AA    | 770  | C    | O4'-C1'-N1 | 7.32  | 114.06      | 108.20   |
| 27  | B8    | 259  | G    | C5-C6-O6   | -7.32 | 124.21      | 128.60   |
| 27  | B8    | 1280 | G    | C5-C6-O6   | -7.32 | 124.21      | 128.60   |
| 27  | B8    | 1423 | G    | O4'-C1'-N9 | 7.32  | 114.06      | 108.20   |
| 27  | B8    | 837  | C    | O4'-C1'-N1 | 7.32  | 114.06      | 108.20   |
| 26  | B7    | 44   | G    | C5-C6-O6   | -7.32 | 124.21      | 128.60   |
| 27  | B8    | 154  | U    | O4'-C1'-N1 | 7.32  | 114.05      | 108.20   |
| 27  | B8    | 2616 | C    | O4'-C1'-N1 | 7.32  | 114.06      | 108.20   |
| 27  | B8    | 1336 | A    | O4'-C1'-N9 | 7.32  | 114.05      | 108.20   |
| 1   | AA    | 358  | U    | O4'-C1'-N1 | 7.31  | 114.05      | 108.20   |
| 27  | B8    | 235  | U    | O4'-C1'-N1 | 7.31  | 114.05      | 108.20   |
| 27  | B8    | 2869 | G    | C5-C6-O6   | -7.31 | 124.21      | 128.60   |
| 1   | AA    | 330  | C    | O4'-C1'-N1 | 7.31  | 114.05      | 108.20   |
| 1   | AA    | 828  | U    | O4'-C1'-N1 | 7.31  | 114.05      | 108.20   |
| 1   | AA    | 1153 | G    | C5-C6-O6   | -7.31 | 124.21      | 128.60   |
| 27  | B8    | 518  | G    | C5-C6-O6   | -7.31 | 124.21      | 128.60   |
| 27  | B8    | 826  | U    | O4'-C1'-N1 | 7.31  | 114.05      | 108.20   |
| 1   | AA    | 670  | G    | C5-C6-O6   | -7.31 | 124.21      | 128.60   |
| 1   | AA    | 218  | U    | O4'-C1'-N1 | 7.31  | 114.05      | 108.20   |
| 1   | AA    | 1459 | G    | C5-C6-O6   | -7.31 | 124.22      | 128.60   |
| 27  | B8    | 196  | A    | O4'-C1'-N9 | 7.31  | 114.05      | 108.20   |
| 27  | B8    | 1863 | G    | C5-C6-O6   | -7.31 | 124.22      | 128.60   |
| 1   | AA    | 1301 | U    | O4'-C1'-N1 | 7.31  | 114.05      | 108.20   |
| 27  | B8    | 494  | G    | O4'-C1'-N9 | 7.31  | 114.05      | 108.20   |
| 27  | B8    | 638  | G    | C5-C6-O6   | -7.31 | 124.22      | 128.60   |
| 27  | B8    | 771  | G    | O4'-C1'-N9 | 7.31  | 114.05      | 108.20   |
| 27  | B8    | 2225 | A    | C4-C5-C6   | 7.31  | 120.65      | 117.00   |
| 27  | B8    | 2256 | G    | C5-C6-O6   | -7.31 | 124.22      | 128.60   |
| 27  | B8    | 2352 | A    | C4-C5-C6   | 7.31  | 120.65      | 117.00   |
| 27  | B8    | 2674 | G    | C5-C6-O6   | -7.31 | 124.22      | 128.60   |
| 27  | B8    | 2836 | U    | O4'-C1'-N1 | 7.31  | 114.05      | 108.20   |
| 26  | B7    | 80   | U    | O4'-C1'-N1 | 7.31  | 114.05      | 108.20   |
| 27  | B8    | 567  | U    | O4'-C1'-N1 | 7.31  | 114.05      | 108.20   |
| 27  | B8    | 2646 | C    | O4'-C1'-N1 | 7.31  | 114.05      | 108.20   |
| 1   | AA    | 516  | U    | O4'-C1'-N1 | 7.30  | 114.04      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 638  | U    | O4'-C1'-N1 | 7.30  | 114.04      | 108.20   |
| 27  | B8    | 11   | C    | O4'-C1'-N1 | 7.30  | 114.04      | 108.20   |
| 27  | B8    | 1623 | G    | C5-C6-O6   | -7.30 | 124.22      | 128.60   |
| 27  | B8    | 1943 | U    | O4'-C1'-N1 | 7.30  | 114.04      | 108.20   |
| 27  | B8    | 2196 | C    | O4'-C1'-N1 | 7.30  | 114.04      | 108.20   |
| 27  | B8    | 135  | U    | O4'-C1'-N1 | 7.30  | 114.04      | 108.20   |
| 1   | AA    | 666  | G    | C5-C6-O6   | -7.30 | 124.22      | 128.60   |
| 3   | AV    | 63   | C    | O4'-C1'-N1 | 7.30  | 114.04      | 108.20   |
| 27  | B8    | 2552 | U    | O4'-C1'-N1 | 7.30  | 114.04      | 108.20   |
| 1   | AA    | 801  | U    | O4'-C1'-N1 | 7.30  | 114.04      | 108.20   |
| 1   | AA    | 1465 | A    | C5-C6-N6   | -7.30 | 117.86      | 123.70   |
| 27  | B8    | 1063 | G    | C5-C6-O6   | -7.30 | 124.22      | 128.60   |
| 1   | AA    | 506  | G    | C5-C6-O6   | -7.30 | 124.22      | 128.60   |
| 27  | B8    | 320  | A    | P-O3'-C3'  | 7.30  | 128.46      | 119.70   |
| 27  | B8    | 2103 | C    | O4'-C1'-N1 | 7.30  | 114.04      | 108.20   |
| 27  | B8    | 2143 | C    | O4'-C1'-N1 | 7.30  | 114.04      | 108.20   |
| 1   | AA    | 562  | U    | P-O3'-C3'  | 7.30  | 128.46      | 119.70   |
| 1   | AA    | 347  | G    | O4'-C1'-N9 | 7.29  | 114.04      | 108.20   |
| 1   | AA    | 371  | A    | O4'-C1'-N9 | 7.29  | 114.04      | 108.20   |
| 26  | B7    | 95   | U    | O4'-C1'-N1 | 7.29  | 114.03      | 108.20   |
| 27  | B8    | 658  | U    | O4'-C1'-N1 | 7.29  | 114.03      | 108.20   |
| 27  | B8    | 939  | G    | C5-C6-O6   | -7.29 | 124.23      | 128.60   |
| 27  | B8    | 1453 | A    | O4'-C1'-N9 | 7.29  | 114.03      | 108.20   |
| 1   | AA    | 971  | G    | C5-C6-O6   | -7.29 | 124.23      | 128.60   |
| 27  | B8    | 1016 | G    | O4'-C1'-N9 | 7.29  | 114.03      | 108.20   |
| 27  | B8    | 1035 | U    | O4'-C1'-N1 | 7.29  | 114.03      | 108.20   |
| 27  | B8    | 1847 | A    | O4'-C1'-N9 | 7.29  | 114.03      | 108.20   |
| 27  | B8    | 2585 | U    | O4'-C1'-N1 | 7.29  | 114.03      | 108.20   |
| 1   | AA    | 833  | G    | C5-C6-O6   | -7.29 | 124.23      | 128.60   |
| 1   | AA    | 887  | G    | C5-C6-O6   | -7.29 | 124.23      | 128.60   |
| 26  | B7    | 2    | G    | C5-C6-O6   | -7.29 | 124.23      | 128.60   |
| 1   | AA    | 103  | U    | O4'-C1'-N1 | 7.29  | 114.03      | 108.20   |
| 1   | AA    | 526  | C    | O4'-C1'-N1 | 7.29  | 114.03      | 108.20   |
| 27  | B8    | 962  | G    | C5-C6-O6   | -7.29 | 124.23      | 128.60   |
| 27  | B8    | 1292 | G    | C5-C6-O6   | -7.29 | 124.23      | 128.60   |
| 27  | B8    | 1484 | U    | O4'-C1'-N1 | 7.29  | 114.03      | 108.20   |
| 1   | AA    | 11   | G    | C5-C6-O6   | -7.29 | 124.23      | 128.60   |
| 1   | AA    | 93   | U    | O4'-C1'-N1 | 7.29  | 114.03      | 108.20   |
| 27  | B8    | 177  | G    | O4'-C1'-N9 | 7.29  | 114.03      | 108.20   |
| 27  | B8    | 289  | G    | C5-C6-O6   | -7.29 | 124.23      | 128.60   |
| 27  | B8    | 1220 | G    | C5-C6-O6   | -7.28 | 124.23      | 128.60   |
| 27  | B8    | 1859 | U    | O4'-C1'-N1 | 7.28  | 114.02      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 133  | U    | O4'-C1'-N1 | 7.28  | 114.02      | 108.20   |
| 27  | B8    | 156  | A    | O4'-C1'-N9 | 7.28  | 114.02      | 108.20   |
| 27  | B8    | 375  | G    | C5-C6-O6   | -7.28 | 124.23      | 128.60   |
| 27  | B8    | 2242 | G    | C5-C6-O6   | -7.28 | 124.23      | 128.60   |
| 27  | B8    | 220  | G    | C5-C6-O6   | -7.28 | 124.23      | 128.60   |
| 27  | B8    | 370  | G    | C5-C6-O6   | -7.28 | 124.23      | 128.60   |
| 27  | B8    | 660  | C    | O4'-C1'-N1 | 7.28  | 114.02      | 108.20   |
| 27  | B8    | 2511 | U    | O4'-C1'-N1 | 7.28  | 114.02      | 108.20   |
| 27  | B8    | 2617 | U    | O4'-C1'-N1 | 7.28  | 114.02      | 108.20   |
| 1   | AA    | 318  | G    | C5-C6-O6   | -7.27 | 124.24      | 128.60   |
| 27  | B8    | 297  | G    | C5-C6-O6   | -7.27 | 124.24      | 128.60   |
| 27  | B8    | 768  | G    | O4'-C1'-N9 | 7.27  | 114.02      | 108.20   |
| 27  | B8    | 2573 | C    | C2-N1-C1'  | 7.27  | 126.80      | 118.80   |
| 1   | AA    | 21   | G    | O4'-C1'-N9 | 7.27  | 114.02      | 108.20   |
| 27  | B8    | 8    | C    | N3-C4-N4   | 7.27  | 123.09      | 118.00   |
| 27  | B8    | 193  | U    | O4'-C1'-N1 | 7.27  | 114.02      | 108.20   |
| 27  | B8    | 2860 | A    | C5-C6-N1   | -7.27 | 114.06      | 117.70   |
| 27  | B8    | 249  | C    | O4'-C1'-N1 | 7.27  | 114.02      | 108.20   |
| 27  | B8    | 1041 | G    | C5-C6-O6   | -7.27 | 124.24      | 128.60   |
| 1   | AA    | 230  | G    | C5-C6-O6   | -7.27 | 124.24      | 128.60   |
| 27  | B8    | 543  | G    | C5-C6-O6   | -7.27 | 124.24      | 128.60   |
| 27  | B8    | 610  | C    | O4'-C1'-N1 | 7.27  | 114.02      | 108.20   |
| 27  | B8    | 874  | G    | C5-C6-O6   | -7.27 | 124.24      | 128.60   |
| 27  | B8    | 1234 | U    | O4'-C1'-N1 | 7.27  | 114.02      | 108.20   |
| 27  | B8    | 1487 | U    | O4'-C1'-N1 | 7.27  | 114.02      | 108.20   |
| 1   | AA    | 94   | G    | C5-C6-O6   | -7.27 | 124.24      | 128.60   |
| 1   | AA    | 830  | G    | C5-C6-O6   | -7.27 | 124.24      | 128.60   |
| 27  | B8    | 1719 | G    | C5-C6-O6   | -7.27 | 124.24      | 128.60   |
| 27  | B8    | 2062 | A    | O4'-C1'-N9 | 7.27  | 114.01      | 108.20   |
| 27  | B8    | 2455 | G    | C5-C6-O6   | -7.27 | 124.24      | 128.60   |
| 27  | B8    | 4    | U    | O4'-C1'-N1 | 7.27  | 114.01      | 108.20   |
| 27  | B8    | 1696 | G    | C5-C6-O6   | -7.26 | 124.24      | 128.60   |
| 27  | B8    | 1878 | G    | C5-C6-O6   | -7.26 | 124.24      | 128.60   |
| 27  | B8    | 2767 | C    | O4'-C1'-N1 | 7.26  | 114.01      | 108.20   |
| 1   | AA    | 564  | C    | O4'-C1'-N1 | 7.26  | 114.01      | 108.20   |
| 1   | AA    | 1124 | G    | C5-C6-O6   | -7.26 | 124.24      | 128.60   |
| 1   | AA    | 1175 | G    | C5-C6-O6   | -7.26 | 124.24      | 128.60   |
| 1   | AA    | 1221 | G    | C5-C6-O6   | -7.26 | 124.24      | 128.60   |
| 27  | B8    | 965  | C    | O4'-C1'-N1 | 7.26  | 114.01      | 108.20   |
| 27  | B8    | 1617 | C    | O4'-C1'-N1 | 7.26  | 114.01      | 108.20   |
| 27  | B8    | 2110 | G    | C5-C6-O6   | -7.26 | 124.24      | 128.60   |
| 1   | AA    | 1527 | U    | O4'-C1'-N1 | 7.26  | 114.01      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 712  | G    | C5-C6-O6   | -7.26 | 124.24      | 128.60   |
| 27  | B8    | 1117 | C    | O4'-C1'-N1 | 7.26  | 114.01      | 108.20   |
| 27  | B8    | 2561 | U    | O4'-C1'-N1 | 7.26  | 114.01      | 108.20   |
| 1   | AA    | 1106 | G    | C5-C6-O6   | -7.26 | 124.25      | 128.60   |
| 27  | B8    | 377  | G    | C5-C6-O6   | -7.26 | 124.25      | 128.60   |
| 27  | B8    | 1895 | C    | O4'-C1'-N1 | 7.26  | 114.00      | 108.20   |
| 27  | B8    | 923  | G    | C5-C6-O6   | -7.25 | 124.25      | 128.60   |
| 27  | B8    | 2458 | G    | C5-C6-O6   | -7.25 | 124.25      | 128.60   |
| 1   | AA    | 625  | U    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 27  | B8    | 1744 | A    | C4-C5-C6   | 7.25  | 120.63      | 117.00   |
| 27  | B8    | 2137 | U    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 1   | AA    | 126  | G    | C5-C6-O6   | -7.25 | 124.25      | 128.60   |
| 1   | AA    | 719  | C    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 1   | AA    | 912  | C    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 27  | B8    | 419  | U    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 27  | B8    | 2106 | U    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 27  | B8    | 2492 | U    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 27  | B8    | 2707 | U    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 1   | AA    | 751  | U    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 1   | AA    | 1241 | G    | C5-C6-O6   | -7.25 | 124.25      | 128.60   |
| 1   | AA    | 684  | U    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 1   | AA    | 866  | C    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 27  | B8    | 1922 | G    | C5-C6-O6   | -7.25 | 124.25      | 128.60   |
| 26  | B7    | 103  | U    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 27  | B8    | 1702 | G    | C5-C6-O6   | -7.25 | 124.25      | 128.60   |
| 27  | B8    | 2102 | G    | C5-C6-O6   | -7.25 | 124.25      | 128.60   |
| 1   | AA    | 947  | G    | C5-C6-O6   | -7.25 | 124.25      | 128.60   |
| 27  | B8    | 1137 | G    | C5-C6-O6   | -7.25 | 124.25      | 128.60   |
| 1   | AA    | 224  | U    | O4'-C1'-N1 | 7.24  | 113.99      | 108.20   |
| 3   | AV    | 53   | G    | O4'-C1'-N9 | 7.24  | 114.00      | 108.20   |
| 27  | B8    | 646  | U    | O4'-C1'-N1 | 7.24  | 113.99      | 108.20   |
| 27  | B8    | 1078 | U    | O4'-C1'-N1 | 7.24  | 113.99      | 108.20   |
| 27  | B8    | 216  | A    | C4-C5-C6   | 7.24  | 120.62      | 117.00   |
| 1   | AA    | 980  | C    | O4'-C1'-N1 | 7.24  | 113.99      | 108.20   |
| 1   | AA    | 1419 | G    | C5-C6-O6   | -7.24 | 124.25      | 128.60   |
| 26  | B7    | 105  | G    | C5-C6-O6   | -7.24 | 124.26      | 128.60   |
| 27  | B8    | 283  | G    | C5-C6-O6   | -7.24 | 124.25      | 128.60   |
| 27  | B8    | 591  | U    | O4'-C1'-N1 | 7.24  | 113.99      | 108.20   |
| 27  | B8    | 710  | U    | O4'-C1'-N1 | 7.24  | 113.99      | 108.20   |
| 27  | B8    | 1074 | G    | C5-C6-O6   | -7.24 | 124.26      | 128.60   |
| 27  | B8    | 1963 | U    | O4'-C1'-N1 | 7.24  | 113.99      | 108.20   |
| 27  | B8    | 2112 | G    | N1-C6-O6   | 7.24  | 124.24      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 780  | A    | C5-C6-N6   | -7.24 | 117.91      | 123.70   |
| 1   | AA    | 1036 | A    | C5-C6-N6   | -7.24 | 117.91      | 123.70   |
| 27  | B8    | 2415 | G    | C5-C6-O6   | -7.24 | 124.26      | 128.60   |
| 1   | AA    | 157  | U    | O4'-C1'-N1 | 7.24  | 113.99      | 108.20   |
| 27  | B8    | 1797 | G    | C5-C6-O6   | -7.24 | 124.26      | 128.60   |
| 1   | AA    | 874  | G    | C5-C6-O6   | -7.24 | 124.26      | 128.60   |
| 27  | B8    | 993  | G    | O4'-C1'-N9 | 7.24  | 113.99      | 108.20   |
| 27  | B8    | 1229 | C    | O4'-C1'-N1 | 7.24  | 113.99      | 108.20   |
| 27  | B8    | 1834 | U    | O4'-C1'-N1 | 7.24  | 113.99      | 108.20   |
| 1   | AA    | 941  | G    | C5-C6-O6   | -7.23 | 124.26      | 128.60   |
| 1   | AA    | 1467 | C    | O4'-C1'-N1 | 7.23  | 113.99      | 108.20   |
| 1   | AA    | 1496 | C    | O4'-C1'-N1 | 7.23  | 113.99      | 108.20   |
| 26  | B7    | 31   | C    | O4'-C1'-N1 | 7.23  | 113.99      | 108.20   |
| 1   | AA    | 31   | G    | C5-C6-O6   | -7.23 | 124.26      | 128.60   |
| 1   | AA    | 288  | A    | C5-C6-N6   | -7.23 | 117.91      | 123.70   |
| 1   | AA    | 757  | U    | O4'-C1'-N1 | 7.23  | 113.98      | 108.20   |
| 27  | B8    | 1506 | U    | O4'-C1'-N1 | 7.23  | 113.99      | 108.20   |
| 27  | B8    | 1840 | G    | C5-C6-O6   | -7.23 | 124.26      | 128.60   |
| 27  | B8    | 2179 | C    | O4'-C1'-N1 | 7.23  | 113.99      | 108.20   |
| 1   | AA    | 841  | C    | O4'-C1'-N1 | 7.23  | 113.98      | 108.20   |
| 1   | AA    | 873  | A    | C4-C5-C6   | 7.23  | 120.61      | 117.00   |
| 27  | B8    | 2399 | G    | C5-C6-O6   | -7.23 | 124.26      | 128.60   |
| 1   | AA    | 1402 | C    | O4'-C1'-N1 | 7.23  | 113.98      | 108.20   |
| 27  | B8    | 2549 | G    | C5-C6-O6   | -7.23 | 124.26      | 128.60   |
| 1   | AA    | 615  | G    | C5-C6-O6   | -7.23 | 124.26      | 128.60   |
| 1   | AA    | 1116 | U    | O4'-C1'-N1 | 7.23  | 113.98      | 108.20   |
| 27  | B8    | 1279 | G    | C5-C6-O6   | -7.23 | 124.26      | 128.60   |
| 27  | B8    | 766  | U    | O4'-C1'-N1 | 7.23  | 113.98      | 108.20   |
| 1   | AA    | 399  | G    | C5-C6-O6   | -7.22 | 124.27      | 128.60   |
| 27  | B8    | 549  | G    | C5-C6-O6   | -7.22 | 124.27      | 128.60   |
| 27  | B8    | 808  | G    | C5-C6-O6   | -7.22 | 124.27      | 128.60   |
| 27  | B8    | 1377 | G    | C5-C6-O6   | -7.22 | 124.27      | 128.60   |
| 27  | B8    | 1662 | U    | O4'-C1'-N1 | 7.22  | 113.98      | 108.20   |
| 1   | AA    | 1083 | U    | O4'-C1'-N1 | 7.22  | 113.98      | 108.20   |
| 26  | B7    | 61   | G    | C5-C6-O6   | -7.22 | 124.27      | 128.60   |
| 27  | B8    | 447  | A    | N1-C6-N6   | 7.22  | 122.93      | 118.60   |
| 27  | B8    | 2236 | U    | O4'-C1'-N1 | 7.22  | 113.98      | 108.20   |
| 1   | AA    | 1313 | U    | O4'-C1'-N1 | 7.22  | 113.97      | 108.20   |
| 27  | B8    | 1346 | G    | C5-C6-O6   | -7.22 | 124.27      | 128.60   |
| 27  | B8    | 2412 | A    | C4-C5-C6   | 7.22  | 120.61      | 117.00   |
| 27  | B8    | 2470 | G    | C5-C6-O6   | -7.22 | 124.27      | 128.60   |
| 3   | AV    | 29   | C    | O4'-C1'-N1 | 7.22  | 113.97      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2578 | G    | C5-C6-O6   | -7.22 | 124.27      | 128.60   |
| 1   | AA    | 46   | G    | C5-C6-O6   | -7.22 | 124.27      | 128.60   |
| 1   | AA    | 1104 | G    | C5-C6-O6   | -7.22 | 124.27      | 128.60   |
| 1   | AA    | 1244 | G    | C5-C6-O6   | -7.22 | 124.27      | 128.60   |
| 27  | B8    | 29   | U    | O4'-C1'-N1 | 7.22  | 113.97      | 108.20   |
| 27  | B8    | 439  | A    | O4'-C1'-N9 | 7.22  | 113.97      | 108.20   |
| 27  | B8    | 500  | G    | C5-C6-O6   | -7.22 | 124.27      | 128.60   |
| 27  | B8    | 542  | C    | O4'-C1'-N1 | 7.22  | 113.97      | 108.20   |
| 27  | B8    | 868  | U    | O4'-C1'-N1 | 7.22  | 113.97      | 108.20   |
| 1   | AA    | 1168 | U    | O4'-C1'-N1 | 7.21  | 113.97      | 108.20   |
| 27  | B8    | 52   | A    | C4-C5-C6   | 7.21  | 120.61      | 117.00   |
| 27  | B8    | 2305 | U    | O4'-C1'-N1 | 7.21  | 113.97      | 108.20   |
| 27  | B8    | 2536 | G    | C5-C6-O6   | -7.21 | 124.27      | 128.60   |
| 27  | B8    | 2759 | G    | C5-C6-O6   | -7.21 | 124.27      | 128.60   |
| 27  | B8    | 962  | G    | O4'-C1'-N9 | 7.21  | 113.97      | 108.20   |
| 27  | B8    | 1469 | A    | C4-C5-C6   | 7.21  | 120.61      | 117.00   |
| 1   | AA    | 1047 | G    | C5-C6-O6   | -7.21 | 124.27      | 128.60   |
| 1   | AA    | 1182 | G    | C5-C6-O6   | -7.21 | 124.28      | 128.60   |
| 27  | B8    | 1310 | G    | C5-C6-O6   | -7.21 | 124.28      | 128.60   |
| 1   | AA    | 1202 | U    | O4'-C1'-N1 | 7.21  | 113.97      | 108.20   |
| 1   | AA    | 1360 | A    | C4-C5-C6   | 7.21  | 120.60      | 117.00   |
| 1   | AA    | 1518 | A    | O4'-C1'-N9 | 7.21  | 113.97      | 108.20   |
| 27  | B8    | 629  | G    | C5-C6-O6   | -7.21 | 124.28      | 128.60   |
| 27  | B8    | 1410 | G    | C5-C6-O6   | -7.21 | 124.28      | 128.60   |
| 27  | B8    | 438  | G    | C5-C6-O6   | -7.21 | 124.28      | 128.60   |
| 27  | B8    | 2087 | G    | O4'-C1'-N9 | 7.21  | 113.96      | 108.20   |
| 1   | AA    | 255  | G    | C5-C6-O6   | -7.20 | 124.28      | 128.60   |
| 1   | AA    | 289  | G    | O4'-C1'-N9 | 7.20  | 113.96      | 108.20   |
| 1   | AA    | 537  | G    | C5-C6-O6   | -7.20 | 124.28      | 128.60   |
| 1   | AA    | 1192 | C    | O4'-C1'-N1 | 7.20  | 113.96      | 108.20   |
| 27  | B8    | 124  | G    | C5-C6-O6   | -7.20 | 124.28      | 128.60   |
| 27  | B8    | 346  | A    | O4'-C1'-N9 | 7.20  | 113.96      | 108.20   |
| 27  | B8    | 1324 | G    | C5-C6-O6   | -7.20 | 124.28      | 128.60   |
| 27  | B8    | 1393 | A    | O4'-C1'-N9 | 7.20  | 113.96      | 108.20   |
| 27  | B8    | 2061 | G    | C5-C6-O6   | -7.20 | 124.28      | 128.60   |
| 1   | AA    | 881  | G    | C5-C6-O6   | -7.20 | 124.28      | 128.60   |
| 27  | B8    | 1959 | G    | C5-C6-O6   | -7.20 | 124.28      | 128.60   |
| 27  | B8    | 2109 | U    | O4'-C1'-N1 | 7.20  | 113.96      | 108.20   |
| 1   | AA    | 736  | C    | O4'-C1'-N1 | 7.20  | 113.96      | 108.20   |
| 1   | AA    | 923  | A    | C5-C6-N6   | -7.20 | 117.94      | 123.70   |
| 27  | B8    | 189  | G    | C5-C6-O6   | -7.20 | 124.28      | 128.60   |
| 27  | B8    | 647  | G    | C5-C6-O6   | -7.20 | 124.28      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 734  | A    | C5-C6-N6   | -7.20 | 117.94      | 123.70   |
| 27  | B8    | 841  | G    | C5-C6-O6   | -7.20 | 124.28      | 128.60   |
| 27  | B8    | 1165 | A    | O4'-C1'-N9 | 7.20  | 113.96      | 108.20   |
| 27  | B8    | 30   | G    | C5-C6-O6   | -7.20 | 124.28      | 128.60   |
| 27  | B8    | 1160 | G    | C5-C6-O6   | -7.20 | 124.28      | 128.60   |
| 1   | AA    | 1135 | U    | O4'-C1'-N1 | 7.20  | 113.96      | 108.20   |
| 27  | B8    | 1899 | A    | C5-C6-N6   | -7.20 | 117.94      | 123.70   |
| 27  | B8    | 2223 | G    | C5-C6-O6   | -7.20 | 124.28      | 128.60   |
| 27  | B8    | 2385 | C    | O4'-C1'-N1 | 7.20  | 113.96      | 108.20   |
| 27  | B8    | 1588 | G    | C5-C6-O6   | -7.19 | 124.28      | 128.60   |
| 27  | B8    | 1620 | G    | C5-C6-O6   | -7.19 | 124.28      | 128.60   |
| 27  | B8    | 1720 | U    | O4'-C1'-N1 | 7.19  | 113.95      | 108.20   |
| 27  | B8    | 2044 | C    | O4'-C1'-N1 | 7.19  | 113.95      | 108.20   |
| 27  | B8    | 956  | G    | C5-C6-O6   | -7.19 | 124.28      | 128.60   |
| 27  | B8    | 2318 | G    | C5-C6-O6   | -7.19 | 124.28      | 128.60   |
| 27  | B8    | 2869 | G    | O4'-C1'-N9 | 7.19  | 113.95      | 108.20   |
| 1   | AA    | 333  | U    | O4'-C1'-N1 | 7.19  | 113.95      | 108.20   |
| 1   | AA    | 1532 | U    | O4'-C1'-N1 | 7.19  | 113.95      | 108.20   |
| 27  | B8    | 201  | C    | N3-C4-N4   | 7.19  | 123.03      | 118.00   |
| 27  | B8    | 206  | U    | O4'-C1'-N1 | 7.19  | 113.95      | 108.20   |
| 1   | AA    | 1322 | C    | O4'-C1'-N1 | 7.19  | 113.95      | 108.20   |
| 27  | B8    | 926  | G    | C5-C6-O6   | -7.19 | 124.29      | 128.60   |
| 1   | AA    | 929  | G    | O4'-C1'-N9 | 7.19  | 113.95      | 108.20   |
| 1   | AA    | 1249 | C    | O4'-C1'-N1 | 7.19  | 113.95      | 108.20   |
| 27  | B8    | 1379 | U    | O4'-C1'-N1 | 7.19  | 113.95      | 108.20   |
| 27  | B8    | 1459 | G    | O4'-C1'-N9 | 7.19  | 113.95      | 108.20   |
| 27  | B8    | 2218 | G    | C5-C6-O6   | -7.19 | 124.29      | 128.60   |
| 27  | B8    | 2490 | G    | C5-C6-O6   | -7.19 | 124.29      | 128.60   |
| 1   | AA    | 952  | U    | O4'-C1'-N1 | 7.19  | 113.95      | 108.20   |
| 27  | B8    | 989  | G    | C5-C6-O6   | -7.19 | 124.29      | 128.60   |
| 27  | B8    | 2737 | G    | C5-C6-O6   | -7.19 | 124.29      | 128.60   |
| 27  | B8    | 1513 | U    | O4'-C1'-N1 | 7.18  | 113.95      | 108.20   |
| 27  | B8    | 1095 | A    | O4'-C1'-N9 | 7.18  | 113.95      | 108.20   |
| 27  | B8    | 1742 | U    | O4'-C1'-N1 | 7.18  | 113.95      | 108.20   |
| 27  | B8    | 1750 | G    | O4'-C1'-N9 | 7.18  | 113.95      | 108.20   |
| 27  | B8    | 1849 | G    | C5-C6-O6   | -7.18 | 124.29      | 128.60   |
| 27  | B8    | 2354 | C    | O4'-C1'-N1 | 7.18  | 113.95      | 108.20   |
| 27  | B8    | 2457 | U    | O4'-C1'-N1 | 7.18  | 113.95      | 108.20   |
| 1   | AA    | 95   | C    | N3-C4-N4   | 7.18  | 123.03      | 118.00   |
| 27  | B8    | 1836 | C    | O4'-C1'-N1 | 7.18  | 113.94      | 108.20   |
| 1   | AA    | 137  | U    | O4'-C1'-N1 | 7.18  | 113.94      | 108.20   |
| 1   | AA    | 181  | A    | C5-C6-N6   | -7.18 | 117.96      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26  | B7    | 5    | U    | O4'-C1'-N1 | 7.18  | 113.94      | 108.20   |
| 26  | B7    | 18   | G    | C5-C6-O6   | -7.18 | 124.29      | 128.60   |
| 27  | B8    | 437  | U    | O4'-C1'-N1 | 7.18  | 113.94      | 108.20   |
| 27  | B8    | 643  | A    | O4'-C1'-N9 | 7.18  | 113.94      | 108.20   |
| 27  | B8    | 740  | C    | O4'-C1'-N1 | 7.18  | 113.94      | 108.20   |
| 1   | AA    | 108  | G    | O4'-C1'-N9 | 7.18  | 113.94      | 108.20   |
| 27  | B8    | 2696 | U    | O4'-C1'-N1 | 7.18  | 113.94      | 108.20   |
| 27  | B8    | 1309 | G    | C5-C6-O6   | -7.17 | 124.30      | 128.60   |
| 27  | B8    | 1373 | A    | C4-C5-C6   | 7.17  | 120.59      | 117.00   |
| 1   | AA    | 957  | U    | O4'-C1'-N1 | 7.17  | 113.94      | 108.20   |
| 1   | AA    | 423  | G    | C5-C6-O6   | -7.17 | 124.30      | 128.60   |
| 27  | B8    | 107  | G    | C5-C6-O6   | -7.17 | 124.30      | 128.60   |
| 27  | B8    | 578  | G    | C5-C6-O6   | -7.17 | 124.30      | 128.60   |
| 27  | B8    | 2398 | U    | O4'-C1'-N1 | 7.17  | 113.94      | 108.20   |
| 27  | B8    | 2693 | G    | C5-C6-O6   | -7.17 | 124.30      | 128.60   |
| 26  | B7    | 12   | C    | O4'-C1'-N1 | 7.17  | 113.94      | 108.20   |
| 1   | AA    | 299  | G    | C5-C6-O6   | -7.17 | 124.30      | 128.60   |
| 1   | AA    | 1084 | G    | C5-C6-O6   | -7.17 | 124.30      | 128.60   |
| 27  | B8    | 2605 | U    | O4'-C1'-N1 | 7.17  | 113.94      | 108.20   |
| 1   | AA    | 906  | A    | C5-C6-N6   | -7.17 | 117.97      | 123.70   |
| 26  | B7    | 120  | U    | O4'-C1'-N1 | 7.17  | 113.93      | 108.20   |
| 27  | B8    | 27   | G    | C5-C6-O6   | -7.17 | 124.30      | 128.60   |
| 27  | B8    | 771  | G    | C5-C6-O6   | -7.17 | 124.30      | 128.60   |
| 27  | B8    | 2586 | U    | O4'-C1'-N1 | 7.17  | 113.93      | 108.20   |
| 27  | B8    | 2881 | U    | O4'-C1'-N1 | 7.17  | 113.93      | 108.20   |
| 27  | B8    | 96   | C    | O4'-C1'-N1 | 7.17  | 113.93      | 108.20   |
| 27  | B8    | 1209 | U    | O4'-C1'-N1 | 7.17  | 113.93      | 108.20   |
| 1   | AA    | 569  | C    | O4'-C1'-N1 | 7.16  | 113.93      | 108.20   |
| 1   | AA    | 979  | C    | O4'-C1'-N1 | 7.16  | 113.93      | 108.20   |
| 1   | AA    | 132  | C    | O4'-C1'-N1 | 7.16  | 113.93      | 108.20   |
| 1   | AA    | 462  | G    | C5-C6-O6   | -7.16 | 124.30      | 128.60   |
| 1   | AA    | 900  | A    | O4'-C1'-N9 | 7.16  | 113.93      | 108.20   |
| 27  | B8    | 24   | G    | C5-C6-O6   | -7.16 | 124.30      | 128.60   |
| 27  | B8    | 636  | G    | C5-C6-O6   | -7.16 | 124.30      | 128.60   |
| 27  | B8    | 2245 | U    | O4'-C1'-N1 | 7.16  | 113.93      | 108.20   |
| 1   | AA    | 514  | C    | O4'-C1'-N1 | 7.16  | 113.93      | 108.20   |
| 1   | AA    | 1404 | C    | O4'-C1'-N1 | 7.16  | 113.93      | 108.20   |
| 27  | B8    | 2000 | C    | O4'-C1'-N1 | 7.16  | 113.93      | 108.20   |
| 27  | B8    | 2259 | U    | O4'-C1'-N1 | 7.16  | 113.93      | 108.20   |
| 27  | B8    | 2846 | G    | C5-C6-O6   | -7.16 | 124.31      | 128.60   |
| 1   | AA    | 295  | C    | O4'-C1'-N1 | 7.16  | 113.93      | 108.20   |
| 27  | B8    | 136  | G    | C5-C6-O6   | -7.16 | 124.31      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 357  | C    | O4'-C1'-N1 | 7.16  | 113.93      | 108.20   |
| 1   | AA    | 442  | G    | C5-C6-O6   | -7.16 | 124.31      | 128.60   |
| 3   | AV    | 51   | G    | C5-C6-O6   | -7.16 | 124.31      | 128.60   |
| 27  | B8    | 511  | U    | O4'-C1'-N1 | 7.16  | 113.92      | 108.20   |
| 27  | B8    | 1053 | C    | N3-C4-N4   | 7.16  | 123.01      | 118.00   |
| 27  | B8    | 2204 | G    | C5-C6-O6   | -7.15 | 124.31      | 128.60   |
| 1   | AA    | 210  | C    | O4'-C1'-N1 | 7.15  | 113.92      | 108.20   |
| 1   | AA    | 1463 | U    | O4'-C1'-N1 | 7.15  | 113.92      | 108.20   |
| 1   | AA    | 445  | G    | C5-C6-O6   | -7.15 | 124.31      | 128.60   |
| 27  | B8    | 1148 | U    | O4'-C1'-N1 | 7.15  | 113.92      | 108.20   |
| 27  | B8    | 2668 | G    | C5-C6-O6   | -7.15 | 124.31      | 128.60   |
| 1   | AA    | 24   | U    | O4'-C1'-N1 | 7.15  | 113.92      | 108.20   |
| 27  | B8    | 1249 | U    | O4'-C1'-N1 | 7.15  | 113.92      | 108.20   |
| 27  | B8    | 2685 | G    | C5-C6-O6   | -7.15 | 124.31      | 128.60   |
| 1   | AA    | 79   | G    | C5-C6-O6   | -7.15 | 124.31      | 128.60   |
| 1   | AA    | 799  | G    | C5-C6-O6   | -7.15 | 124.31      | 128.60   |
| 1   | AA    | 1138 | G    | C5-C6-O6   | -7.15 | 124.31      | 128.60   |
| 1   | AA    | 42   | G    | C5-C6-O6   | -7.14 | 124.31      | 128.60   |
| 1   | AA    | 644  | U    | O4'-C1'-N1 | 7.14  | 113.92      | 108.20   |
| 1   | AA    | 711  | G    | C5-C6-O6   | -7.14 | 124.31      | 128.60   |
| 1   | AA    | 904  | U    | O4'-C1'-N1 | 7.14  | 113.92      | 108.20   |
| 27  | B8    | 1509 | A    | O4'-C1'-N9 | 7.14  | 113.92      | 108.20   |
| 27  | B8    | 1680 | U    | O4'-C1'-N1 | 7.14  | 113.92      | 108.20   |
| 27  | B8    | 2243 | U    | O4'-C1'-N1 | 7.14  | 113.92      | 108.20   |
| 27  | B8    | 2680 | U    | O4'-C1'-N1 | 7.14  | 113.92      | 108.20   |
| 1   | AA    | 39   | G    | O4'-C1'-N9 | 7.14  | 113.92      | 108.20   |
| 26  | B7    | 75   | G    | C5-C6-O6   | -7.14 | 124.31      | 128.60   |
| 27  | B8    | 1380 | G    | C5-C6-O6   | -7.14 | 124.31      | 128.60   |
| 27  | B8    | 2496 | C    | O4'-C1'-N1 | 7.14  | 113.91      | 108.20   |
| 1   | AA    | 375  | U    | O4'-C1'-N1 | 7.14  | 113.91      | 108.20   |
| 27  | B8    | 2593 | U    | O4'-C1'-N1 | 7.14  | 113.91      | 108.20   |
| 27  | B8    | 269  | C    | O4'-C1'-N1 | 7.14  | 113.91      | 108.20   |
| 27  | B8    | 1632 | A    | O4'-C1'-N9 | 7.14  | 113.91      | 108.20   |
| 27  | B8    | 2216 | G    | C5-C6-O6   | -7.14 | 124.32      | 128.60   |
| 27  | B8    | 2277 | G    | O4'-C1'-N9 | 7.14  | 113.91      | 108.20   |
| 1   | AA    | 741  | G    | O4'-C1'-N9 | 7.14  | 113.91      | 108.20   |
| 1   | AA    | 1308 | U    | O4'-C1'-N1 | 7.14  | 113.91      | 108.20   |
| 27  | B8    | 1222 | U    | O4'-C1'-N1 | 7.14  | 113.91      | 108.20   |
| 27  | B8    | 1714 | U    | O4'-C1'-N1 | 7.14  | 113.91      | 108.20   |
| 27  | B8    | 2826 | A    | C5-C6-N6   | -7.14 | 117.99      | 123.70   |
| 1   | AA    | 1397 | C    | O4'-C1'-N1 | 7.13  | 113.91      | 108.20   |
| 26  | B7    | 109  | A    | C5-C6-N6   | -7.13 | 117.99      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 23   | G    | C5-C6-O6   | -7.13 | 124.32      | 128.60   |
| 27  | B8    | 705  | A    | C4-C5-C6   | 7.13  | 120.57      | 117.00   |
| 27  | B8    | 1993 | U    | O4'-C1'-N1 | 7.13  | 113.91      | 108.20   |
| 1   | AA    | 524  | G    | C5-C6-O6   | -7.13 | 124.32      | 128.60   |
| 1   | AA    | 425  | G    | O4'-C1'-N9 | 7.13  | 113.91      | 108.20   |
| 1   | AA    | 921  | U    | O4'-C1'-N1 | 7.13  | 113.91      | 108.20   |
| 27  | B8    | 150  | U    | O4'-C1'-N1 | 7.13  | 113.91      | 108.20   |
| 27  | B8    | 1266 | G    | C5-C6-O6   | -7.13 | 124.32      | 128.60   |
| 27  | B8    | 1891 | G    | C5-C6-O6   | -7.13 | 124.32      | 128.60   |
| 27  | B8    | 2387 | U    | O4'-C1'-N1 | 7.13  | 113.90      | 108.20   |
| 27  | B8    | 2884 | U    | O4'-C1'-N1 | 7.13  | 113.90      | 108.20   |
| 1   | AA    | 993  | G    | O4'-C1'-N9 | 7.13  | 113.90      | 108.20   |
| 27  | B8    | 618  | G    | C5-C6-O6   | -7.13 | 124.32      | 128.60   |
| 27  | B8    | 1128 | G    | C5-C6-O6   | -7.13 | 124.32      | 128.60   |
| 27  | B8    | 1231 | U    | O4'-C1'-N1 | 7.13  | 113.90      | 108.20   |
| 27  | B8    | 2293 | G    | O4'-C1'-N9 | 7.13  | 113.90      | 108.20   |
| 1   | AA    | 1005 | A    | C4-C5-C6   | 7.12  | 120.56      | 117.00   |
| 27  | B8    | 205  | G    | C5-C6-O6   | -7.12 | 124.33      | 128.60   |
| 27  | B8    | 1199 | U    | O4'-C1'-N1 | 7.12  | 113.90      | 108.20   |
| 27  | B8    | 1451 | C    | O4'-C1'-N1 | 7.12  | 113.90      | 108.20   |
| 1   | AA    | 64   | G    | C5-C6-O6   | -7.12 | 124.33      | 128.60   |
| 1   | AA    | 468  | A    | C4-C5-C6   | 7.12  | 120.56      | 117.00   |
| 1   | AA    | 682  | G    | C5-C6-O6   | -7.12 | 124.33      | 128.60   |
| 1   | AA    | 961  | U    | O4'-C1'-N1 | 7.12  | 113.90      | 108.20   |
| 27  | B8    | 1036 | G    | O4'-C1'-N9 | 7.12  | 113.90      | 108.20   |
| 27  | B8    | 1862 | G    | C5-C6-O6   | -7.12 | 124.33      | 128.60   |
| 1   | AA    | 533  | A    | C4-C5-C6   | 7.12  | 120.56      | 117.00   |
| 27  | B8    | 49   | A    | C4-C5-C6   | 7.12  | 120.56      | 117.00   |
| 27  | B8    | 89   | A    | O4'-C1'-N9 | 7.12  | 113.89      | 108.20   |
| 27  | B8    | 1137 | G    | O4'-C1'-N9 | 7.12  | 113.89      | 108.20   |
| 1   | AA    | 674  | G    | O4'-C1'-N9 | 7.11  | 113.89      | 108.20   |
| 1   | AA    | 762  | U    | O4'-C1'-N1 | 7.11  | 113.89      | 108.20   |
| 1   | AA    | 809  | G    | C5-C6-O6   | -7.11 | 124.33      | 128.60   |
| 27  | B8    | 614  | A    | O4'-C1'-N9 | 7.11  | 113.89      | 108.20   |
| 27  | B8    | 1257 | C    | O4'-C1'-N1 | 7.11  | 113.89      | 108.20   |
| 1   | AA    | 121  | U    | O4'-C1'-N1 | 7.11  | 113.89      | 108.20   |
| 1   | AA    | 1464 | U    | O4'-C1'-N1 | 7.11  | 113.89      | 108.20   |
| 1   | AA    | 505  | G    | C5-C6-O6   | -7.11 | 124.33      | 128.60   |
| 26  | B7    | 79   | G    | C5-C6-O6   | -7.11 | 124.34      | 128.60   |
| 27  | B8    | 34   | U    | O4'-C1'-N1 | 7.11  | 113.89      | 108.20   |
| 1   | AA    | 1160 | G    | N1-C6-O6   | 7.11  | 124.16      | 119.90   |
| 27  | B8    | 315  | G    | O4'-C1'-N9 | 7.11  | 113.89      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 639  | U    | O4'-C1'-N1 | 7.11  | 113.89      | 108.20   |
| 27  | B8    | 1004 | U    | O4'-C1'-N1 | 7.11  | 113.89      | 108.20   |
| 27  | B8    | 2074 | U    | O4'-C1'-N1 | 7.11  | 113.89      | 108.20   |
| 1   | AA    | 292  | G    | C5-C6-O6   | -7.10 | 124.34      | 128.60   |
| 1   | AA    | 353  | A    | O4'-C1'-N9 | 7.10  | 113.88      | 108.20   |
| 1   | AA    | 1361 | G    | O4'-C1'-N9 | 7.10  | 113.88      | 108.20   |
| 3   | AV    | 55   | U    | O4'-C1'-N1 | 7.10  | 113.88      | 108.20   |
| 27  | B8    | 2085 | U    | O4'-C1'-N1 | 7.10  | 113.88      | 108.20   |
| 1   | AA    | 891  | U    | O4'-C1'-N1 | 7.10  | 113.88      | 108.20   |
| 27  | B8    | 1079 | C    | O4'-C1'-N1 | 7.10  | 113.88      | 108.20   |
| 27  | B8    | 1582 | C    | O4'-C1'-N1 | 7.10  | 113.88      | 108.20   |
| 27  | B8    | 2580 | U    | O4'-C1'-N1 | 7.10  | 113.88      | 108.20   |
| 1   | AA    | 661  | G    | C5-C6-O6   | -7.10 | 124.34      | 128.60   |
| 27  | B8    | 1711 | A    | O4'-C1'-N9 | 7.10  | 113.88      | 108.20   |
| 27  | B8    | 1882 | U    | O4'-C1'-N1 | 7.10  | 113.88      | 108.20   |
| 27  | B8    | 2231 | U    | O4'-C1'-N1 | 7.10  | 113.88      | 108.20   |
| 27  | B8    | 2800 | A    | C4-C5-C6   | 7.10  | 120.55      | 117.00   |
| 1   | AA    | 88   | U    | O4'-C1'-N1 | 7.10  | 113.88      | 108.20   |
| 27  | B8    | 860  | U    | O4'-C1'-N1 | 7.10  | 113.88      | 108.20   |
| 27  | B8    | 686  | U    | O4'-C1'-N1 | 7.09  | 113.88      | 108.20   |
| 1   | AA    | 809  | G    | O4'-C1'-N9 | 7.09  | 113.87      | 108.20   |
| 1   | AA    | 1504 | G    | C5-C6-O6   | -7.09 | 124.34      | 128.60   |
| 26  | B7    | 102  | G    | C5-C6-O6   | -7.09 | 124.34      | 128.60   |
| 27  | B8    | 5    | A    | C5-C6-N6   | -7.09 | 118.03      | 123.70   |
| 27  | B8    | 495  | G    | C5-C6-O6   | -7.09 | 124.34      | 128.60   |
| 27  | B8    | 2612 | C    | O4'-C1'-N1 | 7.09  | 113.87      | 108.20   |
| 1   | AA    | 982  | U    | O4'-C1'-N1 | 7.09  | 113.87      | 108.20   |
| 1   | AA    | 1387 | G    | C5-C6-O6   | -7.09 | 124.35      | 128.60   |
| 27  | B8    | 323  | C    | C2-N1-C1'  | 7.09  | 126.60      | 118.80   |
| 27  | B8    | 1255 | U    | O4'-C1'-N1 | 7.09  | 113.87      | 108.20   |
| 27  | B8    | 2366 | A    | C4-C5-C6   | 7.09  | 120.54      | 117.00   |
| 27  | B8    | 2768 | U    | O4'-C1'-N1 | 7.09  | 113.87      | 108.20   |
| 3   | AV    | 15   | G    | C5-C6-O6   | -7.09 | 124.35      | 128.60   |
| 1   | AA    | 1194 | U    | O4'-C1'-N1 | 7.09  | 113.87      | 108.20   |
| 1   | AA    | 1448 | C    | N3-C4-N4   | 7.09  | 122.96      | 118.00   |
| 3   | AV    | 40   | G    | C5-C6-O6   | -7.09 | 124.35      | 128.60   |
| 27  | B8    | 59   | U    | O4'-C1'-N1 | 7.09  | 113.87      | 108.20   |
| 1   | AA    | 672  | U    | O4'-C1'-N1 | 7.08  | 113.87      | 108.20   |
| 27  | B8    | 1926 | U    | O4'-C1'-N1 | 7.08  | 113.87      | 108.20   |
| 27  | B8    | 2186 | G    | C5-C6-O6   | -7.08 | 124.35      | 128.60   |
| 1   | AA    | 605  | U    | O4'-C1'-N1 | 7.08  | 113.87      | 108.20   |
| 27  | B8    | 612  | G    | C5-C6-O6   | -7.08 | 124.35      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 915  | C    | O4'-C1'-N1 | 7.08  | 113.87      | 108.20   |
| 1   | AA    | 446  | G    | C5-C6-O6   | -7.08 | 124.35      | 128.60   |
| 1   | AA    | 1526 | G    | C5-C6-O6   | -7.08 | 124.35      | 128.60   |
| 27  | B8    | 459  | U    | O4'-C1'-N1 | 7.08  | 113.86      | 108.20   |
| 27  | B8    | 952  | G    | C5-C6-O6   | -7.08 | 124.35      | 128.60   |
| 27  | B8    | 1475 | G    | C5-C6-O6   | -7.08 | 124.35      | 128.60   |
| 27  | B8    | 2771 | C    | O4'-C1'-N1 | 7.08  | 113.86      | 108.20   |
| 27  | B8    | 310  | A    | C4-C5-C6   | 7.08  | 120.54      | 117.00   |
| 27  | B8    | 1069 | A    | O4'-C1'-N9 | 7.08  | 113.86      | 108.20   |
| 27  | B8    | 1358 | G    | C5-C6-O6   | -7.08 | 124.35      | 128.60   |
| 27  | B8    | 1398 | C    | O4'-C1'-N1 | 7.08  | 113.86      | 108.20   |
| 27  | B8    | 1765 | U    | O4'-C1'-N1 | 7.08  | 113.86      | 108.20   |
| 27  | B8    | 1845 | G    | C5-C6-O6   | -7.08 | 124.35      | 128.60   |
| 27  | B8    | 2107 | G    | C5-C6-O6   | -7.08 | 124.35      | 128.60   |
| 1   | AA    | 495  | A    | C4-C5-C6   | 7.08  | 120.54      | 117.00   |
| 27  | B8    | 1225 | G    | C5-C6-O6   | -7.08 | 124.36      | 128.60   |
| 27  | B8    | 1709 | U    | O4'-C1'-N1 | 7.08  | 113.86      | 108.20   |
| 27  | B8    | 864  | G    | O4'-C1'-N9 | 7.07  | 113.86      | 108.20   |
| 27  | B8    | 2647 | U    | O4'-C1'-N1 | 7.07  | 113.86      | 108.20   |
| 1   | AA    | 460  | A    | O4'-C1'-N9 | 7.07  | 113.86      | 108.20   |
| 27  | B8    | 1210 | G    | C5-C6-O6   | -7.07 | 124.36      | 128.60   |
| 27  | B8    | 1767 | G    | C5-C6-O6   | -7.07 | 124.36      | 128.60   |
| 27  | B8    | 2286 | G    | C5-C6-O6   | -7.07 | 124.36      | 128.60   |
| 27  | B8    | 2405 | G    | C5-C6-O6   | -7.07 | 124.36      | 128.60   |
| 1   | AA    | 1393 | U    | O4'-C1'-N1 | 7.07  | 113.86      | 108.20   |
| 1   | AA    | 1378 | C    | O4'-C1'-N1 | 7.07  | 113.85      | 108.20   |
| 27  | B8    | 2541 | A    | C4-C5-C6   | 7.07  | 120.53      | 117.00   |
| 1   | AA    | 198  | G    | C5-C6-O6   | -7.07 | 124.36      | 128.60   |
| 1   | AA    | 1306 | A    | O4'-C1'-N9 | 7.07  | 113.85      | 108.20   |
| 27  | B8    | 8    | C    | O4'-C1'-N1 | 7.07  | 113.85      | 108.20   |
| 27  | B8    | 1431 | A    | C5-C6-N6   | -7.07 | 118.05      | 123.70   |
| 1   | AA    | 1422 | G    | C5-C6-O6   | -7.06 | 124.36      | 128.60   |
| 27  | B8    | 2452 | C    | O4'-C1'-N1 | 7.06  | 113.85      | 108.20   |
| 1   | AA    | 1365 | G    | C5-C6-O6   | -7.06 | 124.36      | 128.60   |
| 27  | B8    | 803  | U    | O4'-C1'-N1 | 7.06  | 113.85      | 108.20   |
| 27  | B8    | 1350 | C    | O4'-C1'-N1 | 7.06  | 113.85      | 108.20   |
| 27  | B8    | 1633 | G    | C5-C6-O6   | -7.06 | 124.36      | 128.60   |
| 27  | B8    | 1842 | G    | C5-C6-O6   | -7.06 | 124.36      | 128.60   |
| 27  | B8    | 2489 | U    | O4'-C1'-N1 | 7.06  | 113.85      | 108.20   |
| 1   | AA    | 331  | G    | C5-C6-O6   | -7.06 | 124.36      | 128.60   |
| 27  | B8    | 169  | G    | C5-C6-O6   | -7.06 | 124.36      | 128.60   |
| 27  | B8    | 463  | G    | C5-C6-O6   | -7.06 | 124.36      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 776  | G    | C5-C6-O6   | -7.06 | 124.36      | 128.60   |
| 1   | AA    | 745  | G    | C5-C6-O6   | -7.06 | 124.36      | 128.60   |
| 27  | B8    | 576  | U    | O4'-C1'-N1 | 7.06  | 113.84      | 108.20   |
| 27  | B8    | 695  | G    | C5-C6-O6   | -7.06 | 124.36      | 128.60   |
| 27  | B8    | 769  | U    | O4'-C1'-N1 | 7.06  | 113.84      | 108.20   |
| 1   | AA    | 127  | G    | C5-C6-O6   | -7.06 | 124.37      | 128.60   |
| 1   | AA    | 193  | C    | N3-C4-N4   | 7.05  | 122.94      | 118.00   |
| 1   | AA    | 274  | A    | P-O3'-C3'  | 7.05  | 128.16      | 119.70   |
| 1   | AA    | 822  | U    | O4'-C1'-N1 | 7.05  | 113.84      | 108.20   |
| 3   | AV    | 8    | U    | O4'-C1'-N1 | 7.05  | 113.84      | 108.20   |
| 3   | AV    | 44   | G    | C5-C6-O6   | -7.05 | 124.37      | 128.60   |
| 1   | AA    | 1529 | G    | O4'-C1'-N9 | 7.05  | 113.84      | 108.20   |
| 1   | AA    | 381  | C    | O4'-C1'-N1 | 7.05  | 113.84      | 108.20   |
| 27  | B8    | 688  | U    | O4'-C1'-N1 | 7.05  | 113.84      | 108.20   |
| 1   | AA    | 773  | G    | C5-C6-O6   | -7.05 | 124.37      | 128.60   |
| 1   | AA    | 945  | G    | C5-C6-O6   | -7.05 | 124.37      | 128.60   |
| 27  | B8    | 78   | U    | O4'-C1'-N1 | 7.05  | 113.84      | 108.20   |
| 27  | B8    | 323  | C    | O4'-C1'-N1 | 7.05  | 113.84      | 108.20   |
| 27  | B8    | 583  | G    | C5-C6-O6   | -7.05 | 124.37      | 128.60   |
| 27  | B8    | 1930 | G    | P-O3'-C3'  | 7.05  | 128.16      | 119.70   |
| 27  | B8    | 2378 | A    | C5-C6-N1   | -7.05 | 114.17      | 117.70   |
| 1   | AA    | 571  | U    | O4'-C1'-N1 | 7.05  | 113.84      | 108.20   |
| 1   | AA    | 1525 | G    | O4'-C1'-N9 | 7.05  | 113.84      | 108.20   |
| 27  | B8    | 1507 | C    | O4'-C1'-N1 | 7.05  | 113.84      | 108.20   |
| 1   | AA    | 1258 | G    | C5-C6-O6   | -7.05 | 124.37      | 128.60   |
| 27  | B8    | 1982 | U    | O4'-C1'-N1 | 7.05  | 113.84      | 108.20   |
| 27  | B8    | 2852 | G    | O4'-C1'-N9 | 7.05  | 113.84      | 108.20   |
| 1   | AA    | 1023 | U    | O4'-C1'-N1 | 7.04  | 113.84      | 108.20   |
| 1   | AA    | 416  | G    | C5-C6-O6   | -7.04 | 124.37      | 128.60   |
| 1   | AA    | 993  | G    | C5-C6-O6   | -7.04 | 124.37      | 128.60   |
| 27  | B8    | 2    | G    | C5-C6-O6   | -7.04 | 124.37      | 128.60   |
| 27  | B8    | 265  | A    | C5-C6-N6   | -7.04 | 118.06      | 123.70   |
| 26  | B7    | 56   | G    | C5-C6-O6   | -7.04 | 124.38      | 128.60   |
| 27  | B8    | 90   | U    | O4'-C1'-N1 | 7.04  | 113.83      | 108.20   |
| 27  | B8    | 295  | G    | C5-C6-O6   | -7.04 | 124.38      | 128.60   |
| 27  | B8    | 1125 | G    | C5-C6-O6   | -7.04 | 124.38      | 128.60   |
| 27  | B8    | 1292 | G    | O4'-C1'-N9 | 7.04  | 113.83      | 108.20   |
| 27  | B8    | 1401 | G    | C5-C6-O6   | -7.04 | 124.38      | 128.60   |
| 1   | AA    | 1474 | U    | O4'-C1'-N1 | 7.04  | 113.83      | 108.20   |
| 27  | B8    | 469  | G    | C5-C6-O6   | -7.04 | 124.38      | 128.60   |
| 27  | B8    | 1116 | G    | C5-C6-O6   | -7.04 | 124.38      | 128.60   |
| 27  | B8    | 2335 | A    | C4-C5-C6   | 7.04  | 120.52      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | B8    | 2669 | G    | O4'-C1'-N9  | 7.04  | 113.83      | 108.20   |
| 27  | B8    | 926  | G    | O4'-C1'-N9  | 7.04  | 113.83      | 108.20   |
| 27  | B8    | 942  | G    | C5-C6-O6    | -7.04 | 124.38      | 128.60   |
| 27  | B8    | 969  | G    | C5-C6-O6    | -7.04 | 124.38      | 128.60   |
| 27  | B8    | 975  | A    | C4-C5-C6    | 7.04  | 120.52      | 117.00   |
| 1   | AA    | 72   | A    | O4'-C1'-N9  | 7.04  | 113.83      | 108.20   |
| 1   | AA    | 1359 | C    | O4'-C1'-N1  | 7.04  | 113.83      | 108.20   |
| 27  | B8    | 620  | G    | C5-C6-O6    | -7.04 | 124.38      | 128.60   |
| 1   | AA    | 1242 | G    | C5-C6-O6    | -7.03 | 124.38      | 128.60   |
| 1   | AA    | 905  | U    | O4'-C1'-N1  | 7.03  | 113.83      | 108.20   |
| 1   | AA    | 339  | C    | O4'-C1'-N1  | 7.03  | 113.83      | 108.20   |
| 27  | B8    | 427  | U    | O4'-C1'-N1  | 7.03  | 113.83      | 108.20   |
| 27  | B8    | 1825 | U    | O4'-C1'-N1  | 7.03  | 113.82      | 108.20   |
| 27  | B8    | 2326 | C    | O4'-C1'-N1  | 7.03  | 113.82      | 108.20   |
| 1   | AA    | 203  | G    | C5-C6-O6    | -7.03 | 124.38      | 128.60   |
| 1   | AA    | 597  | G    | C5-C6-O6    | -7.03 | 124.38      | 128.60   |
| 1   | AA    | 1064 | G    | C5-C6-O6    | -7.03 | 124.38      | 128.60   |
| 3   | AV    | 69   | U    | O4'-C1'-N1  | 7.03  | 113.82      | 108.20   |
| 27  | B8    | 1024 | G    | C5-C6-O6    | -7.03 | 124.38      | 128.60   |
| 27  | B8    | 535  | G    | C5-C6-O6    | -7.03 | 124.39      | 128.60   |
| 27  | B8    | 1831 | G    | C5-C6-O6    | -7.03 | 124.39      | 128.60   |
| 1   | AA    | 310  | G    | O4'-C1'-N9  | 7.02  | 113.82      | 108.20   |
| 1   | AA    | 829  | G    | C5-C6-O6    | -7.02 | 124.39      | 128.60   |
| 27  | B8    | 303  | G    | C5-C6-O6    | -7.02 | 124.39      | 128.60   |
| 27  | B8    | 930  | G    | C5-C6-O6    | -7.02 | 124.39      | 128.60   |
| 27  | B8    | 974  | G    | C5-C6-O6    | -7.02 | 124.39      | 128.60   |
| 27  | B8    | 1456 | G    | C5-C6-O6    | -7.02 | 124.39      | 128.60   |
| 27  | B8    | 1860 | G    | C5-C6-O6    | -7.02 | 124.39      | 128.60   |
| 27  | B8    | 2244 | U    | O4'-C1'-N1  | 7.02  | 113.82      | 108.20   |
| 1   | AA    | 802  | A    | O4'-C1'-N9  | 7.02  | 113.82      | 108.20   |
| 26  | B7    | 37   | C    | O4'-C1'-N1  | 7.02  | 113.82      | 108.20   |
| 27  | B8    | 514  | A    | O4'-C1'-N9  | 7.02  | 113.82      | 108.20   |
| 27  | B8    | 2645 | G    | C5-C6-O6    | -7.02 | 124.39      | 128.60   |
| 3   | AV    | 35   | G    | C5-C6-O6    | -7.02 | 124.39      | 128.60   |
| 27  | B8    | 573  | U    | O4'-C1'-N1  | 7.02  | 113.82      | 108.20   |
| 27  | B8    | 891  | G    | C1'-O4'-C4' | -7.02 | 104.28      | 109.90   |
| 27  | B8    | 2848 | G    | O4'-C1'-N9  | 7.02  | 113.82      | 108.20   |
| 1   | AA    | 699  | C    | O4'-C1'-N1  | 7.02  | 113.82      | 108.20   |
| 27  | B8    | 188  | G    | C5-C6-O6    | -7.02 | 124.39      | 128.60   |
| 27  | B8    | 1018 | U    | O4'-C1'-N1  | 7.02  | 113.82      | 108.20   |
| 27  | B8    | 1441 | G    | O4'-C1'-N9  | 7.02  | 113.82      | 108.20   |
| 27  | B8    | 2695 | U    | O4'-C1'-N1  | 7.02  | 113.81      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 770  | G    | C5-C6-O6   | -7.02 | 124.39      | 128.60   |
| 27  | B8    | 1567 | G    | C5-C6-O6   | -7.02 | 124.39      | 128.60   |
| 27  | B8    | 2002 | G    | C5-C6-O6   | -7.02 | 124.39      | 128.60   |
| 27  | B8    | 2543 | G    | O4'-C1'-N9 | 7.02  | 113.81      | 108.20   |
| 1   | AA    | 1530 | G    | C5-C6-O6   | -7.02 | 124.39      | 128.60   |
| 27  | B8    | 2307 | G    | N1-C6-O6   | 7.02  | 124.11      | 119.90   |
| 27  | B8    | 2584 | U    | O4'-C1'-N1 | 7.02  | 113.81      | 108.20   |
| 27  | B8    | 2828 | G    | C5-C6-O6   | -7.02 | 124.39      | 128.60   |
| 1   | AA    | 542  | G    | C5-C6-O6   | -7.01 | 124.39      | 128.60   |
| 27  | B8    | 1349 | C    | O4'-C1'-N1 | 7.01  | 113.81      | 108.20   |
| 27  | B8    | 1219 | U    | O4'-C1'-N1 | 7.01  | 113.81      | 108.20   |
| 27  | B8    | 1699 | G    | C5-C6-O6   | -7.01 | 124.39      | 128.60   |
| 27  | B8    | 2267 | A    | C4-C5-C6   | 7.01  | 120.50      | 117.00   |
| 27  | B8    | 2292 | U    | O4'-C1'-N1 | 7.01  | 113.81      | 108.20   |
| 27  | B8    | 2488 | G    | C5-C6-O6   | -7.01 | 124.39      | 128.60   |
| 1   | AA    | 775  | G    | C5-C6-O6   | -7.01 | 124.39      | 128.60   |
| 1   | AA    | 1032 | G    | C5-C6-O6   | -7.01 | 124.39      | 128.60   |
| 27  | B8    | 361  | G    | C5-C6-O6   | -7.01 | 124.39      | 128.60   |
| 27  | B8    | 475  | C    | O4'-C1'-N1 | 7.01  | 113.81      | 108.20   |
| 27  | B8    | 2697 | G    | C5-C6-O6   | -7.01 | 124.39      | 128.60   |
| 1   | AA    | 928  | G    | C5-C6-O6   | -7.01 | 124.39      | 128.60   |
| 27  | B8    | 2547 | A    | O4'-C1'-N9 | 7.01  | 113.81      | 108.20   |
| 1   | AA    | 451  | A    | C5-C6-N6   | -7.01 | 118.09      | 123.70   |
| 27  | B8    | 364  | C    | N3-C4-N4   | 7.01  | 122.90      | 118.00   |
| 27  | B8    | 1516 | G    | C5-C6-O6   | -7.01 | 124.40      | 128.60   |
| 27  | B8    | 1070 | A    | O4'-C1'-N9 | 7.00  | 113.80      | 108.20   |
| 27  | B8    | 1410 | G    | O4'-C1'-N9 | 7.00  | 113.80      | 108.20   |
| 27  | B8    | 2082 | A    | C4-C5-C6   | 7.00  | 120.50      | 117.00   |
| 26  | B7    | 66   | A    | C5-C6-N6   | -7.00 | 118.10      | 123.70   |
| 27  | B8    | 521  | U    | O4'-C1'-N1 | 7.00  | 113.80      | 108.20   |
| 27  | B8    | 1286 | A    | C4-C5-C6   | 7.00  | 120.50      | 117.00   |
| 27  | B8    | 1374 | G    | C5-C6-O6   | -7.00 | 124.40      | 128.60   |
| 1   | AA    | 725  | G    | O4'-C1'-N9 | 7.00  | 113.80      | 108.20   |
| 1   | AA    | 1304 | G    | C5-C6-O6   | -7.00 | 124.40      | 128.60   |
| 1   | AA    | 48   | C    | O4'-C1'-N1 | 7.00  | 113.80      | 108.20   |
| 27  | B8    | 254  | G    | C5-C6-O6   | -7.00 | 124.40      | 128.60   |
| 27  | B8    | 2406 | A    | O4'-C1'-N9 | 7.00  | 113.80      | 108.20   |
| 1   | AA    | 447  | G    | N3-C2-N2   | 7.00  | 124.80      | 119.90   |
| 1   | AA    | 792  | A    | O4'-C1'-N9 | 7.00  | 113.80      | 108.20   |
| 1   | AA    | 1252 | A    | C4-C5-C6   | 7.00  | 120.50      | 117.00   |
| 27  | B8    | 457  | A    | O4'-C1'-N9 | 7.00  | 113.80      | 108.20   |
| 27  | B8    | 630  | G    | C5-C6-O6   | -7.00 | 124.40      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1149 | G    | C5-C6-O6   | -7.00 | 124.40      | 128.60   |
| 27  | B8    | 2545 | G    | C5-C6-O6   | -7.00 | 124.40      | 128.60   |
| 1   | AA    | 155  | A    | C5-C6-N6   | -7.00 | 118.10      | 123.70   |
| 1   | AA    | 1439 | G    | C5-C6-O6   | -7.00 | 124.40      | 128.60   |
| 27  | B8    | 1402 | U    | O4'-C1'-N1 | 7.00  | 113.80      | 108.20   |
| 27  | B8    | 1823 | G    | O4'-C1'-N9 | 7.00  | 113.80      | 108.20   |
| 1   | AA    | 237  | G    | C5-C6-O6   | -6.99 | 124.40      | 128.60   |
| 27  | B8    | 1432 | G    | C5-C6-O6   | -6.99 | 124.40      | 128.60   |
| 27  | B8    | 2700 | A    | O4'-C1'-N9 | 6.99  | 113.80      | 108.20   |
| 1   | AA    | 1295 | U    | O4'-C1'-N1 | 6.99  | 113.79      | 108.20   |
| 26  | B7    | 51   | G    | C5-C6-O6   | -6.99 | 124.41      | 128.60   |
| 1   | AA    | 327  | A    | C4-C5-C6   | 6.99  | 120.50      | 117.00   |
| 1   | AA    | 713  | G    | C5-C6-O6   | -6.99 | 124.41      | 128.60   |
| 1   | AA    | 1190 | G    | C5-C6-O6   | -6.99 | 124.41      | 128.60   |
| 27  | B8    | 785  | G    | C5-C6-O6   | -6.99 | 124.41      | 128.60   |
| 27  | B8    | 1466 | U    | O4'-C1'-N1 | 6.99  | 113.79      | 108.20   |
| 27  | B8    | 2188 | U    | O4'-C1'-N1 | 6.99  | 113.79      | 108.20   |
| 26  | B7    | 96   | G    | C5-C6-O6   | -6.99 | 124.41      | 128.60   |
| 27  | B8    | 1407 | G    | O4'-C1'-N9 | 6.99  | 113.79      | 108.20   |
| 1   | AA    | 273  | U    | O4'-C1'-N1 | 6.99  | 113.79      | 108.20   |
| 3   | AV    | 2    | G    | C5-C6-O6   | -6.99 | 124.41      | 128.60   |
| 27  | B8    | 753  | A    | C4-C5-C6   | 6.99  | 120.49      | 117.00   |
| 27  | B8    | 1767 | G    | O4'-C1'-N9 | 6.99  | 113.79      | 108.20   |
| 27  | B8    | 2393 | U    | O4'-C1'-N1 | 6.99  | 113.79      | 108.20   |
| 1   | AA    | 251  | G    | C5-C6-O6   | -6.98 | 124.41      | 128.60   |
| 1   | AA    | 100  | G    | C5-C6-O6   | -6.98 | 124.41      | 128.60   |
| 1   | AA    | 1035 | A    | C5-C6-N6   | -6.98 | 118.11      | 123.70   |
| 1   | AA    | 1477 | U    | O4'-C1'-N1 | 6.98  | 113.79      | 108.20   |
| 27  | B8    | 306  | U    | O4'-C1'-N1 | 6.98  | 113.79      | 108.20   |
| 27  | B8    | 770  | G    | O4'-C1'-N9 | 6.98  | 113.79      | 108.20   |
| 27  | B8    | 997  | G    | C5-C6-O6   | -6.98 | 124.41      | 128.60   |
| 27  | B8    | 1087 | G    | C5-C6-O6   | -6.98 | 124.41      | 128.60   |
| 27  | B8    | 1120 | G    | C5-C6-O6   | -6.98 | 124.41      | 128.60   |
| 27  | B8    | 1332 | G    | C5-C6-O6   | -6.98 | 124.41      | 128.60   |
| 27  | B8    | 2877 | G    | C5-C6-O6   | -6.98 | 124.41      | 128.60   |
| 1   | AA    | 383  | A    | C4-C5-C6   | 6.98  | 120.49      | 117.00   |
| 27  | B8    | 263  | G    | C5-C6-O6   | -6.98 | 124.41      | 128.60   |
| 27  | B8    | 918  | A    | C4-C5-C6   | 6.98  | 120.49      | 117.00   |
| 27  | B8    | 1619 | G    | C5-C6-O6   | -6.98 | 124.41      | 128.60   |
| 27  | B8    | 2471 | A    | O4'-C1'-N9 | 6.98  | 113.78      | 108.20   |
| 27  | B8    | 327  | G    | C5-C6-O6   | -6.98 | 124.41      | 128.60   |
| 1   | AA    | 55   | A    | C4-C5-C6   | 6.98  | 120.49      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1255 | G    | O4'-C1'-N9 | 6.98  | 113.78      | 108.20   |
| 27  | B8    | 1163 | G    | C5-C6-O6   | -6.98 | 124.41      | 128.60   |
| 27  | B8    | 2049 | G    | C5-C6-O6   | -6.98 | 124.41      | 128.60   |
| 1   | AA    | 72   | A    | C4-C5-C6   | 6.98  | 120.49      | 117.00   |
| 27  | B8    | 1666 | G    | O4'-C1'-N9 | 6.98  | 113.78      | 108.20   |
| 27  | B8    | 1848 | A    | C4-C5-C6   | 6.98  | 120.49      | 117.00   |
| 27  | B8    | 648  | G    | C5-C6-O6   | -6.97 | 124.42      | 128.60   |
| 27  | B8    | 2148 | G    | C5-C6-O6   | -6.97 | 124.42      | 128.60   |
| 1   | AA    | 530  | G    | C5-C6-O6   | -6.97 | 124.42      | 128.60   |
| 1   | AA    | 402  | G    | O4'-C1'-N9 | 6.97  | 113.77      | 108.20   |
| 1   | AA    | 1200 | C    | N3-C4-N4   | 6.97  | 122.88      | 118.00   |
| 27  | B8    | 396  | G    | O4'-C1'-N9 | 6.97  | 113.77      | 108.20   |
| 27  | B8    | 525  | U    | O4'-C1'-N1 | 6.97  | 113.77      | 108.20   |
| 27  | B8    | 537  | G    | C5-C6-O6   | -6.97 | 124.42      | 128.60   |
| 27  | B8    | 2174 | C    | O4'-C1'-N1 | 6.97  | 113.77      | 108.20   |
| 1   | AA    | 710  | G    | O4'-C1'-N9 | 6.96  | 113.77      | 108.20   |
| 27  | B8    | 215  | G    | C5-C6-O6   | -6.96 | 124.42      | 128.60   |
| 27  | B8    | 1363 | C    | O4'-C1'-N1 | 6.96  | 113.77      | 108.20   |
| 1   | AA    | 265  | G    | N1-C6-O6   | 6.96  | 124.08      | 119.90   |
| 27  | B8    | 431  | U    | O4'-C1'-N1 | 6.96  | 113.77      | 108.20   |
| 27  | B8    | 397  | U    | O4'-C1'-N1 | 6.96  | 113.77      | 108.20   |
| 27  | B8    | 1029 | A    | C4-C5-C6   | 6.96  | 120.48      | 117.00   |
| 1   | AA    | 932  | C    | O4'-C1'-N1 | 6.96  | 113.77      | 108.20   |
| 27  | B8    | 407  | G    | O4'-C1'-N9 | 6.96  | 113.77      | 108.20   |
| 1   | AA    | 54   | C    | O4'-C1'-N1 | 6.96  | 113.77      | 108.20   |
| 1   | AA    | 491  | G    | O4'-C1'-N9 | 6.96  | 113.77      | 108.20   |
| 27  | B8    | 1147 | A    | O4'-C1'-N9 | 6.96  | 113.77      | 108.20   |
| 27  | B8    | 1733 | G    | C5-C6-O6   | -6.96 | 124.42      | 128.60   |
| 1   | AA    | 771  | G    | C5-C6-O6   | -6.96 | 124.43      | 128.60   |
| 1   | AA    | 1134 | G    | C5-C6-O6   | -6.96 | 124.43      | 128.60   |
| 27  | B8    | 1205 | A    | O4'-C1'-N9 | 6.96  | 113.77      | 108.20   |
| 27  | B8    | 1371 | G    | C5-C6-O6   | -6.96 | 124.43      | 128.60   |
| 27  | B8    | 1621 | U    | O4'-C1'-N1 | 6.96  | 113.77      | 108.20   |
| 27  | B8    | 2152 | G    | O4'-C1'-N9 | 6.96  | 113.77      | 108.20   |
| 27  | B8    | 2852 | G    | C5-C6-O6   | -6.96 | 124.43      | 128.60   |
| 1   | AA    | 1024 | G    | O4'-C1'-N9 | 6.96  | 113.76      | 108.20   |
| 27  | B8    | 506  | G    | C5-C6-O6   | -6.96 | 124.43      | 128.60   |
| 27  | B8    | 733  | G    | C5-C6-O6   | -6.96 | 124.43      | 128.60   |
| 26  | B7    | 77   | U    | O4'-C1'-N1 | 6.95  | 113.76      | 108.20   |
| 27  | B8    | 1056 | G    | C5-C6-O6   | -6.95 | 124.43      | 128.60   |
| 27  | B8    | 2297 | A    | C4-C5-C6   | 6.95  | 120.48      | 117.00   |
| 27  | B8    | 2484 | G    | O4'-C1'-N9 | 6.95  | 113.76      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2   | AX    | 18   | C    | O4'-C1'-N1 | 6.95  | 113.76      | 108.20   |
| 27  | B8    | 2111 | U    | O4'-C1'-N1 | 6.95  | 113.76      | 108.20   |
| 1   | AA    | 1400 | C    | O4'-C1'-N1 | 6.95  | 113.76      | 108.20   |
| 27  | B8    | 2493 | U    | O4'-C1'-N1 | 6.95  | 113.76      | 108.20   |
| 1   | AA    | 278  | G    | C5-C6-O6   | -6.95 | 124.43      | 128.60   |
| 27  | B8    | 551  | G    | C5-C6-O6   | -6.95 | 124.43      | 128.60   |
| 27  | B8    | 877  | A    | C5-C6-N1   | -6.95 | 114.22      | 117.70   |
| 27  | B8    | 1568 | G    | C5-C6-O6   | -6.95 | 124.43      | 128.60   |
| 27  | B8    | 2291 | U    | O4'-C1'-N1 | 6.95  | 113.76      | 108.20   |
| 27  | B8    | 2379 | G    | C5-C6-O6   | -6.95 | 124.43      | 128.60   |
| 27  | B8    | 2633 | G    | O4'-C1'-N9 | 6.95  | 113.76      | 108.20   |
| 1   | AA    | 729  | A    | O4'-C1'-N9 | 6.95  | 113.76      | 108.20   |
| 27  | B8    | 580  | U    | O4'-C1'-N1 | 6.95  | 113.76      | 108.20   |
| 1   | AA    | 1379 | G    | O4'-C1'-N9 | 6.94  | 113.75      | 108.20   |
| 3   | AV    | 30   | G    | C5-C6-O6   | -6.94 | 124.43      | 128.60   |
| 1   | AA    | 966  | G    | C5-C6-O6   | -6.94 | 124.44      | 128.60   |
| 1   | AA    | 1267 | C    | O4'-C1'-N1 | 6.94  | 113.75      | 108.20   |
| 27  | B8    | 2786 | U    | O4'-C1'-N1 | 6.94  | 113.75      | 108.20   |
| 1   | AA    | 1235 | U    | O4'-C1'-N1 | 6.94  | 113.75      | 108.20   |
| 1   | AA    | 46   | G    | O4'-C1'-N9 | 6.94  | 113.75      | 108.20   |
| 1   | AA    | 656  | G    | C5-C6-O6   | -6.94 | 124.44      | 128.60   |
| 1   | AA    | 1395 | C    | O4'-C1'-N1 | 6.94  | 113.75      | 108.20   |
| 27  | B8    | 794  | A    | C5-C6-N6   | -6.94 | 118.15      | 123.70   |
| 1   | AA    | 716  | A    | O4'-C1'-N9 | 6.94  | 113.75      | 108.20   |
| 27  | B8    | 519  | U    | O4'-C1'-N1 | 6.94  | 113.75      | 108.20   |
| 27  | B8    | 1866 | A    | C4-C5-C6   | 6.94  | 120.47      | 117.00   |
| 27  | B8    | 2361 | G    | O4'-C1'-N9 | 6.94  | 113.75      | 108.20   |
| 27  | B8    | 278  | A    | C4-C5-C6   | 6.93  | 120.47      | 117.00   |
| 27  | B8    | 2193 | G    | C5-C6-O6   | -6.93 | 124.44      | 128.60   |
| 27  | B8    | 2571 | U    | O4'-C1'-N1 | 6.93  | 113.75      | 108.20   |
| 27  | B8    | 2663 | G    | C5-C6-O6   | -6.93 | 124.44      | 128.60   |
| 1   | AA    | 175  | C    | N3-C4-N4   | 6.93  | 122.85      | 118.00   |
| 1   | AA    | 1468 | A    | O4'-C1'-N9 | 6.93  | 113.75      | 108.20   |
| 27  | B8    | 1473 | G    | C5-C6-O6   | -6.93 | 124.44      | 128.60   |
| 27  | B8    | 628  | G    | O4'-C1'-N9 | 6.93  | 113.75      | 108.20   |
| 27  | B8    | 2864 | G    | C5-C6-O6   | -6.93 | 124.44      | 128.60   |
| 27  | B8    | 471  | A    | C4-C5-C6   | 6.93  | 120.46      | 117.00   |
| 27  | B8    | 780  | G    | C5-C6-O6   | -6.93 | 124.44      | 128.60   |
| 27  | B8    | 928  | A    | C5-C6-N6   | -6.93 | 118.16      | 123.70   |
| 27  | B8    | 1750 | G    | C5-C6-O6   | -6.93 | 124.44      | 128.60   |
| 27  | B8    | 2077 | A    | C4-C5-C6   | 6.93  | 120.47      | 117.00   |
| 1   | AA    | 703  | G    | C5-C6-O6   | -6.93 | 124.44      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1177 | G    | C5-C6-O6   | -6.93 | 124.44      | 128.60   |
| 1   | AA    | 563  | A    | C4-C5-C6   | 6.93  | 120.46      | 117.00   |
| 27  | B8    | 494  | G    | C5-C6-O6   | -6.93 | 124.44      | 128.60   |
| 27  | B8    | 2834 | G    | C5-C6-O6   | -6.93 | 124.44      | 128.60   |
| 1   | AA    | 71   | A    | C5-C6-N6   | -6.92 | 118.16      | 123.70   |
| 1   | AA    | 796  | C    | O4'-C1'-N1 | 6.92  | 113.74      | 108.20   |
| 1   | AA    | 1139 | G    | C5-C6-O6   | -6.92 | 124.45      | 128.60   |
| 1   | AA    | 1438 | G    | C5-C6-O6   | -6.92 | 124.44      | 128.60   |
| 27  | B8    | 286  | U    | O4'-C1'-N1 | 6.92  | 113.74      | 108.20   |
| 27  | B8    | 1753 | G    | C5-C6-O6   | -6.92 | 124.44      | 128.60   |
| 27  | B8    | 1903 | G    | C5-C6-O6   | -6.92 | 124.44      | 128.60   |
| 1   | AA    | 603  | U    | O4'-C1'-N1 | 6.92  | 113.74      | 108.20   |
| 1   | AA    | 1088 | G    | C5-C6-O6   | -6.92 | 124.45      | 128.60   |
| 1   | AA    | 1241 | G    | O4'-C1'-N9 | 6.92  | 113.74      | 108.20   |
| 1   | AA    | 310  | G    | C5-C6-O6   | -6.92 | 124.45      | 128.60   |
| 27  | B8    | 2157 | G    | C5-C6-O6   | -6.92 | 124.45      | 128.60   |
| 27  | B8    | 2371 | G    | C5-C6-O6   | -6.92 | 124.45      | 128.60   |
| 27  | B8    | 474  | G    | C5-C6-O6   | -6.92 | 124.45      | 128.60   |
| 27  | B8    | 1322 | A    | O4'-C1'-N9 | 6.92  | 113.74      | 108.20   |
| 27  | B8    | 1814 | G    | C5-C6-O6   | -6.92 | 124.45      | 128.60   |
| 27  | B8    | 2178 | C    | C2-N1-C1'  | 6.92  | 126.41      | 118.80   |
| 1   | AA    | 721  | G    | C5-C6-O6   | -6.92 | 124.45      | 128.60   |
| 26  | B7    | 100  | G    | C5-C6-O6   | -6.92 | 124.45      | 128.60   |
| 27  | B8    | 373  | U    | O4'-C1'-N1 | 6.92  | 113.73      | 108.20   |
| 27  | B8    | 1816 | C    | C6-N1-C1'  | -6.92 | 112.50      | 120.80   |
| 27  | B8    | 2499 | C    | O4'-C1'-N1 | 6.92  | 113.73      | 108.20   |
| 27  | B8    | 2770 | G    | C5-C6-O6   | -6.92 | 124.45      | 128.60   |
| 27  | B8    | 667  | U    | O4'-C1'-N1 | 6.92  | 113.73      | 108.20   |
| 27  | B8    | 1425 | G    | C5-C6-O6   | -6.92 | 124.45      | 128.60   |
| 27  | B8    | 2161 | C    | O4'-C1'-N1 | 6.92  | 113.73      | 108.20   |
| 1   | AA    | 91   | U    | O4'-C1'-N1 | 6.91  | 113.73      | 108.20   |
| 27  | B8    | 889  | C    | O4'-C1'-N1 | 6.91  | 113.73      | 108.20   |
| 27  | B8    | 1178 | C    | O4'-C1'-N1 | 6.91  | 113.73      | 108.20   |
| 27  | B8    | 2570 | G    | C5-C6-O6   | -6.91 | 124.45      | 128.60   |
| 1   | AA    | 194  | C    | O4'-C1'-N1 | 6.91  | 113.73      | 108.20   |
| 27  | B8    | 1133 | A    | P-O3'-C3'  | 6.91  | 127.99      | 119.70   |
| 27  | B8    | 1369 | G    | C5-C6-O6   | -6.91 | 124.45      | 128.60   |
| 27  | B8    | 51   | G    | C5-C6-O6   | -6.91 | 124.45      | 128.60   |
| 27  | B8    | 1516 | G    | O4'-C1'-N9 | 6.91  | 113.73      | 108.20   |
| 27  | B8    | 1763 | G    | C5-C6-O6   | -6.91 | 124.45      | 128.60   |
| 27  | B8    | 1841 | U    | O4'-C1'-N1 | 6.91  | 113.73      | 108.20   |
| 27  | B8    | 2135 | A    | O4'-C1'-N9 | 6.91  | 113.73      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1156 | G    | C5-C6-O6   | -6.91 | 124.45      | 128.60   |
| 1   | AA    | 1492 | A    | C5-C6-N6   | -6.91 | 118.17      | 123.70   |
| 26  | B7    | 7    | G    | O4'-C1'-N9 | 6.91  | 113.73      | 108.20   |
| 27  | B8    | 191  | A    | C4-C5-C6   | 6.91  | 120.45      | 117.00   |
| 27  | B8    | 586  | A    | N1-C6-N6   | 6.91  | 122.75      | 118.60   |
| 27  | B8    | 2372 | U    | O4'-C1'-N1 | 6.91  | 113.73      | 108.20   |
| 27  | B8    | 1361 | G    | C5-C6-O6   | -6.91 | 124.46      | 128.60   |
| 27  | B8    | 1851 | U    | O4'-C1'-N1 | 6.90  | 113.72      | 108.20   |
| 1   | AA    | 384  | G    | C5-C6-O6   | -6.90 | 124.46      | 128.60   |
| 1   | AA    | 601  | G    | O4'-C1'-N9 | 6.90  | 113.72      | 108.20   |
| 1   | AA    | 753  | A    | C4-C5-C6   | 6.90  | 120.45      | 117.00   |
| 1   | AA    | 860  | A    | O4'-C1'-N9 | 6.90  | 113.72      | 108.20   |
| 1   | AA    | 1473 | G    | C5-C6-O6   | -6.90 | 124.46      | 128.60   |
| 27  | B8    | 2429 | G    | C5-C6-O6   | -6.90 | 124.46      | 128.60   |
| 27  | B8    | 2662 | A    | C4-C5-C6   | 6.90  | 120.45      | 117.00   |
| 27  | B8    | 904  | G    | C5-C6-O6   | -6.90 | 124.46      | 128.60   |
| 27  | B8    | 1355 | G    | O4'-C1'-N9 | 6.90  | 113.72      | 108.20   |
| 27  | B8    | 2697 | G    | O4'-C1'-N9 | 6.90  | 113.72      | 108.20   |
| 1   | AA    | 287  | U    | O4'-C1'-N1 | 6.90  | 113.72      | 108.20   |
| 1   | AA    | 988  | G    | C5-C6-O6   | -6.90 | 124.46      | 128.60   |
| 1   | AA    | 1185 | G    | C5-C6-O6   | -6.90 | 124.46      | 128.60   |
| 27  | B8    | 214  | G    | O4'-C1'-N9 | 6.90  | 113.72      | 108.20   |
| 27  | B8    | 1168 | G    | C5-C6-O6   | -6.90 | 124.46      | 128.60   |
| 1   | AA    | 568  | G    | C5-C6-O6   | -6.90 | 124.46      | 128.60   |
| 27  | B8    | 1400 | U    | O4'-C1'-N1 | 6.90  | 113.72      | 108.20   |
| 27  | B8    | 515  | A    | O4'-C1'-N9 | 6.89  | 113.72      | 108.20   |
| 27  | B8    | 545  | U    | O4'-C1'-N1 | 6.89  | 113.72      | 108.20   |
| 27  | B8    | 1776 | G    | C5-C6-O6   | -6.89 | 124.46      | 128.60   |
| 1   | AA    | 714  | G    | C5-C6-O6   | -6.89 | 124.47      | 128.60   |
| 26  | B7    | 96   | G    | O4'-C1'-N9 | 6.89  | 113.71      | 108.20   |
| 27  | B8    | 15   | G    | C5-C6-O6   | -6.89 | 124.46      | 128.60   |
| 27  | B8    | 1831 | G    | O4'-C1'-N9 | 6.89  | 113.72      | 108.20   |
| 27  | B8    | 2374 | C    | O4'-C1'-N1 | 6.89  | 113.71      | 108.20   |
| 27  | B8    | 389  | G    | C5-C6-O6   | -6.89 | 124.47      | 128.60   |
| 27  | B8    | 2031 | A    | O4'-C1'-N9 | 6.89  | 113.71      | 108.20   |
| 1   | AA    | 683  | G    | O4'-C1'-N9 | 6.89  | 113.71      | 108.20   |
| 27  | B8    | 158  | U    | O4'-C1'-N1 | 6.89  | 113.71      | 108.20   |
| 27  | B8    | 718  | A    | C5-C6-N6   | -6.89 | 118.19      | 123.70   |
| 27  | B8    | 2162 | G    | C5-C6-O6   | -6.89 | 124.47      | 128.60   |
| 27  | B8    | 2302 | U    | O4'-C1'-N1 | 6.89  | 113.71      | 108.20   |
| 27  | B8    | 1830 | C    | N3-C4-N4   | 6.89  | 122.82      | 118.00   |
| 27  | B8    | 651  | G    | C5-C6-O6   | -6.89 | 124.47      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | B8    | 1958 | C    | O4'-C1'-N1  | 6.89  | 113.71      | 108.20   |
| 1   | AA    | 151  | A    | C4-C5-C6    | 6.88  | 120.44      | 117.00   |
| 27  | B8    | 1721 | G    | C5-C6-O6    | -6.88 | 124.47      | 128.60   |
| 1   | AA    | 1322 | C    | C2-N1-C1'   | 6.88  | 126.37      | 118.80   |
| 27  | B8    | 1143 | A    | O4'-C1'-N9  | 6.88  | 113.71      | 108.20   |
| 27  | B8    | 2751 | G    | C5-C6-O6    | -6.88 | 124.47      | 128.60   |
| 27  | B8    | 2763 | G    | C5-C6-O6    | -6.88 | 124.47      | 128.60   |
| 1   | AA    | 618  | C    | O4'-C1'-N1  | 6.88  | 113.71      | 108.20   |
| 1   | AA    | 1310 | G    | O4'-C1'-N9  | 6.88  | 113.70      | 108.20   |
| 27  | B8    | 268  | C    | N3-C4-N4    | 6.88  | 122.82      | 118.00   |
| 27  | B8    | 2016 | U    | O4'-C1'-N1  | 6.88  | 113.71      | 108.20   |
| 27  | B8    | 2340 | A    | O4'-C1'-N9  | 6.88  | 113.71      | 108.20   |
| 27  | B8    | 2900 | A    | O4'-C1'-N9  | 6.88  | 113.71      | 108.20   |
| 1   | AA    | 1512 | U    | O4'-C1'-N1  | 6.88  | 113.70      | 108.20   |
| 27  | B8    | 727  | A    | O4'-C1'-N9  | 6.88  | 113.70      | 108.20   |
| 27  | B8    | 1789 | A    | C4-C5-C6    | 6.88  | 120.44      | 117.00   |
| 1   | AA    | 1505 | G    | C5-C6-O6    | -6.88 | 124.47      | 128.60   |
| 1   | AA    | 1529 | G    | C5'-C4'-O4' | 6.88  | 117.35      | 109.10   |
| 1   | AA    | 430  | A    | N1-C6-N6    | 6.88  | 122.73      | 118.60   |
| 1   | AA    | 1137 | C    | O4'-C1'-N1  | 6.88  | 113.70      | 108.20   |
| 1   | AA    | 1368 | A    | O4'-C1'-N9  | 6.88  | 113.70      | 108.20   |
| 27  | B8    | 169  | G    | O4'-C1'-N9  | 6.88  | 113.70      | 108.20   |
| 27  | B8    | 1888 | G    | C5-C6-O6    | -6.88 | 124.47      | 128.60   |
| 27  | B8    | 2116 | G    | C5-C6-O6    | -6.88 | 124.47      | 128.60   |
| 1   | AA    | 903  | G    | O4'-C1'-N9  | 6.88  | 113.70      | 108.20   |
| 27  | B8    | 353  | C    | O4'-C1'-N1  | 6.88  | 113.70      | 108.20   |
| 27  | B8    | 2163 | A    | C4-C5-C6    | 6.88  | 120.44      | 117.00   |
| 1   | AA    | 340  | U    | O4'-C1'-N1  | 6.87  | 113.70      | 108.20   |
| 1   | AA    | 673  | A    | C4-C5-C6    | 6.87  | 120.44      | 117.00   |
| 1   | AA    | 1108 | G    | C5-C6-O6    | -6.87 | 124.47      | 128.60   |
| 27  | B8    | 251  | A    | C4-C5-C6    | 6.87  | 120.44      | 117.00   |
| 27  | B8    | 1777 | U    | O4'-C1'-N1  | 6.87  | 113.70      | 108.20   |
| 27  | B8    | 2159 | G    | C5-C6-O6    | -6.87 | 124.48      | 128.60   |
| 27  | B8    | 2181 | U    | O4'-C1'-N1  | 6.87  | 113.70      | 108.20   |
| 27  | B8    | 67   | U    | O4'-C1'-N1  | 6.87  | 113.70      | 108.20   |
| 27  | B8    | 411  | G    | C5-C6-O6    | -6.87 | 124.48      | 128.60   |
| 27  | B8    | 604  | G    | C5-C6-O6    | -6.87 | 124.48      | 128.60   |
| 27  | B8    | 1730 | C    | O4'-C1'-N1  | 6.87  | 113.70      | 108.20   |
| 27  | B8    | 2721 | A    | O4'-C1'-N9  | 6.87  | 113.70      | 108.20   |
| 27  | B8    | 1600 | C    | O4'-C1'-N1  | 6.87  | 113.70      | 108.20   |
| 27  | B8    | 1757 | A    | O4'-C1'-N9  | 6.87  | 113.70      | 108.20   |
| 1   | AA    | 558  | G    | C5-C6-O6    | -6.87 | 124.48      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1000 | A    | O4'-C1'-N9 | 6.87  | 113.69      | 108.20   |
| 27  | B8    | 2811 | G    | C5-C6-O6   | -6.87 | 124.48      | 128.60   |
| 1   | AA    | 71   | A    | O4'-C1'-N9 | 6.87  | 113.69      | 108.20   |
| 1   | AA    | 346  | G    | C5-C6-O6   | -6.87 | 124.48      | 128.60   |
| 1   | AA    | 464  | U    | O4'-C1'-N1 | 6.87  | 113.69      | 108.20   |
| 1   | AA    | 803  | G    | C5-C6-O6   | -6.87 | 124.48      | 128.60   |
| 1   | AA    | 824  | G    | O4'-C1'-N9 | 6.87  | 113.69      | 108.20   |
| 27  | B8    | 544  | C    | O4'-C1'-N1 | 6.87  | 113.69      | 108.20   |
| 27  | B8    | 2615 | U    | O4'-C1'-N1 | 6.87  | 113.69      | 108.20   |
| 27  | B8    | 2734 | A    | C5-C6-N6   | -6.87 | 118.21      | 123.70   |
| 1   | AA    | 220  | G    | C5-C6-O6   | -6.86 | 124.48      | 128.60   |
| 1   | AA    | 1294 | G    | C5-C6-O6   | -6.86 | 124.48      | 128.60   |
| 27  | B8    | 2587 | A    | C4-C5-C6   | 6.86  | 120.43      | 117.00   |
| 27  | B8    | 2871 | U    | O4'-C1'-N1 | 6.86  | 113.69      | 108.20   |
| 1   | AA    | 1044 | A    | C5-C6-N6   | -6.86 | 118.21      | 123.70   |
| 3   | AV    | 36   | G    | C5-C6-O6   | -6.86 | 124.48      | 128.60   |
| 27  | B8    | 75   | G    | C5-C6-O6   | -6.86 | 124.48      | 128.60   |
| 27  | B8    | 330  | A    | C5-C6-N6   | -6.86 | 118.21      | 123.70   |
| 27  | B8    | 625  | G    | C5-C6-O6   | -6.86 | 124.48      | 128.60   |
| 1   | AA    | 593  | U    | O4'-C1'-N1 | 6.86  | 113.69      | 108.20   |
| 27  | B8    | 917  | A    | C4-C5-C6   | 6.86  | 120.43      | 117.00   |
| 27  | B8    | 1198 | U    | O4'-C1'-N1 | 6.86  | 113.69      | 108.20   |
| 27  | B8    | 2097 | A    | O4'-C1'-N9 | 6.86  | 113.69      | 108.20   |
| 1   | AA    | 95   | C    | O4'-C1'-N1 | 6.86  | 113.69      | 108.20   |
| 27  | B8    | 824  | U    | O4'-C1'-N1 | 6.86  | 113.69      | 108.20   |
| 27  | B8    | 1551 | A    | O4'-C1'-N9 | 6.86  | 113.69      | 108.20   |
| 27  | B8    | 2139 | U    | O4'-C1'-N1 | 6.86  | 113.69      | 108.20   |
| 27  | B8    | 2728 | U    | O4'-C1'-N1 | 6.86  | 113.69      | 108.20   |
| 1   | AA    | 174  | A    | C5-C6-N6   | -6.86 | 118.22      | 123.70   |
| 27  | B8    | 1782 | U    | O4'-C1'-N1 | 6.86  | 113.68      | 108.20   |
| 27  | B8    | 2601 | C    | N3-C4-N4   | 6.86  | 122.80      | 118.00   |
| 1   | AA    | 116  | A    | C4-C5-C6   | 6.85  | 120.43      | 117.00   |
| 1   | AA    | 610  | U    | C2-N1-C1'  | 6.85  | 125.92      | 117.70   |
| 1   | AA    | 935  | A    | C4-C5-C6   | 6.85  | 120.43      | 117.00   |
| 27  | B8    | 912  | C    | O4'-C1'-N1 | 6.85  | 113.68      | 108.20   |
| 27  | B8    | 2217 | G    | O4'-C1'-N9 | 6.85  | 113.68      | 108.20   |
| 27  | B8    | 2532 | G    | C5-C6-O6   | -6.85 | 124.49      | 128.60   |
| 27  | B8    | 2575 | C    | O4'-C1'-N1 | 6.85  | 113.68      | 108.20   |
| 27  | B8    | 2825 | G    | C5-C6-O6   | -6.85 | 124.49      | 128.60   |
| 27  | B8    | 48   | G    | C5-C6-O6   | -6.85 | 124.49      | 128.60   |
| 27  | B8    | 1598 | A    | C5-C6-N6   | -6.85 | 118.22      | 123.70   |
| 1   | AA    | 1115 | U    | O4'-C1'-N1 | 6.85  | 113.68      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 242  | G    | O4'-C1'-N9 | 6.85  | 113.68      | 108.20   |
| 27  | B8    | 744  | U    | O4'-C1'-N1 | 6.85  | 113.68      | 108.20   |
| 27  | B8    | 1556 | C    | O4'-C1'-N1 | 6.85  | 113.68      | 108.20   |
| 27  | B8    | 1603 | A    | C5-C6-N6   | -6.85 | 118.22      | 123.70   |
| 27  | B8    | 2129 | C    | O4'-C1'-N1 | 6.85  | 113.68      | 108.20   |
| 1   | AA    | 924  | C    | N3-C4-N4   | 6.85  | 122.79      | 118.00   |
| 1   | AA    | 1294 | G    | O4'-C1'-N9 | 6.85  | 113.68      | 108.20   |
| 27  | B8    | 340  | A    | C4-C5-C6   | 6.85  | 120.42      | 117.00   |
| 27  | B8    | 1369 | G    | O4'-C1'-N9 | 6.85  | 113.68      | 108.20   |
| 27  | B8    | 2438 | U    | O4'-C1'-N1 | 6.85  | 113.68      | 108.20   |
| 1   | AA    | 591  | U    | O4'-C1'-N1 | 6.85  | 113.68      | 108.20   |
| 27  | B8    | 1984 | G    | O4'-C1'-N9 | 6.85  | 113.68      | 108.20   |
| 1   | AA    | 1453 | G    | C5-C6-O6   | -6.84 | 124.49      | 128.60   |
| 27  | B8    | 489  | G    | C5-C6-O6   | -6.84 | 124.49      | 128.60   |
| 27  | B8    | 971  | G    | C5-C6-O6   | -6.84 | 124.49      | 128.60   |
| 27  | B8    | 1539 | U    | O4'-C1'-N1 | 6.84  | 113.67      | 108.20   |
| 27  | B8    | 277  | G    | C5-C6-O6   | -6.84 | 124.49      | 128.60   |
| 27  | B8    | 704  | G    | C5-C6-O6   | -6.84 | 124.49      | 128.60   |
| 1   | AA    | 437  | U    | O4'-C1'-N1 | 6.84  | 113.67      | 108.20   |
| 26  | B7    | 24   | G    | C5-C6-O6   | -6.84 | 124.50      | 128.60   |
| 26  | B7    | 33   | G    | O4'-C1'-N9 | 6.84  | 113.67      | 108.20   |
| 27  | B8    | 2025 | C    | O4'-C1'-N1 | 6.84  | 113.67      | 108.20   |
| 27  | B8    | 2067 | G    | C5-C6-O6   | -6.84 | 124.50      | 128.60   |
| 1   | AA    | 107  | G    | C5-C6-O6   | -6.84 | 124.50      | 128.60   |
| 1   | AA    | 710  | G    | C5-C6-O6   | -6.84 | 124.50      | 128.60   |
| 1   | AA    | 1489 | G    | C5-C6-O6   | -6.84 | 124.50      | 128.60   |
| 1   | AA    | 1003 | G    | C5-C6-O6   | -6.84 | 124.50      | 128.60   |
| 1   | AA    | 1177 | G    | C5-C6-O6   | -6.84 | 124.50      | 128.60   |
| 27  | B8    | 356  | G    | C5-C6-O6   | -6.84 | 124.50      | 128.60   |
| 27  | B8    | 1120 | G    | O4'-C1'-N9 | 6.84  | 113.67      | 108.20   |
| 27  | B8    | 2253 | G    | C5-C6-O6   | -6.84 | 124.50      | 128.60   |
| 1   | AA    | 1131 | G    | O4'-C1'-N9 | 6.84  | 113.67      | 108.20   |
| 27  | B8    | 2280 | G    | C5-C6-O6   | -6.84 | 124.50      | 128.60   |
| 27  | B8    | 2604 | U    | O4'-C1'-N1 | 6.84  | 113.67      | 108.20   |
| 1   | AA    | 606  | G    | C5-C6-O6   | -6.83 | 124.50      | 128.60   |
| 27  | B8    | 221  | A    | C4-C5-C6   | 6.83  | 120.42      | 117.00   |
| 27  | B8    | 367  | G    | C5-C6-O6   | -6.83 | 124.50      | 128.60   |
| 1   | AA    | 528  | C    | O4'-C1'-N1 | 6.83  | 113.67      | 108.20   |
| 1   | AA    | 1046 | A    | O4'-C1'-N9 | 6.83  | 113.67      | 108.20   |
| 27  | B8    | 178  | G    | O4'-C1'-N9 | 6.83  | 113.67      | 108.20   |
| 27  | B8    | 190  | A    | C4-C5-C6   | 6.83  | 120.42      | 117.00   |
| 27  | B8    | 279  | A    | C4-C5-C6   | 6.83  | 120.42      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 939  | G    | O4'-C1'-N9 | 6.83  | 113.67      | 108.20   |
| 1   | AA    | 2    | A    | O4'-C1'-N9 | 6.83  | 113.67      | 108.20   |
| 27  | B8    | 1915 | U    | O4'-C1'-N1 | 6.83  | 113.67      | 108.20   |
| 27  | B8    | 2479 | U    | O4'-C1'-N1 | 6.83  | 113.67      | 108.20   |
| 1   | AA    | 20   | U    | O4'-C1'-N1 | 6.83  | 113.66      | 108.20   |
| 27  | B8    | 303  | G    | O4'-C1'-N9 | 6.83  | 113.66      | 108.20   |
| 27  | B8    | 787  | C    | N3-C4-N4   | 6.83  | 122.78      | 118.00   |
| 27  | B8    | 1277 | G    | C5-C6-O6   | -6.83 | 124.50      | 128.60   |
| 1   | AA    | 67   | C    | O4'-C1'-N1 | 6.83  | 113.66      | 108.20   |
| 1   | AA    | 690  | G    | C5-C6-O6   | -6.83 | 124.50      | 128.60   |
| 27  | B8    | 971  | G    | O4'-C1'-N9 | 6.83  | 113.66      | 108.20   |
| 1   | AA    | 420  | U    | O4'-C1'-N1 | 6.83  | 113.66      | 108.20   |
| 1   | AA    | 730  | G    | O4'-C1'-N9 | 6.83  | 113.66      | 108.20   |
| 27  | B8    | 1027 | A    | C4-C5-C6   | 6.83  | 120.41      | 117.00   |
| 27  | B8    | 2110 | G    | O4'-C1'-N9 | 6.83  | 113.66      | 108.20   |
| 1   | AA    | 976  | G    | C5-C6-O6   | -6.82 | 124.50      | 128.60   |
| 27  | B8    | 12   | U    | O4'-C1'-N1 | 6.82  | 113.66      | 108.20   |
| 27  | B8    | 669  | G    | C5-C6-O6   | -6.82 | 124.51      | 128.60   |
| 27  | B8    | 1464 | G    | C5-C6-O6   | -6.82 | 124.51      | 128.60   |
| 27  | B8    | 1853 | A    | O4'-C1'-N9 | 6.82  | 113.66      | 108.20   |
| 27  | B8    | 2018 | G    | C5-C6-O6   | -6.82 | 124.51      | 128.60   |
| 27  | B8    | 2242 | G    | O4'-C1'-N9 | 6.82  | 113.66      | 108.20   |
| 27  | B8    | 2271 | G    | C5-C6-O6   | -6.82 | 124.51      | 128.60   |
| 27  | B8    | 2813 | A    | O4'-C1'-N9 | 6.82  | 113.66      | 108.20   |
| 1   | AA    | 589  | U    | O4'-C1'-N1 | 6.82  | 113.66      | 108.20   |
| 27  | B8    | 2867 | G    | C5-C6-O6   | -6.82 | 124.51      | 128.60   |
| 27  | B8    | 1104 | C    | N3-C4-N4   | 6.82  | 122.78      | 118.00   |
| 27  | B8    | 2249 | U    | O4'-C1'-N1 | 6.82  | 113.66      | 108.20   |
| 27  | B8    | 2789 | C    | N3-C4-N4   | 6.82  | 122.77      | 118.00   |
| 1   | AA    | 350  | G    | C5-C6-O6   | -6.82 | 124.51      | 128.60   |
| 27  | B8    | 1807 | G    | C5-C6-O6   | -6.82 | 124.51      | 128.60   |
| 27  | B8    | 1968 | G    | C5-C6-O6   | -6.82 | 124.51      | 128.60   |
| 3   | AV    | 53   | G    | C5-C6-O6   | -6.82 | 124.51      | 128.60   |
| 27  | B8    | 1110 | G    | C5-C6-O6   | -6.82 | 124.51      | 128.60   |
| 27  | B8    | 1989 | G    | C5-C6-O6   | -6.82 | 124.51      | 128.60   |
| 27  | B8    | 2255 | G    | C5-C6-O6   | -6.82 | 124.51      | 128.60   |
| 27  | B8    | 2163 | A    | C5-C6-N6   | -6.81 | 118.25      | 123.70   |
| 27  | B8    | 2769 | U    | O4'-C1'-N1 | 6.81  | 113.65      | 108.20   |
| 1   | AA    | 761  | G    | C5-C6-O6   | -6.81 | 124.51      | 128.60   |
| 3   | AV    | 38   | G    | N1-C6-O6   | 6.81  | 123.99      | 119.90   |
| 26  | B7    | 55   | U    | O4'-C1'-N1 | 6.81  | 113.65      | 108.20   |
| 27  | B8    | 39   | G    | C5-C6-O6   | -6.81 | 124.51      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 596  | U    | O4'-C1'-N1 | 6.81  | 113.65      | 108.20   |
| 27  | B8    | 1149 | G    | O4'-C1'-N9 | 6.81  | 113.65      | 108.20   |
| 27  | B8    | 1407 | G    | C5-C6-O6   | -6.81 | 124.51      | 128.60   |
| 27  | B8    | 2847 | U    | O4'-C1'-N1 | 6.81  | 113.65      | 108.20   |
| 1   | AA    | 1111 | A    | C5-C6-N6   | -6.81 | 118.25      | 123.70   |
| 27  | B8    | 2169 | A    | O4'-C1'-N9 | 6.81  | 113.65      | 108.20   |
| 1   | AA    | 257  | G    | C5-C6-O6   | -6.81 | 124.51      | 128.60   |
| 1   | AA    | 1016 | A    | C5-C6-N1   | -6.81 | 114.30      | 117.70   |
| 27  | B8    | 376  | G    | C5-C6-O6   | -6.81 | 124.52      | 128.60   |
| 27  | B8    | 555  | G    | C5-C6-O6   | -6.81 | 124.51      | 128.60   |
| 27  | B8    | 1364 | G    | C5-C6-O6   | -6.81 | 124.51      | 128.60   |
| 1   | AA    | 814  | A    | C5-C6-N6   | -6.81 | 118.25      | 123.70   |
| 1   | AA    | 1379 | G    | C5-C6-O6   | -6.81 | 124.52      | 128.60   |
| 27  | B8    | 98   | G    | C5-C6-O6   | -6.81 | 124.52      | 128.60   |
| 27  | B8    | 859  | G    | C5-C6-O6   | -6.81 | 124.52      | 128.60   |
| 27  | B8    | 1112 | G    | C5-C6-O6   | -6.81 | 124.52      | 128.60   |
| 27  | B8    | 1217 | U    | O4'-C1'-N1 | 6.81  | 113.65      | 108.20   |
| 27  | B8    | 1333 | G    | C5-C6-O6   | -6.81 | 124.52      | 128.60   |
| 27  | B8    | 1452 | G    | C5-C6-O6   | -6.81 | 124.52      | 128.60   |
| 27  | B8    | 2168 | G    | C5-C6-O6   | -6.81 | 124.52      | 128.60   |
| 27  | B8    | 2661 | G    | O4'-C1'-N9 | 6.81  | 113.65      | 108.20   |
| 27  | B8    | 2898 | U    | O4'-C1'-N1 | 6.81  | 113.64      | 108.20   |
| 1   | AA    | 479  | U    | O4'-C1'-N1 | 6.81  | 113.64      | 108.20   |
| 27  | B8    | 1354 | A    | C4-C5-C6   | 6.81  | 120.40      | 117.00   |
| 27  | B8    | 2120 | G    | C5-C6-O6   | -6.81 | 124.52      | 128.60   |
| 1   | AA    | 229  | U    | O4'-C1'-N1 | 6.80  | 113.64      | 108.20   |
| 1   | AA    | 296  | U    | O4'-C1'-N1 | 6.80  | 113.64      | 108.20   |
| 3   | AV    | 73   | G    | C5-C6-O6   | -6.80 | 124.52      | 128.60   |
| 27  | B8    | 595  | C    | O4'-C1'-N1 | 6.80  | 113.64      | 108.20   |
| 27  | B8    | 1481 | U    | O4'-C1'-N1 | 6.80  | 113.64      | 108.20   |
| 27  | B8    | 1552 | A    | C4-C5-C6   | 6.80  | 120.40      | 117.00   |
| 27  | B8    | 1883 | U    | O4'-C1'-N1 | 6.80  | 113.64      | 108.20   |
| 27  | B8    | 2607 | G    | C5-C6-O6   | -6.80 | 124.52      | 128.60   |
| 27  | B8    | 2784 | U    | O4'-C1'-N1 | 6.80  | 113.64      | 108.20   |
| 1   | AA    | 250  | A    | O4'-C1'-N9 | 6.80  | 113.64      | 108.20   |
| 3   | AV    | 43   | G    | C5-C6-O6   | -6.80 | 124.52      | 128.60   |
| 27  | B8    | 2348 | U    | O4'-C1'-N1 | 6.80  | 113.64      | 108.20   |
| 1   | AA    | 41   | G    | O4'-C1'-N9 | 6.80  | 113.64      | 108.20   |
| 1   | AA    | 844  | G    | C5-C6-O6   | -6.80 | 124.52      | 128.60   |
| 1   | AA    | 1403 | C    | N3-C4-N4   | 6.80  | 122.76      | 118.00   |
| 27  | B8    | 1212 | G    | C5-C6-O6   | -6.80 | 124.52      | 128.60   |
| 27  | B8    | 1710 | G    | C5-C6-O6   | -6.80 | 124.52      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1794 | A    | O4'-C1'-N9 | 6.80  | 113.64      | 108.20   |
| 27  | B8    | 1884 | G    | C5-C6-O6   | -6.80 | 124.52      | 128.60   |
| 27  | B8    | 772  | C    | O4'-C1'-N1 | 6.80  | 113.64      | 108.20   |
| 27  | B8    | 1684 | G    | O4'-C1'-N9 | 6.80  | 113.64      | 108.20   |
| 27  | B8    | 2644 | G    | C5-C6-O6   | -6.80 | 124.52      | 128.60   |
| 27  | B8    | 2848 | G    | C5-C6-O6   | -6.80 | 124.52      | 128.60   |
| 1   | AA    | 319  | G    | O4'-C1'-N9 | 6.80  | 113.64      | 108.20   |
| 1   | AA    | 1036 | A    | C4-C5-C6   | 6.80  | 120.40      | 117.00   |
| 27  | B8    | 512  | G    | C5-C6-O6   | -6.80 | 124.52      | 128.60   |
| 27  | B8    | 1025 | G    | C5-C6-O6   | -6.80 | 124.52      | 128.60   |
| 27  | B8    | 1598 | A    | C4-C5-C6   | 6.80  | 120.40      | 117.00   |
| 27  | B8    | 1784 | A    | P-O3'-C3'  | 6.80  | 127.86      | 119.70   |
| 27  | B8    | 2868 | A    | C4-C5-C6   | 6.80  | 120.40      | 117.00   |
| 27  | B8    | 911  | A    | C5-C6-N6   | -6.79 | 118.26      | 123.70   |
| 1   | AA    | 362  | G    | C5-C6-O6   | -6.79 | 124.52      | 128.60   |
| 1   | AA    | 1231 | G    | O4'-C1'-N9 | 6.79  | 113.64      | 108.20   |
| 27  | B8    | 462  | C    | O4'-C1'-N1 | 6.79  | 113.64      | 108.20   |
| 27  | B8    | 775  | G    | C5-C6-O6   | -6.79 | 124.52      | 128.60   |
| 27  | B8    | 1461 | C    | O4'-C1'-N1 | 6.79  | 113.63      | 108.20   |
| 1   | AA    | 1260 | G    | C5-C6-O6   | -6.79 | 124.53      | 128.60   |
| 27  | B8    | 1138 | G    | C5-C6-O6   | -6.79 | 124.53      | 128.60   |
| 27  | B8    | 1420 | A    | O4'-C1'-N9 | 6.79  | 113.63      | 108.20   |
| 1   | AA    | 850  | U    | O4'-C1'-N1 | 6.79  | 113.63      | 108.20   |
| 1   | AA    | 1330 | U    | O4'-C1'-N1 | 6.79  | 113.63      | 108.20   |
| 27  | B8    | 1743 | G    | N3-C2-N2   | 6.79  | 124.65      | 119.90   |
| 27  | B8    | 2214 | C    | N3-C4-N4   | 6.79  | 122.75      | 118.00   |
| 1   | AA    | 1401 | G    | O4'-C1'-N9 | 6.79  | 113.63      | 108.20   |
| 27  | B8    | 2144 | G    | C5-C6-O6   | -6.79 | 124.53      | 128.60   |
| 1   | AA    | 380  | G    | C5-C6-O6   | -6.79 | 124.53      | 128.60   |
| 1   | AA    | 1436 | U    | O4'-C1'-N1 | 6.79  | 113.63      | 108.20   |
| 1   | AA    | 1273 | C    | N3-C4-N4   | 6.79  | 122.75      | 118.00   |
| 27  | B8    | 199  | A    | C5-C6-N6   | -6.79 | 118.27      | 123.70   |
| 27  | B8    | 313  | G    | C5-C6-O6   | -6.79 | 124.53      | 128.60   |
| 27  | B8    | 1681 | G    | C5-C6-O6   | -6.79 | 124.53      | 128.60   |
| 27  | B8    | 1745 | A    | C5-C6-N6   | -6.79 | 118.27      | 123.70   |
| 1   | AA    | 652  | U    | O4'-C1'-N1 | 6.78  | 113.63      | 108.20   |
| 1   | AA    | 1024 | G    | C5-C6-O6   | -6.78 | 124.53      | 128.60   |
| 1   | AA    | 1297 | G    | C5-C6-O6   | -6.78 | 124.53      | 128.60   |
| 27  | B8    | 2459 | A    | C4-C5-C6   | 6.78  | 120.39      | 117.00   |
| 27  | B8    | 2897 | U    | O4'-C1'-N1 | 6.78  | 113.63      | 108.20   |
| 1   | AA    | 901  | A    | C4-C5-C6   | 6.78  | 120.39      | 117.00   |
| 27  | B8    | 955  | U    | O4'-C1'-N1 | 6.78  | 113.62      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 338  | G    | C5-C6-O6   | -6.78 | 124.53      | 128.60   |
| 27  | B8    | 947  | A    | C5-C6-N6   | -6.78 | 118.28      | 123.70   |
| 27  | B8    | 1869 | G    | C5-C6-O6   | -6.78 | 124.53      | 128.60   |
| 27  | B8    | 1904 | G    | O4'-C1'-N9 | 6.78  | 113.62      | 108.20   |
| 27  | B8    | 2102 | G    | O4'-C1'-N9 | 6.78  | 113.62      | 108.20   |
| 27  | B8    | 2553 | G    | C5-C6-O6   | -6.78 | 124.53      | 128.60   |
| 27  | B8    | 1533 | C    | N3-C4-N4   | 6.78  | 122.75      | 118.00   |
| 27  | B8    | 2204 | G    | O4'-C1'-N9 | 6.78  | 113.62      | 108.20   |
| 1   | AA    | 134  | G    | C5-C6-O6   | -6.78 | 124.53      | 128.60   |
| 1   | AA    | 390  | U    | O4'-C1'-N1 | 6.78  | 113.62      | 108.20   |
| 1   | AA    | 496  | A    | C5-C6-N6   | -6.78 | 118.28      | 123.70   |
| 26  | B7    | 20   | G    | C5-C6-O6   | -6.78 | 124.53      | 128.60   |
| 27  | B8    | 219  | A    | C5-C6-N6   | -6.78 | 118.28      | 123.70   |
| 27  | B8    | 1115 | G    | C5-C6-O6   | -6.78 | 124.53      | 128.60   |
| 27  | B8    | 1467 | U    | O4'-C1'-N1 | 6.78  | 113.62      | 108.20   |
| 27  | B8    | 1584 | U    | O4'-C1'-N1 | 6.78  | 113.62      | 108.20   |
| 1   | AA    | 875  | U    | O4'-C1'-N1 | 6.78  | 113.62      | 108.20   |
| 1   | AA    | 1278 | G    | C5-C6-O6   | -6.78 | 124.53      | 128.60   |
| 27  | B8    | 443  | A    | O4'-C1'-N9 | 6.78  | 113.62      | 108.20   |
| 27  | B8    | 1051 | G    | C5-C6-O6   | -6.78 | 124.53      | 128.60   |
| 27  | B8    | 1775 | U    | O4'-C1'-N1 | 6.78  | 113.62      | 108.20   |
| 1   | AA    | 1017 | U    | O4'-C1'-N1 | 6.77  | 113.62      | 108.20   |
| 27  | B8    | 569  | U    | O4'-C1'-N1 | 6.77  | 113.62      | 108.20   |
| 1   | AA    | 303  | A    | O4'-C1'-N9 | 6.77  | 113.62      | 108.20   |
| 1   | AA    | 354  | G    | C5-C6-O6   | -6.77 | 124.54      | 128.60   |
| 1   | AA    | 817  | C    | O4'-C1'-N1 | 6.77  | 113.62      | 108.20   |
| 27  | B8    | 175  | G    | C5-C6-O6   | -6.77 | 124.54      | 128.60   |
| 27  | B8    | 232  | G    | C5-C6-O6   | -6.77 | 124.54      | 128.60   |
| 27  | B8    | 1159 | U    | O4'-C1'-N1 | 6.77  | 113.62      | 108.20   |
| 27  | B8    | 1423 | G    | C5-C6-O6   | -6.77 | 124.54      | 128.60   |
| 27  | B8    | 1842 | G    | O4'-C1'-N9 | 6.77  | 113.62      | 108.20   |
| 2   | AX    | 14   | G    | C5-C6-O6   | -6.77 | 124.54      | 128.60   |
| 27  | B8    | 1202 | G    | O4'-C1'-N9 | 6.77  | 113.62      | 108.20   |
| 27  | B8    | 1644 | C    | O4'-C1'-N1 | 6.77  | 113.62      | 108.20   |
| 27  | B8    | 899  | A    | O4'-C1'-N9 | 6.77  | 113.61      | 108.20   |
| 27  | B8    | 997  | G    | O4'-C1'-N9 | 6.77  | 113.62      | 108.20   |
| 27  | B8    | 2171 | A    | C5-C6-N6   | -6.77 | 118.28      | 123.70   |
| 1   | AA    | 500  | G    | O4'-C1'-N9 | 6.77  | 113.61      | 108.20   |
| 27  | B8    | 1622 | G    | C5-C6-O6   | -6.77 | 124.54      | 128.60   |
| 27  | B8    | 1687 | G    | O4'-C1'-N9 | 6.77  | 113.61      | 108.20   |
| 27  | B8    | 1872 | A    | O4'-C1'-N9 | 6.77  | 113.61      | 108.20   |
| 27  | B8    | 372  | G    | C5-C6-O6   | -6.77 | 124.54      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1355 | G    | O4'-C1'-N9 | 6.76  | 113.61      | 108.20   |
| 2   | AX    | 20   | G    | C5-C6-O6   | -6.76 | 124.54      | 128.60   |
| 27  | B8    | 1245 | G    | O4'-C1'-N9 | 6.76  | 113.61      | 108.20   |
| 27  | B8    | 1734 | G    | O4'-C1'-N9 | 6.76  | 113.61      | 108.20   |
| 27  | B8    | 2049 | G    | O4'-C1'-N9 | 6.76  | 113.61      | 108.20   |
| 27  | B8    | 2748 | A    | C4-C5-C6   | 6.76  | 120.38      | 117.00   |
| 27  | B8    | 561  | G    | C5-C6-O6   | -6.76 | 124.54      | 128.60   |
| 27  | B8    | 2825 | G    | O4'-C1'-N9 | 6.76  | 113.61      | 108.20   |
| 1   | AA    | 847  | G    | C5-C6-O6   | -6.76 | 124.54      | 128.60   |
| 1   | AA    | 827  | U    | O4'-C1'-N1 | 6.76  | 113.61      | 108.20   |
| 1   | AA    | 1197 | A    | C5-C6-N6   | -6.76 | 118.29      | 123.70   |
| 1   | AA    | 1454 | G    | O4'-C1'-N9 | 6.76  | 113.61      | 108.20   |
| 27  | B8    | 470  | A    | C4-C5-C6   | 6.76  | 120.38      | 117.00   |
| 27  | B8    | 2357 | G    | C5-C6-O6   | -6.76 | 124.55      | 128.60   |
| 1   | AA    | 1381 | U    | O4'-C1'-N1 | 6.76  | 113.61      | 108.20   |
| 27  | B8    | 1857 | G    | C5-C6-O6   | -6.76 | 124.55      | 128.60   |
| 27  | B8    | 2395 | C    | N3-C4-N4   | 6.76  | 122.73      | 118.00   |
| 1   | AA    | 1375 | A    | C4-C5-C6   | 6.76  | 120.38      | 117.00   |
| 27  | B8    | 1703 | G    | C5-C6-O6   | -6.76 | 124.55      | 128.60   |
| 27  | B8    | 1873 | G    | O4'-C1'-N9 | 6.76  | 113.61      | 108.20   |
| 27  | B8    | 56   | A    | C5-C6-N6   | -6.75 | 118.30      | 123.70   |
| 27  | B8    | 458  | G    | C5-C6-O6   | -6.75 | 124.55      | 128.60   |
| 27  | B8    | 2435 | A    | C4-C5-C6   | 6.75  | 120.38      | 117.00   |
| 3   | AV    | 14   | A    | C4-C5-C6   | 6.75  | 120.38      | 117.00   |
| 27  | B8    | 2360 | G    | C5-C6-O6   | -6.75 | 124.55      | 128.60   |
| 27  | B8    | 2656 | U    | O4'-C1'-N1 | 6.75  | 113.60      | 108.20   |
| 27  | B8    | 2844 | G    | C5-C6-O6   | -6.75 | 124.55      | 128.60   |
| 27  | B8    | 2857 | G    | C5-C6-O6   | -6.75 | 124.55      | 128.60   |
| 1   | AA    | 205  | A    | C5-C6-N6   | -6.75 | 118.30      | 123.70   |
| 1   | AA    | 561  | U    | O4'-C1'-N1 | 6.75  | 113.60      | 108.20   |
| 1   | AA    | 642  | A    | C4-C5-C6   | 6.75  | 120.38      | 117.00   |
| 27  | B8    | 221  | A    | C5-C6-N6   | -6.75 | 118.30      | 123.70   |
| 27  | B8    | 371  | A    | C4-C5-C6   | 6.75  | 120.38      | 117.00   |
| 27  | B8    | 2073 | C    | O4'-C1'-N1 | 6.75  | 113.60      | 108.20   |
| 1   | AA    | 881  | G    | O4'-C1'-N9 | 6.75  | 113.60      | 108.20   |
| 1   | AA    | 1529 | G    | C5-C6-O6   | -6.75 | 124.55      | 128.60   |
| 27  | B8    | 2083 | G    | C5-C6-O6   | -6.75 | 124.55      | 128.60   |
| 1   | AA    | 148  | G    | O4'-C1'-N9 | 6.75  | 113.60      | 108.20   |
| 1   | AA    | 714  | G    | O4'-C1'-N9 | 6.75  | 113.60      | 108.20   |
| 1   | AA    | 752  | G    | C5-C6-O6   | -6.75 | 124.55      | 128.60   |
| 1   | AA    | 781  | A    | C4-C5-C6   | 6.75  | 120.38      | 117.00   |
| 27  | B8    | 473  | G    | C5-C6-O6   | -6.75 | 124.55      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2893 | A    | C4-C5-C6   | 6.75  | 120.37      | 117.00   |
| 1   | AA    | 230  | G    | O4'-C1'-N9 | 6.75  | 113.60      | 108.20   |
| 1   | AA    | 919  | A    | C4-C5-C6   | 6.75  | 120.37      | 117.00   |
| 27  | B8    | 49   | A    | O4'-C1'-N9 | 6.75  | 113.60      | 108.20   |
| 27  | B8    | 456  | C    | O4'-C1'-N1 | 6.75  | 113.60      | 108.20   |
| 27  | B8    | 513  | A    | C4-C5-C6   | 6.75  | 120.37      | 117.00   |
| 27  | B8    | 1697 | G    | C5-C6-O6   | -6.75 | 124.55      | 128.60   |
| 1   | AA    | 1398 | A    | C5-C6-N6   | -6.75 | 118.30      | 123.70   |
| 3   | AV    | 45   | G    | C5-C6-O6   | -6.74 | 124.55      | 128.60   |
| 27  | B8    | 633  | A    | C5-C6-N1   | -6.74 | 114.33      | 117.70   |
| 27  | B8    | 1498 | C    | O4'-C1'-N1 | 6.74  | 113.59      | 108.20   |
| 27  | B8    | 2100 | G    | C5-C6-O6   | -6.74 | 124.55      | 128.60   |
| 1   | AA    | 332  | G    | C5-C6-O6   | -6.74 | 124.56      | 128.60   |
| 1   | AA    | 555  | U    | O4'-C1'-N1 | 6.74  | 113.59      | 108.20   |
| 27  | B8    | 256  | A    | C4-C5-C6   | 6.74  | 120.37      | 117.00   |
| 27  | B8    | 1468 | U    | O4'-C1'-N1 | 6.74  | 113.59      | 108.20   |
| 27  | B8    | 1977 | A    | C4-C5-C6   | 6.74  | 120.37      | 117.00   |
| 1   | AA    | 735  | C    | O4'-C1'-N1 | 6.74  | 113.59      | 108.20   |
| 1   | AA    | 950  | U    | O4'-C1'-N1 | 6.74  | 113.59      | 108.20   |
| 1   | AA    | 1060 | U    | O4'-C1'-N1 | 6.74  | 113.59      | 108.20   |
| 1   | AA    | 1516 | G    | C5-C6-O6   | -6.74 | 124.56      | 128.60   |
| 27  | B8    | 1071 | G    | C5-C6-O6   | -6.74 | 124.56      | 128.60   |
| 27  | B8    | 2349 | G    | N1-C6-O6   | 6.74  | 123.94      | 119.90   |
| 1   | AA    | 108  | G    | C5-C6-O6   | -6.74 | 124.56      | 128.60   |
| 1   | AA    | 412  | A    | O4'-C1'-N9 | 6.74  | 113.59      | 108.20   |
| 1   | AA    | 1094 | G    | C5-C6-O6   | -6.74 | 124.56      | 128.60   |
| 1   | AA    | 1316 | G    | C5-C6-O6   | -6.74 | 124.56      | 128.60   |
| 27  | B8    | 491  | G    | C5-C6-O6   | -6.74 | 124.56      | 128.60   |
| 27  | B8    | 835  | C    | N3-C4-N4   | 6.74  | 122.72      | 118.00   |
| 1   | AA    | 282  | A    | N1-C6-N6   | 6.74  | 122.64      | 118.60   |
| 1   | AA    | 700  | G    | C5-C6-O6   | -6.74 | 124.56      | 128.60   |
| 1   | AA    | 1068 | G    | C5-C6-O6   | -6.74 | 124.56      | 128.60   |
| 1   | AA    | 1458 | G    | C5-C6-O6   | -6.74 | 124.56      | 128.60   |
| 27  | B8    | 1339 | G    | C5-C6-O6   | -6.74 | 124.56      | 128.60   |
| 27  | B8    | 2754 | U    | O4'-C1'-N1 | 6.74  | 113.59      | 108.20   |
| 27  | B8    | 2810 | A    | O4'-C1'-N9 | 6.74  | 113.59      | 108.20   |
| 1   | AA    | 907  | A    | C4-C5-C6   | 6.74  | 120.37      | 117.00   |
| 27  | B8    | 1091 | G    | N1-C6-O6   | 6.74  | 123.94      | 119.90   |
| 27  | B8    | 2476 | A    | C4-C5-C6   | 6.74  | 120.37      | 117.00   |
| 1   | AA    | 769  | G    | C5-C6-O6   | -6.73 | 124.56      | 128.60   |
| 27  | B8    | 446  | G    | C5-C6-O6   | -6.73 | 124.56      | 128.60   |
| 27  | B8    | 819  | A    | C4-C5-C6   | 6.73  | 120.37      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 281  | G    | C5-C6-O6   | -6.73 | 124.56      | 128.60   |
| 3   | AV    | 20   | G    | C5-C6-O6   | -6.73 | 124.56      | 128.60   |
| 27  | B8    | 363  | G    | O4'-C1'-N9 | 6.73  | 113.59      | 108.20   |
| 27  | B8    | 2341 | G    | O4'-C1'-N9 | 6.73  | 113.58      | 108.20   |
| 27  | B8    | 2701 | U    | O4'-C1'-N1 | 6.73  | 113.58      | 108.20   |
| 27  | B8    | 1593 | A    | O4'-C1'-N9 | 6.73  | 113.58      | 108.20   |
| 27  | B8    | 1865 | U    | O4'-C1'-N1 | 6.73  | 113.58      | 108.20   |
| 27  | B8    | 2319 | G    | C5-C6-O6   | -6.73 | 124.56      | 128.60   |
| 27  | B8    | 2436 | G    | C5-C6-O6   | -6.73 | 124.56      | 128.60   |
| 27  | B8    | 2831 | G    | C5-C6-O6   | -6.73 | 124.56      | 128.60   |
| 27  | B8    | 652  | U    | O4'-C1'-N1 | 6.73  | 113.58      | 108.20   |
| 27  | B8    | 1311 | G    | C5-C6-O6   | -6.73 | 124.56      | 128.60   |
| 1   | AA    | 1103 | C    | O4'-C1'-N1 | 6.73  | 113.58      | 108.20   |
| 27  | B8    | 359  | G    | C5-C6-O6   | -6.73 | 124.56      | 128.60   |
| 27  | B8    | 608  | A    | C4-C5-C6   | 6.73  | 120.36      | 117.00   |
| 27  | B8    | 1067 | A    | O4'-C1'-N9 | 6.73  | 113.58      | 108.20   |
| 27  | B8    | 1227 | G    | O4'-C1'-N9 | 6.73  | 113.58      | 108.20   |
| 27  | B8    | 1313 | U    | C2-N1-C1'  | 6.73  | 125.77      | 117.70   |
| 27  | B8    | 1955 | U    | O4'-C1'-N1 | 6.73  | 113.58      | 108.20   |
| 27  | B8    | 1715 | G    | C5-C6-O6   | -6.73 | 124.56      | 128.60   |
| 27  | B8    | 2090 | A    | C5-C6-N6   | -6.73 | 118.32      | 123.70   |
| 1   | AA    | 352  | C    | O4'-C1'-N1 | 6.72  | 113.58      | 108.20   |
| 26  | B7    | 107  | G    | C5-C6-O6   | -6.72 | 124.56      | 128.60   |
| 27  | B8    | 426  | C    | N3-C4-N4   | 6.72  | 122.71      | 118.00   |
| 27  | B8    | 747  | U    | O4'-C1'-N1 | 6.72  | 113.58      | 108.20   |
| 27  | B8    | 1434 | A    | O4'-C1'-N9 | 6.72  | 113.58      | 108.20   |
| 27  | B8    | 1807 | G    | O4'-C1'-N9 | 6.72  | 113.58      | 108.20   |
| 27  | B8    | 2742 | G    | C5-C6-O6   | -6.72 | 124.56      | 128.60   |
| 27  | B8    | 704  | G    | O4'-C1'-N9 | 6.72  | 113.58      | 108.20   |
| 1   | AA    | 1076 | U    | O4'-C1'-N1 | 6.72  | 113.58      | 108.20   |
| 1   | AA    | 405  | U    | O4'-C1'-N1 | 6.72  | 113.58      | 108.20   |
| 1   | AA    | 1066 | C    | O4'-C1'-N1 | 6.72  | 113.58      | 108.20   |
| 1   | AA    | 1397 | C    | C2-N1-C1'  | 6.72  | 126.19      | 118.80   |
| 27  | B8    | 332  | A    | C4-C5-C6   | 6.72  | 120.36      | 117.00   |
| 27  | B8    | 381  | G    | C5-C6-O6   | -6.72 | 124.57      | 128.60   |
| 27  | B8    | 642  | U    | O4'-C1'-N1 | 6.72  | 113.58      | 108.20   |
| 27  | B8    | 1382 | G    | C5-C6-O6   | -6.72 | 124.57      | 128.60   |
| 27  | B8    | 2408 | U    | O4'-C1'-N1 | 6.72  | 113.58      | 108.20   |
| 1   | AA    | 211  | G    | O4'-C1'-N9 | 6.72  | 113.57      | 108.20   |
| 1   | AA    | 262  | A    | C4-C5-C6   | 6.72  | 120.36      | 117.00   |
| 27  | B8    | 720  | U    | O4'-C1'-N1 | 6.72  | 113.57      | 108.20   |
| 27  | B8    | 1746 | A    | O4'-C1'-N9 | 6.72  | 113.58      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2670 | A    | O4'-C1'-N9 | 6.72  | 113.57      | 108.20   |
| 1   | AA    | 102  | G    | C5-C6-O6   | -6.72 | 124.57      | 128.60   |
| 1   | AA    | 1165 | U    | O4'-C1'-N1 | 6.72  | 113.57      | 108.20   |
| 27  | B8    | 280  | U    | O4'-C1'-N1 | 6.72  | 113.57      | 108.20   |
| 27  | B8    | 480  | A    | C4-C5-C6   | 6.72  | 120.36      | 117.00   |
| 27  | B8    | 594  | U    | O4'-C1'-N1 | 6.72  | 113.57      | 108.20   |
| 27  | B8    | 842  | U    | O4'-C1'-N1 | 6.72  | 113.57      | 108.20   |
| 1   | AA    | 297  | G    | C5-C6-O6   | -6.71 | 124.57      | 128.60   |
| 1   | AA    | 453  | G    | C5-C6-O6   | -6.71 | 124.57      | 128.60   |
| 1   | AA    | 834  | U    | O4'-C1'-N1 | 6.71  | 113.57      | 108.20   |
| 1   | AA    | 1261 | A    | C4-C5-C6   | 6.71  | 120.36      | 117.00   |
| 27  | B8    | 721  | A    | C5-C6-N1   | -6.71 | 114.34      | 117.70   |
| 27  | B8    | 2353 | G    | C5-C6-O6   | -6.71 | 124.57      | 128.60   |
| 27  | B8    | 2373 | G    | O4'-C1'-N9 | 6.71  | 113.57      | 108.20   |
| 1   | AA    | 10   | A    | O4'-C1'-N9 | 6.71  | 113.57      | 108.20   |
| 27  | B8    | 551  | G    | O4'-C1'-N9 | 6.71  | 113.57      | 108.20   |
| 27  | B8    | 556  | A    | C4-C5-C6   | 6.71  | 120.36      | 117.00   |
| 27  | B8    | 2465 | C    | N3-C4-N4   | 6.71  | 122.70      | 118.00   |
| 1   | AA    | 369  | G    | C5-C6-O6   | -6.71 | 124.57      | 128.60   |
| 3   | AV    | 25   | G    | C5-C6-O6   | -6.71 | 124.57      | 128.60   |
| 27  | B8    | 741  | U    | O4'-C1'-N1 | 6.71  | 113.57      | 108.20   |
| 27  | B8    | 1001 | A    | C4-C5-C6   | 6.71  | 120.36      | 117.00   |
| 27  | B8    | 1573 | G    | O4'-C1'-N9 | 6.71  | 113.57      | 108.20   |
| 27  | B8    | 1724 | G    | C5-C6-O6   | -6.71 | 124.57      | 128.60   |
| 27  | B8    | 2708 | G    | C5-C6-O6   | -6.71 | 124.57      | 128.60   |
| 27  | B8    | 2199 | A    | C4-C5-C6   | 6.71  | 120.36      | 117.00   |
| 1   | AA    | 662  | U    | O4'-C1'-N1 | 6.71  | 113.57      | 108.20   |
| 1   | AA    | 1013 | G    | C5-C6-O6   | -6.71 | 124.57      | 128.60   |
| 27  | B8    | 96   | C    | N3-C4-N4   | 6.71  | 122.70      | 118.00   |
| 27  | B8    | 527  | C    | O4'-C1'-N1 | 6.71  | 113.57      | 108.20   |
| 27  | B8    | 1002 | G    | C5-C6-O6   | -6.71 | 124.58      | 128.60   |
| 27  | B8    | 2517 | C    | O4'-C1'-N1 | 6.71  | 113.57      | 108.20   |
| 1   | AA    | 746  | A    | C5-C6-N6   | -6.71 | 118.33      | 123.70   |
| 3   | AV    | 68   | G    | C5-C6-O6   | -6.71 | 124.58      | 128.60   |
| 27  | B8    | 374  | A    | C4-C5-C6   | 6.71  | 120.35      | 117.00   |
| 27  | B8    | 467  | G    | O4'-C1'-N9 | 6.71  | 113.57      | 108.20   |
| 27  | B8    | 1254 | A    | C4-C5-C6   | 6.71  | 120.35      | 117.00   |
| 27  | B8    | 1267 | U    | O4'-C1'-N1 | 6.71  | 113.56      | 108.20   |
| 27  | B8    | 2886 | A    | C4-C5-C6   | 6.71  | 120.35      | 117.00   |
| 1   | AA    | 1028 | C    | O4'-C1'-N1 | 6.71  | 113.56      | 108.20   |
| 27  | B8    | 1130 | U    | O4'-C1'-N1 | 6.71  | 113.56      | 108.20   |
| 27  | B8    | 2356 | U    | O4'-C1'-N1 | 6.71  | 113.56      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 575  | G    | C5-C6-O6   | -6.70 | 124.58      | 128.60   |
| 27  | B8    | 1839 | G    | C5-C6-O6   | -6.70 | 124.58      | 128.60   |
| 1   | AA    | 76   | G    | O4'-C1'-N9 | 6.70  | 113.56      | 108.20   |
| 26  | B7    | 25   | U    | O4'-C1'-N1 | 6.70  | 113.56      | 108.20   |
| 27  | B8    | 175  | G    | O4'-C1'-N9 | 6.70  | 113.56      | 108.20   |
| 27  | B8    | 1248 | G    | C5-C6-O6   | -6.70 | 124.58      | 128.60   |
| 27  | B8    | 1501 | G    | C5-C6-O6   | -6.70 | 124.58      | 128.60   |
| 27  | B8    | 1664 | A    | C4-C5-C6   | 6.70  | 120.35      | 117.00   |
| 27  | B8    | 1669 | A    | C4-C5-C6   | 6.70  | 120.35      | 117.00   |
| 1   | AA    | 772  | U    | O4'-C1'-N1 | 6.70  | 113.56      | 108.20   |
| 1   | AA    | 909  | A    | C4-C5-C6   | 6.70  | 120.35      | 117.00   |
| 26  | B7    | 52   | A    | O4'-C1'-N9 | 6.70  | 113.56      | 108.20   |
| 27  | B8    | 547  | A    | O4'-C1'-N9 | 6.70  | 113.56      | 108.20   |
| 27  | B8    | 2526 | G    | C5-C6-O6   | -6.70 | 124.58      | 128.60   |
| 27  | B8    | 2808 | G    | C5-C6-O6   | -6.70 | 124.58      | 128.60   |
| 1   | AA    | 1500 | A    | C5-C6-N6   | -6.70 | 118.34      | 123.70   |
| 27  | B8    | 1096 | A    | C4-C5-C6   | 6.70  | 120.35      | 117.00   |
| 27  | B8    | 1674 | G    | C5-C6-O6   | -6.70 | 124.58      | 128.60   |
| 27  | B8    | 1269 | A    | C5-C6-N6   | -6.69 | 118.34      | 123.70   |
| 27  | B8    | 2017 | U    | O4'-C1'-N1 | 6.69  | 113.56      | 108.20   |
| 27  | B8    | 2086 | U    | O4'-C1'-N1 | 6.69  | 113.56      | 108.20   |
| 1   | AA    | 1439 | G    | O4'-C1'-N9 | 6.69  | 113.55      | 108.20   |
| 27  | B8    | 2720 | U    | O4'-C1'-N1 | 6.69  | 113.55      | 108.20   |
| 27  | B8    | 2007 | U    | O4'-C1'-N1 | 6.69  | 113.55      | 108.20   |
| 27  | B8    | 2803 | G    | O4'-C1'-N9 | 6.69  | 113.55      | 108.20   |
| 27  | B8    | 2843 | G    | C5-C6-O6   | -6.69 | 124.58      | 128.60   |
| 1   | AA    | 1252 | A    | O4'-C1'-N9 | 6.69  | 113.55      | 108.20   |
| 27  | B8    | 256  | A    | O4'-C1'-N9 | 6.69  | 113.55      | 108.20   |
| 27  | B8    | 1310 | G    | O4'-C1'-N9 | 6.69  | 113.55      | 108.20   |
| 1   | AA    | 324  | G    | C5-C6-O6   | -6.69 | 124.59      | 128.60   |
| 26  | B7    | 41   | G    | C5-C6-O6   | -6.69 | 124.59      | 128.60   |
| 27  | B8    | 820  | A    | C4-C5-C6   | 6.69  | 120.34      | 117.00   |
| 27  | B8    | 1347 | A    | O4'-C1'-N9 | 6.69  | 113.55      | 108.20   |
| 27  | B8    | 1802 | A    | C4-C5-C6   | 6.69  | 120.34      | 117.00   |
| 1   | AA    | 653  | U    | O4'-C1'-N1 | 6.69  | 113.55      | 108.20   |
| 27  | B8    | 308  | G    | C5-C6-O6   | -6.69 | 124.59      | 128.60   |
| 27  | B8    | 941  | A    | O4'-C1'-N9 | 6.69  | 113.55      | 108.20   |
| 1   | AA    | 1129 | C    | O4'-C1'-N1 | 6.68  | 113.55      | 108.20   |
| 27  | B8    | 1683 | U    | O4'-C1'-N1 | 6.68  | 113.55      | 108.20   |
| 1   | AA    | 927  | G    | C5-C6-O6   | -6.68 | 124.59      | 128.60   |
| 27  | B8    | 907  | G    | C5-C6-O6   | -6.68 | 124.59      | 128.60   |
| 27  | B8    | 1355 | G    | C5-C6-O6   | -6.68 | 124.59      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 787  | A    | O4'-C1'-N9 | 6.68  | 113.54      | 108.20   |
| 1   | AA    | 944  | G    | N3-C2-N2   | 6.68  | 124.58      | 119.90   |
| 1   | AA    | 1089 | G    | C5-C6-O6   | -6.68 | 124.59      | 128.60   |
| 27  | B8    | 622  | G    | C5-C6-O6   | -6.68 | 124.59      | 128.60   |
| 27  | B8    | 1068 | G    | C5-C6-O6   | -6.68 | 124.59      | 128.60   |
| 28  | BA    | 79   | ALA  | N-CA-CB    | 6.68  | 119.45      | 110.10   |
| 1   | AA    | 539  | A    | O4'-C1'-N9 | 6.68  | 113.54      | 108.20   |
| 27  | B8    | 1439 | A    | C4-C5-C6   | 6.68  | 120.34      | 117.00   |
| 27  | B8    | 2797 | U    | O4'-C1'-N1 | 6.68  | 113.54      | 108.20   |
| 1   | AA    | 923  | A    | C4-C5-C6   | 6.68  | 120.34      | 117.00   |
| 26  | B7    | 13   | G    | C5-C6-O6   | -6.68 | 124.59      | 128.60   |
| 27  | B8    | 1036 | G    | C5-C6-O6   | -6.68 | 124.59      | 128.60   |
| 1   | AA    | 563  | A    | C5-C6-N6   | -6.67 | 118.36      | 123.70   |
| 27  | B8    | 830  | G    | C5-C6-O6   | -6.67 | 124.60      | 128.60   |
| 27  | B8    | 1395 | A    | C4-C5-C6   | 6.67  | 120.34      | 117.00   |
| 27  | B8    | 1572 | A    | C4-C5-C6   | 6.67  | 120.34      | 117.00   |
| 27  | B8    | 1920 | C    | N3-C4-N4   | 6.67  | 122.67      | 118.00   |
| 1   | AA    | 1528 | U    | O4'-C1'-N1 | 6.67  | 113.54      | 108.20   |
| 27  | B8    | 2618 | G    | C5-C6-O6   | -6.67 | 124.60      | 128.60   |
| 1   | AA    | 81   | A    | C5-C6-N6   | -6.67 | 118.36      | 123.70   |
| 27  | B8    | 2775 | G    | C5-C6-O6   | -6.67 | 124.60      | 128.60   |
| 27  | B8    | 2885 | G    | C5-C6-O6   | -6.67 | 124.60      | 128.60   |
| 1   | AA    | 1452 | C    | O4'-C1'-N1 | 6.67  | 113.54      | 108.20   |
| 27  | B8    | 709  | U    | O4'-C1'-N1 | 6.67  | 113.54      | 108.20   |
| 27  | B8    | 2566 | A    | C4-C5-C6   | 6.67  | 120.33      | 117.00   |
| 1   | AA    | 534  | U    | O4'-C1'-N1 | 6.67  | 113.53      | 108.20   |
| 1   | AA    | 963  | G    | C5-C6-O6   | -6.67 | 124.60      | 128.60   |
| 27  | B8    | 924  | G    | O4'-C1'-N9 | 6.67  | 113.53      | 108.20   |
| 27  | B8    | 2416 | C    | N3-C4-N4   | 6.67  | 122.67      | 118.00   |
| 27  | B8    | 2809 | A    | O4'-C1'-N9 | 6.67  | 113.53      | 108.20   |
| 27  | B8    | 725  | G    | C5-C6-O6   | -6.67 | 124.60      | 128.60   |
| 27  | B8    | 1242 | U    | O4'-C1'-N1 | 6.67  | 113.53      | 108.20   |
| 27  | B8    | 2133 | G    | C5-C6-O6   | -6.67 | 124.60      | 128.60   |
| 27  | B8    | 2239 | G    | C5-C6-O6   | -6.67 | 124.60      | 128.60   |
| 1   | AA    | 1166 | G    | C5-C6-O6   | -6.67 | 124.60      | 128.60   |
| 1   | AA    | 717  | U    | O4'-C1'-N1 | 6.66  | 113.53      | 108.20   |
| 1   | AA    | 888  | G    | C5-C6-O6   | -6.66 | 124.60      | 128.60   |
| 1   | AA    | 1065 | U    | O4'-C1'-N1 | 6.66  | 113.53      | 108.20   |
| 1   | AA    | 1374 | A    | O4'-C1'-N9 | 6.66  | 113.53      | 108.20   |
| 1   | AA    | 1453 | G    | O4'-C1'-N9 | 6.66  | 113.53      | 108.20   |
| 27  | B8    | 950  | G    | C5-C6-O6   | -6.66 | 124.60      | 128.60   |
| 27  | B8    | 1360 | G    | O4'-C1'-N9 | 6.66  | 113.53      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1459 | G    | C5-C6-O6   | -6.66 | 124.60      | 128.60   |
| 27  | B8    | 2524 | G    | C5-C6-O6   | -6.66 | 124.60      | 128.60   |
| 1   | AA    | 1431 | A    | P-O3'-C3'  | 6.66  | 127.69      | 119.70   |
| 1   | AA    | 1534 | A    | O4'-C1'-N9 | 6.66  | 113.53      | 108.20   |
| 27  | B8    | 126  | A    | O4'-C1'-N9 | 6.66  | 113.53      | 108.20   |
| 27  | B8    | 665  | U    | O4'-C1'-N1 | 6.66  | 113.53      | 108.20   |
| 27  | B8    | 2780 | G    | C5-C6-O6   | -6.66 | 124.60      | 128.60   |
| 1   | AA    | 621  | A    | O4'-C1'-N9 | 6.66  | 113.53      | 108.20   |
| 1   | AA    | 673  | A    | C5-C6-N6   | -6.66 | 118.37      | 123.70   |
| 26  | B7    | 105  | G    | O4'-C1'-N9 | 6.66  | 113.53      | 108.20   |
| 27  | B8    | 159  | G    | C5-C6-O6   | -6.66 | 124.61      | 128.60   |
| 27  | B8    | 528  | A    | O4'-C1'-N9 | 6.66  | 113.53      | 108.20   |
| 27  | B8    | 2192 | U    | O4'-C1'-N1 | 6.66  | 113.53      | 108.20   |
| 1   | AA    | 506  | G    | O4'-C1'-N9 | 6.66  | 113.53      | 108.20   |
| 1   | AA    | 646  | G    | C5-C6-O6   | -6.66 | 124.61      | 128.60   |
| 27  | B8    | 161  | A    | O4'-C1'-N9 | 6.66  | 113.52      | 108.20   |
| 27  | B8    | 969  | G    | O4'-C1'-N9 | 6.66  | 113.53      | 108.20   |
| 27  | B8    | 1824 | G    | C5-C6-O6   | -6.66 | 124.61      | 128.60   |
| 27  | B8    | 1970 | A    | C4-C5-C6   | 6.66  | 120.33      | 117.00   |
| 1   | AA    | 1009 | U    | O4'-C1'-N1 | 6.65  | 113.52      | 108.20   |
| 1   | AA    | 696  | A    | C4-C5-C6   | 6.65  | 120.33      | 117.00   |
| 1   | AA    | 733  | G    | C5-C6-O6   | -6.65 | 124.61      | 128.60   |
| 27  | B8    | 1057 | A    | C4-C5-C6   | 6.65  | 120.33      | 117.00   |
| 27  | B8    | 2284 | A    | C4-C5-C6   | 6.65  | 120.33      | 117.00   |
| 1   | AA    | 63   | C    | N3-C4-N4   | 6.65  | 122.66      | 118.00   |
| 1   | AA    | 520  | A    | C4-C5-C6   | 6.65  | 120.33      | 117.00   |
| 27  | B8    | 1631 | G    | C5-C6-O6   | -6.65 | 124.61      | 128.60   |
| 1   | AA    | 1170 | A    | C4-C5-C6   | 6.65  | 120.32      | 117.00   |
| 27  | B8    | 2227 | A    | O4'-C1'-N9 | 6.65  | 113.52      | 108.20   |
| 1   | AA    | 444  | G    | O4'-C1'-N9 | 6.65  | 113.52      | 108.20   |
| 26  | B7    | 99   | A    | C4-C5-C6   | 6.65  | 120.32      | 117.00   |
| 1   | AA    | 991  | U    | O4'-C1'-N1 | 6.65  | 113.52      | 108.20   |
| 27  | B8    | 548  | G    | C5-C6-O6   | -6.65 | 124.61      | 128.60   |
| 27  | B8    | 664  | G    | C5-C6-O6   | -6.65 | 124.61      | 128.60   |
| 1   | AA    | 797  | C    | N3-C4-N4   | 6.64  | 122.65      | 118.00   |
| 26  | B7    | 72   | G    | C5-C6-O6   | -6.64 | 124.61      | 128.60   |
| 27  | B8    | 2569 | G    | O4'-C1'-N9 | 6.64  | 113.52      | 108.20   |
| 27  | B8    | 99   | U    | C2-N1-C1'  | 6.64  | 125.67      | 117.70   |
| 27  | B8    | 425  | G    | O4'-C1'-N9 | 6.64  | 113.51      | 108.20   |
| 27  | B8    | 821  | A    | O4'-C1'-N9 | 6.64  | 113.51      | 108.20   |
| 27  | B8    | 1015 | U    | O4'-C1'-N1 | 6.64  | 113.51      | 108.20   |
| 27  | B8    | 1026 | G    | C5-C6-O6   | -6.64 | 124.61      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1559 | U    | O4'-C1'-N1 | 6.64  | 113.52      | 108.20   |
| 27  | B8    | 1634 | A    | C4-C5-C6   | 6.64  | 120.32      | 117.00   |
| 27  | B8    | 1643 | G    | O4'-C1'-N9 | 6.64  | 113.51      | 108.20   |
| 1   | AA    | 1483 | A    | C4-C5-C6   | 6.64  | 120.32      | 117.00   |
| 1   | AA    | 1057 | G    | O4'-C1'-N9 | 6.64  | 113.51      | 108.20   |
| 1   | AA    | 1312 | G    | O4'-C1'-N9 | 6.64  | 113.51      | 108.20   |
| 27  | B8    | 869  | G    | C5-C6-O6   | -6.64 | 124.62      | 128.60   |
| 1   | AA    | 194  | C    | N3-C4-N4   | 6.64  | 122.64      | 118.00   |
| 1   | AA    | 270  | A    | O4'-C1'-N9 | 6.64  | 113.51      | 108.20   |
| 1   | AA    | 1400 | C    | C2-N1-C1'  | 6.64  | 126.10      | 118.80   |
| 26  | B7    | 110  | C    | N3-C4-N4   | 6.64  | 122.64      | 118.00   |
| 27  | B8    | 1828 | G    | C5-C6-O6   | -6.64 | 124.62      | 128.60   |
| 27  | B8    | 2285 | C    | N3-C4-N4   | 6.64  | 122.65      | 118.00   |
| 1   | AA    | 254  | G    | C5-C6-O6   | -6.63 | 124.62      | 128.60   |
| 27  | B8    | 166  | U    | O4'-C1'-N1 | 6.63  | 113.51      | 108.20   |
| 27  | B8    | 1935 | G    | C5-C6-O6   | -6.63 | 124.62      | 128.60   |
| 27  | B8    | 2477 | U    | O4'-C1'-N1 | 6.63  | 113.51      | 108.20   |
| 27  | B8    | 2638 | G    | C5-C6-O6   | -6.63 | 124.62      | 128.60   |
| 1   | AA    | 1178 | G    | C5-C6-O6   | -6.63 | 124.62      | 128.60   |
| 1   | AA    | 1362 | A    | O4'-C1'-N9 | 6.63  | 113.51      | 108.20   |
| 1   | AA    | 1531 | A    | C4-C5-C6   | 6.63  | 120.32      | 117.00   |
| 27  | B8    | 1791 | A    | C5-C6-N6   | -6.63 | 118.39      | 123.70   |
| 27  | B8    | 900  | A    | O4'-C1'-N9 | 6.63  | 113.50      | 108.20   |
| 27  | B8    | 2032 | G    | C5-C6-O6   | -6.63 | 124.62      | 128.60   |
| 27  | B8    | 2351 | G    | C5-C6-O6   | -6.63 | 124.62      | 128.60   |
| 27  | B8    | 2890 | G    | C5-C6-O6   | -6.63 | 124.62      | 128.60   |
| 1   | AA    | 180  | U    | O4'-C1'-N1 | 6.63  | 113.50      | 108.20   |
| 1   | AA    | 394  | G    | C5-C6-O6   | -6.63 | 124.62      | 128.60   |
| 27  | B8    | 2551 | C    | O4'-C1'-N1 | 6.63  | 113.50      | 108.20   |
| 27  | B8    | 247  | G    | C5-C6-O6   | -6.63 | 124.62      | 128.60   |
| 27  | B8    | 1017 | G    | C5-C6-O6   | -6.63 | 124.62      | 128.60   |
| 27  | B8    | 1528 | A    | C4-C5-C6   | 6.63  | 120.31      | 117.00   |
| 27  | B8    | 2800 | A    | C5-C6-N6   | -6.63 | 118.40      | 123.70   |
| 1   | AA    | 270  | A    | C4-C5-C6   | 6.63  | 120.31      | 117.00   |
| 1   | AA    | 908  | A    | C4-C5-C6   | 6.63  | 120.31      | 117.00   |
| 27  | B8    | 3    | U    | O4'-C1'-N1 | 6.63  | 113.50      | 108.20   |
| 27  | B8    | 1406 | U    | O4'-C1'-N1 | 6.63  | 113.50      | 108.20   |
| 27  | B8    | 379  | G    | C5-C6-O6   | -6.62 | 124.62      | 128.60   |
| 27  | B8    | 2044 | C    | N3-C4-N4   | 6.62  | 122.64      | 118.00   |
| 27  | B8    | 1089 | A    | C4-C5-C6   | 6.62  | 120.31      | 117.00   |
| 27  | B8    | 2118 | U    | O4'-C1'-N1 | 6.62  | 113.50      | 108.20   |
| 1   | AA    | 480  | U    | O4'-C1'-N1 | 6.62  | 113.50      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1282 | C    | N3-C4-N4   | 6.62  | 122.64      | 118.00   |
| 27  | B8    | 2648 | G    | O4'-C1'-N9 | 6.62  | 113.50      | 108.20   |
| 27  | B8    | 413  | C    | N3-C4-N4   | 6.62  | 122.63      | 118.00   |
| 27  | B8    | 1326 | U    | O4'-C1'-N1 | 6.62  | 113.50      | 108.20   |
| 1   | AA    | 818  | G    | O4'-C1'-N9 | 6.62  | 113.49      | 108.20   |
| 26  | B7    | 69   | G    | N1-C6-O6   | 6.62  | 123.87      | 119.90   |
| 27  | B8    | 1473 | G    | O4'-C1'-N9 | 6.62  | 113.49      | 108.20   |
| 27  | B8    | 2684 | U    | O4'-C1'-N1 | 6.62  | 113.49      | 108.20   |
| 1   | AA    | 429  | U    | P-O3'-C3'  | 6.62  | 127.64      | 119.70   |
| 27  | B8    | 1271 | G    | C5-C6-O6   | -6.62 | 124.63      | 128.60   |
| 27  | B8    | 1426 | G    | C5-C6-O6   | -6.62 | 124.63      | 128.60   |
| 1   | AA    | 596  | A    | O4'-C1'-N9 | 6.62  | 113.49      | 108.20   |
| 1   | AA    | 1517 | G    | C5-C6-O6   | -6.62 | 124.63      | 128.60   |
| 3   | AV    | 5    | A    | O4'-C1'-N9 | 6.62  | 113.49      | 108.20   |
| 27  | B8    | 493  | G    | C5-C6-O6   | -6.62 | 124.63      | 128.60   |
| 27  | B8    | 343  | C    | O4'-C1'-N1 | 6.61  | 113.49      | 108.20   |
| 27  | B8    | 1832 | C    | N3-C4-N4   | 6.61  | 122.63      | 118.00   |
| 27  | B8    | 2435 | A    | C5-C6-N1   | -6.61 | 114.39      | 117.70   |
| 27  | B8    | 2608 | G    | C5-C6-O6   | -6.61 | 124.63      | 128.60   |
| 1   | AA    | 1035 | A    | O4'-C1'-N9 | 6.61  | 113.49      | 108.20   |
| 27  | B8    | 2315 | G    | O4'-C1'-N9 | 6.61  | 113.49      | 108.20   |
| 1   | AA    | 49   | U    | O4'-C1'-N1 | 6.61  | 113.49      | 108.20   |
| 1   | AA    | 231  | U    | O4'-C1'-N1 | 6.61  | 113.49      | 108.20   |
| 1   | AA    | 587  | G    | C5-C6-O6   | -6.61 | 124.63      | 128.60   |
| 1   | AA    | 1370 | G    | O4'-C1'-N9 | 6.61  | 113.49      | 108.20   |
| 27  | B8    | 176  | A    | O4'-C1'-N9 | 6.61  | 113.49      | 108.20   |
| 27  | B8    | 745  | G    | C5-C6-O6   | -6.61 | 124.63      | 128.60   |
| 27  | B8    | 1611 | C    | O4'-C1'-N1 | 6.61  | 113.49      | 108.20   |
| 1   | AA    | 481  | G    | C5-C6-O6   | -6.61 | 124.64      | 128.60   |
| 1   | AA    | 628  | G    | O4'-C1'-N9 | 6.61  | 113.49      | 108.20   |
| 27  | B8    | 1376 | C    | O4'-C1'-N1 | 6.61  | 113.49      | 108.20   |
| 27  | B8    | 1852 | U    | O4'-C1'-N1 | 6.61  | 113.49      | 108.20   |
| 1   | AA    | 1413 | A    | O4'-C1'-N9 | 6.61  | 113.49      | 108.20   |
| 27  | B8    | 228  | C    | O4'-C1'-N1 | 6.61  | 113.48      | 108.20   |
| 27  | B8    | 849  | A    | C5-C6-N6   | -6.61 | 118.41      | 123.70   |
| 27  | B8    | 1100 | C    | N3-C4-N4   | 6.61  | 122.63      | 118.00   |
| 27  | B8    | 1387 | A    | O4'-C1'-N9 | 6.61  | 113.49      | 108.20   |
| 27  | B8    | 1470 | A    | C4-C5-C6   | 6.61  | 120.30      | 117.00   |
| 27  | B8    | 1543 | G    | C5-C6-O6   | -6.61 | 124.64      | 128.60   |
| 27  | B8    | 597  | G    | C5-C6-O6   | -6.61 | 124.64      | 128.60   |
| 27  | B8    | 1965 | C    | O4'-C1'-N1 | 6.61  | 113.48      | 108.20   |
| 1   | AA    | 1213 | A    | C4-C5-C6   | 6.60  | 120.30      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 149  | A    | C4-C5-C6   | 6.60  | 120.30      | 117.00   |
| 27  | B8    | 1501 | G    | O4'-C1'-N9 | 6.60  | 113.48      | 108.20   |
| 27  | B8    | 2842 | G    | C5-C6-O6   | -6.60 | 124.64      | 128.60   |
| 1   | AA    | 145  | G    | O4'-C1'-N9 | 6.60  | 113.48      | 108.20   |
| 1   | AA    | 1014 | A    | C5-C6-N6   | -6.60 | 118.42      | 123.70   |
| 1   | AA    | 1259 | C    | N3-C4-N4   | 6.60  | 122.62      | 118.00   |
| 27  | B8    | 159  | G    | O4'-C1'-N9 | 6.60  | 113.48      | 108.20   |
| 27  | B8    | 522  | A    | C5-C6-N6   | -6.60 | 118.42      | 123.70   |
| 27  | B8    | 728  | G    | C5-C6-O6   | -6.60 | 124.64      | 128.60   |
| 27  | B8    | 1690 | A    | C4-C5-C6   | 6.60  | 120.30      | 117.00   |
| 27  | B8    | 1798 | U    | O4'-C1'-N1 | 6.60  | 113.48      | 108.20   |
| 27  | B8    | 2220 | U    | O4'-C1'-N1 | 6.60  | 113.48      | 108.20   |
| 27  | B8    | 2533 | U    | O4'-C1'-N1 | 6.60  | 113.48      | 108.20   |
| 1   | AA    | 1171 | A    | O4'-C1'-N9 | 6.60  | 113.48      | 108.20   |
| 27  | B8    | 180  | G    | C5-C6-O6   | -6.60 | 124.64      | 128.60   |
| 27  | B8    | 1032 | A    | O4'-C1'-N9 | 6.60  | 113.48      | 108.20   |
| 1   | AA    | 118  | U    | O4'-C1'-N1 | 6.60  | 113.48      | 108.20   |
| 27  | B8    | 2289 | G    | C5-C6-O6   | -6.60 | 124.64      | 128.60   |
| 1   | AA    | 96   | U    | O4'-C1'-N1 | 6.60  | 113.48      | 108.20   |
| 1   | AA    | 478  | A    | O4'-C1'-N9 | 6.60  | 113.48      | 108.20   |
| 1   | AA    | 502  | A    | C5-C6-N6   | -6.60 | 118.42      | 123.70   |
| 1   | AA    | 843  | U    | O4'-C1'-N1 | 6.59  | 113.47      | 108.20   |
| 1   | AA    | 927  | G    | O4'-C1'-N9 | 6.59  | 113.48      | 108.20   |
| 1   | AA    | 1490 | U    | O4'-C1'-N1 | 6.59  | 113.47      | 108.20   |
| 27  | B8    | 998  | C    | N3-C4-N4   | 6.59  | 122.62      | 118.00   |
| 27  | B8    | 1493 | C    | C6-N1-C1'  | -6.59 | 112.89      | 120.80   |
| 27  | B8    | 2877 | G    | O4'-C1'-N9 | 6.59  | 113.47      | 108.20   |
| 27  | B8    | 2879 | A    | C5-C6-N6   | -6.59 | 118.42      | 123.70   |
| 1   | AA    | 1347 | G    | C5-C6-O6   | -6.59 | 124.64      | 128.60   |
| 27  | B8    | 327  | G    | O4'-C1'-N9 | 6.59  | 113.47      | 108.20   |
| 27  | B8    | 756  | A    | C5-C6-N6   | -6.59 | 118.43      | 123.70   |
| 27  | B8    | 891  | G    | C5-C6-O6   | -6.59 | 124.64      | 128.60   |
| 27  | B8    | 1477 | A    | C4-C5-C6   | 6.59  | 120.30      | 117.00   |
| 27  | B8    | 1549 | A    | O4'-C1'-N9 | 6.59  | 113.47      | 108.20   |
| 27  | B8    | 2504 | U    | O4'-C1'-N1 | 6.59  | 113.47      | 108.20   |
| 1   | AA    | 1197 | A    | C4-C5-C6   | 6.59  | 120.30      | 117.00   |
| 27  | B8    | 2048 | G    | C5-C6-O6   | -6.59 | 124.65      | 128.60   |
| 1   | AA    | 696  | A    | O4'-C1'-N9 | 6.59  | 113.47      | 108.20   |
| 1   | AA    | 860  | A    | C4-C5-C6   | 6.59  | 120.30      | 117.00   |
| 1   | AA    | 1418 | A    | C4-C5-C6   | 6.59  | 120.30      | 117.00   |
| 27  | B8    | 1716 | U    | O4'-C1'-N1 | 6.59  | 113.47      | 108.20   |
| 27  | B8    | 2478 | A    | C4-C5-C6   | 6.59  | 120.30      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2668 | G    | O4'-C1'-N9 | 6.59  | 113.47      | 108.20   |
| 27  | B8    | 530  | G    | C5-C6-O6   | -6.59 | 124.65      | 128.60   |
| 27  | B8    | 1182 | G    | O4'-C1'-N9 | 6.59  | 113.47      | 108.20   |
| 27  | B8    | 2149 | U    | O4'-C1'-N1 | 6.59  | 113.47      | 108.20   |
| 27  | B8    | 2865 | U    | O4'-C1'-N1 | 6.59  | 113.47      | 108.20   |
| 1   | AA    | 126  | G    | O4'-C1'-N9 | 6.59  | 113.47      | 108.20   |
| 1   | AA    | 158  | G    | C5-C6-O6   | -6.59 | 124.65      | 128.60   |
| 1   | AA    | 1279 | G    | C5-C6-O6   | -6.59 | 124.65      | 128.60   |
| 27  | B8    | 408  | G    | O4'-C1'-N9 | 6.59  | 113.47      | 108.20   |
| 27  | B8    | 827  | U    | O4'-C1'-N1 | 6.59  | 113.47      | 108.20   |
| 27  | B8    | 1283 | G    | C5-C6-O6   | -6.59 | 124.65      | 128.60   |
| 27  | B8    | 1299 | G    | C5-C6-O6   | -6.59 | 124.65      | 128.60   |
| 27  | B8    | 1383 | A    | O4'-C1'-N9 | 6.59  | 113.47      | 108.20   |
| 27  | B8    | 1485 | U    | O4'-C1'-N1 | 6.59  | 113.47      | 108.20   |
| 27  | B8    | 1514 | G    | C5-C6-O6   | -6.59 | 124.65      | 128.60   |
| 27  | B8    | 1590 | A    | O4'-C1'-N9 | 6.59  | 113.47      | 108.20   |
| 27  | B8    | 2444 | G    | O4'-C1'-N9 | 6.59  | 113.47      | 108.20   |
| 27  | B8    | 1420 | A    | C4-C5-C6   | 6.58  | 120.29      | 117.00   |
| 27  | B8    | 1774 | C    | O4'-C1'-N1 | 6.58  | 113.47      | 108.20   |
| 1   | AA    | 377  | G    | O4'-C1'-N9 | 6.58  | 113.47      | 108.20   |
| 1   | AA    | 588  | G    | C5-C6-O6   | -6.58 | 124.65      | 128.60   |
| 27  | B8    | 74   | A    | C4-C5-C6   | 6.58  | 120.29      | 117.00   |
| 27  | B8    | 443  | A    | C4-C5-C6   | 6.58  | 120.29      | 117.00   |
| 27  | B8    | 577  | G    | C5-C6-O6   | -6.58 | 124.65      | 128.60   |
| 1   | AA    | 595  | A    | C5-C6-N6   | -6.58 | 118.43      | 123.70   |
| 1   | AA    | 1144 | G    | C5-C6-O6   | -6.58 | 124.65      | 128.60   |
| 27  | B8    | 2119 | A    | C4-C5-C6   | 6.58  | 120.29      | 117.00   |
| 27  | B8    | 2121 | G    | C5-C6-O6   | -6.58 | 124.65      | 128.60   |
| 27  | B8    | 2194 | U    | O4'-C1'-N1 | 6.58  | 113.47      | 108.20   |
| 27  | B8    | 2294 | G    | C5-C6-O6   | -6.58 | 124.65      | 128.60   |
| 1   | AA    | 730  | G    | C5-C6-O6   | -6.58 | 124.65      | 128.60   |
| 1   | AA    | 971  | G    | O4'-C1'-N9 | 6.58  | 113.46      | 108.20   |
| 1   | AA    | 1225 | A    | C4-C5-C6   | 6.58  | 120.29      | 117.00   |
| 3   | AV    | 13   | C    | N3-C4-N4   | 6.58  | 122.61      | 118.00   |
| 27  | B8    | 307  | G    | C5-C6-O6   | -6.58 | 124.65      | 128.60   |
| 27  | B8    | 2494 | G    | C5-C6-O6   | -6.58 | 124.65      | 128.60   |
| 1   | AA    | 267  | C    | N3-C4-N4   | 6.58  | 122.60      | 118.00   |
| 27  | B8    | 198  | C    | N3-C4-N4   | 6.58  | 122.61      | 118.00   |
| 27  | B8    | 402  | A    | C4-C5-C6   | 6.58  | 120.29      | 117.00   |
| 27  | B8    | 493  | G    | O4'-C1'-N9 | 6.58  | 113.46      | 108.20   |
| 27  | B8    | 1223 | G    | C5-C6-O6   | -6.58 | 124.65      | 128.60   |
| 27  | B8    | 1352 | U    | O4'-C1'-N1 | 6.58  | 113.46      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1521 | G    | C5-C6-O6   | -6.58 | 124.65      | 128.60   |
| 27  | B8    | 2370 | G    | C5-C6-O6   | -6.58 | 124.65      | 128.60   |
| 1   | AA    | 1258 | G    | O4'-C1'-N9 | 6.58  | 113.46      | 108.20   |
| 27  | B8    | 1936 | A    | C4-C5-C6   | 6.58  | 120.29      | 117.00   |
| 1   | AA    | 253  | A    | O4'-C1'-N9 | 6.58  | 113.46      | 108.20   |
| 27  | B8    | 1047 | G    | C5-C6-O6   | -6.58 | 124.65      | 128.60   |
| 27  | B8    | 1213 | A    | C5-C6-N1   | -6.58 | 114.41      | 117.70   |
| 27  | B8    | 1766 | G    | O4'-C1'-N9 | 6.58  | 113.46      | 108.20   |
| 27  | B8    | 2092 | U    | O4'-C1'-N1 | 6.58  | 113.46      | 108.20   |
| 27  | B8    | 2802 | G    | O4'-C1'-N9 | 6.58  | 113.46      | 108.20   |
| 1   | AA    | 149  | A    | C4-C5-C6   | 6.57  | 120.29      | 117.00   |
| 1   | AA    | 865  | A    | C4-C5-C6   | 6.57  | 120.29      | 117.00   |
| 1   | AA    | 1416 | G    | C5-C6-O6   | -6.57 | 124.66      | 128.60   |
| 27  | B8    | 443  | A    | C5-C6-N6   | -6.57 | 118.44      | 123.70   |
| 27  | B8    | 1031 | G    | O4'-C1'-N9 | 6.57  | 113.46      | 108.20   |
| 27  | B8    | 983  | A    | C4-C5-C6   | 6.57  | 120.29      | 117.00   |
| 27  | B8    | 1045 | C    | N3-C4-N4   | 6.57  | 122.60      | 118.00   |
| 1   | AA    | 315  | A    | O4'-C1'-N9 | 6.57  | 113.46      | 108.20   |
| 1   | AA    | 566  | G    | N1-C6-O6   | 6.57  | 123.84      | 119.90   |
| 1   | AA    | 890  | G    | C5-C6-O6   | -6.57 | 124.66      | 128.60   |
| 1   | AA    | 1432 | G    | C5-C6-O6   | -6.57 | 124.66      | 128.60   |
| 27  | B8    | 359  | G    | O4'-C1'-N9 | 6.57  | 113.46      | 108.20   |
| 27  | B8    | 879  | G    | C5-C6-O6   | -6.57 | 124.66      | 128.60   |
| 27  | B8    | 1604 | C    | N3-C4-N4   | 6.57  | 122.60      | 118.00   |
| 27  | B8    | 2529 | G    | C5-C6-O6   | -6.57 | 124.66      | 128.60   |
| 27  | B8    | 36   | G    | C5-C6-O6   | -6.57 | 124.66      | 128.60   |
| 27  | B8    | 117  | G    | C5-C6-O6   | -6.57 | 124.66      | 128.60   |
| 27  | B8    | 233  | A    | C4-C5-C6   | 6.57  | 120.28      | 117.00   |
| 27  | B8    | 333  | G    | C5-C6-O6   | -6.57 | 124.66      | 128.60   |
| 27  | B8    | 1378 | A    | C4-C5-C6   | 6.57  | 120.28      | 117.00   |
| 3   | AV    | 7    | G    | C5-C6-O6   | -6.57 | 124.66      | 128.60   |
| 27  | B8    | 388  | G    | C5-C6-O6   | -6.57 | 124.66      | 128.60   |
| 27  | B8    | 696  | G    | O4'-C1'-N9 | 6.57  | 113.45      | 108.20   |
| 27  | B8    | 2817 | U    | O4'-C1'-N1 | 6.57  | 113.45      | 108.20   |
| 1   | AA    | 360  | G    | C5-C6-O6   | -6.56 | 124.66      | 128.60   |
| 1   | AA    | 3    | A    | C4-C5-C6   | 6.56  | 120.28      | 117.00   |
| 1   | AA    | 768  | A    | O4'-C1'-N9 | 6.56  | 113.45      | 108.20   |
| 1   | AA    | 994  | A    | C4-C5-C6   | 6.56  | 120.28      | 117.00   |
| 3   | AV    | 49   | C    | O4'-C1'-N1 | 6.56  | 113.45      | 108.20   |
| 27  | B8    | 488  | G    | C5-C6-O6   | -6.56 | 124.66      | 128.60   |
| 27  | B8    | 1186 | G    | O4'-C1'-N9 | 6.56  | 113.45      | 108.20   |
| 27  | B8    | 1508 | A    | O4'-C1'-N9 | 6.56  | 113.45      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1571 | A    | C5-C6-N1   | -6.56 | 114.42      | 117.70   |
| 27  | B8    | 2174 | C    | N3-C4-N4   | 6.56  | 122.59      | 118.00   |
| 27  | B8    | 2190 | G    | O4'-C1'-N9 | 6.56  | 113.45      | 108.20   |
| 27  | B8    | 2740 | A    | O4'-C1'-N9 | 6.56  | 113.45      | 108.20   |
| 1   | AA    | 338  | A    | O4'-C1'-N9 | 6.56  | 113.45      | 108.20   |
| 1   | AA    | 780  | A    | O4'-C1'-N9 | 6.56  | 113.45      | 108.20   |
| 1   | AA    | 1440 | U    | O4'-C1'-N1 | 6.56  | 113.45      | 108.20   |
| 1   | AA    | 14   | U    | O4'-C1'-N1 | 6.56  | 113.45      | 108.20   |
| 1   | AA    | 1001 | C    | N3-C4-N4   | 6.56  | 122.59      | 118.00   |
| 27  | B8    | 53   | A    | C4-C5-C6   | 6.56  | 120.28      | 117.00   |
| 27  | B8    | 113  | U    | O4'-C1'-N1 | 6.56  | 113.45      | 108.20   |
| 27  | B8    | 195  | A    | C4-C5-C6   | 6.56  | 120.28      | 117.00   |
| 27  | B8    | 2659 | G    | C5-C6-O6   | -6.56 | 124.66      | 128.60   |
| 1   | AA    | 63   | C    | O4'-C1'-N1 | 6.56  | 113.45      | 108.20   |
| 1   | AA    | 1355 | G    | C5-C6-O6   | -6.56 | 124.67      | 128.60   |
| 27  | B8    | 664  | G    | O4'-C1'-N9 | 6.56  | 113.45      | 108.20   |
| 27  | B8    | 1073 | A    | C5-C6-N6   | -6.56 | 118.45      | 123.70   |
| 1   | AA    | 16   | A    | C5-C6-N6   | -6.55 | 118.46      | 123.70   |
| 1   | AA    | 504  | C    | N3-C4-N4   | 6.55  | 122.59      | 118.00   |
| 1   | AA    | 598  | U    | O4'-C1'-N1 | 6.55  | 113.44      | 108.20   |
| 1   | AA    | 1303 | C    | O4'-C1'-N1 | 6.55  | 113.44      | 108.20   |
| 27  | B8    | 225  | C    | O4'-C1'-N1 | 6.55  | 113.44      | 108.20   |
| 27  | B8    | 2115 | G    | C5-C6-O6   | -6.55 | 124.67      | 128.60   |
| 27  | B8    | 2862 | G    | O4'-C1'-N9 | 6.55  | 113.44      | 108.20   |
| 27  | B8    | 414  | C    | N3-C4-N4   | 6.55  | 122.59      | 118.00   |
| 27  | B8    | 421  | C    | O4'-C1'-N1 | 6.55  | 113.44      | 108.20   |
| 1   | AA    | 1426 | G    | C5-C6-O6   | -6.55 | 124.67      | 128.60   |
| 27  | B8    | 233  | A    | C5-C6-N6   | -6.55 | 118.46      | 123.70   |
| 27  | B8    | 399  | U    | O4'-C1'-N1 | 6.55  | 113.44      | 108.20   |
| 27  | B8    | 503  | A    | C5-C6-N6   | -6.55 | 118.46      | 123.70   |
| 27  | B8    | 1021 | A    | C4-C5-C6   | 6.55  | 120.28      | 117.00   |
| 27  | B8    | 2822 | G    | C5-C6-O6   | -6.55 | 124.67      | 128.60   |
| 27  | B8    | 1987 | A    | O4'-C1'-N9 | 6.55  | 113.44      | 108.20   |
| 27  | B8    | 95   | A    | C4-C5-C6   | 6.55  | 120.27      | 117.00   |
| 27  | B8    | 298  | G    | C5-C6-O6   | -6.55 | 124.67      | 128.60   |
| 27  | B8    | 880  | G    | C5-C6-O6   | -6.55 | 124.67      | 128.60   |
| 27  | B8    | 1945 | G    | C5-C6-O6   | -6.55 | 124.67      | 128.60   |
| 27  | B8    | 2237 | G    | C5-C6-O6   | -6.55 | 124.67      | 128.60   |
| 27  | B8    | 2311 | A    | C4-C5-C6   | 6.55  | 120.27      | 117.00   |
| 27  | B8    | 2400 | G    | O4'-C1'-N9 | 6.55  | 113.44      | 108.20   |
| 27  | B8    | 2597 | G    | C5-C6-O6   | -6.55 | 124.67      | 128.60   |
| 1   | AA    | 944  | G    | C5-C6-O6   | -6.54 | 124.67      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1305 | G    | C5-C6-O6   | -6.54 | 124.67      | 128.60   |
| 1   | AA    | 1386 | G    | O4'-C1'-N9 | 6.54  | 113.44      | 108.20   |
| 1   | AA    | 1542 | A    | C4-C5-C6   | 6.54  | 120.27      | 117.00   |
| 27  | B8    | 191  | A    | O4'-C1'-N9 | 6.54  | 113.44      | 108.20   |
| 27  | B8    | 2842 | G    | O4'-C1'-N9 | 6.54  | 113.44      | 108.20   |
| 27  | B8    | 1175 | A    | C4-C5-C6   | 6.54  | 120.27      | 117.00   |
| 27  | B8    | 1419 | A    | C4-C5-C6   | 6.54  | 120.27      | 117.00   |
| 27  | B8    | 2328 | A    | C4-C5-C6   | 6.54  | 120.27      | 117.00   |
| 1   | AA    | 35   | G    | C5-C6-O6   | -6.54 | 124.67      | 128.60   |
| 1   | AA    | 307  | C    | O4'-C1'-N1 | 6.54  | 113.43      | 108.20   |
| 27  | B8    | 831  | G    | O4'-C1'-N9 | 6.54  | 113.43      | 108.20   |
| 27  | B8    | 1671 | U    | O4'-C1'-N1 | 6.54  | 113.43      | 108.20   |
| 27  | B8    | 2681 | C    | O4'-C1'-N1 | 6.54  | 113.43      | 108.20   |
| 1   | AA    | 1222 | G    | C5-C6-O6   | -6.54 | 124.68      | 128.60   |
| 3   | AV    | 9    | A    | C4-C5-C6   | 6.54  | 120.27      | 117.00   |
| 27  | B8    | 619  | G    | C5-C6-O6   | -6.54 | 124.68      | 128.60   |
| 27  | B8    | 2872 | A    | C4-C5-C6   | 6.54  | 120.27      | 117.00   |
| 1   | AA    | 226  | G    | C5-C6-O6   | -6.54 | 124.68      | 128.60   |
| 1   | AA    | 691  | G    | C5-C6-O6   | -6.54 | 124.68      | 128.60   |
| 1   | AA    | 693  | G    | C5-C6-O6   | -6.54 | 124.68      | 128.60   |
| 1   | AA    | 1055 | A    | C4-C5-C6   | 6.54  | 120.27      | 117.00   |
| 1   | AA    | 1149 | C    | N3-C4-N4   | 6.54  | 122.58      | 118.00   |
| 26  | B7    | 15   | A    | C4-C5-C6   | 6.54  | 120.27      | 117.00   |
| 27  | B8    | 731  | C    | N3-C4-N4   | 6.54  | 122.58      | 118.00   |
| 27  | B8    | 927  | A    | O4'-C1'-N9 | 6.54  | 113.43      | 108.20   |
| 27  | B8    | 1252 | G    | C5-C6-O6   | -6.54 | 124.68      | 128.60   |
| 27  | B8    | 1946 | U    | O4'-C1'-N1 | 6.54  | 113.43      | 108.20   |
| 27  | B8    | 253  | C    | N3-C4-N4   | 6.54  | 122.58      | 118.00   |
| 27  | B8    | 434  | U    | O4'-C1'-N1 | 6.54  | 113.43      | 108.20   |
| 27  | B8    | 1226 | A    | C4-C5-C6   | 6.54  | 120.27      | 117.00   |
| 27  | B8    | 2112 | G    | O4'-C1'-N9 | 6.54  | 113.43      | 108.20   |
| 1   | AA    | 1077 | G    | C5-C6-O6   | -6.54 | 124.68      | 128.60   |
| 27  | B8    | 174  | U    | O4'-C1'-N1 | 6.54  | 113.43      | 108.20   |
| 27  | B8    | 1412 | U    | O4'-C1'-N1 | 6.54  | 113.43      | 108.20   |
| 27  | B8    | 2010 | G    | C5-C6-O6   | -6.54 | 124.68      | 128.60   |
| 27  | B8    | 2040 | G    | O4'-C1'-N9 | 6.54  | 113.43      | 108.20   |
| 27  | B8    | 2068 | U    | O4'-C1'-N1 | 6.54  | 113.43      | 108.20   |
| 27  | B8    | 2268 | A    | C4-C5-C6   | 6.54  | 120.27      | 117.00   |
| 27  | B8    | 2611 | C    | O4'-C1'-N1 | 6.54  | 113.43      | 108.20   |
| 1   | AA    | 190  | A    | C5-C6-N1   | -6.53 | 114.43      | 117.70   |
| 1   | AA    | 260  | G    | C5-C6-O6   | -6.53 | 124.68      | 128.60   |
| 27  | B8    | 1911 | U    | O4'-C1'-N1 | 6.53  | 113.43      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 43   | G    | C5-C6-O6   | -6.53 | 124.68      | 128.60   |
| 1   | AA    | 86   | G    | C5-C6-O6   | -6.53 | 124.68      | 128.60   |
| 1   | AA    | 92   | U    | O4'-C1'-N1 | 6.53  | 113.42      | 108.20   |
| 1   | AA    | 141  | G    | O4'-C1'-N9 | 6.53  | 113.42      | 108.20   |
| 1   | AA    | 412  | A    | C4-C5-C6   | 6.53  | 120.27      | 117.00   |
| 1   | AA    | 947  | G    | O4'-C1'-N9 | 6.53  | 113.42      | 108.20   |
| 1   | AA    | 1426 | G    | O4'-C1'-N9 | 6.53  | 113.42      | 108.20   |
| 3   | AV    | 50   | G    | C5-C6-O6   | -6.53 | 124.68      | 128.60   |
| 26  | B7    | 119  | A    | O4'-C1'-N9 | 6.53  | 113.42      | 108.20   |
| 1   | AA    | 283  | U    | O4'-C1'-N1 | 6.53  | 113.42      | 108.20   |
| 3   | AV    | 33   | A    | O4'-C1'-N9 | 6.53  | 113.42      | 108.20   |
| 27  | B8    | 2677 | G    | O4'-C1'-N9 | 6.53  | 113.42      | 108.20   |
| 3   | AV    | 37   | G    | C5-C6-O6   | -6.53 | 124.68      | 128.60   |
| 27  | B8    | 35   | G    | O4'-C1'-N9 | 6.53  | 113.42      | 108.20   |
| 27  | B8    | 458  | G    | O4'-C1'-N9 | 6.53  | 113.42      | 108.20   |
| 1   | AA    | 512  | U    | O4'-C1'-N1 | 6.53  | 113.42      | 108.20   |
| 27  | B8    | 93   | G    | C5-C6-O6   | -6.53 | 124.69      | 128.60   |
| 27  | B8    | 476  | G    | C5-C6-O6   | -6.53 | 124.68      | 128.60   |
| 27  | B8    | 888  | C    | O4'-C1'-N1 | 6.53  | 113.42      | 108.20   |
| 27  | B8    | 1811 | G    | C5-C6-O6   | -6.53 | 124.69      | 128.60   |
| 27  | B8    | 2034 | U    | O4'-C1'-N1 | 6.53  | 113.42      | 108.20   |
| 1   | AA    | 183  | C    | O4'-C1'-N1 | 6.52  | 113.42      | 108.20   |
| 1   | AA    | 220  | G    | O4'-C1'-N9 | 6.52  | 113.42      | 108.20   |
| 1   | AA    | 996  | A    | C5-C6-N6   | -6.52 | 118.48      | 123.70   |
| 27  | B8    | 2060 | A    | O4'-C1'-N9 | 6.52  | 113.42      | 108.20   |
| 27  | B8    | 2779 | U    | O4'-C1'-N1 | 6.52  | 113.42      | 108.20   |
| 1   | AA    | 654  | G    | C5-C6-O6   | -6.52 | 124.69      | 128.60   |
| 27  | B8    | 609  | A    | C4-C5-C6   | 6.52  | 120.26      | 117.00   |
| 1   | AA    | 901  | A    | C5-C6-N6   | -6.52 | 118.48      | 123.70   |
| 27  | B8    | 2873 | A    | C4-C5-C6   | 6.52  | 120.26      | 117.00   |
| 1   | AA    | 313  | A    | C4-C5-C6   | 6.52  | 120.26      | 117.00   |
| 1   | AA    | 351  | G    | C5-C6-O6   | -6.52 | 124.69      | 128.60   |
| 1   | AA    | 1002 | G    | O4'-C1'-N9 | 6.52  | 113.42      | 108.20   |
| 26  | B7    | 58   | A    | C4-C5-C6   | 6.52  | 120.26      | 117.00   |
| 27  | B8    | 1408 | G    | C5-C6-O6   | -6.52 | 124.69      | 128.60   |
| 27  | B8    | 1876 | A    | N1-C6-N6   | 6.52  | 122.51      | 118.60   |
| 1   | AA    | 583  | A    | O4'-C1'-N9 | 6.52  | 113.41      | 108.20   |
| 1   | AA    | 592  | G    | O4'-C1'-N9 | 6.52  | 113.42      | 108.20   |
| 1   | AA    | 1387 | G    | O4'-C1'-N9 | 6.52  | 113.41      | 108.20   |
| 26  | B7    | 64   | G    | O4'-C1'-N9 | 6.52  | 113.41      | 108.20   |
| 27  | B8    | 1668 | A    | P-O3'-C3'  | 6.52  | 127.52      | 119.70   |
| 27  | B8    | 2766 | A    | C4-C5-C6   | 6.52  | 120.26      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 776  | G    | O4'-C1'-N9 | 6.52  | 113.41      | 108.20   |
| 27  | B8    | 1577 | C    | N3-C4-N4   | 6.52  | 122.56      | 118.00   |
| 27  | B8    | 544  | C    | C2-N1-C1'  | 6.51  | 125.97      | 118.80   |
| 27  | B8    | 1002 | G    | O4'-C1'-N9 | 6.51  | 113.41      | 108.20   |
| 27  | B8    | 1532 | A    | C5-C6-N6   | -6.51 | 118.49      | 123.70   |
| 26  | B7    | 76   | G    | C5-C6-O6   | -6.51 | 124.69      | 128.60   |
| 27  | B8    | 2627 | G    | C5-C6-O6   | -6.51 | 124.69      | 128.60   |
| 1   | AA    | 44   | A    | O4'-C1'-N9 | 6.51  | 113.41      | 108.20   |
| 1   | AA    | 250  | A    | C4-C5-C6   | 6.51  | 120.25      | 117.00   |
| 1   | AA    | 532  | A    | C4-C5-C6   | 6.51  | 120.26      | 117.00   |
| 1   | AA    | 1222 | G    | O4'-C1'-N9 | 6.51  | 113.41      | 108.20   |
| 1   | AA    | 1434 | A    | O4'-C1'-N9 | 6.51  | 113.41      | 108.20   |
| 27  | B8    | 58   | G    | C5-C6-O6   | -6.51 | 124.69      | 128.60   |
| 27  | B8    | 708  | G    | O4'-C1'-N9 | 6.51  | 113.41      | 108.20   |
| 1   | AA    | 782  | A    | O4'-C1'-N9 | 6.51  | 113.41      | 108.20   |
| 27  | B8    | 213  | A    | C5-C6-N6   | -6.51 | 118.49      | 123.70   |
| 27  | B8    | 315  | G    | C5-C6-O6   | -6.51 | 124.69      | 128.60   |
| 27  | B8    | 855  | G    | C5-C6-O6   | -6.51 | 124.69      | 128.60   |
| 27  | B8    | 95   | A    | C5-C6-N6   | -6.51 | 118.49      | 123.70   |
| 27  | B8    | 424  | G    | O4'-C1'-N9 | 6.51  | 113.41      | 108.20   |
| 27  | B8    | 515  | A    | C5-C6-N6   | -6.51 | 118.49      | 123.70   |
| 27  | B8    | 2524 | G    | O4'-C1'-N9 | 6.51  | 113.41      | 108.20   |
| 1   | AA    | 12   | U    | O4'-C1'-N1 | 6.51  | 113.41      | 108.20   |
| 27  | B8    | 1334 | G    | C5-C6-O6   | -6.51 | 124.70      | 128.60   |
| 27  | B8    | 1564 | C    | N3-C4-N4   | 6.51  | 122.56      | 118.00   |
| 27  | B8    | 1756 | G    | C5-C6-O6   | -6.51 | 124.70      | 128.60   |
| 1   | AA    | 38   | G    | C5-C6-O6   | -6.50 | 124.70      | 128.60   |
| 27  | B8    | 391  | A    | C4-C5-C6   | 6.50  | 120.25      | 117.00   |
| 1   | AA    | 1063 | C    | N3-C4-N4   | 6.50  | 122.55      | 118.00   |
| 1   | AA    | 1219 | A    | C4-C5-C6   | 6.50  | 120.25      | 117.00   |
| 1   | AA    | 1417 | G    | C5-C6-O6   | -6.50 | 124.70      | 128.60   |
| 1   | AA    | 259  | G    | O4'-C1'-N9 | 6.50  | 113.40      | 108.20   |
| 1   | AA    | 731  | G    | O4'-C1'-N9 | 6.50  | 113.40      | 108.20   |
| 27  | B8    | 1026 | G    | O4'-C1'-N9 | 6.50  | 113.40      | 108.20   |
| 27  | B8    | 1531 | C    | N3-C4-N4   | 6.50  | 122.55      | 118.00   |
| 27  | B8    | 2138 | G    | C5-C6-O6   | -6.50 | 124.70      | 128.60   |
| 1   | AA    | 712  | A    | O4'-C1'-N9 | 6.50  | 113.40      | 108.20   |
| 27  | B8    | 400  | G    | N3-C2-N2   | 6.50  | 124.45      | 119.90   |
| 27  | B8    | 2212 | A    | C4-C5-C6   | 6.50  | 120.25      | 117.00   |
| 27  | B8    | 2508 | G    | O4'-C1'-N9 | 6.50  | 113.40      | 108.20   |
| 1   | AA    | 256  | U    | O4'-C1'-N1 | 6.50  | 113.40      | 108.20   |
| 1   | AA    | 1262 | C    | N3-C4-N4   | 6.50  | 122.55      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | B8    | 871  | U    | O4'-C1'-N1  | 6.50  | 113.40      | 108.20   |
| 27  | B8    | 1948 | G    | O4'-C1'-N9  | 6.50  | 113.40      | 108.20   |
| 1   | AA    | 376  | G    | C5-C6-O6    | -6.50 | 124.70      | 128.60   |
| 27  | B8    | 230  | G    | O4'-C1'-N9  | 6.50  | 113.40      | 108.20   |
| 27  | B8    | 1088 | A    | O4'-C1'-N9  | 6.50  | 113.40      | 108.20   |
| 27  | B8    | 1702 | G    | O4'-C1'-N9  | 6.50  | 113.40      | 108.20   |
| 1   | AA    | 472  | U    | O4'-C1'-N1  | 6.50  | 113.40      | 108.20   |
| 1   | AA    | 1263 | C    | N3-C4-N4    | 6.50  | 122.55      | 118.00   |
| 27  | B8    | 560  | C    | N3-C4-N4    | 6.50  | 122.55      | 118.00   |
| 27  | B8    | 1700 | A    | C4-C5-C6    | 6.50  | 120.25      | 117.00   |
| 27  | B8    | 2282 | G    | C5-C6-O6    | -6.50 | 124.70      | 128.60   |
| 1   | AA    | 82   | G    | C5-C6-O6    | -6.49 | 124.70      | 128.60   |
| 1   | AA    | 262  | A    | C5-C6-N6    | -6.49 | 118.50      | 123.70   |
| 1   | AA    | 305  | G    | C5-C6-O6    | -6.49 | 124.70      | 128.60   |
| 1   | AA    | 926  | G    | C5-C6-O6    | -6.49 | 124.70      | 128.60   |
| 27  | B8    | 689  | A    | C5-C6-N6    | -6.49 | 118.50      | 123.70   |
| 27  | B8    | 872  | U    | O4'-C1'-N1  | 6.49  | 113.39      | 108.20   |
| 27  | B8    | 876  | C    | C5'-C4'-O4' | 6.49  | 116.89      | 109.10   |
| 27  | B8    | 1471 | G    | C5-C6-O6    | -6.49 | 124.70      | 128.60   |
| 27  | B8    | 2432 | A    | C4-C5-C6    | 6.49  | 120.25      | 117.00   |
| 27  | B8    | 2611 | C    | N3-C4-N4    | 6.49  | 122.55      | 118.00   |
| 27  | B8    | 412  | A    | C4-C5-C6    | 6.49  | 120.25      | 117.00   |
| 27  | B8    | 1819 | A    | C4-C5-C6    | 6.49  | 120.25      | 117.00   |
| 1   | AA    | 475  | C    | N3-C4-N4    | 6.49  | 122.54      | 118.00   |
| 1   | AA    | 694  | A    | C4-C5-C6    | 6.49  | 120.25      | 117.00   |
| 1   | AA    | 789  | U    | O4'-C1'-N1  | 6.49  | 113.39      | 108.20   |
| 27  | B8    | 973  | A    | C4-C5-C6    | 6.49  | 120.25      | 117.00   |
| 27  | B8    | 1237 | A    | C4-C5-C6    | 6.49  | 120.25      | 117.00   |
| 27  | B8    | 1613 | G    | O4'-C1'-N9  | 6.49  | 113.39      | 108.20   |
| 27  | B8    | 2051 | A    | C5-C6-N6    | -6.49 | 118.51      | 123.70   |
| 27  | B8    | 2537 | U    | O4'-C1'-N1  | 6.49  | 113.39      | 108.20   |
| 27  | B8    | 2774 | C    | N3-C4-N4    | 6.49  | 122.54      | 118.00   |
| 27  | B8    | 2821 | A    | C4-C5-C6    | 6.49  | 120.25      | 117.00   |
| 27  | B8    | 2573 | C    | C6-N1-C1'   | -6.49 | 113.01      | 120.80   |
| 1   | AA    | 1079 | G    | C5-C6-O6    | -6.49 | 124.71      | 128.60   |
| 27  | B8    | 2127 | G    | C5-C6-O6    | -6.49 | 124.71      | 128.60   |
| 27  | B8    | 2816 | G    | C5-C6-O6    | -6.49 | 124.71      | 128.60   |
| 27  | B8    | 2863 | C    | N3-C4-N4    | 6.49  | 122.54      | 118.00   |
| 1   | AA    | 597  | G    | O4'-C1'-N9  | 6.49  | 113.39      | 108.20   |
| 27  | B8    | 305  | C    | N3-C4-N4    | 6.49  | 122.54      | 118.00   |
| 27  | B8    | 1527 | G    | C5-C6-O6    | -6.49 | 124.71      | 128.60   |
| 1   | AA    | 410  | G    | O4'-C1'-N9  | 6.48  | 113.39      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1938 | A    | O4'-C1'-N9 | 6.48  | 113.39      | 108.20   |
| 1   | AA    | 187  | G    | C5-C6-O6   | -6.48 | 124.71      | 128.60   |
| 1   | AA    | 208  | U    | O4'-C1'-N1 | 6.48  | 113.39      | 108.20   |
| 27  | B8    | 532  | A    | C5-C6-N6   | -6.48 | 118.51      | 123.70   |
| 27  | B8    | 712  | G    | O4'-C1'-N9 | 6.48  | 113.39      | 108.20   |
| 27  | B8    | 1524 | G    | C5-C6-O6   | -6.48 | 124.71      | 128.60   |
| 27  | B8    | 1580 | A    | C4-C5-C6   | 6.48  | 120.24      | 117.00   |
| 27  | B8    | 2014 | A    | C4-C5-C6   | 6.48  | 120.24      | 117.00   |
| 27  | B8    | 2665 | A    | C4-C5-C6   | 6.48  | 120.24      | 117.00   |
| 27  | B8    | 2887 | A    | C4-C5-C6   | 6.48  | 120.24      | 117.00   |
| 1   | AA    | 574  | A    | C4-C5-C6   | 6.48  | 120.24      | 117.00   |
| 1   | AA    | 1123 | U    | O4'-C1'-N1 | 6.48  | 113.39      | 108.20   |
| 1   | AA    | 1415 | G    | C5-C6-O6   | -6.48 | 124.71      | 128.60   |
| 27  | B8    | 1263 | U    | O4'-C1'-N1 | 6.48  | 113.38      | 108.20   |
| 27  | B8    | 1371 | G    | O4'-C1'-N9 | 6.48  | 113.39      | 108.20   |
| 27  | B8    | 2154 | A    | C4-C5-C6   | 6.48  | 120.24      | 117.00   |
| 1   | AA    | 1111 | A    | C4-C5-C6   | 6.48  | 120.24      | 117.00   |
| 3   | AV    | 9    | A    | C5-C6-N6   | -6.48 | 118.52      | 123.70   |
| 26  | B7    | 46   | A    | C5-C6-N1   | -6.48 | 114.46      | 117.70   |
| 27  | B8    | 889  | C    | C2-N1-C1'  | 6.48  | 125.93      | 118.80   |
| 1   | AA    | 550  | G    | O4'-C1'-N9 | 6.48  | 113.38      | 108.20   |
| 1   | AA    | 737  | C    | N3-C4-N4   | 6.48  | 122.53      | 118.00   |
| 27  | B8    | 365  | U    | O4'-C1'-N1 | 6.48  | 113.38      | 108.20   |
| 27  | B8    | 570  | G    | C5-C6-O6   | -6.48 | 124.71      | 128.60   |
| 27  | B8    | 1578 | U    | O4'-C1'-N1 | 6.48  | 113.38      | 108.20   |
| 27  | B8    | 1648 | U    | O4'-C1'-N1 | 6.48  | 113.38      | 108.20   |
| 27  | B8    | 2568 | U    | O4'-C1'-N1 | 6.48  | 113.38      | 108.20   |
| 27  | B8    | 1066 | U    | O4'-C1'-N1 | 6.48  | 113.38      | 108.20   |
| 27  | B8    | 1483 | G    | C5-C6-O6   | -6.48 | 124.71      | 128.60   |
| 27  | B8    | 1872 | A    | C4-C5-C6   | 6.48  | 120.24      | 117.00   |
| 1   | AA    | 768  | A    | C4-C5-C6   | 6.47  | 120.24      | 117.00   |
| 1   | AA    | 1541 | U    | P-O3'-C3'  | 6.47  | 127.47      | 119.70   |
| 27  | B8    | 582  | A    | C5-C6-N6   | -6.47 | 118.52      | 123.70   |
| 27  | B8    | 1314 | C    | O4'-C1'-N1 | 6.47  | 113.38      | 108.20   |
| 27  | B8    | 2256 | G    | O4'-C1'-N9 | 6.47  | 113.38      | 108.20   |
| 27  | B8    | 2560 | A    | C5-C6-N1   | -6.47 | 114.46      | 117.70   |
| 1   | AA    | 133  | U    | O4'-C1'-N1 | 6.47  | 113.38      | 108.20   |
| 1   | AA    | 159  | G    | C5-C6-O6   | -6.47 | 124.72      | 128.60   |
| 27  | B8    | 982  | C    | C2-N1-C1'  | 6.47  | 125.92      | 118.80   |
| 27  | B8    | 1048 | A    | C4-C5-C6   | 6.47  | 120.24      | 117.00   |
| 27  | B8    | 1392 | A    | C4-C5-C6   | 6.47  | 120.24      | 117.00   |
| 27  | B8    | 2721 | A    | C4-C5-C6   | 6.47  | 120.24      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1306 | A    | C4-C5-C6   | 6.47  | 120.23      | 117.00   |
| 27  | B8    | 1121 | C    | N3-C4-N4   | 6.47  | 122.53      | 118.00   |
| 27  | B8    | 1166 | G    | C5-C6-O6   | -6.47 | 124.72      | 128.60   |
| 1   | AA    | 1434 | A    | C4-C5-C6   | 6.47  | 120.23      | 117.00   |
| 26  | B7    | 74   | U    | O4'-C1'-N1 | 6.47  | 113.38      | 108.20   |
| 27  | B8    | 882  | G    | C5-C6-O6   | -6.47 | 124.72      | 128.60   |
| 27  | B8    | 2662 | A    | C5-C6-N6   | -6.47 | 118.52      | 123.70   |
| 1   | AA    | 263  | A    | C4-C5-C6   | 6.47  | 120.23      | 117.00   |
| 1   | AA    | 541  | G    | O4'-C1'-N9 | 6.47  | 113.38      | 108.20   |
| 1   | AA    | 1324 | A    | C4-C5-C6   | 6.47  | 120.23      | 117.00   |
| 1   | AA    | 1459 | G    | O4'-C1'-N9 | 6.47  | 113.37      | 108.20   |
| 27  | B8    | 212  | G    | O4'-C1'-N9 | 6.47  | 113.37      | 108.20   |
| 27  | B8    | 1667 | G    | C5-C6-O6   | -6.47 | 124.72      | 128.60   |
| 1   | AA    | 6    | G    | C5-C6-O6   | -6.47 | 124.72      | 128.60   |
| 1   | AA    | 139  | A    | O4'-C1'-N9 | 6.47  | 113.37      | 108.20   |
| 1   | AA    | 886  | G    | C5-C6-O6   | -6.47 | 124.72      | 128.60   |
| 1   | AA    | 1488 | G    | C5-C6-O6   | -6.47 | 124.72      | 128.60   |
| 27  | B8    | 19   | A    | C5-C6-N6   | -6.47 | 118.53      | 123.70   |
| 27  | B8    | 2122 | U    | O4'-C1'-N1 | 6.47  | 113.37      | 108.20   |
| 1   | AA    | 477  | C    | N3-C4-N4   | 6.46  | 122.53      | 118.00   |
| 27  | B8    | 54   | G    | C5-C6-O6   | -6.46 | 124.72      | 128.60   |
| 27  | B8    | 207  | A    | O4'-C1'-N9 | 6.46  | 113.37      | 108.20   |
| 27  | B8    | 752  | A    | C4-C5-C6   | 6.46  | 120.23      | 117.00   |
| 27  | B8    | 1453 | A    | C4-C5-C6   | 6.46  | 120.23      | 117.00   |
| 27  | B8    | 1700 | A    | C5-C6-N6   | -6.46 | 118.53      | 123.70   |
| 27  | B8    | 277  | G    | O4'-C1'-N9 | 6.46  | 113.37      | 108.20   |
| 27  | B8    | 2735 | G    | C5-C6-O6   | -6.46 | 124.72      | 128.60   |
| 1   | AA    | 125  | U    | O4'-C1'-N1 | 6.46  | 113.37      | 108.20   |
| 1   | AA    | 247  | G    | C5-C6-O6   | -6.46 | 124.72      | 128.60   |
| 27  | B8    | 600  | G    | C5-C6-O6   | -6.46 | 124.72      | 128.60   |
| 27  | B8    | 1020 | A    | O4'-C1'-N9 | 6.46  | 113.37      | 108.20   |
| 27  | B8    | 2033 | A    | C4-C5-C6   | 6.46  | 120.23      | 117.00   |
| 27  | B8    | 2271 | G    | O4'-C1'-N9 | 6.46  | 113.37      | 108.20   |
| 27  | B8    | 2838 | G    | O4'-C1'-N9 | 6.46  | 113.37      | 108.20   |
| 1   | AA    | 540  | G    | O4'-C1'-N9 | 6.46  | 113.37      | 108.20   |
| 1   | AA    | 894  | G    | O4'-C1'-N9 | 6.46  | 113.37      | 108.20   |
| 3   | AV    | 19   | G    | C5-C6-O6   | -6.46 | 124.72      | 128.60   |
| 5   | A0    | 166  | TYR  | CB-CG-CD2  | -6.46 | 117.12      | 121.00   |
| 27  | B8    | 503  | A    | C4-C5-C6   | 6.46  | 120.23      | 117.00   |
| 27  | B8    | 1713 | A    | C4-C5-C6   | 6.46  | 120.23      | 117.00   |
| 27  | B8    | 2499 | C    | N3-C4-N4   | 6.46  | 122.52      | 118.00   |
| 1   | AA    | 138  | G    | O4'-C1'-N9 | 6.46  | 113.37      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 337  | G    | O4'-C1'-N9 | 6.46  | 113.37      | 108.20   |
| 1   | AA    | 756  | C    | N3-C4-N4   | 6.46  | 122.52      | 118.00   |
| 27  | B8    | 452  | G    | C5-C6-O6   | -6.46 | 124.72      | 128.60   |
| 27  | B8    | 1875 | G    | C5-C6-O6   | -6.46 | 124.72      | 128.60   |
| 27  | B8    | 2482 | A    | C4-C5-C6   | 6.46  | 120.23      | 117.00   |
| 27  | B8    | 2595 | G    | C5-C6-O6   | -6.46 | 124.72      | 128.60   |
| 1   | AA    | 19   | A    | C4-C5-C6   | 6.46  | 120.23      | 117.00   |
| 1   | AA    | 262  | A    | C5-C6-N1   | -6.46 | 114.47      | 117.70   |
| 1   | AA    | 818  | G    | C5-C6-O6   | -6.46 | 124.73      | 128.60   |
| 1   | AA    | 826  | C    | O4'-C1'-N1 | 6.46  | 113.37      | 108.20   |
| 27  | B8    | 110  | G    | O4'-C1'-N9 | 6.46  | 113.36      | 108.20   |
| 27  | B8    | 352  | A    | C4-C5-C6   | 6.46  | 120.23      | 117.00   |
| 27  | B8    | 592  | A    | O4'-C1'-N9 | 6.46  | 113.36      | 108.20   |
| 27  | B8    | 1189 | A    | C4-C5-C6   | 6.46  | 120.23      | 117.00   |
| 27  | B8    | 1589 | U    | O4'-C1'-N1 | 6.46  | 113.37      | 108.20   |
| 27  | B8    | 662  | G    | O4'-C1'-N9 | 6.46  | 113.36      | 108.20   |
| 1   | AA    | 1248 | A    | O4'-C1'-N9 | 6.45  | 113.36      | 108.20   |
| 27  | B8    | 2729 | G    | O4'-C1'-N9 | 6.45  | 113.36      | 108.20   |
| 1   | AA    | 557  | G    | C5-C6-O6   | -6.45 | 124.73      | 128.60   |
| 27  | B8    | 167  | A    | C4-C5-C6   | 6.45  | 120.23      | 117.00   |
| 27  | B8    | 1178 | C    | N3-C4-N4   | 6.45  | 122.52      | 118.00   |
| 1   | AA    | 628  | G    | C5-C6-O6   | -6.45 | 124.73      | 128.60   |
| 27  | B8    | 1283 | G    | O4'-C1'-N9 | 6.45  | 113.36      | 108.20   |
| 27  | B8    | 2190 | G    | C5-C6-O6   | -6.45 | 124.73      | 128.60   |
| 1   | AA    | 682  | G    | O4'-C1'-N9 | 6.45  | 113.36      | 108.20   |
| 1   | AA    | 1438 | G    | O4'-C1'-N9 | 6.45  | 113.36      | 108.20   |
| 26  | B7    | 119  | A    | C4-C5-C6   | 6.45  | 120.22      | 117.00   |
| 27  | B8    | 104  | A    | C5-C6-N6   | -6.45 | 118.54      | 123.70   |
| 27  | B8    | 114  | U    | O4'-C1'-N1 | 6.45  | 113.36      | 108.20   |
| 27  | B8    | 1535 | A    | C4-C5-C6   | 6.45  | 120.22      | 117.00   |
| 27  | B8    | 1862 | G    | O4'-C1'-N9 | 6.45  | 113.36      | 108.20   |
| 27  | B8    | 2811 | G    | O4'-C1'-N9 | 6.45  | 113.36      | 108.20   |
| 27  | B8    | 2895 | G    | O4'-C1'-N9 | 6.45  | 113.36      | 108.20   |
| 1   | AA    | 1441 | A    | O4'-C1'-N9 | 6.45  | 113.36      | 108.20   |
| 26  | B7    | 35   | C    | C2-N1-C1'  | 6.45  | 125.89      | 118.80   |
| 27  | B8    | 1235 | G    | C5-C6-O6   | -6.45 | 124.73      | 128.60   |
| 27  | B8    | 1315 | C    | N3-C4-N4   | 6.45  | 122.51      | 118.00   |
| 27  | B8    | 2544 | G    | O4'-C1'-N9 | 6.45  | 113.36      | 108.20   |
| 27  | B8    | 713  | G    | C5-C6-O6   | -6.44 | 124.73      | 128.60   |
| 27  | B8    | 866  | A    | C4-C5-C6   | 6.44  | 120.22      | 117.00   |
| 27  | B8    | 1930 | G    | C5-C6-O6   | -6.44 | 124.73      | 128.60   |
| 1   | AA    | 419  | C    | N3-C4-N4   | 6.44  | 122.51      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1127 | G    | C5-C6-O6   | -6.44 | 124.73      | 128.60   |
| 27  | B8    | 196  | A    | C4-C5-C6   | 6.44  | 120.22      | 117.00   |
| 27  | B8    | 801  | G    | C5-C6-O6   | -6.44 | 124.73      | 128.60   |
| 27  | B8    | 2464 | G    | O4'-C1'-N9 | 6.44  | 113.35      | 108.20   |
| 1   | AA    | 128  | G    | C5-C6-O6   | -6.44 | 124.74      | 128.60   |
| 1   | AA    | 498  | A    | C4-C5-C6   | 6.44  | 120.22      | 117.00   |
| 1   | AA    | 915  | A    | C5-C6-N6   | -6.44 | 118.55      | 123.70   |
| 1   | AA    | 1039 | G    | O4'-C1'-N9 | 6.44  | 113.35      | 108.20   |
| 1   | AA    | 1173 | U    | O4'-C1'-N1 | 6.44  | 113.35      | 108.20   |
| 27  | B8    | 782  | A    | C4-C5-C6   | 6.44  | 120.22      | 117.00   |
| 27  | B8    | 1703 | G    | O4'-C1'-N9 | 6.44  | 113.35      | 108.20   |
| 27  | B8    | 2706 | A    | C4-C5-C6   | 6.44  | 120.22      | 117.00   |
| 1   | AA    | 1062 | U    | O4'-C1'-N1 | 6.44  | 113.35      | 108.20   |
| 27  | B8    | 264  | C    | O4'-C1'-N1 | 6.44  | 113.35      | 108.20   |
| 27  | B8    | 406  | G    | O4'-C1'-N9 | 6.44  | 113.35      | 108.20   |
| 27  | B8    | 2130 | U    | O4'-C1'-N1 | 6.44  | 113.35      | 108.20   |
| 1   | AA    | 459  | A    | C4-C5-C6   | 6.44  | 120.22      | 117.00   |
| 1   | AA    | 865  | A    | O4'-C1'-N9 | 6.44  | 113.35      | 108.20   |
| 1   | AA    | 1406 | U    | O4'-C1'-N1 | 6.44  | 113.35      | 108.20   |
| 27  | B8    | 37   | C    | N3-C4-N4   | 6.43  | 122.50      | 118.00   |
| 27  | B8    | 522  | A    | O4'-C1'-N9 | 6.43  | 113.35      | 108.20   |
| 27  | B8    | 716  | A    | C4-C5-C6   | 6.43  | 120.22      | 117.00   |
| 27  | B8    | 2546 | U    | O4'-C1'-N1 | 6.43  | 113.35      | 108.20   |
| 1   | AA    | 536  | C    | O4'-C1'-N1 | 6.43  | 113.35      | 108.20   |
| 27  | B8    | 330  | A    | C4-C5-C6   | 6.43  | 120.22      | 117.00   |
| 27  | B8    | 1730 | C    | C2-N1-C1'  | 6.43  | 125.88      | 118.80   |
| 27  | B8    | 2150 | C    | N3-C4-N4   | 6.43  | 122.50      | 118.00   |
| 27  | B8    | 2269 | G    | C5-C6-O6   | -6.43 | 124.74      | 128.60   |
| 1   | AA    | 355  | C    | N3-C4-N4   | 6.43  | 122.50      | 118.00   |
| 27  | B8    | 1170 | C    | N3-C4-N4   | 6.43  | 122.50      | 118.00   |
| 27  | B8    | 1773 | A    | C5-C6-N6   | -6.43 | 118.56      | 123.70   |
| 1   | AA    | 371  | A    | C5-C6-N6   | -6.43 | 118.56      | 123.70   |
| 1   | AA    | 376  | G    | O4'-C1'-N9 | 6.43  | 113.34      | 108.20   |
| 1   | AA    | 974  | A    | C4-C5-C6   | 6.43  | 120.22      | 117.00   |
| 1   | AA    | 1324 | A    | O4'-C1'-N9 | 6.43  | 113.34      | 108.20   |
| 27  | B8    | 975  | A    | O4'-C1'-N9 | 6.43  | 113.34      | 108.20   |
| 27  | B8    | 1436 | G    | C5-C6-O6   | -6.43 | 124.74      | 128.60   |
| 27  | B8    | 1922 | G    | O4'-C1'-N9 | 6.43  | 113.34      | 108.20   |
| 27  | B8    | 2035 | G    | C5-C6-O6   | -6.43 | 124.74      | 128.60   |
| 27  | B8    | 2309 | A    | C4-C5-C6   | 6.43  | 120.22      | 117.00   |
| 27  | B8    | 2444 | G    | C5-C6-O6   | -6.43 | 124.74      | 128.60   |
| 1   | AA    | 1172 | C    | N3-C4-N4   | 6.43  | 122.50      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | AV    | 46   | G    | C5-C6-O6   | -6.43 | 124.74      | 128.60   |
| 1   | AA    | 1    | A    | C4-C5-C6   | 6.43  | 120.21      | 117.00   |
| 1   | AA    | 692  | U    | O4'-C1'-N1 | 6.43  | 113.34      | 108.20   |
| 27  | B8    | 581  | C    | N3-C4-N4   | 6.43  | 122.50      | 118.00   |
| 27  | B8    | 1565 | C    | O4'-C1'-N1 | 6.43  | 113.34      | 108.20   |
| 27  | B8    | 1755 | A    | O4'-C1'-N9 | 6.43  | 113.34      | 108.20   |
| 27  | B8    | 2793 | C    | O4'-C1'-N1 | 6.43  | 113.34      | 108.20   |
| 1   | AA    | 695  | A    | C4-C5-C6   | 6.42  | 120.21      | 117.00   |
| 1   | AA    | 1018 | G    | C5-C6-O6   | -6.42 | 124.75      | 128.60   |
| 1   | AA    | 1403 | C    | O4'-C1'-N1 | 6.42  | 113.34      | 108.20   |
| 27  | B8    | 107  | G    | O4'-C1'-N9 | 6.42  | 113.34      | 108.20   |
| 27  | B8    | 1275 | A    | C4-C5-C6   | 6.42  | 120.21      | 117.00   |
| 27  | B8    | 2365 | G    | C5-C6-O6   | -6.42 | 124.75      | 128.60   |
| 1   | AA    | 581  | G    | O4'-C1'-N9 | 6.42  | 113.34      | 108.20   |
| 1   | AA    | 389  | A    | C4-C5-C6   | 6.42  | 120.21      | 117.00   |
| 1   | AA    | 581  | G    | C5-C6-O6   | -6.42 | 124.75      | 128.60   |
| 27  | B8    | 276  | U    | C2-N1-C1'  | 6.42  | 125.41      | 117.70   |
| 27  | B8    | 1211 | C    | C2-N1-C1'  | 6.42  | 125.86      | 118.80   |
| 27  | B8    | 1300 | G    | C5-C6-O6   | -6.42 | 124.75      | 128.60   |
| 27  | B8    | 1898 | U    | O4'-C1'-N1 | 6.42  | 113.34      | 108.20   |
| 1   | AA    | 309  | A    | O4'-C1'-N9 | 6.42  | 113.34      | 108.20   |
| 3   | AV    | 64   | U    | O4'-C1'-N1 | 6.42  | 113.34      | 108.20   |
| 27  | B8    | 189  | G    | O4'-C1'-N9 | 6.42  | 113.34      | 108.20   |
| 27  | B8    | 324  | A    | O4'-C1'-N9 | 6.42  | 113.34      | 108.20   |
| 27  | B8    | 1717 | A    | C4-C5-C6   | 6.42  | 120.21      | 117.00   |
| 27  | B8    | 2899 | A    | O4'-C1'-N9 | 6.42  | 113.34      | 108.20   |
| 1   | AA    | 2    | A    | C4-C5-C6   | 6.42  | 120.21      | 117.00   |
| 1   | AA    | 219  | U    | O4'-C1'-N1 | 6.42  | 113.33      | 108.20   |
| 1   | AA    | 433  | G    | C5-C6-O6   | -6.42 | 124.75      | 128.60   |
| 27  | B8    | 105  | C    | N3-C4-N4   | 6.42  | 122.49      | 118.00   |
| 27  | B8    | 685  | A    | C5-C6-N6   | -6.42 | 118.56      | 123.70   |
| 27  | B8    | 802  | A    | C4-C5-C6   | 6.42  | 120.21      | 117.00   |
| 27  | B8    | 1787 | A    | C5-C6-N6   | -6.42 | 118.56      | 123.70   |
| 1   | AA    | 447  | G    | C5-C6-O6   | -6.42 | 124.75      | 128.60   |
| 1   | AA    | 448  | A    | O4'-C1'-N9 | 6.42  | 113.33      | 108.20   |
| 3   | AV    | 22   | A    | C4-C5-C6   | 6.42  | 120.21      | 117.00   |
| 27  | B8    | 300  | A    | C4-C5-C6   | 6.42  | 120.21      | 117.00   |
| 1   | AA    | 1266 | G    | C5-C6-O6   | -6.42 | 124.75      | 128.60   |
| 3   | AV    | 56   | U    | O4'-C1'-N1 | 6.42  | 113.33      | 108.20   |
| 27  | B8    | 28   | A    | C5-C6-N6   | -6.42 | 118.57      | 123.70   |
| 27  | B8    | 349  | U    | O4'-C1'-N1 | 6.42  | 113.33      | 108.20   |
| 27  | B8    | 1086 | A    | C5-C6-N1   | -6.42 | 114.49      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 38   | G    | O4'-C1'-N9 | 6.41  | 113.33      | 108.20   |
| 27  | B8    | 1599 | U    | O4'-C1'-N1 | 6.41  | 113.33      | 108.20   |
| 27  | B8    | 1770 | G    | C5-C6-O6   | -6.41 | 124.75      | 128.60   |
| 27  | B8    | 2265 | U    | O4'-C1'-N1 | 6.41  | 113.33      | 108.20   |
| 27  | B8    | 2505 | G    | O4'-C1'-N9 | 6.41  | 113.33      | 108.20   |
| 1   | AA    | 1179 | A    | C4-C5-C6   | 6.41  | 120.21      | 117.00   |
| 27  | B8    | 10   | A    | C4-C5-C6   | 6.41  | 120.21      | 117.00   |
| 27  | B8    | 1260 | A    | C5-C6-N6   | -6.41 | 118.57      | 123.70   |
| 1   | AA    | 192  | A    | C5-C6-N6   | -6.41 | 118.57      | 123.70   |
| 27  | B8    | 1916 | A    | O4'-C1'-N9 | 6.41  | 113.33      | 108.20   |
| 26  | B7    | 2    | G    | O4'-C1'-N9 | 6.41  | 113.33      | 108.20   |
| 27  | B8    | 755  | U    | O4'-C1'-N1 | 6.41  | 113.33      | 108.20   |
| 27  | B8    | 899  | A    | C5-C6-N6   | -6.41 | 118.57      | 123.70   |
| 27  | B8    | 1000 | A    | C4-C5-C6   | 6.41  | 120.20      | 117.00   |
| 27  | B8    | 2045 | C    | N3-C4-N4   | 6.41  | 122.49      | 118.00   |
| 27  | B8    | 2791 | G    | C5-C6-O6   | -6.41 | 124.75      | 128.60   |
| 3   | AV    | 27   | A    | C4-C5-C6   | 6.41  | 120.20      | 117.00   |
| 27  | B8    | 356  | G    | O4'-C1'-N9 | 6.41  | 113.33      | 108.20   |
| 27  | B8    | 1476 | U    | O4'-C1'-N1 | 6.41  | 113.33      | 108.20   |
| 1   | AA    | 1191 | A    | C4-C5-C6   | 6.41  | 120.20      | 117.00   |
| 27  | B8    | 1639 | C    | N3-C4-N4   | 6.41  | 122.48      | 118.00   |
| 27  | B8    | 1757 | A    | C4-C5-C6   | 6.41  | 120.20      | 117.00   |
| 27  | B8    | 1259 | G    | O4'-C1'-N9 | 6.40  | 113.32      | 108.20   |
| 27  | B8    | 1808 | A    | C4-C5-C6   | 6.40  | 120.20      | 117.00   |
| 27  | B8    | 2170 | A    | C4-C5-C6   | 6.40  | 120.20      | 117.00   |
| 1   | AA    | 21   | G    | C5-C6-O6   | -6.40 | 124.76      | 128.60   |
| 1   | AA    | 399  | G    | O4'-C1'-N9 | 6.40  | 113.32      | 108.20   |
| 27  | B8    | 299  | A    | C4-C5-C6   | 6.40  | 120.20      | 117.00   |
| 27  | B8    | 2284 | A    | C5-C6-N6   | -6.40 | 118.58      | 123.70   |
| 1   | AA    | 482  | A    | C5-C6-N6   | -6.40 | 118.58      | 123.70   |
| 1   | AA    | 1138 | G    | O4'-C1'-N9 | 6.40  | 113.32      | 108.20   |
| 1   | AA    | 1268 | G    | C5-C6-O6   | -6.40 | 124.76      | 128.60   |
| 26  | B7    | 42   | C    | O4'-C1'-N1 | 6.40  | 113.32      | 108.20   |
| 27  | B8    | 1642 | G    | O4'-C1'-N9 | 6.40  | 113.32      | 108.20   |
| 27  | B8    | 1713 | A    | C5-C6-N6   | -6.40 | 118.58      | 123.70   |
| 27  | B8    | 1929 | G    | C5-C6-O6   | -6.40 | 124.76      | 128.60   |
| 27  | B8    | 2013 | A    | C4-C5-C6   | 6.40  | 120.20      | 117.00   |
| 27  | B8    | 707  | G    | O4'-C1'-N9 | 6.40  | 113.32      | 108.20   |
| 27  | B8    | 711  | G    | O4'-C1'-N9 | 6.40  | 113.32      | 108.20   |
| 27  | B8    | 1874 | C    | N3-C4-N4   | 6.40  | 122.48      | 118.00   |
| 1   | AA    | 228  | A    | C4-C5-C6   | 6.40  | 120.20      | 117.00   |
| 1   | AA    | 421  | U    | C2-N1-C1'  | 6.40  | 125.38      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 556  | C    | N3-C4-N4   | 6.40  | 122.48      | 118.00   |
| 1   | AA    | 893  | C    | N3-C4-N4   | 6.40  | 122.48      | 118.00   |
| 1   | AA    | 1399 | C    | O4'-C1'-N1 | 6.40  | 113.32      | 108.20   |
| 3   | AV    | 77   | A    | C4-C5-C6   | 6.40  | 120.20      | 117.00   |
| 27  | B8    | 55   | G    | C5-C6-O6   | -6.40 | 124.76      | 128.60   |
| 27  | B8    | 1285 | A    | C4-C5-C6   | 6.40  | 120.20      | 117.00   |
| 27  | B8    | 1787 | A    | C4-C5-C6   | 6.40  | 120.20      | 117.00   |
| 27  | B8    | 2175 | C    | P-O3'-C3'  | 6.40  | 127.38      | 119.70   |
| 1   | AA    | 608  | A    | O4'-C1'-N9 | 6.40  | 113.32      | 108.20   |
| 27  | B8    | 1103 | A    | C4-C5-C6   | 6.40  | 120.20      | 117.00   |
| 1   | AA    | 1011 | C    | O4'-C1'-N1 | 6.39  | 113.31      | 108.20   |
| 1   | AA    | 1331 | G    | C5-C6-O6   | -6.39 | 124.76      | 128.60   |
| 27  | B8    | 28   | A    | O4'-C1'-N9 | 6.39  | 113.32      | 108.20   |
| 27  | B8    | 317  | G    | C5-C6-O6   | -6.39 | 124.76      | 128.60   |
| 27  | B8    | 1027 | A    | C5-C6-N6   | -6.39 | 118.58      | 123.70   |
| 27  | B8    | 1132 | U    | O4'-C1'-N1 | 6.39  | 113.32      | 108.20   |
| 27  | B8    | 1781 | U    | O4'-C1'-N1 | 6.39  | 113.31      | 108.20   |
| 27  | B8    | 2655 | G    | C5-C6-O6   | -6.39 | 124.76      | 128.60   |
| 1   | AA    | 378  | G    | C5-C6-O6   | -6.39 | 124.76      | 128.60   |
| 1   | AA    | 1491 | G    | C5-C6-O6   | -6.39 | 124.76      | 128.60   |
| 27  | B8    | 1309 | G    | O4'-C1'-N9 | 6.39  | 113.31      | 108.20   |
| 27  | B8    | 2446 | G    | C5-C6-O6   | -6.39 | 124.76      | 128.60   |
| 27  | B8    | 1953 | A    | C4-C5-C6   | 6.39  | 120.19      | 117.00   |
| 27  | B8    | 2793 | C    | N3-C4-N4   | 6.39  | 122.47      | 118.00   |
| 1   | AA    | 52   | C    | N3-C4-N4   | 6.39  | 122.47      | 118.00   |
| 1   | AA    | 343  | U    | O4'-C1'-N1 | 6.39  | 113.31      | 108.20   |
| 1   | AA    | 990  | C    | O4'-C1'-N1 | 6.39  | 113.31      | 108.20   |
| 26  | B7    | 112  | G    | O4'-C1'-N9 | 6.39  | 113.31      | 108.20   |
| 27  | B8    | 418  | C    | N3-C4-N4   | 6.39  | 122.47      | 118.00   |
| 27  | B8    | 449  | A    | C4-C5-C6   | 6.39  | 120.19      | 117.00   |
| 27  | B8    | 748  | G    | C5-C6-O6   | -6.39 | 124.77      | 128.60   |
| 27  | B8    | 1346 | G    | O4'-C1'-N9 | 6.39  | 113.31      | 108.20   |
| 27  | B8    | 2800 | A    | O4'-C1'-N9 | 6.39  | 113.31      | 108.20   |
| 1   | AA    | 1507 | A    | C4-C5-C6   | 6.39  | 120.19      | 117.00   |
| 1   | AA    | 1493 | A    | C4-C5-C6   | 6.39  | 120.19      | 117.00   |
| 27  | B8    | 1341 | G    | C5-C6-O6   | -6.39 | 124.77      | 128.60   |
| 27  | B8    | 1980 | G    | C5-C6-O6   | -6.39 | 124.77      | 128.60   |
| 1   | AA    | 147  | G    | O4'-C1'-N9 | 6.38  | 113.31      | 108.20   |
| 27  | B8    | 595  | C    | N3-C4-N4   | 6.38  | 122.47      | 118.00   |
| 27  | B8    | 1712 | U    | O4'-C1'-N1 | 6.38  | 113.31      | 108.20   |
| 27  | B8    | 2901 | C    | N3-C4-N4   | 6.38  | 122.47      | 118.00   |
| 1   | AA    | 202  | G    | C5-C6-O6   | -6.38 | 124.77      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 629  | A    | C4-C5-C6   | 6.38  | 120.19      | 117.00   |
| 1   | AA    | 1499 | A    | C4-C5-C6   | 6.38  | 120.19      | 117.00   |
| 27  | B8    | 2776 | A    | C4-C5-C6   | 6.38  | 120.19      | 117.00   |
| 1   | AA    | 109  | A    | C4-C5-C6   | 6.38  | 120.19      | 117.00   |
| 1   | AA    | 495  | A    | C5-C6-N1   | -6.38 | 114.51      | 117.70   |
| 1   | AA    | 1423 | G    | O4'-C1'-N9 | 6.38  | 113.31      | 108.20   |
| 27  | B8    | 64   | A    | C5-C6-N1   | -6.38 | 114.51      | 117.70   |
| 27  | B8    | 655  | A    | O4'-C1'-N9 | 6.38  | 113.31      | 108.20   |
| 27  | B8    | 1122 | G    | C5-C6-O6   | -6.38 | 124.77      | 128.60   |
| 27  | B8    | 1359 | A    | O4'-C1'-N9 | 6.38  | 113.31      | 108.20   |
| 27  | B8    | 2062 | A    | C4-C5-C6   | 6.38  | 120.19      | 117.00   |
| 27  | B8    | 2258 | C    | O4'-C1'-N1 | 6.38  | 113.31      | 108.20   |
| 27  | B8    | 2686 | G    | O4'-C1'-N9 | 6.38  | 113.31      | 108.20   |
| 1   | AA    | 987  | G    | O4'-C1'-N9 | 6.38  | 113.30      | 108.20   |
| 1   | AA    | 1110 | A    | C4-C5-C6   | 6.38  | 120.19      | 117.00   |
| 27  | B8    | 260  | G    | O4'-C1'-N9 | 6.38  | 113.30      | 108.20   |
| 1   | AA    | 1112 | C    | O4'-C1'-N1 | 6.38  | 113.30      | 108.20   |
| 3   | AV    | 30   | G    | O4'-C1'-N9 | 6.38  | 113.30      | 108.20   |
| 1   | AA    | 77   | A    | C5-C6-N6   | -6.38 | 118.60      | 123.70   |
| 1   | AA    | 270  | A    | C5-C6-N6   | -6.38 | 118.60      | 123.70   |
| 27  | B8    | 219  | A    | C4-C5-C6   | 6.38  | 120.19      | 117.00   |
| 27  | B8    | 329  | G    | C5-C6-O6   | -6.38 | 124.77      | 128.60   |
| 27  | B8    | 2602 | A    | C4-C5-C6   | 6.38  | 120.19      | 117.00   |
| 27  | B8    | 2606 | C    | N3-C4-N4   | 6.38  | 122.46      | 118.00   |
| 27  | B8    | 2900 | A    | C5-C6-N6   | -6.38 | 118.60      | 123.70   |
| 1   | AA    | 28   | A    | O4'-C1'-N9 | 6.38  | 113.30      | 108.20   |
| 27  | B8    | 2406 | A    | C4-C5-C6   | 6.38  | 120.19      | 117.00   |
| 1   | AA    | 53   | A    | O4'-C1'-N9 | 6.37  | 113.30      | 108.20   |
| 1   | AA    | 776  | G    | O4'-C1'-N9 | 6.37  | 113.30      | 108.20   |
| 1   | AA    | 1095 | U    | O4'-C1'-N1 | 6.37  | 113.30      | 108.20   |
| 27  | B8    | 243  | U    | O4'-C1'-N1 | 6.37  | 113.30      | 108.20   |
| 27  | B8    | 1664 | A    | C5-C6-N6   | -6.37 | 118.60      | 123.70   |
| 27  | B8    | 2632 | A    | C5-C6-N6   | -6.37 | 118.60      | 123.70   |
| 1   | AA    | 176  | C    | N3-C4-N4   | 6.37  | 122.46      | 118.00   |
| 1   | AA    | 742  | G    | C5-C6-O6   | -6.37 | 124.78      | 128.60   |
| 27  | B8    | 571  | U    | O4'-C1'-N1 | 6.37  | 113.30      | 108.20   |
| 27  | B8    | 1921 | G    | O4'-C1'-N9 | 6.37  | 113.30      | 108.20   |
| 27  | B8    | 2297 | A    | C5-C6-N1   | -6.37 | 114.51      | 117.70   |
| 41  | BM    | 43   | ALA  | N-CA-CB    | 6.37  | 119.02      | 110.10   |
| 1   | AA    | 386  | C    | O4'-C1'-N1 | 6.37  | 113.30      | 108.20   |
| 1   | AA    | 455  | G    | O4'-C1'-N9 | 6.37  | 113.30      | 108.20   |
| 1   | AA    | 941  | G    | O4'-C1'-N9 | 6.37  | 113.29      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1244 | G    | O4'-C1'-N9 | 6.37  | 113.30      | 108.20   |
| 1   | AA    | 1534 | A    | C4-C5-C6   | 6.37  | 120.18      | 117.00   |
| 27  | B8    | 13   | A    | C5-C6-N6   | -6.37 | 118.61      | 123.70   |
| 27  | B8    | 2442 | C    | N3-C4-N4   | 6.37  | 122.46      | 118.00   |
| 27  | B8    | 2451 | A    | O4'-C1'-N9 | 6.37  | 113.30      | 108.20   |
| 27  | B8    | 2113 | U    | O4'-C1'-N1 | 6.37  | 113.29      | 108.20   |
| 26  | B7    | 101  | A    | C5-C6-N6   | -6.37 | 118.61      | 123.70   |
| 27  | B8    | 1098 | A    | C4-C5-C6   | 6.37  | 120.18      | 117.00   |
| 27  | B8    | 1692 | U    | O4'-C1'-N1 | 6.37  | 113.29      | 108.20   |
| 27  | B8    | 1745 | A    | C4-C5-C6   | 6.37  | 120.18      | 117.00   |
| 27  | B8    | 2079 | U    | O4'-C1'-N1 | 6.37  | 113.29      | 108.20   |
| 1   | AA    | 1496 | C    | N3-C4-N4   | 6.36  | 122.45      | 118.00   |
| 27  | B8    | 420  | C    | N3-C4-N4   | 6.36  | 122.45      | 118.00   |
| 27  | B8    | 1861 | G    | O4'-C1'-N9 | 6.36  | 113.29      | 108.20   |
| 27  | B8    | 1880 | U    | O4'-C1'-N1 | 6.36  | 113.29      | 108.20   |
| 27  | B8    | 2434 | A    | C4-C5-C6   | 6.36  | 120.18      | 117.00   |
| 27  | B8    | 881  | G    | C5-C6-O6   | -6.36 | 124.78      | 128.60   |
| 27  | B8    | 1823 | G    | C5-C6-O6   | -6.36 | 124.78      | 128.60   |
| 27  | B8    | 2030 | A    | C4-C5-C6   | 6.36  | 120.18      | 117.00   |
| 27  | B8    | 2358 | A    | C4-C5-C6   | 6.36  | 120.18      | 117.00   |
| 1   | AA    | 1105 | A    | O4'-C1'-N9 | 6.36  | 113.29      | 108.20   |
| 1   | AA    | 1480 | A    | O4'-C1'-N9 | 6.36  | 113.29      | 108.20   |
| 27  | B8    | 284  | U    | O4'-C1'-N1 | 6.36  | 113.29      | 108.20   |
| 27  | B8    | 403  | U    | O4'-C1'-N1 | 6.36  | 113.29      | 108.20   |
| 27  | B8    | 1061 | U    | C6-N1-C1'  | -6.36 | 112.30      | 121.20   |
| 27  | B8    | 1317 | G    | O4'-C1'-N9 | 6.36  | 113.29      | 108.20   |
| 27  | B8    | 1689 | A    | C4-C5-C6   | 6.36  | 120.18      | 117.00   |
| 1   | AA    | 312  | C    | N3-C4-N4   | 6.36  | 122.45      | 118.00   |
| 1   | AA    | 1332 | A    | O4'-C1'-N9 | 6.36  | 113.29      | 108.20   |
| 1   | AA    | 1338 | G    | C5-C6-O6   | -6.36 | 124.78      | 128.60   |
| 1   | AA    | 1456 | A    | C4-C5-C6   | 6.36  | 120.18      | 117.00   |
| 26  | B7    | 39   | A    | C5-C6-N6   | -6.36 | 118.61      | 123.70   |
| 27  | B8    | 16   | C    | N3-C4-N4   | 6.36  | 122.45      | 118.00   |
| 27  | B8    | 45   | G    | O4'-C1'-N9 | 6.36  | 113.29      | 108.20   |
| 27  | B8    | 428  | A    | C4-C5-C6   | 6.36  | 120.18      | 117.00   |
| 27  | B8    | 547  | A    | C4-C5-C6   | 6.36  | 120.18      | 117.00   |
| 27  | B8    | 2732 | G    | O4'-C1'-N9 | 6.36  | 113.29      | 108.20   |
| 1   | AA    | 1072 | G    | O4'-C1'-N9 | 6.36  | 113.28      | 108.20   |
| 3   | AV    | 12   | G    | C5-C6-O6   | -6.36 | 124.79      | 128.60   |
| 27  | B8    | 1347 | A    | C5-C6-N1   | -6.36 | 114.52      | 117.70   |
| 27  | B8    | 2076 | U    | C2-N1-C1'  | 6.36  | 125.33      | 117.70   |
| 1   | AA    | 1074 | G    | C5-C6-O6   | -6.35 | 124.79      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1207 | C    | N3-C4-N4   | 6.35  | 122.45      | 118.00   |
| 27  | B8    | 2850 | A    | C4-C5-C6   | 6.35  | 120.18      | 117.00   |
| 1   | AA    | 595  | A    | C4-C5-C6   | 6.35  | 120.18      | 117.00   |
| 1   | AA    | 777  | A    | C4-C5-C6   | 6.35  | 120.18      | 117.00   |
| 1   | AA    | 989  | U    | O4'-C1'-N1 | 6.35  | 113.28      | 108.20   |
| 27  | B8    | 255  | A    | C4-C5-C6   | 6.35  | 120.18      | 117.00   |
| 27  | B8    | 390  | U    | O4'-C1'-N1 | 6.35  | 113.28      | 108.20   |
| 27  | B8    | 999  | U    | O4'-C1'-N1 | 6.35  | 113.28      | 108.20   |
| 27  | B8    | 2517 | C    | N3-C4-N4   | 6.35  | 122.45      | 118.00   |
| 1   | AA    | 517  | G    | C5-C6-O6   | -6.35 | 124.79      | 128.60   |
| 27  | B8    | 101  | A    | C4-C5-C6   | 6.35  | 120.18      | 117.00   |
| 27  | B8    | 1187 | G    | C5-C6-O6   | -6.35 | 124.79      | 128.60   |
| 27  | B8    | 1203 | U    | O4'-C1'-N1 | 6.35  | 113.28      | 108.20   |
| 1   | AA    | 676  | A    | C5-C6-N1   | -6.35 | 114.53      | 117.70   |
| 1   | AA    | 866  | C    | N3-C4-N4   | 6.35  | 122.44      | 118.00   |
| 1   | AA    | 1206 | G    | O4'-C1'-N9 | 6.35  | 113.28      | 108.20   |
| 27  | B8    | 575  | A    | C5-C6-N1   | -6.35 | 114.53      | 117.70   |
| 27  | B8    | 607  | U    | O4'-C1'-N1 | 6.35  | 113.28      | 108.20   |
| 27  | B8    | 863  | A    | C4-C5-C6   | 6.35  | 120.17      | 117.00   |
| 27  | B8    | 1163 | G    | O4'-C1'-N9 | 6.35  | 113.28      | 108.20   |
| 27  | B8    | 2006 | C    | N3-C4-N4   | 6.35  | 122.44      | 118.00   |
| 1   | AA    | 128  | G    | O4'-C1'-N9 | 6.35  | 113.28      | 108.20   |
| 1   | AA    | 318  | G    | O4'-C1'-N9 | 6.35  | 113.28      | 108.20   |
| 1   | AA    | 367  | U    | O4'-C1'-N1 | 6.35  | 113.28      | 108.20   |
| 27  | B8    | 217  | A    | C4-C5-C6   | 6.35  | 120.17      | 117.00   |
| 27  | B8    | 242  | G    | C5-C6-O6   | -6.35 | 124.79      | 128.60   |
| 27  | B8    | 2173 | A    | C4-C5-C6   | 6.35  | 120.17      | 117.00   |
| 1   | AA    | 146  | G    | O4'-C1'-N9 | 6.35  | 113.28      | 108.20   |
| 1   | AA    | 1219 | A    | C5-C6-N6   | -6.35 | 118.62      | 123.70   |
| 27  | B8    | 417  | C    | N3-C4-N4   | 6.35  | 122.44      | 118.00   |
| 27  | B8    | 752  | A    | O4'-C1'-N9 | 6.35  | 113.28      | 108.20   |
| 27  | B8    | 1288 | G    | C5-C6-O6   | -6.35 | 124.79      | 128.60   |
| 27  | B8    | 2261 | C    | N3-C4-N4   | 6.35  | 122.44      | 118.00   |
| 27  | B8    | 2425 | A    | C4-C5-C6   | 6.35  | 120.17      | 117.00   |
| 1   | AA    | 155  | A    | O4'-C1'-N9 | 6.34  | 113.28      | 108.20   |
| 1   | AA    | 162  | A    | C5-C6-N1   | -6.34 | 114.53      | 117.70   |
| 1   | AA    | 1475 | G    | C5-C6-O6   | -6.34 | 124.79      | 128.60   |
| 27  | B8    | 227  | A    | C4-C5-C6   | 6.34  | 120.17      | 117.00   |
| 27  | B8    | 1669 | A    | C5-C6-N1   | -6.34 | 114.53      | 117.70   |
| 27  | B8    | 1802 | A    | C5-C6-N1   | -6.34 | 114.53      | 117.70   |
| 27  | B8    | 268  | C    | O4'-C1'-N1 | 6.34  | 113.27      | 108.20   |
| 27  | B8    | 1197 | G    | C5-C6-O6   | -6.34 | 124.79      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1754 | A    | C4-C5-C6   | 6.34  | 120.17      | 117.00   |
| 27  | B8    | 2127 | G    | O4'-C1'-N9 | 6.34  | 113.27      | 108.20   |
| 32  | BD    | 31   | ALA  | N-CA-CB    | 6.34  | 118.98      | 110.10   |
| 1   | AA    | 1530 | G    | O4'-C1'-N9 | 6.34  | 113.27      | 108.20   |
| 27  | B8    | 635  | C    | N3-C4-N4   | 6.34  | 122.44      | 118.00   |
| 27  | B8    | 938  | G    | O4'-C1'-N9 | 6.34  | 113.27      | 108.20   |
| 27  | B8    | 1368 | G    | O4'-C1'-N9 | 6.34  | 113.27      | 108.20   |
| 27  | B8    | 1886 | U    | O4'-C1'-N1 | 6.34  | 113.27      | 108.20   |
| 27  | B8    | 1962 | C    | N3-C4-N4   | 6.34  | 122.44      | 118.00   |
| 27  | B8    | 492  | A    | C4-C5-C6   | 6.34  | 120.17      | 117.00   |
| 27  | B8    | 1465 | G    | O4'-C1'-N9 | 6.34  | 113.27      | 108.20   |
| 27  | B8    | 1548 | A    | O4'-C1'-N9 | 6.34  | 113.27      | 108.20   |
| 27  | B8    | 2015 | A    | O4'-C1'-N9 | 6.34  | 113.27      | 108.20   |
| 27  | B8    | 2072 | C    | N3-C4-N4   | 6.34  | 122.44      | 118.00   |
| 27  | B8    | 857  | G    | C5-C6-O6   | -6.34 | 124.80      | 128.60   |
| 27  | B8    | 1573 | G    | C5-C6-O6   | -6.34 | 124.80      | 128.60   |
| 27  | B8    | 2262 | U    | O4'-C1'-N1 | 6.34  | 113.27      | 108.20   |
| 1   | AA    | 47   | C    | N3-C4-N4   | 6.34  | 122.44      | 118.00   |
| 1   | AA    | 74   | A    | O4'-C1'-N9 | 6.34  | 113.27      | 108.20   |
| 1   | AA    | 1180 | A    | C4-C5-C6   | 6.34  | 120.17      | 117.00   |
| 1   | AA    | 1199 | U    | O4'-C1'-N1 | 6.34  | 113.27      | 108.20   |
| 27  | B8    | 142  | A    | O4'-C1'-N9 | 6.34  | 113.27      | 108.20   |
| 27  | B8    | 186  | G    | O4'-C1'-N9 | 6.34  | 113.27      | 108.20   |
| 27  | B8    | 728  | G    | O4'-C1'-N9 | 6.34  | 113.27      | 108.20   |
| 27  | B8    | 1498 | C    | N3-C4-N4   | 6.34  | 122.44      | 118.00   |
| 27  | B8    | 1860 | G    | O4'-C1'-N9 | 6.34  | 113.27      | 108.20   |
| 27  | B8    | 1918 | A    | C5-C6-N6   | -6.34 | 118.63      | 123.70   |
| 27  | B8    | 1996 | C    | N3-C4-N4   | 6.33  | 122.43      | 118.00   |
| 27  | B8    | 2575 | C    | N3-C4-N4   | 6.33  | 122.43      | 118.00   |
| 3   | AV    | 71   | C    | N3-C4-N4   | 6.33  | 122.43      | 118.00   |
| 27  | B8    | 1613 | G    | C5-C6-O6   | -6.33 | 124.80      | 128.60   |
| 27  | B8    | 2352 | A    | C5-C6-N1   | -6.33 | 114.53      | 117.70   |
| 1   | AA    | 408  | A    | C4-C5-C6   | 6.33  | 120.17      | 117.00   |
| 1   | AA    | 1030 | U    | C2-N1-C1'  | 6.33  | 125.30      | 117.70   |
| 27  | B8    | 138  | U    | O4'-C1'-N1 | 6.33  | 113.27      | 108.20   |
| 27  | B8    | 237  | C    | N3-C4-N4   | 6.33  | 122.43      | 118.00   |
| 27  | B8    | 2165 | C    | O4'-C1'-N1 | 6.33  | 113.27      | 108.20   |
| 27  | B8    | 2168 | G    | O4'-C1'-N9 | 6.33  | 113.27      | 108.20   |
| 27  | B8    | 2322 | A    | C4-C5-C6   | 6.33  | 120.17      | 117.00   |
| 27  | B8    | 91   | A    | C4-C5-C6   | 6.33  | 120.17      | 117.00   |
| 27  | B8    | 529  | A    | C4-C5-C6   | 6.33  | 120.17      | 117.00   |
| 27  | B8    | 1780 | A    | O4'-C1'-N9 | 6.33  | 113.26      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2666 | C    | C6-N1-C1'  | -6.33 | 113.20      | 120.80   |
| 1   | AA    | 869  | G    | C5-C6-O6   | -6.33 | 124.80      | 128.60   |
| 27  | B8    | 54   | G    | O4'-C1'-N9 | 6.33  | 113.26      | 108.20   |
| 27  | B8    | 185  | G    | O4'-C1'-N9 | 6.33  | 113.26      | 108.20   |
| 27  | B8    | 216  | A    | O4'-C1'-N9 | 6.33  | 113.26      | 108.20   |
| 27  | B8    | 1557 | C    | O4'-C1'-N1 | 6.33  | 113.26      | 108.20   |
| 27  | B8    | 1724 | G    | O4'-C1'-N9 | 6.33  | 113.26      | 108.20   |
| 27  | B8    | 2787 | C    | N3-C4-N4   | 6.33  | 122.43      | 118.00   |
| 1   | AA    | 284  | C    | N3-C4-N4   | 6.33  | 122.43      | 118.00   |
| 1   | AA    | 586  | C    | N3-C4-N4   | 6.33  | 122.43      | 118.00   |
| 1   | AA    | 727  | G    | C5-C6-O6   | -6.33 | 124.80      | 128.60   |
| 1   | AA    | 1189 | U    | O4'-C1'-N1 | 6.33  | 113.26      | 108.20   |
| 27  | B8    | 699  | A    | C4-C5-C6   | 6.33  | 120.16      | 117.00   |
| 1   | AA    | 461  | A    | C4-C5-C6   | 6.33  | 120.16      | 117.00   |
| 1   | AA    | 814  | A    | C4-C5-C6   | 6.33  | 120.16      | 117.00   |
| 1   | AA    | 1360 | A    | C5-C6-N6   | -6.33 | 118.64      | 123.70   |
| 26  | B7    | 75   | G    | O4'-C1'-N9 | 6.33  | 113.26      | 108.20   |
| 27  | B8    | 619  | G    | O4'-C1'-N9 | 6.33  | 113.26      | 108.20   |
| 1   | AA    | 204  | G    | O4'-C1'-N9 | 6.32  | 113.26      | 108.20   |
| 27  | B8    | 87   | U    | O4'-C1'-N1 | 6.32  | 113.26      | 108.20   |
| 27  | B8    | 909  | A    | O4'-C1'-N9 | 6.32  | 113.26      | 108.20   |
| 27  | B8    | 1264 | A    | C5-C6-N6   | -6.32 | 118.64      | 123.70   |
| 27  | B8    | 2065 | C    | N3-C4-N4   | 6.32  | 122.43      | 118.00   |
| 1   | AA    | 830  | G    | O4'-C1'-N9 | 6.32  | 113.26      | 108.20   |
| 27  | B8    | 750  | A    | C4-C5-C6   | 6.32  | 120.16      | 117.00   |
| 27  | B8    | 644  | A    | C4-C5-C6   | 6.32  | 120.16      | 117.00   |
| 1   | AA    | 70   | U    | O4'-C1'-N1 | 6.32  | 113.25      | 108.20   |
| 27  | B8    | 577  | G    | O4'-C1'-N9 | 6.32  | 113.25      | 108.20   |
| 1   | AA    | 738  | C    | N3-C4-N4   | 6.32  | 122.42      | 118.00   |
| 1   | AA    | 1513 | A    | C5-C6-N6   | -6.32 | 118.65      | 123.70   |
| 27  | B8    | 732  | C    | N3-C4-N4   | 6.32  | 122.42      | 118.00   |
| 27  | B8    | 1496 | A    | C5-C6-N6   | -6.32 | 118.65      | 123.70   |
| 27  | B8    | 2101 | A    | O4'-C1'-N9 | 6.32  | 113.25      | 108.20   |
| 27  | B8    | 2134 | A    | C4-C5-C6   | 6.32  | 120.16      | 117.00   |
| 1   | AA    | 892  | A    | O4'-C1'-N9 | 6.32  | 113.25      | 108.20   |
| 1   | AA    | 1501 | C    | O4'-C1'-N1 | 6.32  | 113.25      | 108.20   |
| 27  | B8    | 479  | A    | C4-C5-C6   | 6.32  | 120.16      | 117.00   |
| 27  | B8    | 1509 | A    | C4-C5-C6   | 6.32  | 120.16      | 117.00   |
| 27  | B8    | 1738 | G    | C5-C6-O6   | -6.32 | 124.81      | 128.60   |
| 27  | B8    | 2733 | A    | C4-C5-C6   | 6.31  | 120.16      | 117.00   |
| 1   | AA    | 177  | G    | N1-C6-O6   | 6.31  | 123.69      | 119.90   |
| 1   | AA    | 803  | G    | O4'-C1'-N9 | 6.31  | 113.25      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1119 | C    | N3-C4-N4   | 6.31  | 122.42      | 118.00   |
| 1   | AA    | 1489 | G    | O4'-C1'-N9 | 6.31  | 113.25      | 108.20   |
| 27  | B8    | 726  | G    | C5-C6-O6   | -6.31 | 124.81      | 128.60   |
| 27  | B8    | 1227 | G    | C5-C6-O6   | -6.31 | 124.81      | 128.60   |
| 27  | B8    | 1345 | C    | N3-C4-N4   | 6.31  | 122.42      | 118.00   |
| 27  | B8    | 2033 | A    | O4'-C1'-N9 | 6.31  | 113.25      | 108.20   |
| 27  | B8    | 656  | G    | O4'-C1'-N9 | 6.31  | 113.25      | 108.20   |
| 27  | B8    | 1635 | A    | C4-C5-C6   | 6.31  | 120.16      | 117.00   |
| 27  | B8    | 2215 | C    | N3-C4-N4   | 6.31  | 122.42      | 118.00   |
| 27  | B8    | 2709 | G    | O4'-C1'-N9 | 6.31  | 113.25      | 108.20   |
| 1   | AA    | 573  | A    | C4-C5-C6   | 6.31  | 120.16      | 117.00   |
| 1   | AA    | 614  | C    | N3-C4-N4   | 6.31  | 122.42      | 118.00   |
| 1   | AA    | 1455 | G    | O4'-C1'-N9 | 6.31  | 113.25      | 108.20   |
| 1   | AA    | 1498 | U    | O4'-C1'-N1 | 6.31  | 113.25      | 108.20   |
| 3   | AV    | 34   | U    | O4'-C1'-N1 | 6.31  | 113.25      | 108.20   |
| 27  | B8    | 881  | G    | O4'-C1'-N9 | 6.31  | 113.25      | 108.20   |
| 27  | B8    | 1737 | G    | C5-C6-O6   | -6.31 | 124.81      | 128.60   |
| 1   | AA    | 245  | U    | O4'-C1'-N1 | 6.31  | 113.25      | 108.20   |
| 27  | B8    | 684  | G    | C5-C6-O6   | -6.31 | 124.81      | 128.60   |
| 27  | B8    | 797  | G    | O4'-C1'-N9 | 6.31  | 113.25      | 108.20   |
| 26  | B7    | 53   | A    | O4'-C1'-N9 | 6.31  | 113.25      | 108.20   |
| 27  | B8    | 1269 | A    | C4-C5-C6   | 6.31  | 120.15      | 117.00   |
| 1   | AA    | 101  | A    | C4-C5-C6   | 6.30  | 120.15      | 117.00   |
| 1   | AA    | 247  | G    | O4'-C1'-N9 | 6.30  | 113.24      | 108.20   |
| 1   | AA    | 868  | C    | N3-C4-N4   | 6.30  | 122.41      | 118.00   |
| 27  | B8    | 294  | A    | C5-C6-N6   | -6.30 | 118.66      | 123.70   |
| 27  | B8    | 2331 | G    | C5-C6-O6   | -6.30 | 124.82      | 128.60   |
| 27  | B8    | 2788 | C    | N3-C4-N4   | 6.30  | 122.41      | 118.00   |
| 1   | AA    | 468  | A    | C5-C6-N1   | -6.30 | 114.55      | 117.70   |
| 26  | B7    | 94   | A    | O4'-C1'-N9 | 6.30  | 113.24      | 108.20   |
| 27  | B8    | 109  | C    | N3-C4-N4   | 6.30  | 122.41      | 118.00   |
| 27  | B8    | 2154 | A    | C5-C6-N6   | -6.30 | 118.66      | 123.70   |
| 27  | B8    | 2899 | A    | C4-C5-C6   | 6.30  | 120.15      | 117.00   |
| 1   | AA    | 739  | C    | N3-C4-N4   | 6.30  | 122.41      | 118.00   |
| 1   | AA    | 859  | G    | O4'-C1'-N9 | 6.30  | 113.24      | 108.20   |
| 1   | AA    | 895  | G    | C5-C6-O6   | -6.30 | 124.82      | 128.60   |
| 1   | AA    | 1291 | U    | O4'-C1'-N1 | 6.30  | 113.24      | 108.20   |
| 3   | AV    | 74   | A    | O4'-C1'-N9 | 6.30  | 113.24      | 108.20   |
| 27  | B8    | 2089 | C    | N3-C4-N4   | 6.30  | 122.41      | 118.00   |
| 27  | B8    | 2551 | C    | N3-C4-N4   | 6.30  | 122.41      | 118.00   |
| 27  | B8    | 2667 | C    | N3-C4-N4   | 6.30  | 122.41      | 118.00   |
| 27  | B8    | 2682 | A    | C4-C5-C6   | 6.30  | 120.15      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2904 | U    | O4'-C1'-N1 | 6.30  | 113.24      | 108.20   |
| 1   | AA    | 1345 | U    | O4'-C1'-N1 | 6.30  | 113.24      | 108.20   |
| 27  | B8    | 1041 | G    | O4'-C1'-N9 | 6.30  | 113.24      | 108.20   |
| 27  | B8    | 2675 | A    | C5-C6-N1   | -6.30 | 114.55      | 117.70   |
| 1   | AA    | 205  | A    | C4-C5-C6   | 6.30  | 120.15      | 117.00   |
| 27  | B8    | 132  | G    | O4'-C1'-N9 | 6.30  | 113.24      | 108.20   |
| 1   | AA    | 1447 | A    | C5-C6-N1   | -6.30 | 114.55      | 117.70   |
| 27  | B8    | 111  | A    | C4-C5-C6   | 6.30  | 120.15      | 117.00   |
| 27  | B8    | 535  | G    | O4'-C1'-N9 | 6.30  | 113.24      | 108.20   |
| 27  | B8    | 1287 | A    | O4'-C1'-N9 | 6.30  | 113.24      | 108.20   |
| 27  | B8    | 1972 | G    | C5-C6-O6   | -6.30 | 124.82      | 128.60   |
| 1   | AA    | 106  | C    | N3-C4-N4   | 6.29  | 122.41      | 118.00   |
| 1   | AA    | 675  | A    | C4-C5-C6   | 6.29  | 120.15      | 117.00   |
| 27  | B8    | 936  | A    | C4-C5-C6   | 6.29  | 120.15      | 117.00   |
| 27  | B8    | 2151 | U    | O4'-C1'-N1 | 6.29  | 113.24      | 108.20   |
| 27  | B8    | 2591 | C    | N3-C4-N4   | 6.29  | 122.41      | 118.00   |
| 1   | AA    | 81   | A    | C4-C5-C6   | 6.29  | 120.15      | 117.00   |
| 1   | AA    | 432  | A    | C4-C5-C6   | 6.29  | 120.15      | 117.00   |
| 1   | AA    | 937  | A    | C4-C5-C6   | 6.29  | 120.15      | 117.00   |
| 27  | B8    | 1469 | A    | O4'-C1'-N9 | 6.29  | 113.23      | 108.20   |
| 27  | B8    | 2216 | G    | O4'-C1'-N9 | 6.29  | 113.23      | 108.20   |
| 1   | AA    | 397  | A    | C4-C5-C6   | 6.29  | 120.15      | 117.00   |
| 1   | AA    | 509  | A    | C4-C5-C6   | 6.29  | 120.15      | 117.00   |
| 1   | AA    | 932  | C    | N3-C4-N4   | 6.29  | 122.40      | 118.00   |
| 26  | B7    | 8    | C    | N3-C4-N4   | 6.29  | 122.40      | 118.00   |
| 27  | B8    | 711  | G    | C5-C6-O6   | -6.29 | 124.83      | 128.60   |
| 27  | B8    | 1847 | A    | C4-C5-C6   | 6.29  | 120.15      | 117.00   |
| 1   | AA    | 299  | G    | O4'-C1'-N9 | 6.29  | 113.23      | 108.20   |
| 1   | AA    | 320  | A    | C5-C6-N6   | -6.29 | 118.67      | 123.70   |
| 1   | AA    | 1437 | A    | C5-C6-N6   | -6.29 | 118.67      | 123.70   |
| 27  | B8    | 1698 | A    | C4-C5-C6   | 6.29  | 120.14      | 117.00   |
| 27  | B8    | 2430 | A    | C5-C6-N6   | -6.29 | 118.67      | 123.70   |
| 1   | AA    | 1000 | A    | C5-C6-N6   | -6.29 | 118.67      | 123.70   |
| 1   | AA    | 1028 | C    | N3-C4-N4   | 6.29  | 122.40      | 118.00   |
| 3   | AV    | 76   | C    | N3-C4-N4   | 6.29  | 122.40      | 118.00   |
| 27  | B8    | 298  | G    | N3-C2-N2   | 6.29  | 124.30      | 119.90   |
| 27  | B8    | 438  | G    | O4'-C1'-N9 | 6.29  | 113.23      | 108.20   |
| 27  | B8    | 641  | U    | O4'-C1'-N1 | 6.29  | 113.23      | 108.20   |
| 27  | B8    | 1117 | C    | N3-C4-N4   | 6.29  | 122.40      | 118.00   |
| 27  | B8    | 1214 | A    | O4'-C1'-N9 | 6.29  | 113.23      | 108.20   |
| 27  | B8    | 1279 | G    | O4'-C1'-N9 | 6.29  | 113.23      | 108.20   |
| 27  | B8    | 2042 | A    | C4-C5-C6   | 6.29  | 120.14      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2353 | G    | O4'-C1'-N9 | 6.29  | 113.23      | 108.20   |
| 1   | AA    | 645  | G    | O4'-C1'-N9 | 6.29  | 113.23      | 108.20   |
| 27  | B8    | 2218 | G    | O4'-C1'-N9 | 6.29  | 113.23      | 108.20   |
| 27  | B8    | 2266 | A    | C4-C5-C6   | 6.29  | 120.14      | 117.00   |
| 1   | AA    | 199  | A    | C5-C6-N6   | -6.29 | 118.67      | 123.70   |
| 1   | AA    | 255  | G    | O4'-C1'-N9 | 6.29  | 113.23      | 108.20   |
| 1   | AA    | 765  | G    | C5-C6-O6   | -6.29 | 124.83      | 128.60   |
| 1   | AA    | 886  | G    | O4'-C1'-N9 | 6.29  | 113.23      | 108.20   |
| 1   | AA    | 934  | C    | N3-C4-C5   | -6.29 | 119.39      | 121.90   |
| 1   | AA    | 1397 | C    | N3-C4-N4   | 6.29  | 122.40      | 118.00   |
| 27  | B8    | 25   | U    | O4'-C1'-N1 | 6.29  | 113.23      | 108.20   |
| 27  | B8    | 484  | C    | N3-C4-N4   | 6.29  | 122.40      | 118.00   |
| 27  | B8    | 675  | A    | C4-C5-C6   | 6.29  | 120.14      | 117.00   |
| 27  | B8    | 681  | G    | O4'-C1'-N9 | 6.29  | 113.23      | 108.20   |
| 1   | AA    | 161  | A    | C4-C5-C6   | 6.28  | 120.14      | 117.00   |
| 1   | AA    | 1102 | A    | C4-C5-C6   | 6.28  | 120.14      | 117.00   |
| 1   | AA    | 1488 | G    | O4'-C1'-N9 | 6.28  | 113.23      | 108.20   |
| 27  | B8    | 886  | A    | C4-C5-C6   | 6.28  | 120.14      | 117.00   |
| 27  | B8    | 982  | C    | O4'-C1'-N1 | 6.28  | 113.23      | 108.20   |
| 27  | B8    | 1244 | A    | O4'-C1'-N9 | 6.28  | 113.23      | 108.20   |
| 27  | B8    | 1593 | A    | C4-C5-C6   | 6.28  | 120.14      | 117.00   |
| 27  | B8    | 2050 | C    | O4'-C1'-N1 | 6.28  | 113.23      | 108.20   |
| 27  | B8    | 2827 | C    | N3-C4-N4   | 6.28  | 122.40      | 118.00   |
| 27  | B8    | 125  | A    | C4-C5-C6   | 6.28  | 120.14      | 117.00   |
| 27  | B8    | 1928 | A    | C4-C5-C6   | 6.28  | 120.14      | 117.00   |
| 27  | B8    | 2205 | A    | O4'-C1'-N9 | 6.28  | 113.23      | 108.20   |
| 27  | B8    | 2738 | A    | C5-C6-N1   | -6.28 | 114.56      | 117.70   |
| 27  | B8    | 379  | G    | O4'-C1'-N9 | 6.28  | 113.22      | 108.20   |
| 27  | B8    | 482  | A    | C4-C5-C6   | 6.28  | 120.14      | 117.00   |
| 27  | B8    | 505  | A    | C4-C5-C6   | 6.28  | 120.14      | 117.00   |
| 27  | B8    | 572  | A    | C4-C5-C6   | 6.28  | 120.14      | 117.00   |
| 27  | B8    | 1104 | C    | N3-C4-C5   | -6.28 | 119.39      | 121.90   |
| 27  | B8    | 2407 | A    | C4-C5-C6   | 6.28  | 120.14      | 117.00   |
| 27  | B8    | 2612 | C    | N3-C4-N4   | 6.28  | 122.40      | 118.00   |
| 27  | B8    | 2008 | C    | N3-C4-N4   | 6.28  | 122.39      | 118.00   |
| 1   | AA    | 214  | C    | N3-C4-N4   | 6.28  | 122.39      | 118.00   |
| 1   | AA    | 1398 | A    | C4-C5-C6   | 6.28  | 120.14      | 117.00   |
| 27  | B8    | 1695 | G    | C5-C6-O6   | -6.28 | 124.83      | 128.60   |
| 27  | B8    | 2351 | G    | N3-C2-N2   | 6.28  | 124.30      | 119.90   |
| 27  | B8    | 2745 | C    | N3-C4-N4   | 6.28  | 122.39      | 118.00   |
| 27  | B8    | 2748 | A    | O4'-C1'-N9 | 6.28  | 113.22      | 108.20   |
| 1   | AA    | 1415 | G    | O4'-C1'-N9 | 6.28  | 113.22      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 6    | A    | C4-C5-C6   | 6.28  | 120.14      | 117.00   |
| 27  | B8    | 188  | G    | O4'-C1'-N9 | 6.28  | 113.22      | 108.20   |
| 27  | B8    | 251  | A    | C5-C6-N1   | -6.28 | 114.56      | 117.70   |
| 27  | B8    | 1246 | A    | O4'-C1'-N9 | 6.28  | 113.22      | 108.20   |
| 27  | B8    | 1579 | A    | C5-C6-N6   | -6.28 | 118.68      | 123.70   |
| 27  | B8    | 1596 | A    | O4'-C1'-N9 | 6.28  | 113.22      | 108.20   |
| 27  | B8    | 1668 | A    | C4-C5-C6   | 6.28  | 120.14      | 117.00   |
| 27  | B8    | 1864 | U    | O4'-C1'-N1 | 6.28  | 113.22      | 108.20   |
| 3   | AV    | 68   | G    | O4'-C1'-N9 | 6.27  | 113.22      | 108.20   |
| 26  | B7    | 50   | A    | O4'-C1'-N9 | 6.27  | 113.22      | 108.20   |
| 27  | B8    | 1124 | G    | O4'-C1'-N9 | 6.27  | 113.22      | 108.20   |
| 27  | B8    | 1353 | A    | O4'-C1'-N9 | 6.27  | 113.22      | 108.20   |
| 27  | B8    | 1813 | G    | O4'-C1'-N9 | 6.27  | 113.22      | 108.20   |
| 27  | B8    | 1988 | G    | O4'-C1'-N9 | 6.27  | 113.22      | 108.20   |
| 27  | B8    | 2745 | C    | O4'-C1'-N1 | 6.27  | 113.22      | 108.20   |
| 1   | AA    | 179  | A    | C4-C5-C6   | 6.27  | 120.14      | 117.00   |
| 1   | AA    | 670  | G    | O4'-C1'-N9 | 6.27  | 113.22      | 108.20   |
| 1   | AA    | 1525 | G    | C5-C6-O6   | -6.27 | 124.84      | 128.60   |
| 2   | AX    | 22   | A    | C4-C5-C6   | 6.27  | 120.14      | 117.00   |
| 27  | B8    | 671  | C    | N3-C4-N4   | 6.27  | 122.39      | 118.00   |
| 27  | B8    | 2518 | A    | C5-C6-N6   | -6.27 | 118.68      | 123.70   |
| 27  | B8    | 2558 | C    | N3-C4-N4   | 6.27  | 122.39      | 118.00   |
| 1   | AA    | 334  | C    | N3-C4-N4   | 6.27  | 122.39      | 118.00   |
| 1   | AA    | 990  | C    | N3-C4-N4   | 6.27  | 122.39      | 118.00   |
| 1   | AA    | 1066 | C    | N3-C4-N4   | 6.27  | 122.39      | 118.00   |
| 27  | B8    | 136  | G    | O4'-C1'-N9 | 6.27  | 113.22      | 108.20   |
| 27  | B8    | 707  | G    | C5-C6-O6   | -6.27 | 124.84      | 128.60   |
| 1   | AA    | 40   | C    | N3-C4-N4   | 6.27  | 122.39      | 118.00   |
| 1   | AA    | 958  | A    | C4-C5-C6   | 6.27  | 120.14      | 117.00   |
| 1   | AA    | 1361 | G    | C5-C6-O6   | -6.27 | 124.84      | 128.60   |
| 27  | B8    | 892  | A    | C4-C5-C6   | 6.27  | 120.14      | 117.00   |
| 27  | B8    | 1582 | C    | N3-C4-N4   | 6.27  | 122.39      | 118.00   |
| 27  | B8    | 2335 | A    | O4'-C1'-N9 | 6.27  | 113.22      | 108.20   |
| 27  | B8    | 2391 | G    | C5-C6-O6   | -6.27 | 124.84      | 128.60   |
| 27  | B8    | 2855 | C    | N3-C4-N4   | 6.27  | 122.39      | 118.00   |
| 1   | AA    | 1145 | A    | C5-C6-N1   | -6.27 | 114.57      | 117.70   |
| 27  | B8    | 1127 | A    | C5-C6-N6   | -6.27 | 118.69      | 123.70   |
| 27  | B8    | 1673 | G    | C5-C6-O6   | -6.27 | 124.84      | 128.60   |
| 27  | B8    | 2715 | C    | N3-C4-N4   | 6.27  | 122.39      | 118.00   |
| 1   | AA    | 357  | G    | C5-C6-O6   | -6.27 | 124.84      | 128.60   |
| 27  | B8    | 1085 | A    | C5-C6-N6   | -6.27 | 118.69      | 123.70   |
| 27  | B8    | 1433 | A    | O4'-C1'-N9 | 6.27  | 113.21      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2579 | C    | N3-C4-N4   | 6.27  | 122.39      | 118.00   |
| 1   | AA    | 130  | A    | C4-C5-C6   | 6.26  | 120.13      | 117.00   |
| 1   | AA    | 1357 | A    | C4-C5-C6   | 6.26  | 120.13      | 117.00   |
| 26  | B7    | 20   | G    | O4'-C1'-N9 | 6.26  | 113.21      | 108.20   |
| 27  | B8    | 583  | G    | O4'-C1'-N9 | 6.26  | 113.21      | 108.20   |
| 27  | B8    | 861  | A    | C5-C6-N6   | -6.26 | 118.69      | 123.70   |
| 27  | B8    | 1927 | A    | C5-C6-N1   | -6.26 | 114.57      | 117.70   |
| 27  | B8    | 1969 | A    | C4-C5-C6   | 6.26  | 120.13      | 117.00   |
| 27  | B8    | 2274 | A    | C5-C6-N6   | -6.26 | 118.69      | 123.70   |
| 27  | B8    | 2516 | A    | O4'-C1'-N9 | 6.26  | 113.21      | 108.20   |
| 1   | AA    | 313  | A    | O4'-C1'-N9 | 6.26  | 113.21      | 108.20   |
| 1   | AA    | 1422 | G    | O4'-C1'-N9 | 6.26  | 113.21      | 108.20   |
| 27  | B8    | 1705 | A    | C5-C6-N6   | -6.26 | 118.69      | 123.70   |
| 1   | AA    | 266  | G    | C5-C6-O6   | -6.26 | 124.84      | 128.60   |
| 1   | AA    | 838  | G    | O4'-C1'-N9 | 6.26  | 113.21      | 108.20   |
| 1   | AA    | 962  | C    | N3-C4-N4   | 6.26  | 122.38      | 118.00   |
| 1   | AA    | 1363 | A    | C4-C5-C6   | 6.26  | 120.13      | 117.00   |
| 27  | B8    | 651  | G    | O4'-C1'-N9 | 6.26  | 113.21      | 108.20   |
| 27  | B8    | 1957 | C    | N3-C4-N4   | 6.26  | 122.38      | 118.00   |
| 27  | B8    | 2771 | C    | N3-C4-N4   | 6.26  | 122.38      | 118.00   |
| 1   | AA    | 576  | C    | O4'-C1'-N1 | 6.26  | 113.21      | 108.20   |
| 27  | B8    | 38   | A    | C4-C5-C6   | 6.26  | 120.13      | 117.00   |
| 27  | B8    | 177  | G    | C5-C6-O6   | -6.26 | 124.84      | 128.60   |
| 27  | B8    | 2736 | A    | C4-C5-C6   | 6.26  | 120.13      | 117.00   |
| 1   | AA    | 300  | A    | C5-C6-N6   | -6.26 | 118.69      | 123.70   |
| 27  | B8    | 1434 | A    | C5-C6-N6   | -6.26 | 118.69      | 123.70   |
| 27  | B8    | 2513 | A    | C5-C6-N1   | -6.26 | 114.57      | 117.70   |
| 1   | AA    | 338  | A    | C4-C5-C6   | 6.26  | 120.13      | 117.00   |
| 1   | AA    | 746  | A    | C4-C5-C6   | 6.26  | 120.13      | 117.00   |
| 1   | AA    | 1014 | A    | C4-C5-C6   | 6.26  | 120.13      | 117.00   |
| 1   | AA    | 1420 | U    | O4'-C1'-N1 | 6.26  | 113.20      | 108.20   |
| 26  | B7    | 115  | A    | C5-C6-N6   | -6.26 | 118.69      | 123.70   |
| 27  | B8    | 1143 | A    | C5-C6-N6   | -6.26 | 118.69      | 123.70   |
| 27  | B8    | 2253 | G    | O4'-C1'-N9 | 6.26  | 113.20      | 108.20   |
| 27  | B8    | 2274 | A    | C4-C5-C6   | 6.26  | 120.13      | 117.00   |
| 1   | AA    | 1129 | C    | N3-C4-N4   | 6.25  | 122.38      | 118.00   |
| 27  | B8    | 2631 | G    | O4'-C1'-N9 | 6.25  | 113.20      | 108.20   |
| 27  | B8    | 2778 | A    | C4-C5-C6   | 6.25  | 120.13      | 117.00   |
| 1   | AA    | 758  | C    | N3-C4-N4   | 6.25  | 122.38      | 118.00   |
| 27  | B8    | 1187 | G    | O4'-C1'-N9 | 6.25  | 113.20      | 108.20   |
| 27  | B8    | 1228 | G    | O4'-C1'-N9 | 6.25  | 113.20      | 108.20   |
| 1   | AA    | 23   | C    | N3-C4-N4   | 6.25  | 122.38      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 98   | A    | C4-C5-C6   | 6.25  | 120.13      | 117.00   |
| 27  | B8    | 1088 | A    | C4-C5-C6   | 6.25  | 120.13      | 117.00   |
| 27  | B8    | 1901 | A    | C4-C5-C6   | 6.25  | 120.13      | 117.00   |
| 27  | B8    | 2222 | C    | N3-C4-N4   | 6.25  | 122.38      | 118.00   |
| 27  | B8    | 2843 | G    | O4'-C1'-N9 | 6.25  | 113.20      | 108.20   |
| 27  | B8    | 1900 | A    | C5-C6-N1   | -6.25 | 114.58      | 117.70   |
| 1   | AA    | 988  | G    | O4'-C1'-N9 | 6.25  | 113.20      | 108.20   |
| 1   | AA    | 1038 | C    | N3-C4-N4   | 6.25  | 122.38      | 118.00   |
| 26  | B7    | 27   | C    | N3-C4-N4   | 6.25  | 122.37      | 118.00   |
| 27  | B8    | 182  | A    | C4-C5-C6   | 6.25  | 120.12      | 117.00   |
| 27  | B8    | 246  | C    | N3-C4-N4   | 6.25  | 122.37      | 118.00   |
| 27  | B8    | 966  | G    | O4'-C1'-N9 | 6.25  | 113.20      | 108.20   |
| 27  | B8    | 1867 | G    | O4'-C1'-N9 | 6.25  | 113.20      | 108.20   |
| 27  | B8    | 2043 | C    | N3-C4-N4   | 6.25  | 122.37      | 118.00   |
| 28  | BA    | 314  | GLN  | CB-CA-C    | 6.25  | 122.89      | 110.40   |
| 1   | AA    | 51   | A    | C4-C5-C6   | 6.25  | 120.12      | 117.00   |
| 1   | AA    | 848  | C    | N3-C4-N4   | 6.25  | 122.37      | 118.00   |
| 1   | AA    | 1269 | A    | C5-C6-N6   | -6.25 | 118.70      | 123.70   |
| 27  | B8    | 1367 | A    | O4'-C1'-N9 | 6.25  | 113.20      | 108.20   |
| 27  | B8    | 2316 | G    | O4'-C1'-N9 | 6.25  | 113.20      | 108.20   |
| 28  | BA    | 401  | PHE  | N-CA-CB    | 6.25  | 121.84      | 110.60   |
| 1   | AA    | 1022 | A    | C5-C6-N1   | -6.25 | 114.58      | 117.70   |
| 27  | B8    | 33   | C    | N3-C4-N4   | 6.25  | 122.37      | 118.00   |
| 27  | B8    | 2105 | U    | O4'-C1'-N1 | 6.25  | 113.20      | 108.20   |
| 27  | B8    | 2439 | A    | C4-C5-C6   | 6.25  | 120.12      | 117.00   |
| 1   | AA    | 9    | G    | O4'-C1'-N9 | 6.24  | 113.19      | 108.20   |
| 1   | AA    | 607  | A    | C4-C5-C6   | 6.24  | 120.12      | 117.00   |
| 1   | AA    | 858  | G    | C5-C6-O6   | -6.24 | 124.85      | 128.60   |
| 1   | AA    | 1053 | G    | C5-C6-O6   | -6.24 | 124.85      | 128.60   |
| 26  | B7    | 84   | G    | O4'-C1'-N9 | 6.24  | 113.19      | 108.20   |
| 27  | B8    | 378  | C    | N3-C4-N4   | 6.24  | 122.37      | 118.00   |
| 27  | B8    | 402  | A    | O4'-C1'-N9 | 6.24  | 113.19      | 108.20   |
| 27  | B8    | 509  | C    | N3-C4-C5   | -6.24 | 119.40      | 121.90   |
| 27  | B8    | 1482 | G    | O4'-C1'-N9 | 6.24  | 113.19      | 108.20   |
| 27  | B8    | 2613 | U    | O4'-C1'-N1 | 6.24  | 113.19      | 108.20   |
| 27  | B8    | 2646 | C    | N3-C4-N4   | 6.24  | 122.37      | 118.00   |
| 1   | AA    | 864  | A    | C4-C5-C6   | 6.24  | 120.12      | 117.00   |
| 27  | B8    | 1557 | C    | N3-C4-N4   | 6.24  | 122.37      | 118.00   |
| 27  | B8    | 1871 | A    | C4-C5-C6   | 6.24  | 120.12      | 117.00   |
| 1   | AA    | 1445 | U    | O4'-C1'-N1 | 6.24  | 113.19      | 108.20   |
| 27  | B8    | 42   | A    | O4'-C1'-N9 | 6.24  | 113.19      | 108.20   |
| 27  | B8    | 670  | A    | C4-C5-C6   | 6.24  | 120.12      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 759  | G    | O4'-C1'-N9 | 6.24  | 113.19      | 108.20   |
| 27  | B8    | 1240 | U    | O4'-C1'-N1 | 6.24  | 113.19      | 108.20   |
| 27  | B8    | 1620 | G    | O4'-C1'-N9 | 6.24  | 113.19      | 108.20   |
| 27  | B8    | 1659 | G    | O4'-C1'-N9 | 6.24  | 113.19      | 108.20   |
| 1   | AA    | 1048 | G    | O4'-C1'-N9 | 6.24  | 113.19      | 108.20   |
| 1   | AA    | 1231 | G    | C5-C6-O6   | -6.24 | 124.86      | 128.60   |
| 27  | B8    | 984  | A    | C4-C5-C6   | 6.24  | 120.12      | 117.00   |
| 27  | B8    | 1510 | G    | O4'-C1'-N9 | 6.24  | 113.19      | 108.20   |
| 27  | B8    | 1687 | G    | C5-C6-O6   | -6.24 | 124.86      | 128.60   |
| 27  | B8    | 2726 | A    | C4-C5-C6   | 6.24  | 120.12      | 117.00   |
| 1   | AA    | 624  | C    | N3-C4-N4   | 6.24  | 122.37      | 118.00   |
| 1   | AA    | 675  | A    | O4'-C1'-N9 | 6.24  | 113.19      | 108.20   |
| 1   | AA    | 845  | A    | C4-C5-C6   | 6.24  | 120.12      | 117.00   |
| 27  | B8    | 195  | A    | C5-C6-N6   | -6.24 | 118.71      | 123.70   |
| 27  | B8    | 986  | C    | N3-C4-N4   | 6.24  | 122.37      | 118.00   |
| 27  | B8    | 1638 | C    | N3-C4-N4   | 6.24  | 122.37      | 118.00   |
| 27  | B8    | 1885 | A    | C4-C5-C6   | 6.24  | 120.12      | 117.00   |
| 27  | B8    | 2719 | G    | C5-C6-O6   | -6.24 | 124.86      | 128.60   |
| 1   | AA    | 415  | A    | C4-C5-C6   | 6.24  | 120.12      | 117.00   |
| 1   | AA    | 1288 | A    | C4-C5-C6   | 6.24  | 120.12      | 117.00   |
| 1   | AA    | 1385 | G    | O4'-C1'-N9 | 6.24  | 113.19      | 108.20   |
| 26  | B7    | 53   | A    | C4-C5-C6   | 6.24  | 120.12      | 117.00   |
| 27  | B8    | 415  | A    | C5-C6-N6   | -6.24 | 118.71      | 123.70   |
| 27  | B8    | 1356 | G    | C5-C6-O6   | -6.24 | 124.86      | 128.60   |
| 26  | B7    | 3    | C    | N3-C4-N4   | 6.23  | 122.36      | 118.00   |
| 27  | B8    | 123  | G    | O4'-C1'-N9 | 6.23  | 113.19      | 108.20   |
| 27  | B8    | 705  | A    | C5-C6-N6   | -6.23 | 118.71      | 123.70   |
| 27  | B8    | 1131 | G    | C5-C6-O6   | -6.23 | 124.86      | 128.60   |
| 27  | B8    | 1275 | A    | C5-C6-N6   | -6.23 | 118.71      | 123.70   |
| 27  | B8    | 1490 | A    | C4-C5-C6   | 6.23  | 120.12      | 117.00   |
| 27  | B8    | 1793 | C    | N3-C4-N4   | 6.23  | 122.36      | 118.00   |
| 1   | AA    | 887  | G    | O4'-C1'-N9 | 6.23  | 113.19      | 108.20   |
| 1   | AA    | 1080 | A    | C5-C6-N6   | -6.23 | 118.71      | 123.70   |
| 27  | B8    | 210  | C    | N3-C4-N4   | 6.23  | 122.36      | 118.00   |
| 27  | B8    | 696  | G    | C5-C6-O6   | -6.23 | 124.86      | 128.60   |
| 27  | B8    | 1144 | A    | C4-C5-C6   | 6.23  | 120.12      | 117.00   |
| 27  | B8    | 1726 | C    | N3-C4-N4   | 6.23  | 122.36      | 118.00   |
| 27  | B8    | 2088 | A    | O4'-C1'-N9 | 6.23  | 113.19      | 108.20   |
| 27  | B8    | 2178 | C    | P-O3'-C3'  | 6.23  | 127.18      | 119.70   |
| 27  | B8    | 2463 | C    | N3-C4-N4   | 6.23  | 122.36      | 118.00   |
| 27  | B8    | 2495 | G    | O4'-C1'-N9 | 6.23  | 113.19      | 108.20   |
| 1   | AA    | 27   | G    | O4'-C1'-N9 | 6.23  | 113.19      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 316  | C    | N3-C4-N4   | 6.23  | 122.36      | 118.00   |
| 1   | AA    | 435  | A    | C4-C5-C6   | 6.23  | 120.11      | 117.00   |
| 1   | AA    | 626  | G    | O4'-C1'-N9 | 6.23  | 113.18      | 108.20   |
| 3   | AV    | 27   | A    | C5-C6-N6   | -6.23 | 118.72      | 123.70   |
| 27  | B8    | 77   | G    | O4'-C1'-N9 | 6.23  | 113.18      | 108.20   |
| 27  | B8    | 429  | A    | C4-C5-C6   | 6.23  | 120.11      | 117.00   |
| 27  | B8    | 718  | A    | C4-C5-C6   | 6.23  | 120.11      | 117.00   |
| 27  | B8    | 2660 | A    | C4-C5-C6   | 6.23  | 120.11      | 117.00   |
| 1   | AA    | 139  | A    | C5-C6-N6   | -6.23 | 118.72      | 123.70   |
| 27  | B8    | 126  | A    | C4-C5-C6   | 6.23  | 120.11      | 117.00   |
| 27  | B8    | 565  | C    | N3-C4-N4   | 6.23  | 122.36      | 118.00   |
| 27  | B8    | 2886 | A    | O4'-C1'-N9 | 6.23  | 113.18      | 108.20   |
| 1   | AA    | 171  | A    | C4-C5-C6   | 6.23  | 120.11      | 117.00   |
| 1   | AA    | 852  | G    | C5-C6-O6   | -6.23 | 124.86      | 128.60   |
| 1   | AA    | 1482 | G    | C5-C6-O6   | -6.23 | 124.86      | 128.60   |
| 1   | AA    | 1502 | A    | C4-C5-C6   | 6.23  | 120.11      | 117.00   |
| 27  | B8    | 2795 | C    | N3-C4-N4   | 6.23  | 122.36      | 118.00   |
| 28  | BA    | 249  | ALA  | N-CA-CB    | 6.23  | 118.82      | 110.10   |
| 27  | B8    | 152  | A    | C5-C6-N6   | -6.23 | 118.72      | 123.70   |
| 27  | B8    | 2018 | G    | O4'-C1'-N9 | 6.23  | 113.18      | 108.20   |
| 1   | AA    | 77   | A    | C4-C5-C6   | 6.22  | 120.11      | 117.00   |
| 1   | AA    | 474  | G    | O4'-C1'-N9 | 6.22  | 113.18      | 108.20   |
| 27  | B8    | 52   | A    | C5-C6-N1   | -6.22 | 114.59      | 117.70   |
| 27  | B8    | 621  | A    | O4'-C1'-N9 | 6.22  | 113.18      | 108.20   |
| 27  | B8    | 1317 | G    | C5-C6-O6   | -6.22 | 124.86      | 128.60   |
| 27  | B8    | 1387 | A    | C5-C6-N6   | -6.22 | 118.72      | 123.70   |
| 27  | B8    | 1618 | A    | C4-C5-C6   | 6.22  | 120.11      | 117.00   |
| 27  | B8    | 2632 | A    | C4-C5-C6   | 6.22  | 120.11      | 117.00   |
| 1   | AA    | 98   | A    | C5-C6-N6   | -6.22 | 118.72      | 123.70   |
| 1   | AA    | 1281 | C    | O4'-C1'-N1 | 6.22  | 113.18      | 108.20   |
| 27  | B8    | 111  | A    | O4'-C1'-N9 | 6.22  | 113.18      | 108.20   |
| 27  | B8    | 822  | G    | O4'-C1'-N9 | 6.22  | 113.18      | 108.20   |
| 27  | B8    | 831  | G    | C5-C6-O6   | -6.22 | 124.87      | 128.60   |
| 27  | B8    | 878  | A    | C4-C5-C6   | 6.22  | 120.11      | 117.00   |
| 27  | B8    | 2225 | A    | C5-C6-N1   | -6.22 | 114.59      | 117.70   |
| 1   | AA    | 32   | A    | C4-C5-C6   | 6.22  | 120.11      | 117.00   |
| 1   | AA    | 33   | A    | C4-C5-C6   | 6.22  | 120.11      | 117.00   |
| 1   | AA    | 623  | C    | N3-C4-N4   | 6.22  | 122.36      | 118.00   |
| 27  | B8    | 377  | G    | O4'-C1'-N9 | 6.22  | 113.18      | 108.20   |
| 27  | B8    | 1084 | A    | C4-C5-C6   | 6.22  | 120.11      | 117.00   |
| 27  | B8    | 1464 | G    | O4'-C1'-N9 | 6.22  | 113.18      | 108.20   |
| 27  | B8    | 2003 | A    | C4-C5-C6   | 6.22  | 120.11      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 15   | G    | O4'-C1'-N9 | 6.22  | 113.17      | 108.20   |
| 1   | AA    | 326  | G    | C5-C6-O6   | -6.22 | 124.87      | 128.60   |
| 1   | AA    | 1158 | C    | C2-N1-C1'  | 6.22  | 125.64      | 118.80   |
| 5   | A0    | 166  | TYR  | CB-CG-CD1  | 6.22  | 124.73      | 121.00   |
| 27  | B8    | 347  | A    | C5-C6-N6   | -6.22 | 118.72      | 123.70   |
| 27  | B8    | 1331 | G    | C5-C6-O6   | -6.22 | 124.87      | 128.60   |
| 27  | B8    | 1696 | G    | O4'-C1'-N9 | 6.22  | 113.18      | 108.20   |
| 27  | B8    | 1934 | C    | N3-C4-N4   | 6.22  | 122.35      | 118.00   |
| 27  | B8    | 2392 | A    | C4-C5-C6   | 6.22  | 120.11      | 117.00   |
| 27  | B8    | 2577 | A    | C4-C5-C6   | 6.22  | 120.11      | 117.00   |
| 27  | B8    | 2753 | A    | C4-C5-C6   | 6.22  | 120.11      | 117.00   |
| 27  | B8    | 2816 | G    | O4'-C1'-N9 | 6.22  | 113.18      | 108.20   |
| 1   | AA    | 144  | G    | O4'-C1'-N9 | 6.22  | 113.17      | 108.20   |
| 1   | AA    | 1274 | A    | O4'-C1'-N9 | 6.22  | 113.17      | 108.20   |
| 1   | AA    | 1276 | G    | O4'-C1'-N9 | 6.22  | 113.17      | 108.20   |
| 27  | B8    | 629  | G    | O4'-C1'-N9 | 6.22  | 113.17      | 108.20   |
| 27  | B8    | 1762 | A    | C4-C5-C6   | 6.22  | 120.11      | 117.00   |
| 27  | B8    | 2704 | C    | N3-C4-N4   | 6.22  | 122.35      | 118.00   |
| 1   | AA    | 192  | A    | C4-C5-C6   | 6.22  | 120.11      | 117.00   |
| 1   | AA    | 713  | G    | O4'-C1'-N9 | 6.22  | 113.17      | 108.20   |
| 1   | AA    | 732  | C    | N3-C4-N4   | 6.22  | 122.35      | 118.00   |
| 1   | AA    | 1046 | A    | C5-C6-N6   | -6.22 | 118.73      | 123.70   |
| 1   | AA    | 1526 | G    | O4'-C1'-N9 | 6.22  | 113.17      | 108.20   |
| 27  | B8    | 386  | G    | C5-C6-O6   | -6.22 | 124.87      | 128.60   |
| 27  | B8    | 1205 | A    | C4-C5-C6   | 6.22  | 120.11      | 117.00   |
| 1   | AA    | 10   | A    | C4-C5-C6   | 6.21  | 120.11      | 117.00   |
| 1   | AA    | 16   | A    | C4-C5-C6   | 6.21  | 120.11      | 117.00   |
| 1   | AA    | 463  | U    | O4'-C1'-N1 | 6.21  | 113.17      | 108.20   |
| 1   | AA    | 1224 | U    | O4'-C1'-N1 | 6.21  | 113.17      | 108.20   |
| 27  | B8    | 267  | C    | N3-C4-N4   | 6.21  | 122.35      | 118.00   |
| 27  | B8    | 323  | C    | C6-N1-C1'  | -6.21 | 113.34      | 120.80   |
| 27  | B8    | 454  | A    | C4-C5-C6   | 6.21  | 120.11      | 117.00   |
| 27  | B8    | 1722 | A    | C5-C6-N1   | -6.21 | 114.59      | 117.70   |
| 27  | B8    | 1892 | C    | N3-C4-N4   | 6.21  | 122.35      | 118.00   |
| 27  | B8    | 1966 | A    | C4-C5-C6   | 6.21  | 120.11      | 117.00   |
| 1   | AA    | 621  | A    | C4-C5-C6   | 6.21  | 120.11      | 117.00   |
| 2   | AX    | 21   | A    | C4-C5-C6   | 6.21  | 120.11      | 117.00   |
| 27  | B8    | 1244 | A    | C5-C6-N6   | -6.21 | 118.73      | 123.70   |
| 1   | AA    | 681  | A    | C5-C6-N1   | -6.21 | 114.59      | 117.70   |
| 1   | AA    | 745  | G    | O4'-C1'-N9 | 6.21  | 113.17      | 108.20   |
| 1   | AA    | 964  | A    | C4-C5-C6   | 6.21  | 120.11      | 117.00   |
| 27  | B8    | 680  | C    | N3-C4-N4   | 6.21  | 122.35      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 925  | A    | C5-C6-N1   | -6.21 | 114.59      | 117.70   |
| 27  | B8    | 1054 | A    | C4-C5-C6   | 6.21  | 120.11      | 117.00   |
| 27  | B8    | 1321 | A    | C4-C5-C6   | 6.21  | 120.11      | 117.00   |
| 27  | B8    | 2126 | A    | C4-C5-C6   | 6.21  | 120.11      | 117.00   |
| 27  | B8    | 2738 | A    | C4-C5-C6   | 6.21  | 120.11      | 117.00   |
| 27  | B8    | 2792 | A    | C4-C5-C6   | 6.21  | 120.11      | 117.00   |
| 27  | B8    | 360  | U    | O4'-C1'-N1 | 6.21  | 113.17      | 108.20   |
| 27  | B8    | 1713 | A    | C5-C6-N1   | -6.21 | 114.60      | 117.70   |
| 27  | B8    | 2879 | A    | C4-C5-C6   | 6.21  | 120.11      | 117.00   |
| 1   | AA    | 227  | G    | O4'-C1'-N9 | 6.21  | 113.17      | 108.20   |
| 1   | AA    | 359  | G    | O4'-C1'-N9 | 6.21  | 113.17      | 108.20   |
| 1   | AA    | 1057 | G    | C5-C6-O6   | -6.21 | 124.88      | 128.60   |
| 1   | AA    | 1092 | A    | C4-C5-C6   | 6.21  | 120.10      | 117.00   |
| 27  | B8    | 563  | A    | C4-C5-C6   | 6.21  | 120.10      | 117.00   |
| 27  | B8    | 1969 | A    | O4'-C1'-N9 | 6.21  | 113.17      | 108.20   |
| 27  | B8    | 2071 | A    | C4-C5-C6   | 6.21  | 120.10      | 117.00   |
| 27  | B8    | 2114 | A    | C4-C5-C6   | 6.21  | 120.10      | 117.00   |
| 27  | B8    | 2223 | G    | O4'-C1'-N9 | 6.21  | 113.17      | 108.20   |
| 27  | B8    | 2649 | C    | N3-C4-N4   | 6.21  | 122.34      | 118.00   |
| 1   | AA    | 599  | C    | N3-C4-N4   | 6.21  | 122.34      | 118.00   |
| 1   | AA    | 855  | U    | O4'-C1'-N1 | 6.21  | 113.16      | 108.20   |
| 27  | B8    | 117  | G    | O4'-C1'-N9 | 6.21  | 113.16      | 108.20   |
| 27  | B8    | 119  | A    | O4'-C1'-N9 | 6.21  | 113.16      | 108.20   |
| 27  | B8    | 840  | C    | N3-C4-N4   | 6.21  | 122.34      | 118.00   |
| 27  | B8    | 1052 | C    | N3-C4-N4   | 6.21  | 122.34      | 118.00   |
| 1   | AA    | 285  | C    | N3-C4-N4   | 6.20  | 122.34      | 118.00   |
| 1   | AA    | 349  | A    | C5-C6-N1   | -6.20 | 114.60      | 117.70   |
| 1   | AA    | 524  | G    | O4'-C1'-N9 | 6.20  | 113.16      | 108.20   |
| 27  | B8    | 1301 | A    | C4-C5-C6   | 6.20  | 120.10      | 117.00   |
| 27  | B8    | 1316 | U    | O4'-C1'-N1 | 6.20  | 113.16      | 108.20   |
| 27  | B8    | 2038 | G    | C5-C6-O6   | -6.20 | 124.88      | 128.60   |
| 27  | B8    | 2273 | A    | C4-C5-C6   | 6.20  | 120.10      | 117.00   |
| 1   | AA    | 363  | A    | C4-C5-C6   | 6.20  | 120.10      | 117.00   |
| 27  | B8    | 384  | A    | C4-C5-C6   | 6.20  | 120.10      | 117.00   |
| 27  | B8    | 2764 | A    | C4-C5-C6   | 6.20  | 120.10      | 117.00   |
| 1   | AA    | 112  | G    | C5-C6-O6   | -6.20 | 124.88      | 128.60   |
| 27  | B8    | 1586 | A    | C4-C5-C6   | 6.20  | 120.10      | 117.00   |
| 27  | B8    | 1916 | A    | C4-C5-C6   | 6.20  | 120.10      | 117.00   |
| 27  | B8    | 2491 | U    | O4'-C1'-N1 | 6.20  | 113.16      | 108.20   |
| 1   | AA    | 186  | C    | N3-C4-N4   | 6.20  | 122.34      | 118.00   |
| 1   | AA    | 494  | G    | C5-C6-O6   | -6.20 | 124.88      | 128.60   |
| 1   | AA    | 895  | G    | O4'-C1'-N9 | 6.20  | 113.16      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 964  | A    | C5-C6-N6   | -6.20 | 118.74      | 123.70   |
| 1   | AA    | 1236 | A    | C5-C6-N6   | -6.20 | 118.74      | 123.70   |
| 27  | B8    | 326  | G    | O4'-C1'-N9 | 6.20  | 113.16      | 108.20   |
| 1   | AA    | 1256 | A    | C4-C5-C6   | 6.20  | 120.10      | 117.00   |
| 1   | AA    | 1357 | A    | C5-C6-N6   | -6.20 | 118.74      | 123.70   |
| 27  | B8    | 1253 | A    | C4-C5-C6   | 6.20  | 120.10      | 117.00   |
| 1   | AA    | 1421 | G    | C5-C6-O6   | -6.20 | 124.88      | 128.60   |
| 1   | AA    | 1457 | G    | O4'-C1'-N9 | 6.20  | 113.16      | 108.20   |
| 27  | B8    | 26   | G    | C5-C6-O6   | -6.20 | 124.88      | 128.60   |
| 27  | B8    | 2614 | A    | C4-C5-C6   | 6.20  | 120.10      | 117.00   |
| 27  | B8    | 2706 | A    | O4'-C1'-N9 | 6.20  | 113.16      | 108.20   |
| 1   | AA    | 538  | G    | O4'-C1'-N9 | 6.19  | 113.16      | 108.20   |
| 1   | AA    | 741  | G    | C5-C6-O6   | -6.19 | 124.88      | 128.60   |
| 27  | B8    | 21   | A    | C4-C5-C6   | 6.19  | 120.10      | 117.00   |
| 27  | B8    | 1022 | G    | O4'-C1'-N9 | 6.19  | 113.16      | 108.20   |
| 1   | AA    | 129  | A    | O4'-C1'-N9 | 6.19  | 113.16      | 108.20   |
| 1   | AA    | 1122 | U    | O4'-C1'-N1 | 6.19  | 113.15      | 108.20   |
| 27  | B8    | 160  | A    | C4-C5-C6   | 6.19  | 120.10      | 117.00   |
| 27  | B8    | 461  | C    | N3-C4-N4   | 6.19  | 122.33      | 118.00   |
| 27  | B8    | 1737 | G    | P-O3'-C3'  | 6.19  | 127.13      | 119.70   |
| 27  | B8    | 2168 | G    | N3-C2-N2   | 6.19  | 124.23      | 119.90   |
| 27  | B8    | 2354 | C    | N3-C4-N4   | 6.19  | 122.33      | 118.00   |
| 27  | B8    | 2557 | G    | O4'-C1'-N9 | 6.19  | 113.15      | 108.20   |
| 1   | AA    | 622  | A    | O4'-C1'-N9 | 6.19  | 113.15      | 108.20   |
| 1   | AA    | 777  | A    | O4'-C1'-N9 | 6.19  | 113.15      | 108.20   |
| 1   | AA    | 940  | C    | N3-C4-N4   | 6.19  | 122.33      | 118.00   |
| 26  | B7    | 49   | C    | N3-C4-N4   | 6.19  | 122.33      | 118.00   |
| 27  | B8    | 730  | A    | C4-C5-C6   | 6.19  | 120.09      | 117.00   |
| 27  | B8    | 1704 | C    | N3-C4-N4   | 6.19  | 122.33      | 118.00   |
| 1   | AA    | 86   | G    | O4'-C1'-N9 | 6.19  | 113.15      | 108.20   |
| 1   | AA    | 577  | G    | O4'-C1'-N9 | 6.19  | 113.15      | 108.20   |
| 27  | B8    | 661  | A    | C4-C5-C6   | 6.19  | 120.09      | 117.00   |
| 27  | B8    | 1095 | A    | C5-C6-N6   | -6.19 | 118.75      | 123.70   |
| 27  | B8    | 2080 | A    | C4-C5-C6   | 6.19  | 120.09      | 117.00   |
| 27  | B8    | 2184 | A    | C5-C6-N6   | -6.19 | 118.75      | 123.70   |
| 1   | AA    | 865  | A    | C5-C6-N6   | -6.19 | 118.75      | 123.70   |
| 27  | B8    | 1042 | G    | O4'-C1'-N9 | 6.19  | 113.15      | 108.20   |
| 27  | B8    | 2741 | A    | C4-C5-C6   | 6.19  | 120.09      | 117.00   |
| 1   | AA    | 460  | A    | C5-C6-N1   | -6.19 | 114.61      | 117.70   |
| 27  | B8    | 1413 | A    | C5-C6-N6   | -6.19 | 118.75      | 123.70   |
| 27  | B8    | 1422 | G    | O4'-C1'-N9 | 6.19  | 113.15      | 108.20   |
| 27  | B8    | 1544 | A    | C4-C5-C6   | 6.19  | 120.09      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | B8    | 1644 | C    | N3-C4-N4    | 6.19  | 122.33      | 118.00   |
| 27  | B8    | 2453 | A    | C5-C6-N6    | -6.19 | 118.75      | 123.70   |
| 1   | AA    | 66   | A    | C4-C5-C6    | 6.18  | 120.09      | 117.00   |
| 26  | B7    | 29   | A    | C5-C6-N6    | -6.18 | 118.75      | 123.70   |
| 27  | B8    | 68   | G    | O4'-C1'-N9  | 6.18  | 113.15      | 108.20   |
| 27  | B8    | 168  | G    | O4'-C1'-N9  | 6.18  | 113.15      | 108.20   |
| 27  | B8    | 491  | G    | C5'-C4'-O4' | 6.18  | 116.52      | 109.10   |
| 27  | B8    | 1818 | U    | O4'-C1'-N1  | 6.18  | 113.15      | 108.20   |
| 27  | B8    | 1900 | A    | C4-C5-C6    | 6.18  | 120.09      | 117.00   |
| 1   | AA    | 35   | G    | O4'-C1'-N9  | 6.18  | 113.15      | 108.20   |
| 1   | AA    | 373  | A    | C4-C5-C6    | 6.18  | 120.09      | 117.00   |
| 1   | AA    | 1418 | A    | C5-C6-N6    | -6.18 | 118.75      | 123.70   |
| 27  | B8    | 415  | A    | C4-C5-C6    | 6.18  | 120.09      | 117.00   |
| 27  | B8    | 465  | G    | C5-C6-O6    | -6.18 | 124.89      | 128.60   |
| 27  | B8    | 1144 | A    | C5-C6-N6    | -6.18 | 118.75      | 123.70   |
| 27  | B8    | 165  | A    | C4-C5-C6    | 6.18  | 120.09      | 117.00   |
| 27  | B8    | 1504 | A    | C4-C5-C6    | 6.18  | 120.09      | 117.00   |
| 27  | B8    | 2025 | C    | N3-C4-C5    | -6.18 | 119.43      | 121.90   |
| 1   | AA    | 431  | A    | O4'-C1'-N9  | 6.18  | 113.14      | 108.20   |
| 1   | AA    | 1153 | G    | O4'-C1'-N9  | 6.18  | 113.14      | 108.20   |
| 27  | B8    | 71   | A    | C4-C5-C6    | 6.18  | 120.09      | 117.00   |
| 27  | B8    | 1008 | A    | C4-C5-C6    | 6.18  | 120.09      | 117.00   |
| 1   | AA    | 1344 | C    | N3-C4-N4    | 6.18  | 122.32      | 118.00   |
| 27  | B8    | 2    | G    | O4'-C1'-N9  | 6.18  | 113.14      | 108.20   |
| 27  | B8    | 293  | U    | O4'-C1'-N1  | 6.18  | 113.14      | 108.20   |
| 27  | B8    | 2330 | G    | O4'-C1'-N9  | 6.18  | 113.14      | 108.20   |
| 27  | B8    | 2746 | U    | O4'-C1'-N1  | 6.18  | 113.14      | 108.20   |
| 1   | AA    | 181  | A    | O4'-C1'-N9  | 6.18  | 113.14      | 108.20   |
| 1   | AA    | 466  | A    | C4-C5-C6    | 6.18  | 120.09      | 117.00   |
| 27  | B8    | 33   | C    | O4'-C1'-N1  | 6.18  | 113.14      | 108.20   |
| 27  | B8    | 197  | A    | C4-C5-C6    | 6.18  | 120.09      | 117.00   |
| 27  | B8    | 655  | A    | C5-C6-N6    | -6.18 | 118.76      | 123.70   |
| 27  | B8    | 816  | C    | N3-C4-N4    | 6.18  | 122.32      | 118.00   |
| 27  | B8    | 1069 | A    | C4-C5-C6    | 6.18  | 120.09      | 117.00   |
| 27  | B8    | 1810 | A    | C4-C5-C6    | 6.18  | 120.09      | 117.00   |
| 27  | B8    | 2488 | G    | O4'-C1'-N9  | 6.18  | 113.14      | 108.20   |
| 1   | AA    | 236  | A    | C4-C5-C6    | 6.17  | 120.09      | 117.00   |
| 1   | AA    | 1044 | A    | C4-C5-C6    | 6.17  | 120.09      | 117.00   |
| 1   | AA    | 1309 | G    | O4'-C1'-N9  | 6.17  | 113.14      | 108.20   |
| 27  | B8    | 172  | A    | O4'-C1'-N9  | 6.17  | 113.14      | 108.20   |
| 27  | B8    | 368  | A    | C4-C5-C6    | 6.17  | 120.09      | 117.00   |
| 27  | B8    | 620  | G    | O4'-C1'-N9  | 6.17  | 113.14      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1543 | G    | O4'-C1'-N9 | 6.17  | 113.14      | 108.20   |
| 27  | B8    | 2375 | G    | C5-C6-O6   | -6.17 | 124.89      | 128.60   |
| 27  | B8    | 2461 | A    | C4-C5-C6   | 6.17  | 120.09      | 117.00   |
| 27  | B8    | 2512 | C    | N3-C4-N4   | 6.17  | 122.32      | 118.00   |
| 27  | B8    | 2810 | A    | C4-C5-C6   | 6.17  | 120.09      | 117.00   |
| 1   | AA    | 872  | A    | C4-C5-C6   | 6.17  | 120.09      | 117.00   |
| 1   | AA    | 879  | C    | N3-C4-N4   | 6.17  | 122.32      | 118.00   |
| 1   | AA    | 1093 | A    | C4-C5-C6   | 6.17  | 120.09      | 117.00   |
| 1   | AA    | 1099 | G    | C5-C6-O6   | -6.17 | 124.90      | 128.60   |
| 27  | B8    | 389  | G    | O4'-C1'-N9 | 6.17  | 113.14      | 108.20   |
| 27  | B8    | 947  | A    | C4-C5-C6   | 6.17  | 120.09      | 117.00   |
| 27  | B8    | 2047 | C    | N3-C4-N4   | 6.17  | 122.32      | 118.00   |
| 1   | AA    | 294  | U    | O4'-C1'-N1 | 6.17  | 113.14      | 108.20   |
| 1   | AA    | 1449 | C    | N3-C4-N4   | 6.17  | 122.32      | 118.00   |
| 27  | B8    | 282  | A    | C5-C6-N1   | -6.17 | 114.61      | 117.70   |
| 27  | B8    | 689  | A    | C4-C5-C6   | 6.17  | 120.09      | 117.00   |
| 27  | B8    | 815  | C    | N3-C4-N4   | 6.17  | 122.32      | 118.00   |
| 27  | B8    | 876  | C    | N3-C4-N4   | 6.17  | 122.32      | 118.00   |
| 27  | B8    | 1755 | A    | C5-C6-N6   | -6.17 | 118.76      | 123.70   |
| 27  | B8    | 2428 | G    | O4'-C1'-N9 | 6.17  | 113.14      | 108.20   |
| 1   | AA    | 749  | A    | O4'-C1'-N9 | 6.17  | 113.14      | 108.20   |
| 27  | B8    | 730  | A    | C5-C6-N6   | -6.17 | 118.76      | 123.70   |
| 1   | AA    | 265  | G    | O4'-C1'-N9 | 6.17  | 113.13      | 108.20   |
| 1   | AA    | 650  | G    | C5-C6-O6   | -6.17 | 124.90      | 128.60   |
| 1   | AA    | 664  | G    | C5-C6-O6   | -6.17 | 124.90      | 128.60   |
| 1   | AA    | 1359 | C    | N3-C4-N4   | 6.17  | 122.32      | 118.00   |
| 27  | B8    | 1039 | A    | C4-C5-C6   | 6.17  | 120.08      | 117.00   |
| 27  | B8    | 1425 | G    | O4'-C1'-N9 | 6.17  | 113.14      | 108.20   |
| 27  | B8    | 2402 | U    | O4'-C1'-N1 | 6.17  | 113.13      | 108.20   |
| 1   | AA    | 328  | C    | O4'-C1'-N1 | 6.17  | 113.13      | 108.20   |
| 1   | AA    | 456  | A    | C5-C6-N1   | -6.17 | 114.62      | 117.70   |
| 1   | AA    | 630  | A    | C4-C5-C6   | 6.17  | 120.08      | 117.00   |
| 11  | AG    | 161  | PHE  | CB-CG-CD2  | -6.17 | 116.48      | 120.80   |
| 26  | B7    | 11   | C    | O4'-C1'-N1 | 6.17  | 113.13      | 108.20   |
| 27  | B8    | 606  | U    | O4'-C1'-N1 | 6.17  | 113.13      | 108.20   |
| 27  | B8    | 614  | A    | C4-C5-C6   | 6.17  | 120.08      | 117.00   |
| 27  | B8    | 2386 | A    | C5-C6-N6   | -6.17 | 118.77      | 123.70   |
| 27  | B8    | 2403 | C    | N3-C4-N4   | 6.17  | 122.32      | 118.00   |
| 27  | B8    | 2765 | A    | C4-C5-C6   | 6.17  | 120.08      | 117.00   |
| 1   | AA    | 442  | G    | O4'-C1'-N9 | 6.17  | 113.13      | 108.20   |
| 18  | AN    | 52   | ARG  | NE-CZ-NH1  | 6.17  | 123.38      | 120.30   |
| 27  | B8    | 492  | A    | O4'-C1'-N9 | 6.17  | 113.13      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2420 | C    | N3-C4-N4   | 6.17  | 122.31      | 118.00   |
| 26  | B7    | 85   | G    | O4'-C1'-N9 | 6.16  | 113.13      | 108.20   |
| 26  | B7    | 104  | A    | C5-C6-N6   | -6.16 | 118.77      | 123.70   |
| 27  | B8    | 690  | G    | C5-C6-O6   | -6.16 | 124.90      | 128.60   |
| 27  | B8    | 1022 | G    | C5-C6-O6   | -6.16 | 124.90      | 128.60   |
| 27  | B8    | 1885 | A    | O4'-C1'-N9 | 6.16  | 113.13      | 108.20   |
| 27  | B8    | 2152 | G    | C5-C6-O6   | -6.16 | 124.90      | 128.60   |
| 27  | B8    | 2581 | G    | C5-C6-O6   | -6.16 | 124.90      | 128.60   |
| 1   | AA    | 1377 | A    | C4-C5-C6   | 6.16  | 120.08      | 117.00   |
| 1   | AA    | 36   | C    | N3-C4-N4   | 6.16  | 122.31      | 118.00   |
| 1   | AA    | 754  | C    | C2-N1-C1'  | 6.16  | 125.58      | 118.80   |
| 1   | AA    | 981  | U    | O4'-C1'-N1 | 6.16  | 113.13      | 108.20   |
| 1   | AA    | 1297 | G    | O4'-C1'-N9 | 6.16  | 113.13      | 108.20   |
| 27  | B8    | 833  | A    | C4-C5-C6   | 6.16  | 120.08      | 117.00   |
| 27  | B8    | 1062 | G    | O4'-C1'-N9 | 6.16  | 113.13      | 108.20   |
| 27  | B8    | 2147 | A    | C4-C5-C6   | 6.16  | 120.08      | 117.00   |
| 1   | AA    | 142  | G    | O4'-C1'-N9 | 6.16  | 113.13      | 108.20   |
| 1   | AA    | 306  | A    | C4-C5-C6   | 6.16  | 120.08      | 117.00   |
| 1   | AA    | 313  | A    | C5-C6-N6   | -6.16 | 118.77      | 123.70   |
| 1   | AA    | 832  | G    | O4'-C1'-N9 | 6.16  | 113.13      | 108.20   |
| 1   | AA    | 937  | A    | O4'-C1'-N9 | 6.16  | 113.13      | 108.20   |
| 1   | AA    | 956  | U    | O4'-C1'-N1 | 6.16  | 113.13      | 108.20   |
| 1   | AA    | 1022 | A    | C4-C5-C6   | 6.16  | 120.08      | 117.00   |
| 27  | B8    | 663  | G    | O4'-C1'-N9 | 6.16  | 113.13      | 108.20   |
| 27  | B8    | 2166 | U    | O4'-C1'-N1 | 6.16  | 113.13      | 108.20   |
| 27  | B8    | 2882 | A    | C5-C6-N1   | -6.16 | 114.62      | 117.70   |
| 1   | AA    | 1251 | A    | O4'-C1'-N9 | 6.16  | 113.13      | 108.20   |
| 27  | B8    | 988  | A    | C4-C5-C6   | 6.16  | 120.08      | 117.00   |
| 27  | B8    | 1133 | A    | C4-C5-C6   | 6.16  | 120.08      | 117.00   |
| 27  | B8    | 1251 | C    | N3-C4-N4   | 6.16  | 122.31      | 118.00   |
| 1   | AA    | 33   | A    | C5-C6-N6   | -6.16 | 118.78      | 123.70   |
| 1   | AA    | 410  | G    | N3-C2-N2   | 6.16  | 124.21      | 119.90   |
| 1   | AA    | 1096 | C    | N3-C4-N4   | 6.16  | 122.31      | 118.00   |
| 1   | AA    | 1339 | A    | C5-C6-N1   | -6.16 | 114.62      | 117.70   |
| 27  | B8    | 1918 | A    | C4-C5-C6   | 6.16  | 120.08      | 117.00   |
| 27  | B8    | 2267 | A    | C5-C6-N6   | -6.16 | 118.78      | 123.70   |
| 1   | AA    | 862  | C    | N3-C4-N4   | 6.15  | 122.31      | 118.00   |
| 27  | B8    | 644  | A    | C5-C6-N6   | -6.15 | 118.78      | 123.70   |
| 27  | B8    | 789  | A    | C4-C5-C6   | 6.15  | 120.08      | 117.00   |
| 1   | AA    | 764  | C    | N3-C4-N4   | 6.15  | 122.31      | 118.00   |
| 1   | AA    | 1098 | C    | N3-C4-N4   | 6.15  | 122.31      | 118.00   |
| 1   | AA    | 1242 | G    | O4'-C1'-N9 | 6.15  | 113.12      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1434 | A    | C5-C6-N6   | -6.15 | 118.78      | 123.70   |
| 27  | B8    | 1608 | A    | C5-C6-N1   | -6.15 | 114.62      | 117.70   |
| 27  | B8    | 2531 | A    | C5-C6-N1   | -6.15 | 114.62      | 117.70   |
| 1   | AA    | 908  | A    | O4'-C1'-N9 | 6.15  | 113.12      | 108.20   |
| 1   | AA    | 1128 | C    | N3-C4-C5   | -6.15 | 119.44      | 121.90   |
| 26  | B7    | 34   | A    | O4'-C1'-N9 | 6.15  | 113.12      | 108.20   |
| 27  | B8    | 342  | A    | C4-C5-C6   | 6.15  | 120.08      | 117.00   |
| 27  | B8    | 472  | A    | C4-C5-C6   | 6.15  | 120.08      | 117.00   |
| 27  | B8    | 927  | A    | C4-C5-C6   | 6.15  | 120.08      | 117.00   |
| 27  | B8    | 1307 | A    | O4'-C1'-N9 | 6.15  | 113.12      | 108.20   |
| 27  | B8    | 1417 | C    | N3-C4-N4   | 6.15  | 122.31      | 118.00   |
| 27  | B8    | 1897 | G    | O4'-C1'-N9 | 6.15  | 113.12      | 108.20   |
| 27  | B8    | 2037 | A    | O4'-C1'-N9 | 6.15  | 113.12      | 108.20   |
| 27  | B8    | 2388 | A    | C4-C5-C6   | 6.15  | 120.08      | 117.00   |
| 27  | B8    | 2481 | G    | C5-C6-O6   | -6.15 | 124.91      | 128.60   |
| 1   | AA    | 1061 | G    | O4'-C1'-N9 | 6.15  | 113.12      | 108.20   |
| 27  | B8    | 792  | A    | C4-C5-C6   | 6.15  | 120.07      | 117.00   |
| 27  | B8    | 953  | G    | O4'-C1'-N9 | 6.15  | 113.12      | 108.20   |
| 27  | B8    | 1805 | A    | O4'-C1'-N9 | 6.15  | 113.12      | 108.20   |
| 27  | B8    | 2717 | C    | N3-C4-N4   | 6.15  | 122.30      | 118.00   |
| 1   | AA    | 311  | C    | N3-C4-N4   | 6.15  | 122.30      | 118.00   |
| 26  | B7    | 91   | C    | N3-C4-N4   | 6.15  | 122.30      | 118.00   |
| 27  | B8    | 1204 | A    | C4-C5-C6   | 6.15  | 120.07      | 117.00   |
| 27  | B8    | 1950 | G    | C5-C6-O6   | -6.15 | 124.91      | 128.60   |
| 27  | B8    | 2228 | G    | O4'-C1'-N9 | 6.15  | 113.12      | 108.20   |
| 27  | B8    | 2873 | A    | C5-C6-N6   | -6.15 | 118.78      | 123.70   |
| 1   | AA    | 80   | A    | C4-C5-C6   | 6.15  | 120.07      | 117.00   |
| 27  | B8    | 122  | G    | O4'-C1'-N9 | 6.15  | 113.12      | 108.20   |
| 1   | AA    | 211  | G    | C5-C6-O6   | -6.14 | 124.91      | 128.60   |
| 1   | AA    | 898  | G    | C5-C6-O6   | -6.14 | 124.91      | 128.60   |
| 27  | B8    | 146  | A    | O4'-C1'-N9 | 6.14  | 113.12      | 108.20   |
| 27  | B8    | 258  | G    | O4'-C1'-N9 | 6.14  | 113.11      | 108.20   |
| 27  | B8    | 325  | G    | O4'-C1'-N9 | 6.14  | 113.11      | 108.20   |
| 27  | B8    | 1063 | G    | O4'-C1'-N9 | 6.14  | 113.11      | 108.20   |
| 27  | B8    | 1603 | A    | C4-C5-C6   | 6.14  | 120.07      | 117.00   |
| 27  | B8    | 2411 | A    | C4-C5-C6   | 6.14  | 120.07      | 117.00   |
| 1   | AA    | 321  | A    | O4'-C1'-N9 | 6.14  | 113.11      | 108.20   |
| 1   | AA    | 779  | C    | N3-C4-N4   | 6.14  | 122.30      | 118.00   |
| 1   | AA    | 1156 | G    | N3-C2-N2   | 6.14  | 124.20      | 119.90   |
| 1   | AA    | 1435 | G    | O4'-C1'-N9 | 6.14  | 113.11      | 108.20   |
| 27  | B8    | 218  | A    | C4-C5-C6   | 6.14  | 120.07      | 117.00   |
| 27  | B8    | 367  | G    | O4'-C1'-N9 | 6.14  | 113.11      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 160  | A    | C4-C5-C6   | 6.14  | 120.07      | 117.00   |
| 1   | AA    | 743  | A    | C4-C5-C6   | 6.14  | 120.07      | 117.00   |
| 1   | AA    | 790  | A    | C4-C5-C6   | 6.14  | 120.07      | 117.00   |
| 1   | AA    | 1374 | A    | C5-C6-N6   | -6.14 | 118.79      | 123.70   |
| 26  | B7    | 27   | C    | P-O5'-C5'  | 6.14  | 130.72      | 120.90   |
| 27  | B8    | 309  | A    | C4-C5-C6   | 6.14  | 120.07      | 117.00   |
| 27  | B8    | 354  | A    | C5-C6-N1   | -6.14 | 114.63      | 117.70   |
| 27  | B8    | 910  | A    | C4-C5-C6   | 6.14  | 120.07      | 117.00   |
| 1   | AA    | 297  | G    | O4'-C1'-N9 | 6.14  | 113.11      | 108.20   |
| 27  | B8    | 73   | A    | O4'-C1'-N9 | 6.14  | 113.11      | 108.20   |
| 27  | B8    | 144  | A    | C4-C5-C6   | 6.14  | 120.07      | 117.00   |
| 27  | B8    | 226  | A    | C5-C6-N6   | -6.14 | 118.79      | 123.70   |
| 27  | B8    | 920  | A    | O4'-C1'-N9 | 6.14  | 113.11      | 108.20   |
| 27  | B8    | 1561 | C    | N3-C4-N4   | 6.14  | 122.30      | 118.00   |
| 27  | B8    | 1924 | C    | N3-C4-N4   | 6.14  | 122.30      | 118.00   |
| 1   | AA    | 393  | A    | C4-C5-C6   | 6.13  | 120.07      | 117.00   |
| 1   | AA    | 873  | A    | C5-C6-N1   | -6.13 | 114.63      | 117.70   |
| 26  | B7    | 86   | G    | O4'-C1'-N9 | 6.13  | 113.11      | 108.20   |
| 26  | B7    | 87   | U    | O4'-C1'-N1 | 6.13  | 113.11      | 108.20   |
| 27  | B8    | 585  | G    | N3-C2-N2   | 6.13  | 124.19      | 119.90   |
| 27  | B8    | 1287 | A    | C4-C5-C6   | 6.13  | 120.07      | 117.00   |
| 27  | B8    | 1358 | G    | O4'-C1'-N9 | 6.13  | 113.11      | 108.20   |
| 27  | B8    | 1495 | A    | C4-C5-C6   | 6.13  | 120.07      | 117.00   |
| 1   | AA    | 572  | A    | C4-C5-C6   | 6.13  | 120.07      | 117.00   |
| 1   | AA    | 675  | A    | C5-C6-N6   | -6.13 | 118.79      | 123.70   |
| 27  | B8    | 152  | A    | C4-C5-C6   | 6.13  | 120.07      | 117.00   |
| 27  | B8    | 1877 | A    | C4-C5-C6   | 6.13  | 120.07      | 117.00   |
| 1   | AA    | 189  | A    | C4-C5-C6   | 6.13  | 120.07      | 117.00   |
| 1   | AA    | 471  | U    | O4'-C1'-N1 | 6.13  | 113.11      | 108.20   |
| 1   | AA    | 763  | G    | O4'-C1'-N9 | 6.13  | 113.11      | 108.20   |
| 1   | AA    | 817  | C    | N3-C4-C5   | -6.13 | 119.45      | 121.90   |
| 1   | AA    | 1088 | G    | O4'-C1'-N9 | 6.13  | 113.11      | 108.20   |
| 27  | B8    | 353  | C    | N3-C4-N4   | 6.13  | 122.29      | 118.00   |
| 27  | B8    | 592  | A    | C5-C6-N1   | -6.13 | 114.63      | 117.70   |
| 27  | B8    | 1134 | A    | C4-C5-C6   | 6.13  | 120.06      | 117.00   |
| 27  | B8    | 1253 | A    | C5-C6-N1   | -6.13 | 114.63      | 117.70   |
| 27  | B8    | 1431 | A    | C4-C5-C6   | 6.13  | 120.07      | 117.00   |
| 27  | B8    | 1994 | C    | N3-C4-N4   | 6.13  | 122.29      | 118.00   |
| 27  | B8    | 896  | A    | C4-C5-C6   | 6.13  | 120.06      | 117.00   |
| 1   | AA    | 560  | A    | C4-C5-C6   | 6.13  | 120.06      | 117.00   |
| 3   | AV    | 58   | A    | C4-C5-C6   | 6.13  | 120.06      | 117.00   |
| 26  | B7    | 92   | C    | N3-C4-N4   | 6.13  | 122.29      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 510  | C    | N3-C4-N4   | 6.13  | 122.29      | 118.00   |
| 27  | B8    | 915  | C    | N3-C4-N4   | 6.13  | 122.29      | 118.00   |
| 27  | B8    | 1752 | C    | N3-C4-C5   | -6.13 | 119.45      | 121.90   |
| 27  | B8    | 2688 | G    | C5-C6-O6   | -6.13 | 124.92      | 128.60   |
| 1   | AA    | 724  | G    | O4'-C1'-N9 | 6.13  | 113.10      | 108.20   |
| 1   | AA    | 968  | A    | C4-C5-C6   | 6.13  | 120.06      | 117.00   |
| 1   | AA    | 1318 | A    | C4-C5-C6   | 6.13  | 120.06      | 117.00   |
| 27  | B8    | 743  | A    | C5-C6-N6   | -6.13 | 118.80      | 123.70   |
| 27  | B8    | 1574 | C    | N3-C4-N4   | 6.13  | 122.29      | 118.00   |
| 27  | B8    | 1654 | A    | C4-C5-C6   | 6.13  | 120.06      | 117.00   |
| 27  | B8    | 1673 | G    | O4'-C1'-N9 | 6.13  | 113.10      | 108.20   |
| 27  | B8    | 2470 | G    | O4'-C1'-N9 | 6.13  | 113.10      | 108.20   |
| 27  | B8    | 30   | G    | O4'-C1'-N9 | 6.12  | 113.10      | 108.20   |
| 27  | B8    | 409  | G    | O4'-C1'-N9 | 6.12  | 113.10      | 108.20   |
| 27  | B8    | 2405 | G    | N3-C2-N2   | 6.12  | 124.19      | 119.90   |
| 1   | AA    | 206  | C    | N3-C4-N4   | 6.12  | 122.29      | 118.00   |
| 1   | AA    | 536  | C    | N3-C4-N4   | 6.12  | 122.29      | 118.00   |
| 1   | AA    | 629  | A    | O4'-C1'-N9 | 6.12  | 113.10      | 108.20   |
| 1   | AA    | 742  | G    | O4'-C1'-N9 | 6.12  | 113.10      | 108.20   |
| 1   | AA    | 1319 | A    | C4-C5-C6   | 6.12  | 120.06      | 117.00   |
| 1   | AA    | 1408 | A    | O4'-C1'-N9 | 6.12  | 113.10      | 108.20   |
| 1   | AA    | 1479 | C    | N3-C4-C5   | -6.12 | 119.45      | 121.90   |
| 27  | B8    | 584  | C    | N3-C4-N4   | 6.12  | 122.29      | 118.00   |
| 27  | B8    | 858  | G    | C5-C6-O6   | -6.12 | 124.92      | 128.60   |
| 27  | B8    | 911  | A    | C4-C5-C6   | 6.12  | 120.06      | 117.00   |
| 27  | B8    | 1039 | A    | O4'-C1'-N9 | 6.12  | 113.10      | 108.20   |
| 1   | AA    | 1275 | A    | C4-C5-C6   | 6.12  | 120.06      | 117.00   |
| 1   | AA    | 1441 | A    | C4-C5-C6   | 6.12  | 120.06      | 117.00   |
| 3   | AV    | 70   | G    | O4'-C1'-N9 | 6.12  | 113.10      | 108.20   |
| 27  | B8    | 93   | G    | O4'-C1'-N9 | 6.12  | 113.10      | 108.20   |
| 27  | B8    | 795  | C    | N3-C4-N4   | 6.12  | 122.28      | 118.00   |
| 27  | B8    | 1262 | A    | C4-C5-C6   | 6.12  | 120.06      | 117.00   |
| 27  | B8    | 1529 | G    | C5-C6-O6   | -6.12 | 124.93      | 128.60   |
| 27  | B8    | 1876 | A    | O4'-C1'-N9 | 6.12  | 113.10      | 108.20   |
| 27  | B8    | 2095 | A    | C4-C5-C6   | 6.12  | 120.06      | 117.00   |
| 1   | AA    | 909  | A    | O4'-C1'-N9 | 6.12  | 113.10      | 108.20   |
| 27  | B8    | 666  | A    | C5-C6-N6   | -6.12 | 118.80      | 123.70   |
| 1   | AA    | 173  | U    | O4'-C1'-N1 | 6.12  | 113.09      | 108.20   |
| 1   | AA    | 201  | G    | C5-C6-O6   | -6.12 | 124.93      | 128.60   |
| 1   | AA    | 416  | G    | O4'-C1'-N9 | 6.12  | 113.09      | 108.20   |
| 1   | AA    | 1019 | A    | C4-C5-C6   | 6.12  | 120.06      | 117.00   |
| 27  | B8    | 94   | A    | O4'-C1'-N9 | 6.12  | 113.09      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1186 | G    | C5-C6-O6   | -6.12 | 124.93      | 128.60   |
| 27  | B8    | 1288 | G    | O4'-C1'-N9 | 6.12  | 113.09      | 108.20   |
| 27  | B8    | 1393 | A    | C4-C5-C6   | 6.12  | 120.06      | 117.00   |
| 27  | B8    | 1517 | G    | O4'-C1'-N9 | 6.12  | 113.09      | 108.20   |
| 27  | B8    | 1579 | A    | C4-C5-C6   | 6.12  | 120.06      | 117.00   |
| 1   | AA    | 131  | A    | C4-C5-C6   | 6.12  | 120.06      | 117.00   |
| 27  | B8    | 65   | U    | O4'-C1'-N1 | 6.12  | 113.09      | 108.20   |
| 27  | B8    | 1299 | G    | O4'-C1'-N9 | 6.12  | 113.09      | 108.20   |
| 27  | B8    | 1991 | U    | O4'-C1'-N1 | 6.12  | 113.09      | 108.20   |
| 1   | AA    | 238  | A    | C4-C5-C6   | 6.12  | 120.06      | 117.00   |
| 1   | AA    | 295  | C    | N3-C4-N4   | 6.12  | 122.28      | 118.00   |
| 1   | AA    | 309  | A    | C5-C6-N6   | -6.12 | 118.81      | 123.70   |
| 1   | AA    | 579  | A    | C4-C5-C6   | 6.12  | 120.06      | 117.00   |
| 1   | AA    | 784  | A    | C4-C5-C6   | 6.12  | 120.06      | 117.00   |
| 27  | B8    | 1072 | C    | N3-C4-N4   | 6.12  | 122.28      | 118.00   |
| 27  | B8    | 1354 | A    | C5-C6-N6   | -6.12 | 118.81      | 123.70   |
| 27  | B8    | 2773 | C    | N3-C4-N4   | 6.12  | 122.28      | 118.00   |
| 1   | AA    | 119  | A    | C5-C6-N1   | -6.11 | 114.64      | 117.70   |
| 1   | AA    | 942  | G    | C5-C6-O6   | -6.11 | 124.93      | 128.60   |
| 1   | AA    | 1167 | A    | C5-C6-N6   | -6.11 | 118.81      | 123.70   |
| 1   | AA    | 1254 | A    | C5-C6-N1   | -6.11 | 114.64      | 117.70   |
| 27  | B8    | 73   | A    | C4-C5-C6   | 6.11  | 120.06      | 117.00   |
| 27  | B8    | 1366 | A    | C4-C5-C6   | 6.11  | 120.06      | 117.00   |
| 27  | B8    | 2227 | A    | C4-C5-C6   | 6.11  | 120.06      | 117.00   |
| 27  | B8    | 2711 | A    | C5-C6-N6   | -6.11 | 118.81      | 123.70   |
| 1   | AA    | 545  | C    | N3-C4-N4   | 6.11  | 122.28      | 118.00   |
| 1   | AA    | 953  | G    | O4'-C1'-N9 | 6.11  | 113.09      | 108.20   |
| 27  | B8    | 1215 | G    | O4'-C1'-N9 | 6.11  | 113.09      | 108.20   |
| 27  | B8    | 1590 | A    | C5-C6-N6   | -6.11 | 118.81      | 123.70   |
| 27  | B8    | 2333 | A    | C5-C6-N6   | -6.11 | 118.81      | 123.70   |
| 27  | B8    | 2700 | A    | C5-C6-N6   | -6.11 | 118.81      | 123.70   |
| 1   | AA    | 404  | G    | O4'-C1'-N9 | 6.11  | 113.09      | 108.20   |
| 1   | AA    | 1131 | G    | C5-C6-O6   | -6.11 | 124.93      | 128.60   |
| 1   | AA    | 1150 | A    | C4-C5-C6   | 6.11  | 120.06      | 117.00   |
| 1   | AA    | 1451 | U    | O4'-C1'-N1 | 6.11  | 113.09      | 108.20   |
| 27  | B8    | 19   | A    | O4'-C1'-N9 | 6.11  | 113.09      | 108.20   |
| 27  | B8    | 127  | A    | C5-C6-N6   | -6.11 | 118.81      | 123.70   |
| 27  | B8    | 200  | U    | O4'-C1'-N1 | 6.11  | 113.09      | 108.20   |
| 27  | B8    | 502  | A    | C5-C6-N6   | -6.11 | 118.81      | 123.70   |
| 27  | B8    | 1505 | A    | C4-C5-C6   | 6.11  | 120.06      | 117.00   |
| 27  | B8    | 2361 | G    | C5-C6-O6   | -6.11 | 124.93      | 128.60   |
| 27  | B8    | 996  | A    | C4-C5-C6   | 6.11  | 120.06      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1168 | G    | O4'-C1'-N9 | 6.11  | 113.09      | 108.20   |
| 27  | B8    | 1179 | G    | O4'-C1'-N9 | 6.11  | 113.09      | 108.20   |
| 27  | B8    | 1359 | A    | C4-C5-C6   | 6.11  | 120.05      | 117.00   |
| 26  | B7    | 62   | C    | N3-C4-N4   | 6.11  | 122.28      | 118.00   |
| 27  | B8    | 151  | C    | N3-C4-C5   | -6.11 | 119.46      | 121.90   |
| 27  | B8    | 155  | A    | C5-C6-N1   | -6.11 | 114.65      | 117.70   |
| 27  | B8    | 1718 | G    | C5-C6-O6   | -6.11 | 124.94      | 128.60   |
| 27  | B8    | 1739 | A    | O4'-C1'-N9 | 6.11  | 113.09      | 108.20   |
| 27  | B8    | 2037 | A    | C5-C6-N6   | -6.11 | 118.81      | 123.70   |
| 27  | B8    | 2237 | G    | N3-C2-N2   | 6.11  | 124.17      | 119.90   |
| 27  | B8    | 2336 | A    | C4-C5-C6   | 6.11  | 120.05      | 117.00   |
| 27  | B8    | 2622 | U    | O4'-C1'-N1 | 6.11  | 113.09      | 108.20   |
| 27  | B8    | 2799 | A    | C4-C5-C6   | 6.11  | 120.05      | 117.00   |
| 1   | AA    | 8    | A    | C4-C5-C6   | 6.11  | 120.05      | 117.00   |
| 1   | AA    | 8    | A    | O4'-C1'-N9 | 6.11  | 113.08      | 108.20   |
| 1   | AA    | 42   | G    | O4'-C1'-N9 | 6.11  | 113.08      | 108.20   |
| 1   | AA    | 1052 | U    | O4'-C1'-N1 | 6.11  | 113.08      | 108.20   |
| 1   | AA    | 1487 | G    | C5-C6-O6   | -6.11 | 124.94      | 128.60   |
| 26  | B7    | 78   | A    | C5-C6-N6   | -6.11 | 118.81      | 123.70   |
| 27  | B8    | 575  | A    | C4-C5-C6   | 6.11  | 120.05      | 117.00   |
| 27  | B8    | 616  | A    | C4-C5-C6   | 6.11  | 120.05      | 117.00   |
| 27  | B8    | 845  | A    | C4-C5-C6   | 6.11  | 120.05      | 117.00   |
| 27  | B8    | 1365 | A    | C4-C5-C6   | 6.11  | 120.05      | 117.00   |
| 27  | B8    | 2042 | A    | C5-C6-N6   | -6.11 | 118.81      | 123.70   |
| 27  | B8    | 2576 | G    | C5-C6-O6   | -6.11 | 124.94      | 128.60   |
| 1   | AA    | 1074 | G    | O4'-C1'-N9 | 6.10  | 113.08      | 108.20   |
| 27  | B8    | 1433 | A    | C4-C5-C6   | 6.10  | 120.05      | 117.00   |
| 27  | B8    | 2864 | G    | O4'-C1'-N9 | 6.10  | 113.08      | 108.20   |
| 1   | AA    | 238  | A    | C5-C6-N6   | -6.10 | 118.82      | 123.70   |
| 27  | B8    | 372  | G    | O4'-C1'-N9 | 6.10  | 113.08      | 108.20   |
| 27  | B8    | 613  | A    | C4-C5-C6   | 6.10  | 120.05      | 117.00   |
| 27  | B8    | 637  | A    | C4-C5-C6   | 6.10  | 120.05      | 117.00   |
| 27  | B8    | 793  | A    | C4-C5-C6   | 6.10  | 120.05      | 117.00   |
| 27  | B8    | 885  | C    | N3-C4-N4   | 6.10  | 122.27      | 118.00   |
| 27  | B8    | 960  | A    | C4-C5-C6   | 6.10  | 120.05      | 117.00   |
| 27  | B8    | 1192 | G    | O4'-C1'-N9 | 6.10  | 113.08      | 108.20   |
| 27  | B8    | 1318 | U    | O4'-C1'-N1 | 6.10  | 113.08      | 108.20   |
| 27  | B8    | 1583 | A    | O4'-C1'-N9 | 6.10  | 113.08      | 108.20   |
| 27  | B8    | 2598 | A    | C5-C6-N6   | -6.10 | 118.82      | 123.70   |
| 26  | B7    | 58   | A    | C5-C6-N6   | -6.10 | 118.82      | 123.70   |
| 27  | B8    | 1550 | C    | N3-C4-N4   | 6.10  | 122.27      | 118.00   |
| 27  | B8    | 1868 | C    | N3-C4-N4   | 6.10  | 122.27      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 252  | U    | O4'-C1'-N1 | 6.10  | 113.08      | 108.20   |
| 1   | AA    | 722  | G    | C5-C6-O6   | -6.10 | 124.94      | 128.60   |
| 1   | AA    | 918  | A    | C4-C5-C6   | 6.10  | 120.05      | 117.00   |
| 26  | B7    | 101  | A    | O4'-C1'-N9 | 6.10  | 113.08      | 108.20   |
| 27  | B8    | 474  | G    | O4'-C1'-N9 | 6.10  | 113.08      | 108.20   |
| 27  | B8    | 859  | G    | N3-C2-N2   | 6.10  | 124.17      | 119.90   |
| 27  | B8    | 988  | A    | O4'-C1'-N9 | 6.10  | 113.08      | 108.20   |
| 1   | AA    | 202  | G    | O4'-C1'-N9 | 6.10  | 113.08      | 108.20   |
| 1   | AA    | 840  | C    | O4'-C1'-N1 | 6.10  | 113.08      | 108.20   |
| 27  | B8    | 342  | A    | C5-C6-N6   | -6.10 | 118.82      | 123.70   |
| 27  | B8    | 825  | A    | O4'-C1'-N9 | 6.10  | 113.08      | 108.20   |
| 27  | B8    | 861  | A    | O4'-C1'-N9 | 6.10  | 113.08      | 108.20   |
| 27  | B8    | 1640 | A    | C5-C6-N6   | -6.10 | 118.82      | 123.70   |
| 27  | B8    | 1932 | A    | O4'-C1'-N9 | 6.10  | 113.08      | 108.20   |
| 27  | B8    | 2885 | G    | O4'-C1'-N9 | 6.10  | 113.08      | 108.20   |
| 1   | AA    | 18   | C    | N3-C4-N4   | 6.10  | 122.27      | 118.00   |
| 1   | AA    | 718  | A    | C4-C5-C6   | 6.10  | 120.05      | 117.00   |
| 1   | AA    | 726  | C    | N3-C4-N4   | 6.10  | 122.27      | 118.00   |
| 27  | B8    | 630  | G    | O4'-C1'-N9 | 6.10  | 113.08      | 108.20   |
| 1   | AA    | 360  | G    | O4'-C1'-N9 | 6.09  | 113.08      | 108.20   |
| 1   | AA    | 975  | A    | C4-C5-C6   | 6.09  | 120.05      | 117.00   |
| 1   | AA    | 975  | A    | O4'-C1'-N9 | 6.09  | 113.08      | 108.20   |
| 1   | AA    | 1514 | G    | O4'-C1'-N9 | 6.09  | 113.08      | 108.20   |
| 27  | B8    | 883  | G    | C5-C6-O6   | -6.09 | 124.94      | 128.60   |
| 27  | B8    | 1373 | A    | O4'-C1'-N9 | 6.09  | 113.08      | 108.20   |
| 27  | B8    | 1512 | C    | N3-C4-N4   | 6.09  | 122.27      | 118.00   |
| 27  | B8    | 1973 | G    | O4'-C1'-N9 | 6.09  | 113.08      | 108.20   |
| 27  | B8    | 2589 | A    | C4-C5-C6   | 6.09  | 120.05      | 117.00   |
| 27  | B8    | 2896 | C    | N3-C4-N4   | 6.09  | 122.27      | 118.00   |
| 27  | B8    | 2252 | G    | C5-C6-O6   | -6.09 | 124.94      | 128.60   |
| 1   | AA    | 761  | G    | O4'-C1'-N9 | 6.09  | 113.07      | 108.20   |
| 1   | AA    | 919  | A    | C5-C6-N1   | -6.09 | 114.66      | 117.70   |
| 1   | AA    | 1476 | A    | C5-C6-N1   | -6.09 | 114.65      | 117.70   |
| 27  | B8    | 626  | A    | C4-C5-C6   | 6.09  | 120.05      | 117.00   |
| 27  | B8    | 818  | G    | C5-C6-O6   | -6.09 | 124.95      | 128.60   |
| 27  | B8    | 2186 | G    | O4'-C1'-N9 | 6.09  | 113.07      | 108.20   |
| 27  | B8    | 2727 | A    | C4-C5-C6   | 6.09  | 120.05      | 117.00   |
| 1   | AA    | 427  | U    | O4'-C1'-N1 | 6.09  | 113.07      | 108.20   |
| 1   | AA    | 1195 | C    | N3-C4-N4   | 6.09  | 122.26      | 118.00   |
| 27  | B8    | 964  | C    | N3-C4-N4   | 6.09  | 122.26      | 118.00   |
| 27  | B8    | 1512 | C    | O4'-C1'-N1 | 6.09  | 113.07      | 108.20   |
| 27  | B8    | 1525 | A    | C4-C5-C6   | 6.09  | 120.04      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2117 | A    | C4-C5-C6   | 6.09  | 120.05      | 117.00   |
| 27  | B8    | 2283 | C    | N3-C4-N4   | 6.09  | 122.26      | 118.00   |
| 27  | B8    | 2288 | A    | C4-C5-C6   | 6.09  | 120.05      | 117.00   |
| 45  | BQ    | 23   | TYR  | CB-CG-CD1  | -6.09 | 117.35      | 121.00   |
| 1   | AA    | 596  | A    | C4-C5-C6   | 6.09  | 120.04      | 117.00   |
| 1   | AA    | 831  | A    | O4'-C1'-N9 | 6.09  | 113.07      | 108.20   |
| 1   | AA    | 1437 | A    | C4-C5-C6   | 6.09  | 120.04      | 117.00   |
| 1   | AA    | 1458 | G    | O4'-C1'-N9 | 6.09  | 113.07      | 108.20   |
| 26  | B7    | 113  | C    | N3-C4-N4   | 6.09  | 122.26      | 118.00   |
| 27  | B8    | 337  | C    | N3-C4-N4   | 6.09  | 122.26      | 118.00   |
| 27  | B8    | 722  | A    | C4-C5-C6   | 6.09  | 120.04      | 117.00   |
| 27  | B8    | 1014 | A    | O4'-C1'-N9 | 6.09  | 113.07      | 108.20   |
| 27  | B8    | 2207 | C    | N3-C4-N4   | 6.09  | 122.26      | 118.00   |
| 1   | AA    | 649  | A    | O4'-C1'-N9 | 6.09  | 113.07      | 108.20   |
| 27  | B8    | 761  | A    | C5-C6-N6   | -6.09 | 118.83      | 123.70   |
| 27  | B8    | 1061 | U    | O4'-C1'-N1 | 6.09  | 113.07      | 108.20   |
| 27  | B8    | 1080 | A    | O4'-C1'-N9 | 6.09  | 113.07      | 108.20   |
| 27  | B8    | 2345 | G    | C5-C6-O6   | -6.09 | 124.95      | 128.60   |
| 1   | AA    | 1185 | G    | O4'-C1'-N9 | 6.08  | 113.07      | 108.20   |
| 27  | B8    | 2670 | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 1   | AA    | 527  | G    | O4'-C1'-N9 | 6.08  | 113.07      | 108.20   |
| 1   | AA    | 1508 | A    | O4'-C1'-N9 | 6.08  | 113.07      | 108.20   |
| 27  | B8    | 435  | C    | O4'-C1'-N1 | 6.08  | 113.07      | 108.20   |
| 27  | B8    | 790  | U    | O4'-C1'-N1 | 6.08  | 113.07      | 108.20   |
| 27  | B8    | 918  | A    | C5-C6-N1   | -6.08 | 114.66      | 117.70   |
| 27  | B8    | 1156 | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 27  | B8    | 2566 | A    | C5-C6-N1   | -6.08 | 114.66      | 117.70   |
| 27  | B8    | 2658 | C    | N3-C4-N4   | 6.08  | 122.26      | 118.00   |
| 1   | AA    | 53   | A    | C5-C6-N6   | -6.08 | 118.84      | 123.70   |
| 1   | AA    | 221  | C    | N3-C4-N4   | 6.08  | 122.26      | 118.00   |
| 1   | AA    | 403  | C    | N3-C4-N4   | 6.08  | 122.26      | 118.00   |
| 1   | AA    | 483  | C    | N3-C4-N4   | 6.08  | 122.26      | 118.00   |
| 1   | AA    | 539  | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 1   | AA    | 1229 | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 27  | B8    | 362  | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 27  | B8    | 858  | G    | O4'-C1'-N9 | 6.08  | 113.06      | 108.20   |
| 27  | B8    | 1626 | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 27  | B8    | 1630 | A    | O4'-C1'-N9 | 6.08  | 113.07      | 108.20   |
| 1   | AA    | 151  | A    | C5-C6-N1   | -6.08 | 114.66      | 117.70   |
| 27  | B8    | 925  | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 27  | B8    | 1566 | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 27  | B8    | 2627 | G    | O4'-C1'-N9 | 6.08  | 113.06      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 155  | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 1   | AA    | 695  | A    | C5-C6-N6   | -6.08 | 118.84      | 123.70   |
| 1   | AA    | 1245 | C    | N3-C4-N4   | 6.08  | 122.25      | 118.00   |
| 1   | AA    | 1285 | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 27  | B8    | 477  | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 27  | B8    | 985  | C    | N3-C4-N4   | 6.08  | 122.25      | 118.00   |
| 27  | B8    | 1151 | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 27  | B8    | 1268 | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 27  | B8    | 1846 | G    | O4'-C1'-N9 | 6.08  | 113.06      | 108.20   |
| 27  | B8    | 2300 | C    | N3-C4-N4   | 6.08  | 122.25      | 118.00   |
| 27  | B8    | 2494 | G    | O4'-C1'-N9 | 6.08  | 113.06      | 108.20   |
| 27  | B8    | 2792 | A    | P-O3'-C3'  | 6.08  | 127.00      | 119.70   |
| 27  | B8    | 1020 | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 27  | B8    | 1735 | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 27  | B8    | 2156 | G    | O4'-C1'-N9 | 6.08  | 113.06      | 108.20   |
| 27  | B8    | 2826 | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 1   | AA    | 1146 | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 1   | AA    | 1226 | C    | O4'-C1'-N1 | 6.08  | 113.06      | 108.20   |
| 1   | AA    | 1314 | C    | N3-C4-N4   | 6.08  | 122.25      | 118.00   |
| 11  | AG    | 161  | PHE  | CB-CG-CD1  | 6.08  | 125.05      | 120.80   |
| 27  | B8    | 1298 | C    | N3-C4-N4   | 6.08  | 122.25      | 118.00   |
| 27  | B8    | 1424 | G    | O4'-C1'-N9 | 6.08  | 113.06      | 108.20   |
| 27  | B8    | 1551 | A    | C5-C6-N1   | -6.08 | 114.66      | 117.70   |
| 27  | B8    | 2433 | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 27  | B8    | 2560 | A    | C4-C5-C6   | 6.08  | 120.04      | 117.00   |
| 1   | AA    | 683  | G    | C5-C6-O6   | -6.07 | 124.95      | 128.60   |
| 1   | AA    | 1151 | A    | C4-C5-C6   | 6.07  | 120.04      | 117.00   |
| 1   | AA    | 1503 | A    | C4-C5-C6   | 6.07  | 120.04      | 117.00   |
| 26  | B7    | 45   | A    | O4'-C1'-N9 | 6.07  | 113.06      | 108.20   |
| 27  | B8    | 262  | A    | C4-C5-C6   | 6.07  | 120.04      | 117.00   |
| 27  | B8    | 450  | G    | C5-C6-O6   | -6.07 | 124.96      | 128.60   |
| 27  | B8    | 2323 | G    | O4'-C1'-N9 | 6.07  | 113.06      | 108.20   |
| 1   | AA    | 445  | G    | O4'-C1'-N9 | 6.07  | 113.06      | 108.20   |
| 27  | B8    | 676  | A    | O4'-C1'-N9 | 6.07  | 113.06      | 108.20   |
| 27  | B8    | 2572 | A    | C4-C5-C6   | 6.07  | 120.04      | 117.00   |
| 1   | AA    | 1102 | A    | C5-C6-N1   | -6.07 | 114.67      | 117.70   |
| 1   | AA    | 1287 | A    | C4-C5-C6   | 6.07  | 120.03      | 117.00   |
| 1   | AA    | 1299 | A    | C4-C5-C6   | 6.07  | 120.03      | 117.00   |
| 1   | AA    | 1372 | U    | O4'-C1'-N1 | 6.07  | 113.06      | 108.20   |
| 1   | AA    | 1407 | C    | N3-C4-N4   | 6.07  | 122.25      | 118.00   |
| 27  | B8    | 513  | A    | C5-C6-N6   | -6.07 | 118.84      | 123.70   |
| 27  | B8    | 829  | A    | P-O3'-C3'  | 6.07  | 126.98      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1206 | G    | O4'-C1'-N9 | 6.07  | 113.06      | 108.20   |
| 27  | B8    | 2513 | A    | C4-C5-C6   | 6.07  | 120.03      | 117.00   |
| 1   | AA    | 1    | A    | O4'-C1'-N9 | 6.07  | 113.06      | 108.20   |
| 1   | AA    | 116  | A    | O4'-C1'-N9 | 6.07  | 113.06      | 108.20   |
| 1   | AA    | 531  | U    | O4'-C1'-N1 | 6.07  | 113.06      | 108.20   |
| 27  | B8    | 255  | A    | C5-C6-N6   | -6.07 | 118.84      | 123.70   |
| 27  | B8    | 263  | G    | O4'-C1'-N9 | 6.07  | 113.06      | 108.20   |
| 27  | B8    | 2370 | G    | O4'-C1'-N9 | 6.07  | 113.06      | 108.20   |
| 1   | AA    | 182  | A    | C4-C5-C6   | 6.07  | 120.03      | 117.00   |
| 1   | AA    | 514  | C    | N3-C4-N4   | 6.07  | 122.25      | 118.00   |
| 1   | AA    | 1201 | A    | C4-C5-C6   | 6.07  | 120.03      | 117.00   |
| 26  | B7    | 29   | A    | C4-C5-C6   | 6.07  | 120.03      | 117.00   |
| 27  | B8    | 737  | C    | N3-C4-N4   | 6.07  | 122.25      | 118.00   |
| 27  | B8    | 1470 | A    | C5-C6-N6   | -6.07 | 118.85      | 123.70   |
| 27  | B8    | 1829 | A    | C5-C6-N6   | -6.07 | 118.85      | 123.70   |
| 27  | B8    | 2238 | G    | C5-C6-O6   | -6.07 | 124.96      | 128.60   |
| 27  | B8    | 2287 | A    | C4-C5-C6   | 6.07  | 120.03      | 117.00   |
| 1   | AA    | 473  | U    | O4'-C1'-N1 | 6.07  | 113.05      | 108.20   |
| 1   | AA    | 501  | C    | N3-C4-N4   | 6.07  | 122.25      | 118.00   |
| 1   | AA    | 1188 | A    | C4-C5-C6   | 6.07  | 120.03      | 117.00   |
| 27  | B8    | 168  | G    | C5-C6-O6   | -6.07 | 124.96      | 128.60   |
| 27  | B8    | 182  | A    | C5-C6-N1   | -6.07 | 114.67      | 117.70   |
| 27  | B8    | 1640 | A    | C4-C5-C6   | 6.07  | 120.03      | 117.00   |
| 27  | B8    | 1672 | A    | C4-C5-C6   | 6.07  | 120.03      | 117.00   |
| 27  | B8    | 2376 | A    | C4-C5-C6   | 6.07  | 120.03      | 117.00   |
| 1   | AA    | 28   | A    | C4-C5-C6   | 6.06  | 120.03      | 117.00   |
| 1   | AA    | 181  | A    | C4-C5-C6   | 6.06  | 120.03      | 117.00   |
| 1   | AA    | 1487 | G    | O4'-C1'-N9 | 6.06  | 113.05      | 108.20   |
| 27  | B8    | 725  | G    | O4'-C1'-N9 | 6.06  | 113.05      | 108.20   |
| 27  | B8    | 1641 | A    | C5-C6-N1   | -6.06 | 114.67      | 117.70   |
| 27  | B8    | 2084 | C    | N3-C4-N4   | 6.06  | 122.25      | 118.00   |
| 27  | B8    | 2158 | A    | C4-C5-C6   | 6.06  | 120.03      | 117.00   |
| 1   | AA    | 253  | A    | C5-C6-N6   | -6.06 | 118.85      | 123.70   |
| 27  | B8    | 381  | G    | O4'-C1'-N9 | 6.06  | 113.05      | 108.20   |
| 27  | B8    | 788  | A    | C4-C5-C6   | 6.06  | 120.03      | 117.00   |
| 27  | B8    | 2380 | C    | N3-C4-N4   | 6.06  | 122.24      | 118.00   |
| 27  | B8    | 2503 | A    | C4-C5-C6   | 6.06  | 120.03      | 117.00   |
| 27  | B8    | 2742 | G    | O4'-C1'-N9 | 6.06  | 113.05      | 108.20   |
| 1   | AA    | 1468 | A    | C5-C6-N1   | -6.06 | 114.67      | 117.70   |
| 27  | B8    | 631  | A    | C4-C5-C6   | 6.06  | 120.03      | 117.00   |
| 27  | B8    | 2399 | G    | O4'-C1'-N9 | 6.06  | 113.05      | 108.20   |
| 1   | AA    | 1397 | C    | C6-N1-C1'  | -6.06 | 113.53      | 120.80   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 451  | U    | O4'-C1'-N1 | 6.06  | 113.05      | 108.20   |
| 27  | B8    | 1229 | C    | N3-C4-N4   | 6.06  | 122.24      | 118.00   |
| 27  | B8    | 1285 | A    | C5-C6-N6   | -6.06 | 118.85      | 123.70   |
| 27  | B8    | 2230 | G    | O4'-C1'-N9 | 6.06  | 113.05      | 108.20   |
| 27  | B8    | 2346 | A    | C4-C5-C6   | 6.06  | 120.03      | 117.00   |
| 27  | B8    | 2437 | G    | O4'-C1'-N9 | 6.06  | 113.05      | 108.20   |
| 27  | B8    | 2565 | A    | C4-C5-C6   | 6.06  | 120.03      | 117.00   |
| 1   | AA    | 235  | C    | N3-C4-N4   | 6.06  | 122.24      | 118.00   |
| 1   | AA    | 470  | C    | N3-C4-N4   | 6.06  | 122.24      | 118.00   |
| 1   | AA    | 831  | A    | C4-C5-C6   | 6.06  | 120.03      | 117.00   |
| 26  | B7    | 60   | C    | N3-C4-N4   | 6.06  | 122.24      | 118.00   |
| 27  | B8    | 461  | C    | O4'-C1'-N1 | 6.06  | 113.05      | 108.20   |
| 27  | B8    | 1095 | A    | C4-C5-C6   | 6.06  | 120.03      | 117.00   |
| 27  | B8    | 1755 | A    | C4-C5-C6   | 6.06  | 120.03      | 117.00   |
| 1   | AA    | 385  | C    | N3-C4-N4   | 6.06  | 122.24      | 118.00   |
| 1   | AA    | 782  | A    | C4-C5-C6   | 6.06  | 120.03      | 117.00   |
| 27  | B8    | 1560 | G    | O4'-C1'-N9 | 6.06  | 113.05      | 108.20   |
| 27  | B8    | 2629 | U    | O4'-C1'-N1 | 6.06  | 113.05      | 108.20   |
| 27  | B8    | 2760 | C    | N3-C4-N4   | 6.06  | 122.24      | 118.00   |
| 1   | AA    | 502  | A    | C4-C5-C6   | 6.05  | 120.03      | 117.00   |
| 1   | AA    | 1164 | G    | O4'-C1'-N9 | 6.05  | 113.04      | 108.20   |
| 1   | AA    | 1207 | G    | O4'-C1'-N9 | 6.05  | 113.04      | 108.20   |
| 3   | AV    | 60   | A    | O4'-C1'-N9 | 6.05  | 113.04      | 108.20   |
| 27  | B8    | 248  | G    | O4'-C1'-N9 | 6.05  | 113.04      | 108.20   |
| 27  | B8    | 1508 | A    | C4-C5-C6   | 6.05  | 120.03      | 117.00   |
| 27  | B8    | 1597 | A    | C4-C5-C6   | 6.05  | 120.03      | 117.00   |
| 27  | B8    | 1849 | G    | O4'-C1'-N9 | 6.05  | 113.04      | 108.20   |
| 27  | B8    | 2562 | U    | O4'-C1'-N1 | 6.05  | 113.04      | 108.20   |
| 1   | AA    | 816  | A    | C4-C5-C6   | 6.05  | 120.03      | 117.00   |
| 26  | B7    | 39   | A    | C4-C5-C6   | 6.05  | 120.03      | 117.00   |
| 27  | B8    | 28   | A    | C4-C5-C6   | 6.05  | 120.03      | 117.00   |
| 27  | B8    | 818  | G    | N3-C2-N2   | 6.05  | 124.14      | 119.90   |
| 1   | AA    | 1152 | A    | C4-C5-C6   | 6.05  | 120.03      | 117.00   |
| 1   | AA    | 1257 | A    | C4-C5-C6   | 6.05  | 120.03      | 117.00   |
| 26  | B7    | 59   | A    | C4-C5-C6   | 6.05  | 120.03      | 117.00   |
| 26  | B7    | 63   | C    | N3-C4-C5   | -6.05 | 119.48      | 121.90   |
| 27  | B8    | 216  | A    | C5-C6-N1   | -6.05 | 114.67      | 117.70   |
| 27  | B8    | 734  | A    | C4-C5-C6   | 6.05  | 120.03      | 117.00   |
| 27  | B8    | 1067 | A    | C4-C5-C6   | 6.05  | 120.03      | 117.00   |
| 27  | B8    | 1268 | A    | O4'-C1'-N9 | 6.05  | 113.04      | 108.20   |
| 27  | B8    | 2144 | G    | O4'-C1'-N9 | 6.05  | 113.04      | 108.20   |
| 1   | AA    | 679  | C    | N3-C4-C5   | -6.05 | 119.48      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 996  | A    | C4-C5-C6   | 6.05  | 120.03      | 117.00   |
| 27  | B8    | 149  | A    | C5-C6-N6   | -6.05 | 118.86      | 123.70   |
| 27  | B8    | 1918 | A    | O4'-C1'-N9 | 6.05  | 113.04      | 108.20   |
| 27  | B8    | 2730 | C    | N3-C4-N4   | 6.05  | 122.23      | 118.00   |
| 1   | AA    | 883  | C    | N3-C4-N4   | 6.05  | 122.23      | 118.00   |
| 1   | AA    | 1465 | A    | C4-C5-C6   | 6.05  | 120.02      | 117.00   |
| 27  | B8    | 1983 | G    | C5-C6-O6   | -6.05 | 124.97      | 128.60   |
| 27  | B8    | 2070 | A    | O4'-C1'-N9 | 6.05  | 113.04      | 108.20   |
| 27  | B8    | 2692 | G    | O4'-C1'-N9 | 6.05  | 113.04      | 108.20   |
| 1   | AA    | 977  | A    | C4-C5-C6   | 6.05  | 120.02      | 117.00   |
| 27  | B8    | 1077 | A    | C4-C5-C6   | 6.05  | 120.02      | 117.00   |
| 27  | B8    | 1336 | A    | C4-C5-C6   | 6.05  | 120.02      | 117.00   |
| 27  | B8    | 1811 | G    | O4'-C1'-N9 | 6.05  | 113.04      | 108.20   |
| 27  | B8    | 1942 | C    | O4'-C1'-N1 | 6.05  | 113.04      | 108.20   |
| 27  | B8    | 2197 | U    | O4'-C1'-N1 | 6.05  | 113.04      | 108.20   |
| 1   | AA    | 515  | G    | O4'-C1'-N9 | 6.04  | 113.04      | 108.20   |
| 1   | AA    | 1004 | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |
| 27  | B8    | 184  | C    | N3-C4-N4   | 6.04  | 122.23      | 118.00   |
| 27  | B8    | 781  | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |
| 1   | AA    | 30   | U    | O4'-C1'-N1 | 6.04  | 113.03      | 108.20   |
| 27  | B8    | 13   | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |
| 27  | B8    | 751  | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |
| 27  | B8    | 1385 | A    | C5-C6-N1   | -6.04 | 114.68      | 117.70   |
| 27  | B8    | 1677 | A    | C5-C6-N6   | -6.04 | 118.87      | 123.70   |
| 27  | B8    | 1803 | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |
| 1   | AA    | 440  | C    | N3-C4-N4   | 6.04  | 122.23      | 118.00   |
| 1   | AA    | 794  | A    | O4'-C1'-N9 | 6.04  | 113.03      | 108.20   |
| 27  | B8    | 56   | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |
| 27  | B8    | 167  | A    | C5-C6-N6   | -6.04 | 118.87      | 123.70   |
| 27  | B8    | 508  | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |
| 27  | B8    | 987  | C    | N3-C4-N4   | 6.04  | 122.23      | 118.00   |
| 27  | B8    | 1038 | G    | O4'-C1'-N9 | 6.04  | 113.03      | 108.20   |
| 27  | B8    | 1304 | A    | O4'-C1'-N9 | 6.04  | 113.03      | 108.20   |
| 27  | B8    | 1855 | U    | O4'-C1'-N1 | 6.04  | 113.03      | 108.20   |
| 27  | B8    | 2184 | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |
| 27  | B8    | 2270 | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |
| 27  | B8    | 2505 | G    | C5-C6-O6   | -6.04 | 124.97      | 128.60   |
| 1   | AA    | 10   | A    | C5-C6-N6   | -6.04 | 118.87      | 123.70   |
| 1   | AA    | 97   | G    | C5-C6-O6   | -6.04 | 124.98      | 128.60   |
| 1   | AA    | 663  | A    | C5-C6-N1   | -6.04 | 114.68      | 117.70   |
| 1   | AA    | 718  | A    | O4'-C1'-N9 | 6.04  | 113.03      | 108.20   |
| 27  | B8    | 324  | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 34   | C    | N3-C4-N4   | 6.04  | 122.23      | 118.00   |
| 1   | AA    | 1091 | U    | O4'-C1'-N1 | 6.04  | 113.03      | 108.20   |
| 1   | AA    | 1316 | G    | P-O3'-C3'  | 6.04  | 126.95      | 119.70   |
| 2   | AX    | 18   | C    | N3-C4-N4   | 6.04  | 122.23      | 118.00   |
| 27  | B8    | 344  | A    | O4'-C1'-N9 | 6.04  | 113.03      | 108.20   |
| 27  | B8    | 1526 | C    | N3-C4-N4   | 6.04  | 122.23      | 118.00   |
| 27  | B8    | 2171 | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |
| 27  | B8    | 2183 | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |
| 27  | B8    | 2263 | C    | N3-C4-N4   | 6.04  | 122.23      | 118.00   |
| 27  | B8    | 2385 | C    | N3-C4-N4   | 6.04  | 122.23      | 118.00   |
| 1   | AA    | 315  | A    | C5-C6-N1   | -6.04 | 114.68      | 117.70   |
| 27  | B8    | 957  | C    | N3-C4-N4   | 6.04  | 122.23      | 118.00   |
| 27  | B8    | 1055 | G    | O4'-C1'-N9 | 6.04  | 113.03      | 108.20   |
| 27  | B8    | 1204 | A    | C5-C6-N6   | -6.04 | 118.87      | 123.70   |
| 1   | AA    | 53   | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |
| 1   | AA    | 365  | U    | O4'-C1'-N1 | 6.04  | 113.03      | 108.20   |
| 1   | AA    | 459  | A    | C5-C6-N1   | -6.04 | 114.68      | 117.70   |
| 27  | B8    | 439  | A    | C5-C6-N1   | -6.04 | 114.68      | 117.70   |
| 27  | B8    | 1236 | G    | C5-C6-O6   | -6.04 | 124.98      | 128.60   |
| 27  | B8    | 1344 | U    | O4'-C1'-N1 | 6.04  | 113.03      | 108.20   |
| 27  | B8    | 1383 | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |
| 27  | B8    | 2048 | G    | O4'-C1'-N9 | 6.04  | 113.03      | 108.20   |
| 27  | B8    | 2281 | A    | C5-C6-N6   | -6.04 | 118.87      | 123.70   |
| 27  | B8    | 2507 | C    | N3-C4-N4   | 6.04  | 122.22      | 118.00   |
| 27  | B8    | 2634 | A    | C4-C5-C6   | 6.04  | 120.02      | 117.00   |
| 28  | BA    | 383  | PHE  | CB-CG-CD2  | 6.04  | 125.02      | 120.80   |
| 1   | AA    | 223  | A    | C4-C5-C6   | 6.03  | 120.02      | 117.00   |
| 1   | AA    | 383  | A    | C5-C6-N1   | -6.03 | 114.68      | 117.70   |
| 1   | AA    | 435  | A    | O4'-C1'-N9 | 6.03  | 113.03      | 108.20   |
| 1   | AA    | 755  | G    | O4'-C1'-N9 | 6.03  | 113.03      | 108.20   |
| 1   | AA    | 1167 | A    | O4'-C1'-N9 | 6.03  | 113.03      | 108.20   |
| 1   | AA    | 1404 | C    | N3-C4-N4   | 6.03  | 122.22      | 118.00   |
| 1   | AA    | 1473 | G    | O4'-C1'-N9 | 6.03  | 113.03      | 108.20   |
| 27  | B8    | 187  | G    | O4'-C1'-N9 | 6.03  | 113.03      | 108.20   |
| 27  | B8    | 291  | G    | O4'-C1'-N9 | 6.03  | 113.03      | 108.20   |
| 27  | B8    | 432  | A    | C4-C5-C6   | 6.03  | 120.02      | 117.00   |
| 27  | B8    | 945  | A    | C4-C5-C6   | 6.03  | 120.02      | 117.00   |
| 27  | B8    | 1190 | G    | O4'-C1'-N9 | 6.03  | 113.03      | 108.20   |
| 27  | B8    | 1532 | A    | C4-C5-C6   | 6.03  | 120.02      | 117.00   |
| 27  | B8    | 1894 | C    | N3-C4-N4   | 6.03  | 122.22      | 118.00   |
| 27  | B8    | 2279 | G    | O4'-C1'-N9 | 6.03  | 113.03      | 108.20   |
| 27  | B8    | 2471 | A    | C5-C6-N6   | -6.03 | 118.87      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2900 | A    | C4-C5-C6   | 6.03  | 120.02      | 117.00   |
| 1   | AA    | 228  | A    | C5-C6-N6   | -6.03 | 118.87      | 123.70   |
| 27  | B8    | 1233 | C    | N3-C4-N4   | 6.03  | 122.22      | 118.00   |
| 27  | B8    | 2117 | A    | O4'-C1'-N9 | 6.03  | 113.03      | 108.20   |
| 1   | AA    | 493  | A    | C5-C6-N6   | -6.03 | 118.88      | 123.70   |
| 1   | AA    | 979  | C    | N3-C4-N4   | 6.03  | 122.22      | 118.00   |
| 27  | B8    | 320  | A    | C4-C5-C6   | 6.03  | 120.02      | 117.00   |
| 27  | B8    | 453  | A    | C4-C5-C6   | 6.03  | 120.02      | 117.00   |
| 27  | B8    | 541  | A    | C4-C5-C6   | 6.03  | 120.02      | 117.00   |
| 1   | AA    | 1114 | C    | N3-C4-N4   | 6.03  | 122.22      | 118.00   |
| 1   | AA    | 1140 | C    | N3-C4-C5   | -6.03 | 119.49      | 121.90   |
| 27  | B8    | 1314 | C    | N3-C4-N4   | 6.03  | 122.22      | 118.00   |
| 27  | B8    | 1524 | G    | O4'-C1'-N9 | 6.03  | 113.02      | 108.20   |
| 27  | B8    | 2369 | A    | C5-C6-N6   | -6.03 | 118.88      | 123.70   |
| 1   | AA    | 16   | A    | C5-C6-N1   | -6.03 | 114.69      | 117.70   |
| 1   | AA    | 706  | A    | C4-C5-C6   | 6.03  | 120.01      | 117.00   |
| 1   | AA    | 1209 | C    | N3-C4-N4   | 6.03  | 122.22      | 118.00   |
| 27  | B8    | 572  | A    | C5-C6-N6   | -6.03 | 118.88      | 123.70   |
| 27  | B8    | 991  | C    | N3-C4-C5   | -6.03 | 119.49      | 121.90   |
| 27  | B8    | 1591 | A    | O4'-C1'-N9 | 6.03  | 113.02      | 108.20   |
| 27  | B8    | 1735 | A    | O4'-C1'-N9 | 6.03  | 113.02      | 108.20   |
| 27  | B8    | 1791 | A    | C4-C5-C6   | 6.03  | 120.01      | 117.00   |
| 27  | B8    | 2031 | A    | C4-C5-C6   | 6.03  | 120.01      | 117.00   |
| 27  | B8    | 2534 | A    | C4-C5-C6   | 6.03  | 120.01      | 117.00   |
| 27  | B8    | 2541 | A    | C5-C6-N6   | -6.03 | 118.88      | 123.70   |
| 3   | AV    | 75   | C    | N3-C4-C5   | -6.03 | 119.49      | 121.90   |
| 27  | B8    | 94   | A    | C4-C5-C6   | 6.03  | 120.01      | 117.00   |
| 27  | B8    | 222  | A    | C4-C5-C6   | 6.03  | 120.01      | 117.00   |
| 27  | B8    | 522  | A    | C4-C5-C6   | 6.03  | 120.01      | 117.00   |
| 27  | B8    | 678  | C    | N3-C4-N4   | 6.03  | 122.22      | 118.00   |
| 27  | B8    | 937  | C    | N3-C4-N4   | 6.03  | 122.22      | 118.00   |
| 27  | B8    | 1084 | A    | C5-C6-N1   | -6.03 | 114.69      | 117.70   |
| 27  | B8    | 1261 | C    | N3-C4-N4   | 6.03  | 122.22      | 118.00   |
| 27  | B8    | 2138 | G    | O4'-C1'-N9 | 6.03  | 113.02      | 108.20   |
| 1   | AA    | 179  | A    | C5-C6-N1   | -6.02 | 114.69      | 117.70   |
| 1   | AA    | 499  | A    | C4-C5-C6   | 6.02  | 120.01      | 117.00   |
| 1   | AA    | 519  | C    | N3-C4-C5   | -6.02 | 119.49      | 121.90   |
| 27  | B8    | 68   | G    | C5-C6-O6   | -6.02 | 124.99      | 128.60   |
| 1   | AA    | 336  | A    | C5-C6-N1   | -6.02 | 114.69      | 117.70   |
| 1   | AA    | 493  | A    | C4-C5-C6   | 6.02  | 120.01      | 117.00   |
| 1   | AA    | 892  | A    | C4-C5-C6   | 6.02  | 120.01      | 117.00   |
| 1   | AA    | 1443 | C    | N3-C4-N4   | 6.02  | 122.22      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 736  | C    | N3-C4-N4   | 6.02  | 122.22      | 118.00   |
| 27  | B8    | 892  | A    | C5-C6-N6   | -6.02 | 118.88      | 123.70   |
| 27  | B8    | 2371 | G    | O4'-C1'-N9 | 6.02  | 113.02      | 108.20   |
| 1   | AA    | 984  | C    | N3-C4-N4   | 6.02  | 122.22      | 118.00   |
| 27  | B8    | 786  | C    | N3-C4-N4   | 6.02  | 122.22      | 118.00   |
| 27  | B8    | 1676 | A    | C5-C6-N6   | -6.02 | 118.88      | 123.70   |
| 1   | AA    | 59   | A    | C4-C5-C6   | 6.02  | 120.01      | 117.00   |
| 1   | AA    | 320  | A    | O4'-C1'-N9 | 6.02  | 113.02      | 108.20   |
| 1   | AA    | 1542 | A    | O4'-C1'-N9 | 6.02  | 113.02      | 108.20   |
| 3   | AV    | 33   | A    | C4-C5-C6   | 6.02  | 120.01      | 117.00   |
| 26  | B7    | 38   | C    | N3-C4-N4   | 6.02  | 122.21      | 118.00   |
| 27  | B8    | 172  | A    | C4-C5-C6   | 6.02  | 120.01      | 117.00   |
| 27  | B8    | 322  | A    | C5-C6-N1   | -6.02 | 114.69      | 117.70   |
| 27  | B8    | 1084 | A    | C5-C6-N6   | -6.02 | 118.89      | 123.70   |
| 27  | B8    | 2054 | A    | C4-C5-C6   | 6.02  | 120.01      | 117.00   |
| 27  | B8    | 2679 | A    | O4'-C1'-N9 | 6.02  | 113.02      | 108.20   |
| 1   | AA    | 547  | A    | C4-C5-C6   | 6.02  | 120.01      | 117.00   |
| 1   | AA    | 1246 | A    | O4'-C1'-N9 | 6.02  | 113.01      | 108.20   |
| 27  | B8    | 173  | A    | O4'-C1'-N9 | 6.02  | 113.01      | 108.20   |
| 27  | B8    | 468  | G    | O4'-C1'-N9 | 6.02  | 113.01      | 108.20   |
| 27  | B8    | 743  | A    | O4'-C1'-N9 | 6.02  | 113.01      | 108.20   |
| 27  | B8    | 1571 | A    | O4'-C1'-N9 | 6.02  | 113.02      | 108.20   |
| 27  | B8    | 2516 | A    | C5-C6-N6   | -6.02 | 118.89      | 123.70   |
| 1   | AA    | 329  | A    | C4-C5-C6   | 6.02  | 120.01      | 117.00   |
| 3   | AV    | 16   | C    | O4'-C1'-N1 | 6.02  | 113.01      | 108.20   |
| 27  | B8    | 231  | A    | C4-C5-C6   | 6.02  | 120.01      | 117.00   |
| 27  | B8    | 726  | G    | O4'-C1'-N9 | 6.02  | 113.01      | 108.20   |
| 27  | B8    | 2178 | C    | C6-N1-C1'  | -6.02 | 113.58      | 120.80   |
| 1   | AA    | 356  | A    | C5-C6-N6   | -6.01 | 118.89      | 123.70   |
| 1   | AA    | 1130 | A    | C5-C6-N6   | -6.01 | 118.89      | 123.70   |
| 3   | AV    | 4    | C    | N3-C4-N4   | 6.01  | 122.21      | 118.00   |
| 27  | B8    | 20   | C    | N3-C4-N4   | 6.01  | 122.21      | 118.00   |
| 27  | B8    | 148  | U    | O4'-C1'-N1 | 6.01  | 113.01      | 108.20   |
| 27  | B8    | 231  | A    | C5-C6-N1   | -6.01 | 114.69      | 117.70   |
| 27  | B8    | 341  | C    | N3-C4-N4   | 6.01  | 122.21      | 118.00   |
| 27  | B8    | 506  | G    | O4'-C1'-N9 | 6.01  | 113.01      | 108.20   |
| 27  | B8    | 1029 | A    | C5-C6-N1   | -6.01 | 114.69      | 117.70   |
| 27  | B8    | 1336 | A    | C5-C6-N6   | -6.01 | 118.89      | 123.70   |
| 27  | B8    | 1632 | A    | C4-C5-C6   | 6.01  | 120.01      | 117.00   |
| 27  | B8    | 1913 | A    | C4-C5-C6   | 6.01  | 120.01      | 117.00   |
| 27  | B8    | 2224 | G    | C5-C6-O6   | -6.01 | 124.99      | 128.60   |
| 3   | AV    | 50   | G    | O4'-C1'-N9 | 6.01  | 113.01      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 760  | G    | O4'-C1'-N9 | 6.01  | 113.01      | 108.20   |
| 27  | B8    | 1384 | A    | C5-C6-N6   | -6.01 | 118.89      | 123.70   |
| 27  | B8    | 2531 | A    | C4-C5-C6   | 6.01  | 120.01      | 117.00   |
| 1   | AA    | 400  | C    | N3-C4-N4   | 6.01  | 122.21      | 118.00   |
| 1   | AA    | 969  | A    | O4'-C1'-N9 | 6.01  | 113.01      | 108.20   |
| 27  | B8    | 262  | A    | C5-C6-N1   | -6.01 | 114.69      | 117.70   |
| 27  | B8    | 979  | A    | C4-C5-C6   | 6.01  | 120.01      | 117.00   |
| 27  | B8    | 1302 | A    | C5-C6-N1   | -6.01 | 114.69      | 117.70   |
| 27  | B8    | 1541 | C    | N3-C4-N4   | 6.01  | 122.21      | 118.00   |
| 27  | B8    | 1665 | A    | C4-C5-C6   | 6.01  | 120.01      | 117.00   |
| 27  | B8    | 1998 | A    | C4-C5-C6   | 6.01  | 120.00      | 117.00   |
| 27  | B8    | 2327 | A    | C4-C5-C6   | 6.01  | 120.01      | 117.00   |
| 27  | B8    | 2377 | A    | C4-C5-C6   | 6.01  | 120.01      | 117.00   |
| 27  | B8    | 2453 | A    | C4-C5-C6   | 6.01  | 120.01      | 117.00   |
| 1   | AA    | 82   | G    | O4'-C1'-N9 | 6.01  | 113.01      | 108.20   |
| 1   | AA    | 120  | A    | C4-C5-C6   | 6.01  | 120.00      | 117.00   |
| 1   | AA    | 237  | G    | O4'-C1'-N9 | 6.01  | 113.01      | 108.20   |
| 27  | B8    | 599  | A    | C5-C6-N6   | -6.01 | 118.89      | 123.70   |
| 27  | B8    | 975  | A    | C5-C6-N1   | -6.01 | 114.69      | 117.70   |
| 27  | B8    | 2278 | A    | C5-C6-N6   | -6.01 | 118.89      | 123.70   |
| 27  | B8    | 2475 | C    | N3-C4-C5   | -6.01 | 119.50      | 121.90   |
| 27  | B8    | 2653 | U    | O4'-C1'-N1 | 6.01  | 113.01      | 108.20   |
| 27  | B8    | 742  | A    | C5-C6-N6   | -6.01 | 118.89      | 123.70   |
| 27  | B8    | 1086 | A    | O4'-C1'-N9 | 6.01  | 113.01      | 108.20   |
| 27  | B8    | 1678 | A    | C4-C5-C6   | 6.01  | 120.00      | 117.00   |
| 27  | B8    | 2349 | G    | O4'-C1'-N9 | 6.01  | 113.01      | 108.20   |
| 27  | B8    | 2678 | C    | N3-C4-N4   | 6.01  | 122.21      | 118.00   |
| 27  | B8    | 2831 | G    | O4'-C1'-N9 | 6.01  | 113.01      | 108.20   |
| 1   | AA    | 1200 | C    | O4'-C1'-N1 | 6.01  | 113.01      | 108.20   |
| 1   | AA    | 1521 | C    | N3-C4-N4   | 6.01  | 122.20      | 118.00   |
| 27  | B8    | 259  | G    | O4'-C1'-N9 | 6.01  | 113.01      | 108.20   |
| 27  | B8    | 1297 | C    | N3-C4-N4   | 6.01  | 122.20      | 118.00   |
| 27  | B8    | 1821 | A    | O4'-C1'-N9 | 6.01  | 113.00      | 108.20   |
| 28  | BA    | 383  | PHE  | CB-CG-CD1  | -6.01 | 116.59      | 120.80   |
| 1   | AA    | 174  | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 27  | B8    | 921  | C    | N3-C4-N4   | 6.00  | 122.20      | 118.00   |
| 27  | B8    | 1822 | C    | N3-C4-N4   | 6.00  | 122.20      | 118.00   |
| 27  | B8    | 1958 | C    | N3-C4-N4   | 6.00  | 122.20      | 118.00   |
| 27  | B8    | 2635 | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 1   | AA    | 704  | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 27  | B8    | 236  | C    | N3-C4-N4   | 6.00  | 122.20      | 118.00   |
| 27  | B8    | 311  | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 698  | C    | N3-C4-N4   | 6.00  | 122.20      | 118.00   |
| 27  | B8    | 991  | C    | N3-C4-N4   | 6.00  | 122.20      | 118.00   |
| 27  | B8    | 1174 | U    | O4'-C1'-N1 | 6.00  | 113.00      | 108.20   |
| 27  | B8    | 2381 | A    | C5-C6-N6   | -6.00 | 118.90      | 123.70   |
| 27  | B8    | 2679 | A    | C5-C6-N6   | -6.00 | 118.90      | 123.70   |
| 1   | AA    | 143  | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 1   | AA    | 418  | C    | N3-C4-N4   | 6.00  | 122.20      | 118.00   |
| 1   | AA    | 502  | A    | O4'-C1'-N9 | 6.00  | 113.00      | 108.20   |
| 1   | AA    | 602  | A    | O4'-C1'-N9 | 6.00  | 113.00      | 108.20   |
| 1   | AA    | 1502 | A    | O4'-C1'-N9 | 6.00  | 113.00      | 108.20   |
| 27  | B8    | 83   | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 27  | B8    | 213  | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 27  | B8    | 492  | A    | C5-C6-N6   | -6.00 | 118.90      | 123.70   |
| 27  | B8    | 504  | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 27  | B8    | 820  | A    | O4'-C1'-N9 | 6.00  | 113.00      | 108.20   |
| 27  | B8    | 995  | C    | C2-N1-C1'  | 6.00  | 125.40      | 118.80   |
| 27  | B8    | 2094 | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 1   | AA    | 831  | A    | C5-C6-N6   | -6.00 | 118.90      | 123.70   |
| 27  | B8    | 2142 | A    | C5-C6-N6   | -6.00 | 118.90      | 123.70   |
| 27  | B8    | 2301 | C    | N3-C4-N4   | 6.00  | 122.20      | 118.00   |
| 27  | B8    | 2486 | C    | N3-C4-N4   | 6.00  | 122.20      | 118.00   |
| 1   | AA    | 374  | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 26  | B7    | 35   | C    | C6-N1-C1'  | -6.00 | 113.60      | 120.80   |
| 27  | B8    | 289  | G    | O4'-C1'-N9 | 6.00  | 113.00      | 108.20   |
| 27  | B8    | 423  | A    | C5-C6-N6   | -6.00 | 118.90      | 123.70   |
| 27  | B8    | 677  | A    | O4'-C1'-N9 | 6.00  | 113.00      | 108.20   |
| 27  | B8    | 808  | G    | O4'-C1'-N9 | 6.00  | 113.00      | 108.20   |
| 27  | B8    | 2211 | A    | C5-C6-N6   | -6.00 | 118.90      | 123.70   |
| 27  | B8    | 2485 | G    | O4'-C1'-N9 | 6.00  | 113.00      | 108.20   |
| 27  | B8    | 2814 | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 1   | AA    | 286  | C    | N3-C4-N4   | 6.00  | 122.20      | 118.00   |
| 1   | AA    | 364  | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 1   | AA    | 422  | C    | O4'-C1'-N1 | 6.00  | 113.00      | 108.20   |
| 1   | AA    | 715  | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 1   | AA    | 1394 | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 27  | B8    | 447  | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 27  | B8    | 602  | A    | C5-C6-N6   | -6.00 | 118.90      | 123.70   |
| 27  | B8    | 623  | C    | N3-C4-N4   | 6.00  | 122.20      | 118.00   |
| 27  | B8    | 1342 | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 27  | B8    | 1795 | C    | N3-C4-C5   | -6.00 | 119.50      | 121.90   |
| 27  | B8    | 2497 | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 1   | AA    | 465  | A    | C5-C6-N6   | -6.00 | 118.90      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 208  | C    | N3-C4-N4   | 6.00  | 122.20      | 118.00   |
| 27  | B8    | 743  | A    | C4-C5-C6   | 6.00  | 120.00      | 117.00   |
| 27  | B8    | 1593 | A    | C5-C6-N6   | -6.00 | 118.90      | 123.70   |
| 1   | AA    | 673  | A    | O4'-C1'-N9 | 5.99  | 113.00      | 108.20   |
| 3   | AV    | 36   | G    | O4'-C1'-N9 | 5.99  | 113.00      | 108.20   |
| 27  | B8    | 44   | A    | C4-C5-C6   | 5.99  | 120.00      | 117.00   |
| 27  | B8    | 693  | A    | C5-C6-N6   | -5.99 | 118.91      | 123.70   |
| 27  | B8    | 896  | A    | O4'-C1'-N9 | 5.99  | 113.00      | 108.20   |
| 27  | B8    | 1779 | U    | O4'-C1'-N1 | 5.99  | 113.00      | 108.20   |
| 27  | B8    | 2564 | A    | C4-C5-C6   | 5.99  | 120.00      | 117.00   |
| 27  | B8    | 2853 | C    | N3-C4-N4   | 5.99  | 122.20      | 118.00   |
| 1   | AA    | 327  | A    | C5-C6-N1   | -5.99 | 114.70      | 117.70   |
| 27  | B8    | 347  | A    | C4-C5-C6   | 5.99  | 120.00      | 117.00   |
| 27  | B8    | 1350 | C    | N3-C4-N4   | 5.99  | 122.19      | 118.00   |
| 27  | B8    | 1932 | A    | C4-C5-C6   | 5.99  | 120.00      | 117.00   |
| 27  | B8    | 2643 | G    | O4'-C1'-N9 | 5.99  | 112.99      | 108.20   |
| 1   | AA    | 328  | C    | N3-C4-N4   | 5.99  | 122.19      | 118.00   |
| 1   | AA    | 356  | A    | O4'-C1'-N9 | 5.99  | 112.99      | 108.20   |
| 1   | AA    | 817  | C    | N3-C4-N4   | 5.99  | 122.19      | 118.00   |
| 2   | AX    | 16   | C    | N3-C4-N4   | 5.99  | 122.19      | 118.00   |
| 27  | B8    | 183  | C    | N3-C4-N4   | 5.99  | 122.19      | 118.00   |
| 27  | B8    | 1193 | G    | O4'-C1'-N9 | 5.99  | 112.99      | 108.20   |
| 27  | B8    | 1361 | G    | O4'-C1'-N9 | 5.99  | 112.99      | 108.20   |
| 27  | B8    | 2381 | A    | C4-C5-C6   | 5.99  | 120.00      | 117.00   |
| 27  | B8    | 2461 | A    | O4'-C1'-N9 | 5.99  | 112.99      | 108.20   |
| 1   | AA    | 374  | A    | O4'-C1'-N9 | 5.99  | 112.99      | 108.20   |
| 1   | AA    | 641  | U    | O4'-C1'-N1 | 5.99  | 112.99      | 108.20   |
| 1   | AA    | 1035 | A    | C4-C5-C6   | 5.99  | 119.99      | 117.00   |
| 1   | AA    | 1369 | C    | N3-C4-N4   | 5.99  | 122.19      | 118.00   |
| 27  | B8    | 643  | A    | C4-C5-C6   | 5.99  | 119.99      | 117.00   |
| 27  | B8    | 912  | C    | N3-C4-N4   | 5.99  | 122.19      | 118.00   |
| 27  | B8    | 1166 | G    | O4'-C1'-N9 | 5.99  | 112.99      | 108.20   |
| 27  | B8    | 1801 | A    | C4-C5-C6   | 5.99  | 120.00      | 117.00   |
| 27  | B8    | 1836 | C    | N3-C4-N4   | 5.99  | 122.19      | 118.00   |
| 27  | B8    | 1890 | A    | C4-C5-C6   | 5.99  | 119.99      | 117.00   |
| 27  | B8    | 2024 | G    | O4'-C1'-N9 | 5.99  | 112.99      | 108.20   |
| 27  | B8    | 2363 | G    | O4'-C1'-N9 | 5.99  | 112.99      | 108.20   |
| 27  | B8    | 2461 | A    | C5-C6-N6   | -5.99 | 118.91      | 123.70   |
| 27  | B8    | 2616 | C    | N3-C4-N4   | 5.99  | 122.19      | 118.00   |
| 27  | B8    | 2752 | C    | N3-C4-N4   | 5.99  | 122.19      | 118.00   |
| 27  | B8    | 2755 | C    | N3-C4-N4   | 5.99  | 122.19      | 118.00   |
| 26  | B7    | 116  | G    | O4'-C1'-N9 | 5.99  | 112.99      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 292  | G    | O4'-C1'-N9  | 5.99  | 112.99      | 108.20   |
| 1   | AA    | 1147 | C    | N3-C4-N4    | 5.99  | 122.19      | 118.00   |
| 27  | B8    | 1403 | A    | C4-C5-C6    | 5.99  | 119.99      | 117.00   |
| 27  | B8    | 1433 | A    | C5-C6-N1    | -5.99 | 114.71      | 117.70   |
| 27  | B8    | 1448 | G    | O4'-C1'-N9  | 5.99  | 112.99      | 108.20   |
| 27  | B8    | 2101 | A    | C4-C5-C6    | 5.99  | 119.99      | 117.00   |
| 1   | AA    | 766  | A    | C4-C5-C6    | 5.98  | 119.99      | 117.00   |
| 26  | B7    | 82   | U    | O4'-C1'-N1  | 5.98  | 112.99      | 108.20   |
| 27  | B8    | 439  | A    | C4-C5-C6    | 5.98  | 119.99      | 117.00   |
| 27  | B8    | 1064 | C    | N3-C4-N4    | 5.98  | 122.19      | 118.00   |
| 27  | B8    | 1290 | C    | N3-C4-N4    | 5.98  | 122.19      | 118.00   |
| 27  | B8    | 1844 | C    | N3-C4-N4    | 5.98  | 122.19      | 118.00   |
| 1   | AA    | 1105 | A    | C5-C6-N6    | -5.98 | 118.91      | 123.70   |
| 27  | B8    | 190  | A    | C5-C6-N6    | -5.98 | 118.92      | 123.70   |
| 27  | B8    | 1783 | A    | C4-C5-C6    | 5.98  | 119.99      | 117.00   |
| 27  | B8    | 2198 | A    | C5-C6-N6    | -5.98 | 118.91      | 123.70   |
| 27  | B8    | 2530 | A    | C1'-O4'-C4' | -5.98 | 105.11      | 109.90   |
| 45  | BQ    | 23   | TYR  | CB-CG-CD2   | 5.98  | 124.59      | 121.00   |
| 1   | AA    | 120  | A    | C5-C6-N6    | -5.98 | 118.92      | 123.70   |
| 1   | AA    | 232  | G    | C5-C6-O6    | -5.98 | 125.01      | 128.60   |
| 1   | AA    | 878  | A    | C4-C5-C6    | 5.98  | 119.99      | 117.00   |
| 1   | AA    | 1287 | A    | C5-C6-N6    | -5.98 | 118.92      | 123.70   |
| 27  | B8    | 501  | A    | C4-C5-C6    | 5.98  | 119.99      | 117.00   |
| 27  | B8    | 1404 | C    | N3-C4-N4    | 5.98  | 122.19      | 118.00   |
| 27  | B8    | 2027 | G    | O4'-C1'-N9  | 5.98  | 112.98      | 108.20   |
| 27  | B8    | 47   | C    | N3-C4-N4    | 5.98  | 122.19      | 118.00   |
| 27  | B8    | 589  | U    | O4'-C1'-N1  | 5.98  | 112.98      | 108.20   |
| 27  | B8    | 2503 | A    | C5-C6-N6    | -5.98 | 118.92      | 123.70   |
| 1   | AA    | 182  | A    | O4'-C1'-N9  | 5.98  | 112.98      | 108.20   |
| 1   | AA    | 303  | A    | C4-C5-C6    | 5.98  | 119.99      | 117.00   |
| 1   | AA    | 1032 | G    | O4'-C1'-N9  | 5.98  | 112.98      | 108.20   |
| 1   | AA    | 1103 | C    | N3-C4-N4    | 5.98  | 122.18      | 118.00   |
| 27  | B8    | 538  | A    | O4'-C1'-N9  | 5.98  | 112.98      | 108.20   |
| 27  | B8    | 1152 | C    | N3-C4-N4    | 5.98  | 122.18      | 118.00   |
| 27  | B8    | 1278 | C    | N3-C4-N4    | 5.98  | 122.18      | 118.00   |
| 27  | B8    | 1938 | A    | C4-C5-C6    | 5.98  | 119.99      | 117.00   |
| 1   | AA    | 366  | A    | C4-C5-C6    | 5.97  | 119.99      | 117.00   |
| 1   | AA    | 451  | A    | C4-C5-C6    | 5.97  | 119.99      | 117.00   |
| 1   | AA    | 686  | U    | O4'-C1'-N1  | 5.97  | 112.98      | 108.20   |
| 1   | AA    | 1155 | A    | O4'-C1'-N9  | 5.97  | 112.98      | 108.20   |
| 26  | B7    | 99   | A    | C5-C6-N1    | -5.97 | 114.71      | 117.70   |
| 1   | AA    | 288  | A    | C4-C5-C6    | 5.97  | 119.99      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 609  | A    | C4-C5-C6   | 5.97  | 119.99      | 117.00   |
| 1   | AA    | 743  | A    | C5-C6-N6   | -5.97 | 118.92      | 123.70   |
| 1   | AA    | 1104 | G    | O4'-C1'-N9 | 5.97  | 112.98      | 108.20   |
| 1   | AA    | 1371 | G    | C5-C6-O6   | -5.97 | 125.02      | 128.60   |
| 27  | B8    | 481  | G    | C5-C6-O6   | -5.97 | 125.02      | 128.60   |
| 27  | B8    | 540  | C    | N3-C4-N4   | 5.97  | 122.18      | 118.00   |
| 27  | B8    | 550  | C    | N3-C4-C5   | -5.97 | 119.51      | 121.90   |
| 27  | B8    | 777  | G    | O4'-C1'-N9 | 5.97  | 112.98      | 108.20   |
| 27  | B8    | 802  | A    | C5-C6-N1   | -5.97 | 114.71      | 117.70   |
| 27  | B8    | 1091 | G    | C5-C6-O6   | -5.97 | 125.02      | 128.60   |
| 27  | B8    | 1430 | G    | O4'-C1'-N9 | 5.97  | 112.98      | 108.20   |
| 27  | B8    | 2135 | A    | C4-C5-C6   | 5.97  | 119.99      | 117.00   |
| 27  | B8    | 2221 | G    | O4'-C1'-N9 | 5.97  | 112.98      | 108.20   |
| 27  | B8    | 2758 | A    | C5-C6-N6   | -5.97 | 118.92      | 123.70   |
| 1   | AA    | 391  | G    | O4'-C1'-N9 | 5.97  | 112.98      | 108.20   |
| 27  | B8    | 1413 | A    | C4-C5-C6   | 5.97  | 119.98      | 117.00   |
| 27  | B8    | 1587 | G    | C5-C6-O6   | -5.97 | 125.02      | 128.60   |
| 27  | B8    | 2846 | G    | O4'-C1'-N9 | 5.97  | 112.98      | 108.20   |
| 1   | AA    | 716  | A    | C5-C6-N1   | -5.97 | 114.72      | 117.70   |
| 1   | AA    | 877  | G    | O4'-C1'-N9 | 5.97  | 112.98      | 108.20   |
| 1   | AA    | 1181 | G    | C5-C6-O6   | -5.97 | 125.02      | 128.60   |
| 1   | AA    | 1428 | A    | C4-C5-C6   | 5.97  | 119.98      | 117.00   |
| 27  | B8    | 241  | A    | C4-C5-C6   | 5.97  | 119.98      | 117.00   |
| 27  | B8    | 1165 | A    | C5-C6-N1   | -5.97 | 114.72      | 117.70   |
| 27  | B8    | 1854 | A    | O4'-C1'-N9 | 5.97  | 112.98      | 108.20   |
| 27  | B8    | 2099 | U    | O4'-C1'-N1 | 5.97  | 112.97      | 108.20   |
| 27  | B8    | 2172 | U    | O4'-C1'-N1 | 5.97  | 112.97      | 108.20   |
| 27  | B8    | 2211 | A    | C4-C5-C6   | 5.97  | 119.98      | 117.00   |
| 27  | B8    | 2241 | A    | C4-C5-C6   | 5.97  | 119.98      | 117.00   |
| 27  | B8    | 2350 | C    | N3-C4-N4   | 5.97  | 122.18      | 118.00   |
| 27  | B8    | 130  | C    | N3-C4-N4   | 5.97  | 122.18      | 118.00   |
| 27  | B8    | 270  | A    | C4-C5-C6   | 5.97  | 119.98      | 117.00   |
| 27  | B8    | 892  | A    | O4'-C1'-N9 | 5.97  | 112.97      | 108.20   |
| 27  | B8    | 2588 | G    | O4'-C1'-N9 | 5.97  | 112.97      | 108.20   |
| 1   | AA    | 184  | G    | O4'-C1'-N9 | 5.97  | 112.97      | 108.20   |
| 1   | AA    | 1170 | A    | C5-C6-N6   | -5.97 | 118.93      | 123.70   |
| 1   | AA    | 1196 | A    | C4-C5-C6   | 5.97  | 119.98      | 117.00   |
| 27  | B8    | 1070 | A    | C4-C5-C6   | 5.97  | 119.98      | 117.00   |
| 27  | B8    | 2176 | A    | O4'-C1'-N9 | 5.97  | 112.97      | 108.20   |
| 27  | B8    | 2723 | C    | N3-C4-N4   | 5.97  | 122.18      | 118.00   |
| 1   | AA    | 1059 | C    | N3-C4-N4   | 5.96  | 122.18      | 118.00   |
| 1   | AA    | 1325 | C    | N3-C4-N4   | 5.96  | 122.17      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1518 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 27  | B8    | 586  | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 27  | B8    | 1367 | A    | C5-C6-N6   | -5.96 | 118.93      | 123.70   |
| 27  | B8    | 2196 | C    | N3-C4-N4   | 5.96  | 122.18      | 118.00   |
| 27  | B8    | 2382 | G    | O4'-C1'-N9 | 5.96  | 112.97      | 108.20   |
| 27  | B8    | 2888 | C    | N3-C4-N4   | 5.96  | 122.17      | 118.00   |
| 1   | AA    | 1284 | C    | N3-C4-N4   | 5.96  | 122.17      | 118.00   |
| 27  | B8    | 1247 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 1   | AA    | 702  | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 1   | AA    | 1081 | A    | C5-C6-N6   | -5.96 | 118.93      | 123.70   |
| 1   | AA    | 1108 | G    | O4'-C1'-N9 | 5.96  | 112.97      | 108.20   |
| 1   | AA    | 1251 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 27  | B8    | 103  | A    | O4'-C1'-N9 | 5.96  | 112.97      | 108.20   |
| 27  | B8    | 281  | C    | N3-C4-N4   | 5.96  | 122.17      | 118.00   |
| 27  | B8    | 528  | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 27  | B8    | 603  | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 27  | B8    | 804  | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 27  | B8    | 878  | A    | C5-C6-N6   | -5.96 | 118.93      | 123.70   |
| 27  | B8    | 1919 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 27  | B8    | 2094 | A    | C5-C6-N6   | -5.96 | 118.93      | 123.70   |
| 46  | BR    | 3    | ALA  | N-CA-CB    | 5.96  | 118.45      | 110.10   |
| 1   | AA    | 793  | U    | O4'-C1'-N1 | 5.96  | 112.97      | 108.20   |
| 27  | B8    | 452  | G    | O4'-C1'-N9 | 5.96  | 112.97      | 108.20   |
| 27  | B8    | 1471 | G    | O4'-C1'-N9 | 5.96  | 112.97      | 108.20   |
| 1   | AA    | 225  | C    | N3-C4-N4   | 5.96  | 122.17      | 118.00   |
| 1   | AA    | 1169 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 1   | AA    | 1239 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 1   | AA    | 1519 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 27  | B8    | 750  | A    | C5-C6-N6   | -5.96 | 118.93      | 123.70   |
| 27  | B8    | 1118 | C    | N3-C4-N4   | 5.96  | 122.17      | 118.00   |
| 27  | B8    | 1634 | A    | C5-C6-N1   | -5.96 | 114.72      | 117.70   |
| 27  | B8    | 1650 | A    | C5-C6-N6   | -5.96 | 118.93      | 123.70   |
| 27  | B8    | 2037 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 27  | B8    | 2143 | C    | N3-C4-N4   | 5.96  | 122.17      | 118.00   |
| 27  | B8    | 2426 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 1   | AA    | 496  | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 1   | AA    | 899  | C    | N3-C4-C5   | -5.96 | 119.52      | 121.90   |
| 1   | AA    | 1082 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 1   | AA    | 1163 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 1   | AA    | 1500 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 27  | B8    | 297  | G    | O4'-C1'-N9 | 5.96  | 112.97      | 108.20   |
| 27  | B8    | 391  | A    | C5-C6-N6   | -5.96 | 118.94      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 936  | A    | C5-C6-N6   | -5.96 | 118.94      | 123.70   |
| 27  | B8    | 1754 | A    | C5-C6-N6   | -5.96 | 118.94      | 123.70   |
| 27  | B8    | 1778 | U    | O4'-C1'-N1 | 5.96  | 112.97      | 108.20   |
| 27  | B8    | 1829 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 27  | B8    | 2590 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 27  | B8    | 2796 | U    | O4'-C1'-N1 | 5.96  | 112.97      | 108.20   |
| 1   | AA    | 241  | G    | O4'-C1'-N9 | 5.96  | 112.96      | 108.20   |
| 1   | AA    | 456  | A    | O4'-C1'-N9 | 5.96  | 112.96      | 108.20   |
| 1   | AA    | 469  | C    | N3-C4-N4   | 5.96  | 122.17      | 118.00   |
| 1   | AA    | 1502 | A    | C5-C6-N1   | -5.96 | 114.72      | 117.70   |
| 27  | B8    | 108  | G    | O4'-C1'-N9 | 5.96  | 112.96      | 108.20   |
| 27  | B8    | 282  | A    | O4'-C1'-N9 | 5.96  | 112.96      | 108.20   |
| 27  | B8    | 346  | A    | C5-C6-N1   | -5.96 | 114.72      | 117.70   |
| 27  | B8    | 653  | U    | C2-N1-C1'  | 5.96  | 124.85      | 117.70   |
| 27  | B8    | 1286 | A    | C5-C6-N1   | -5.96 | 114.72      | 117.70   |
| 27  | B8    | 2278 | A    | C4-C5-C6   | 5.96  | 119.98      | 117.00   |
| 1   | AA    | 80   | A    | C5-C6-N1   | -5.95 | 114.72      | 117.70   |
| 1   | AA    | 681  | A    | C4-C5-C6   | 5.95  | 119.98      | 117.00   |
| 27  | B8    | 89   | A    | C4-C5-C6   | 5.95  | 119.98      | 117.00   |
| 27  | B8    | 361  | G    | O4'-C1'-N9 | 5.95  | 112.96      | 108.20   |
| 27  | B8    | 1826 | G    | O4'-C1'-N9 | 5.95  | 112.96      | 108.20   |
| 1   | AA    | 243  | A    | C4-C5-C6   | 5.95  | 119.98      | 117.00   |
| 27  | B8    | 905  | A    | C4-C5-C6   | 5.95  | 119.98      | 117.00   |
| 27  | B8    | 1866 | A    | C5-C6-N6   | -5.95 | 118.94      | 123.70   |
| 1   | AA    | 129  | A    | C4-C5-C6   | 5.95  | 119.98      | 117.00   |
| 1   | AA    | 600  | A    | O4'-C1'-N9 | 5.95  | 112.96      | 108.20   |
| 1   | AA    | 767  | A    | C4-C5-C6   | 5.95  | 119.98      | 117.00   |
| 1   | AA    | 1163 | A    | O4'-C1'-N9 | 5.95  | 112.96      | 108.20   |
| 27  | B8    | 147  | C    | N3-C4-N4   | 5.95  | 122.17      | 118.00   |
| 27  | B8    | 156  | A    | C4-C5-C6   | 5.95  | 119.97      | 117.00   |
| 27  | B8    | 179  | C    | N3-C4-N4   | 5.95  | 122.17      | 118.00   |
| 27  | B8    | 456  | C    | N3-C4-C5   | -5.95 | 119.52      | 121.90   |
| 27  | B8    | 980  | A    | C4-C5-C6   | 5.95  | 119.97      | 117.00   |
| 27  | B8    | 1065 | U    | O4'-C1'-N1 | 5.95  | 112.96      | 108.20   |
| 27  | B8    | 1637 | A    | C5-C6-N1   | -5.95 | 114.72      | 117.70   |
| 27  | B8    | 2175 | C    | N3-C4-N4   | 5.95  | 122.17      | 118.00   |
| 27  | B8    | 2448 | A    | C4-C5-C6   | 5.95  | 119.97      | 117.00   |
| 1   | AA    | 613  | C    | N3-C4-N4   | 5.95  | 122.17      | 118.00   |
| 1   | AA    | 1520 | C    | N3-C4-N4   | 5.95  | 122.16      | 118.00   |
| 27  | B8    | 102  | U    | O4'-C1'-N1 | 5.95  | 112.96      | 108.20   |
| 27  | B8    | 254  | G    | O4'-C1'-N9 | 5.95  | 112.96      | 108.20   |
| 27  | B8    | 637  | A    | C5-C6-N6   | -5.95 | 118.94      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 806  | C    | N3-C4-N4   | 5.95  | 122.16      | 118.00   |
| 27  | B8    | 2854 | G    | O4'-C1'-N9 | 5.95  | 112.96      | 108.20   |
| 1   | AA    | 28   | A    | C5-C6-N6   | -5.95 | 118.94      | 123.70   |
| 1   | AA    | 282  | A    | C4-C5-C6   | 5.95  | 119.97      | 117.00   |
| 26  | B7    | 21   | G    | O4'-C1'-N9 | 5.95  | 112.96      | 108.20   |
| 27  | B8    | 611  | C    | N3-C4-N4   | 5.95  | 122.16      | 118.00   |
| 1   | AA    | 156  | C    | N3-C4-N4   | 5.95  | 122.16      | 118.00   |
| 1   | AA    | 363  | A    | O4'-C1'-N9 | 5.95  | 112.96      | 108.20   |
| 1   | AA    | 546  | A    | C4-C5-C6   | 5.95  | 119.97      | 117.00   |
| 27  | B8    | 60   | G    | O4'-C1'-N9 | 5.95  | 112.96      | 108.20   |
| 27  | B8    | 564  | C    | N3-C4-N4   | 5.95  | 122.16      | 118.00   |
| 27  | B8    | 706  | A    | C4-C5-C6   | 5.95  | 119.97      | 117.00   |
| 27  | B8    | 1856 | U    | O4'-C1'-N1 | 5.95  | 112.96      | 108.20   |
| 27  | B8    | 2679 | A    | C4-C5-C6   | 5.95  | 119.97      | 117.00   |
| 1   | AA    | 271  | C    | N3-C4-N4   | 5.94  | 122.16      | 118.00   |
| 1   | AA    | 314  | C    | N3-C4-N4   | 5.94  | 122.16      | 118.00   |
| 1   | AA    | 826  | C    | N3-C4-C5   | -5.94 | 119.52      | 121.90   |
| 1   | AA    | 912  | C    | N3-C4-N4   | 5.94  | 122.16      | 118.00   |
| 27  | B8    | 1676 | A    | C4-C5-C6   | 5.94  | 119.97      | 117.00   |
| 27  | B8    | 2294 | G    | O4'-C1'-N9 | 5.94  | 112.95      | 108.20   |
| 1   | AA    | 320  | A    | C4-C5-C6   | 5.94  | 119.97      | 117.00   |
| 22  | AR    | 4    | PHE  | CB-CG-CD1  | 5.94  | 124.96      | 120.80   |
| 27  | B8    | 923  | G    | O4'-C1'-N9 | 5.94  | 112.95      | 108.20   |
| 27  | B8    | 1270 | C    | N3-C4-N4   | 5.94  | 122.16      | 118.00   |
| 27  | B8    | 1272 | A    | C4-C5-C6   | 5.94  | 119.97      | 117.00   |
| 27  | B8    | 1845 | G    | O4'-C1'-N9 | 5.94  | 112.95      | 108.20   |
| 27  | B8    | 2374 | C    | N3-C4-N4   | 5.94  | 122.16      | 118.00   |
| 27  | B8    | 2770 | G    | O4'-C1'-N9 | 5.94  | 112.95      | 108.20   |
| 1   | AA    | 73   | C    | N3-C4-N4   | 5.94  | 122.16      | 118.00   |
| 1   | AA    | 874  | G    | O4'-C1'-N9 | 5.94  | 112.95      | 108.20   |
| 26  | B7    | 28   | C    | N3-C4-N4   | 5.94  | 122.16      | 118.00   |
| 27  | B8    | 401  | A    | C4-C5-C6   | 5.94  | 119.97      | 117.00   |
| 27  | B8    | 1042 | G    | C5-C6-O6   | -5.94 | 125.03      | 128.60   |
| 27  | B8    | 1817 | G    | C5-C6-O6   | -5.94 | 125.04      | 128.60   |
| 27  | B8    | 2053 | G    | O4'-C1'-N9 | 5.94  | 112.95      | 108.20   |
| 27  | B8    | 2171 | A    | O4'-C1'-N9 | 5.94  | 112.95      | 108.20   |
| 27  | B8    | 841  | G    | O4'-C1'-N9 | 5.94  | 112.95      | 108.20   |
| 27  | B8    | 2129 | C    | C2-N1-C1'  | 5.94  | 125.33      | 118.80   |
| 1   | AA    | 130  | A    | P-O3'-C3'  | 5.94  | 126.83      | 119.70   |
| 1   | AA    | 637  | C    | N3-C4-N4   | 5.94  | 122.16      | 118.00   |
| 1   | AA    | 900  | A    | C4-C5-C6   | 5.94  | 119.97      | 117.00   |
| 1   | AA    | 1340 | A    | O4'-C1'-N9 | 5.94  | 112.95      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 706  | A    | O4'-C1'-N9 | 5.94  | 112.95      | 108.20   |
| 27  | B8    | 1080 | A    | C4-C5-C6   | 5.94  | 119.97      | 117.00   |
| 27  | B8    | 1082 | U    | O4'-C1'-N1 | 5.94  | 112.95      | 108.20   |
| 27  | B8    | 1507 | C    | N3-C4-N4   | 5.94  | 122.16      | 118.00   |
| 27  | B8    | 1730 | C    | C6-N1-C1'  | -5.94 | 113.67      | 120.80   |
| 27  | B8    | 1810 | A    | C5-C6-N6   | -5.94 | 118.95      | 123.70   |
| 1   | AA    | 269  | C    | N3-C4-N4   | 5.93  | 122.15      | 118.00   |
| 1   | AA    | 478  | A    | C5-C6-N6   | -5.93 | 118.95      | 123.70   |
| 1   | AA    | 559  | A    | C4-C5-C6   | 5.93  | 119.97      | 117.00   |
| 1   | AA    | 832  | G    | C5-C6-O6   | -5.93 | 125.04      | 128.60   |
| 1   | AA    | 893  | C    | N3-C4-C5   | -5.93 | 119.53      | 121.90   |
| 1   | AA    | 922  | G    | C5-C6-O6   | -5.93 | 125.04      | 128.60   |
| 1   | AA    | 1230 | C    | N3-C4-N4   | 5.93  | 122.15      | 118.00   |
| 1   | AA    | 1269 | A    | O4'-C1'-N9 | 5.93  | 112.95      | 108.20   |
| 1   | AA    | 1501 | C    | N3-C4-N4   | 5.93  | 122.15      | 118.00   |
| 3   | AV    | 60   | A    | C4-C5-C6   | 5.93  | 119.97      | 117.00   |
| 27  | B8    | 14   | A    | C4-C5-C6   | 5.93  | 119.97      | 117.00   |
| 27  | B8    | 346  | A    | C4-C5-C6   | 5.93  | 119.97      | 117.00   |
| 27  | B8    | 538  | A    | C4-C5-C6   | 5.93  | 119.97      | 117.00   |
| 27  | B8    | 582  | A    | C4-C5-C6   | 5.93  | 119.97      | 117.00   |
| 27  | B8    | 690  | G    | O4'-C1'-N9 | 5.93  | 112.95      | 108.20   |
| 27  | B8    | 1158 | C    | N3-C4-N4   | 5.93  | 122.15      | 118.00   |
| 27  | B8    | 1216 | G    | O4'-C1'-N9 | 5.93  | 112.95      | 108.20   |
| 27  | B8    | 2880 | C    | N3-C4-N4   | 5.93  | 122.15      | 118.00   |
| 1   | AA    | 78   | A    | O4'-C1'-N9 | 5.93  | 112.95      | 108.20   |
| 1   | AA    | 816  | A    | O4'-C1'-N9 | 5.93  | 112.95      | 108.20   |
| 1   | AA    | 1160 | G    | O4'-C1'-N9 | 5.93  | 112.95      | 108.20   |
| 27  | B8    | 89   | A    | C5-C6-N1   | -5.93 | 114.73      | 117.70   |
| 27  | B8    | 400  | G    | O4'-C1'-N9 | 5.93  | 112.95      | 108.20   |
| 27  | B8    | 1000 | A    | O4'-C1'-N9 | 5.93  | 112.94      | 108.20   |
| 27  | B8    | 1150 | C    | N3-C4-N4   | 5.93  | 122.15      | 118.00   |
| 27  | B8    | 2284 | A    | O4'-C1'-N9 | 5.93  | 112.95      | 108.20   |
| 27  | B8    | 2574 | G    | O4'-C1'-N9 | 5.93  | 112.95      | 108.20   |
| 1   | AA    | 574  | A    | C5-C6-N6   | -5.93 | 118.95      | 123.70   |
| 1   | AA    | 1272 | G    | O4'-C1'-N9 | 5.93  | 112.94      | 108.20   |
| 1   | AA    | 1333 | A    | C4-C5-C6   | 5.93  | 119.97      | 117.00   |
| 27  | B8    | 104  | A    | C4-C5-C6   | 5.93  | 119.97      | 117.00   |
| 27  | B8    | 287  | G    | O4'-C1'-N9 | 5.93  | 112.94      | 108.20   |
| 27  | B8    | 2281 | A    | C4-C5-C6   | 5.93  | 119.97      | 117.00   |
| 27  | B8    | 2600 | A    | O4'-C1'-N9 | 5.93  | 112.94      | 108.20   |
| 1   | AA    | 596  | A    | C5-C6-N6   | -5.93 | 118.96      | 123.70   |
| 27  | B8    | 340  | A    | O4'-C1'-N9 | 5.93  | 112.94      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 844  | A    | C4-C5-C6   | 5.93  | 119.96      | 117.00   |
| 27  | B8    | 1392 | A    | O4'-C1'-N9 | 5.93  | 112.94      | 108.20   |
| 27  | B8    | 1572 | A    | C5-C6-N6   | -5.93 | 118.96      | 123.70   |
| 27  | B8    | 2826 | A    | O4'-C1'-N9 | 5.93  | 112.94      | 108.20   |
| 27  | B8    | 2837 | A    | C4-C5-C6   | 5.93  | 119.97      | 117.00   |
| 1   | AA    | 915  | A    | C4-C5-C6   | 5.93  | 119.96      | 117.00   |
| 1   | AA    | 948  | C    | N3-C4-N4   | 5.93  | 122.15      | 118.00   |
| 27  | B8    | 483  | A    | C4-C5-C6   | 5.93  | 119.96      | 117.00   |
| 27  | B8    | 2397 | G    | C5-C6-O6   | -5.93 | 125.04      | 128.60   |
| 27  | B8    | 2753 | A    | C5-C6-N6   | -5.93 | 118.96      | 123.70   |
| 27  | B8    | 2902 | C    | N3-C4-N4   | 5.93  | 122.15      | 118.00   |
| 1   | AA    | 554  | A    | O4'-C1'-N9 | 5.93  | 112.94      | 108.20   |
| 1   | AA    | 735  | C    | N3-C4-N4   | 5.93  | 122.15      | 118.00   |
| 1   | AA    | 768  | A    | C5-C6-N6   | -5.93 | 118.96      | 123.70   |
| 1   | AA    | 829  | G    | O4'-C1'-N9 | 5.93  | 112.94      | 108.20   |
| 27  | B8    | 84   | A    | C4-C5-C6   | 5.93  | 119.96      | 117.00   |
| 27  | B8    | 862  | G    | O4'-C1'-N9 | 5.93  | 112.94      | 108.20   |
| 27  | B8    | 1127 | A    | C5-C6-N1   | -5.93 | 114.74      | 117.70   |
| 27  | B8    | 1224 | U    | O4'-C1'-N1 | 5.93  | 112.94      | 108.20   |
| 27  | B8    | 2019 | A    | C4-C5-C6   | 5.93  | 119.96      | 117.00   |
| 1   | AA    | 1110 | A    | C5-C6-N6   | -5.92 | 118.96      | 123.70   |
| 1   | AA    | 1223 | C    | N3-C4-N4   | 5.92  | 122.15      | 118.00   |
| 1   | AA    | 1234 | C    | N3-C4-N4   | 5.92  | 122.15      | 118.00   |
| 1   | AA    | 1306 | A    | C5-C6-N6   | -5.92 | 118.96      | 123.70   |
| 3   | AV    | 22   | A    | C5-C6-N6   | -5.92 | 118.96      | 123.70   |
| 27  | B8    | 83   | A    | C5-C6-N6   | -5.92 | 118.96      | 123.70   |
| 27  | B8    | 357  | C    | N3-C4-N4   | 5.92  | 122.15      | 118.00   |
| 27  | B8    | 1128 | G    | O4'-C1'-N9 | 5.92  | 112.94      | 108.20   |
| 1   | AA    | 532  | A    | O4'-C1'-N9 | 5.92  | 112.94      | 108.20   |
| 1   | AA    | 1137 | C    | C2-N1-C1'  | 5.92  | 125.32      | 118.80   |
| 27  | B8    | 632  | A    | C4-C5-C6   | 5.92  | 119.96      | 117.00   |
| 27  | B8    | 2031 | A    | C5-C6-N6   | -5.92 | 118.96      | 123.70   |
| 1   | AA    | 655  | A    | C4-C5-C6   | 5.92  | 119.96      | 117.00   |
| 1   | AA    | 1151 | A    | C5-C6-N6   | -5.92 | 118.96      | 123.70   |
| 1   | AA    | 1175 | G    | O4'-C1'-N9 | 5.92  | 112.94      | 108.20   |
| 1   | AA    | 1450 | U    | O4'-C1'-N1 | 5.92  | 112.94      | 108.20   |
| 27  | B8    | 152  | A    | O4'-C1'-N9 | 5.92  | 112.94      | 108.20   |
| 27  | B8    | 322  | A    | C4-C5-C6   | 5.92  | 119.96      | 117.00   |
| 27  | B8    | 739  | A    | C4-C5-C6   | 5.92  | 119.96      | 117.00   |
| 27  | B8    | 981  | A    | C4-C5-C6   | 5.92  | 119.96      | 117.00   |
| 27  | B8    | 1200 | C    | N3-C4-N4   | 5.92  | 122.14      | 118.00   |
| 27  | B8    | 1264 | A    | C4-C5-C6   | 5.92  | 119.96      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1265 | A    | C4-C5-C6   | 5.92  | 119.96      | 117.00   |
| 27  | B8    | 1356 | G    | O4'-C1'-N9 | 5.92  | 112.94      | 108.20   |
| 27  | B8    | 1399 | C    | N3-C4-N4   | 5.92  | 122.14      | 118.00   |
| 27  | B8    | 1740 | G    | O4'-C1'-N9 | 5.92  | 112.94      | 108.20   |
| 27  | B8    | 1905 | C    | N3-C4-N4   | 5.92  | 122.14      | 118.00   |
| 27  | B8    | 1927 | A    | C4-C5-C6   | 5.92  | 119.96      | 117.00   |
| 27  | B8    | 1999 | C    | N3-C4-N4   | 5.92  | 122.14      | 118.00   |
| 27  | B8    | 2466 | C    | N3-C4-N4   | 5.92  | 122.14      | 118.00   |
| 1   | AA    | 842  | U    | C2-N1-C1'  | 5.92  | 124.80      | 117.70   |
| 27  | B8    | 274  | C    | N3-C4-N4   | 5.92  | 122.14      | 118.00   |
| 27  | B8    | 323  | C    | N3-C4-N4   | 5.92  | 122.14      | 118.00   |
| 27  | B8    | 902  | C    | N3-C4-N4   | 5.92  | 122.14      | 118.00   |
| 27  | B8    | 2600 | A    | C5-C6-N6   | -5.92 | 118.96      | 123.70   |
| 27  | B8    | 513  | A    | O4'-C1'-N9 | 5.92  | 112.93      | 108.20   |
| 27  | B8    | 756  | A    | C4-C5-C6   | 5.92  | 119.96      | 117.00   |
| 27  | B8    | 954  | G    | O4'-C1'-N9 | 5.92  | 112.94      | 108.20   |
| 27  | B8    | 1129 | A    | O4'-C1'-N9 | 5.92  | 112.94      | 108.20   |
| 27  | B8    | 1889 | A    | C4-C5-C6   | 5.92  | 119.96      | 117.00   |
| 27  | B8    | 1941 | C    | N3-C4-N4   | 5.92  | 122.14      | 118.00   |
| 27  | B8    | 1953 | A    | C5-C6-N1   | -5.92 | 114.74      | 117.70   |
| 27  | B8    | 1998 | A    | O4'-C1'-N9 | 5.92  | 112.94      | 108.20   |
| 27  | B8    | 2859 | G    | C5-C6-O6   | -5.92 | 125.05      | 128.60   |
| 1   | AA    | 59   | A    | C5-C6-N6   | -5.92 | 118.97      | 123.70   |
| 1   | AA    | 1162 | C    | N3-C4-N4   | 5.92  | 122.14      | 118.00   |
| 1   | AA    | 1432 | G    | N3-C2-N2   | 5.92  | 124.04      | 119.90   |
| 27  | B8    | 84   | A    | C5-C6-N6   | -5.92 | 118.97      | 123.70   |
| 27  | B8    | 310  | A    | C5-C6-N1   | -5.92 | 114.74      | 117.70   |
| 27  | B8    | 460  | A    | C4-C5-C6   | 5.92  | 119.96      | 117.00   |
| 27  | B8    | 1010 | A    | C4-C5-C6   | 5.92  | 119.96      | 117.00   |
| 27  | B8    | 1556 | C    | N3-C4-C5   | -5.92 | 119.53      | 121.90   |
| 27  | B8    | 1805 | A    | C4-C5-C6   | 5.92  | 119.96      | 117.00   |
| 27  | B8    | 2767 | C    | N3-C4-N4   | 5.92  | 122.14      | 118.00   |
| 27  | B8    | 2887 | A    | C5-C6-N6   | -5.92 | 118.97      | 123.70   |
| 1   | AA    | 796  | C    | N3-C4-N4   | 5.92  | 122.14      | 118.00   |
| 27  | B8    | 19   | A    | C4-C5-C6   | 5.92  | 119.96      | 117.00   |
| 1   | AA    | 344  | A    | C4-C5-C6   | 5.91  | 119.96      | 117.00   |
| 1   | AA    | 581  | G    | N3-C2-N2   | 5.91  | 124.04      | 119.90   |
| 1   | AA    | 896  | C    | N3-C4-N4   | 5.91  | 122.14      | 118.00   |
| 26  | B7    | 119  | A    | C5-C6-N6   | -5.91 | 118.97      | 123.70   |
| 27  | B8    | 650  | C    | N3-C4-N4   | 5.91  | 122.14      | 118.00   |
| 27  | B8    | 1998 | A    | C5-C6-N6   | -5.91 | 118.97      | 123.70   |
| 27  | B8    | 2317 | A    | C5-C6-N6   | -5.91 | 118.97      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2435 | A    | O4'-C1'-N9 | 5.91  | 112.93      | 108.20   |
| 27  | B8    | 2589 | A    | C5-C6-N1   | -5.91 | 114.74      | 117.70   |
| 27  | B8    | 2725 | A    | C4-C5-C6   | 5.91  | 119.96      | 117.00   |
| 27  | B8    | 2813 | A    | C4-C5-C6   | 5.91  | 119.96      | 117.00   |
| 1   | AA    | 136  | C    | N3-C4-N4   | 5.91  | 122.14      | 118.00   |
| 1   | AA    | 1229 | A    | C5-C6-N6   | -5.91 | 118.97      | 123.70   |
| 1   | AA    | 1329 | A    | C4-C5-C6   | 5.91  | 119.96      | 117.00   |
| 27  | B8    | 794  | A    | C4-C5-C6   | 5.91  | 119.96      | 117.00   |
| 27  | B8    | 814  | C    | N3-C4-N4   | 5.91  | 122.14      | 118.00   |
| 1   | AA    | 309  | A    | C4-C5-C6   | 5.91  | 119.96      | 117.00   |
| 1   | AA    | 1236 | A    | C5-C6-N1   | -5.91 | 114.75      | 117.70   |
| 1   | AA    | 1524 | C    | N3-C4-N4   | 5.91  | 122.14      | 118.00   |
| 27  | B8    | 103  | A    | C4-C5-C6   | 5.91  | 119.96      | 117.00   |
| 27  | B8    | 838  | C    | N3-C4-N4   | 5.91  | 122.14      | 118.00   |
| 27  | B8    | 1247 | A    | C5-C6-N1   | -5.91 | 114.75      | 117.70   |
| 27  | B8    | 1592 | C    | N3-C4-N4   | 5.91  | 122.14      | 118.00   |
| 27  | B8    | 1745 | A    | C5-C6-N1   | -5.91 | 114.75      | 117.70   |
| 27  | B8    | 1863 | G    | O4'-C1'-N9 | 5.91  | 112.93      | 108.20   |
| 27  | B8    | 1936 | A    | C5-C6-N6   | -5.91 | 118.97      | 123.70   |
| 27  | B8    | 1960 | A    | C4-C5-C6   | 5.91  | 119.95      | 117.00   |
| 1   | AA    | 539  | A    | C5-C6-N6   | -5.91 | 118.97      | 123.70   |
| 1   | AA    | 985  | C    | N3-C4-N4   | 5.91  | 122.14      | 118.00   |
| 1   | AA    | 1188 | A    | C5-C6-N6   | -5.91 | 118.97      | 123.70   |
| 1   | AA    | 1322 | C    | C6-N1-C1'  | -5.91 | 113.71      | 120.80   |
| 27  | B8    | 5    | A    | C4-C5-C6   | 5.91  | 119.95      | 117.00   |
| 27  | B8    | 97   | C    | N3-C4-N4   | 5.91  | 122.14      | 118.00   |
| 27  | B8    | 422  | A    | C4-C5-C6   | 5.91  | 119.95      | 117.00   |
| 27  | B8    | 627  | A    | C4-C5-C6   | 5.91  | 119.95      | 117.00   |
| 27  | B8    | 2662 | A    | C5-C6-N1   | -5.91 | 114.75      | 117.70   |
| 27  | B8    | 2829 | A    | C4-C5-C6   | 5.91  | 119.95      | 117.00   |
| 1   | AA    | 131  | A    | C5-C6-N1   | -5.91 | 114.75      | 117.70   |
| 1   | AA    | 1019 | A    | O4'-C1'-N9 | 5.91  | 112.93      | 108.20   |
| 27  | B8    | 435  | C    | N3-C4-C5   | -5.91 | 119.54      | 121.90   |
| 27  | B8    | 1450 | G    | O4'-C1'-N9 | 5.91  | 112.93      | 108.20   |
| 27  | B8    | 2545 | G    | O4'-C1'-N9 | 5.91  | 112.93      | 108.20   |
| 1   | AA    | 321  | A    | C5-C6-N1   | -5.91 | 114.75      | 117.70   |
| 1   | AA    | 1067 | A    | C4-C5-C6   | 5.91  | 119.95      | 117.00   |
| 27  | B8    | 1243 | C    | N3-C4-N4   | 5.91  | 122.13      | 118.00   |
| 27  | B8    | 2009 | A    | O4'-C1'-N9 | 5.91  | 112.92      | 108.20   |
| 27  | B8    | 2147 | A    | C5-C6-N6   | -5.91 | 118.98      | 123.70   |
| 1   | AA    | 794  | A    | C4-C5-C6   | 5.90  | 119.95      | 117.00   |
| 1   | AA    | 1067 | A    | C5-C6-N1   | -5.90 | 114.75      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1250 | A    | C5-C6-N6   | -5.90 | 118.98      | 123.70   |
| 27  | B8    | 1109 | C    | N3-C4-N4   | 5.90  | 122.13      | 118.00   |
| 27  | B8    | 1677 | A    | C4-C5-C6   | 5.90  | 119.95      | 117.00   |
| 1   | AA    | 328  | C    | C2-N1-C1'  | 5.90  | 125.29      | 118.80   |
| 27  | B8    | 128  | C    | N3-C4-N4   | 5.90  | 122.13      | 118.00   |
| 27  | B8    | 471  | A    | C5-C6-N1   | -5.90 | 114.75      | 117.70   |
| 27  | B8    | 599  | A    | C5-C6-N1   | -5.90 | 114.75      | 117.70   |
| 27  | B8    | 812  | C    | N3-C4-N4   | 5.90  | 122.13      | 118.00   |
| 27  | B8    | 978  | G    | O4'-C1'-N9 | 5.90  | 112.92      | 108.20   |
| 27  | B8    | 1039 | A    | C5-C6-N6   | -5.90 | 118.98      | 123.70   |
| 27  | B8    | 1155 | A    | C4-C5-C6   | 5.90  | 119.95      | 117.00   |
| 27  | B8    | 1241 | A    | C4-C5-C6   | 5.90  | 119.95      | 117.00   |
| 27  | B8    | 1788 | C    | N3-C4-N4   | 5.90  | 122.13      | 118.00   |
| 1   | AA    | 192  | A    | C5-C6-N1   | -5.90 | 114.75      | 117.70   |
| 1   | AA    | 396  | C    | N3-C4-N4   | 5.90  | 122.13      | 118.00   |
| 1   | AA    | 462  | G    | O4'-C1'-N9 | 5.90  | 112.92      | 108.20   |
| 1   | AA    | 1171 | A    | C4-C5-C6   | 5.90  | 119.95      | 117.00   |
| 1   | AA    | 1364 | U    | C2-N1-C1'  | 5.90  | 124.78      | 117.70   |
| 1   | AA    | 1480 | A    | C4-C5-C6   | 5.90  | 119.95      | 117.00   |
| 27  | B8    | 211  | C    | N3-C4-N4   | 5.90  | 122.13      | 118.00   |
| 27  | B8    | 749  | A    | C5-C6-N6   | -5.90 | 118.98      | 123.70   |
| 27  | B8    | 789  | A    | C5-C6-N6   | -5.90 | 118.98      | 123.70   |
| 27  | B8    | 994  | C    | N3-C4-N4   | 5.90  | 122.13      | 118.00   |
| 27  | B8    | 1114 | C    | N3-C4-N4   | 5.90  | 122.13      | 118.00   |
| 27  | B8    | 1334 | G    | O4'-C1'-N9 | 5.90  | 112.92      | 108.20   |
| 27  | B8    | 1586 | A    | C5-C6-N6   | -5.90 | 118.98      | 123.70   |
| 27  | B8    | 1615 | C    | O4'-C1'-N1 | 5.90  | 112.92      | 108.20   |
| 27  | B8    | 2191 | A    | C4-C5-C6   | 5.90  | 119.95      | 117.00   |
| 27  | B8    | 2710 | C    | N3-C4-N4   | 5.90  | 122.13      | 118.00   |
| 1   | AA    | 11   | G    | O4'-C1'-N9 | 5.90  | 112.92      | 108.20   |
| 1   | AA    | 1082 | A    | C5-C6-N1   | -5.90 | 114.75      | 117.70   |
| 27  | B8    | 181  | A    | O4'-C1'-N9 | 5.90  | 112.92      | 108.20   |
| 27  | B8    | 404  | A    | C4-C5-C6   | 5.90  | 119.95      | 117.00   |
| 27  | B8    | 624  | C    | N3-C4-C5   | -5.90 | 119.54      | 121.90   |
| 1   | AA    | 336  | A    | C4-C5-C6   | 5.90  | 119.95      | 117.00   |
| 27  | B8    | 1194 | A    | C5-C6-N6   | -5.90 | 118.98      | 123.70   |
| 27  | B8    | 1289 | C    | N3-C4-N4   | 5.90  | 122.13      | 118.00   |
| 27  | B8    | 1760 | C    | N3-C4-N4   | 5.90  | 122.13      | 118.00   |
| 27  | B8    | 2013 | A    | C5-C6-N6   | -5.90 | 118.98      | 123.70   |
| 27  | B8    | 2133 | G    | O4'-C1'-N9 | 5.90  | 112.92      | 108.20   |
| 27  | B8    | 2170 | A    | C5-C6-N6   | -5.90 | 118.98      | 123.70   |
| 27  | B8    | 2873 | A    | O4'-C1'-N9 | 5.90  | 112.92      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 800  | G    | C5-C6-O6   | -5.90 | 125.06      | 128.60   |
| 1   | AA    | 899  | C    | N3-C4-N4   | 5.90  | 122.13      | 118.00   |
| 27  | B8    | 2810 | A    | C5-C6-N6   | -5.90 | 118.98      | 123.70   |
| 1   | AA    | 323  | U    | O4'-C1'-N1 | 5.89  | 112.92      | 108.20   |
| 1   | AA    | 386  | C    | N3-C4-N4   | 5.89  | 122.13      | 118.00   |
| 1   | AA    | 958  | A    | C5-C6-N1   | -5.89 | 114.75      | 117.70   |
| 1   | AA    | 1208 | C    | N3-C4-N4   | 5.89  | 122.13      | 118.00   |
| 1   | AA    | 1374 | A    | C4-C5-C6   | 5.89  | 119.95      | 117.00   |
| 1   | AA    | 1446 | A    | C4-C5-C6   | 5.89  | 119.95      | 117.00   |
| 27  | B8    | 38   | A    | C5-C6-N6   | -5.89 | 118.98      | 123.70   |
| 27  | B8    | 322  | A    | C5-C6-N6   | -5.89 | 118.98      | 123.70   |
| 27  | B8    | 1208 | C    | N3-C4-N4   | 5.89  | 122.13      | 118.00   |
| 27  | B8    | 1978 | A    | C5-C6-N6   | -5.89 | 118.98      | 123.70   |
| 27  | B8    | 2308 | G    | C5-C6-O6   | -5.89 | 125.06      | 128.60   |
| 27  | B8    | 2547 | A    | C4-C5-C6   | 5.89  | 119.95      | 117.00   |
| 1   | AA    | 183  | C    | C2-N1-C1'  | 5.89  | 125.28      | 118.80   |
| 1   | AA    | 938  | A    | C5-C6-N6   | -5.89 | 118.99      | 123.70   |
| 1   | AA    | 1031 | C    | N3-C4-C5   | -5.89 | 119.54      | 121.90   |
| 27  | B8    | 295  | G    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |
| 27  | B8    | 602  | A    | C4-C5-C6   | 5.89  | 119.95      | 117.00   |
| 27  | B8    | 1191 | G    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |
| 27  | B8    | 1230 | A    | C5-C6-N6   | -5.89 | 118.99      | 123.70   |
| 27  | B8    | 1544 | A    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |
| 27  | B8    | 2075 | U    | O4'-C1'-N1 | 5.89  | 112.91      | 108.20   |
| 1   | AA    | 68   | G    | C5-C6-O6   | -5.89 | 125.06      | 128.60   |
| 1   | AA    | 1214 | C    | O4'-C1'-N1 | 5.89  | 112.91      | 108.20   |
| 1   | AA    | 1410 | A    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |
| 27  | B8    | 21   | A    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |
| 27  | B8    | 1446 | C    | N3-C4-N4   | 5.89  | 122.12      | 118.00   |
| 27  | B8    | 1553 | A    | C4-C5-C6   | 5.89  | 119.94      | 117.00   |
| 27  | B8    | 2837 | A    | C5-C6-N6   | -5.89 | 118.99      | 123.70   |
| 1   | AA    | 1049 | U    | O4'-C1'-N1 | 5.89  | 112.91      | 108.20   |
| 1   | AA    | 1427 | C    | N3-C4-N4   | 5.89  | 122.12      | 118.00   |
| 1   | AA    | 1429 | A    | C4-C5-C6   | 5.89  | 119.94      | 117.00   |
| 3   | AV    | 59   | A    | C4-C5-C6   | 5.89  | 119.94      | 117.00   |
| 26  | B7    | 118  | C    | N3-C4-N4   | 5.89  | 122.12      | 118.00   |
| 27  | B8    | 382  | A    | C4-C5-C6   | 5.89  | 119.94      | 117.00   |
| 27  | B8    | 605  | G    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |
| 27  | B8    | 855  | G    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |
| 27  | B8    | 910  | A    | C5-C6-N1   | -5.89 | 114.75      | 117.70   |
| 27  | B8    | 989  | G    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |
| 27  | B8    | 1090 | A    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1294 | U    | O4'-C1'-N1 | 5.89  | 112.91      | 108.20   |
| 27  | B8    | 1639 | C    | O4'-C1'-N1 | 5.89  | 112.91      | 108.20   |
| 27  | B8    | 1741 | C    | N3-C4-N4   | 5.89  | 122.12      | 118.00   |
| 27  | B8    | 2317 | A    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |
| 1   | AA    | 7    | A    | C4-C5-C6   | 5.89  | 119.94      | 117.00   |
| 27  | B8    | 904  | G    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |
| 27  | B8    | 1623 | G    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |
| 27  | B8    | 2132 | U    | C2-N1-C1'  | 5.89  | 124.77      | 117.70   |
| 1   | AA    | 414  | A    | C4-C5-C6   | 5.89  | 119.94      | 117.00   |
| 1   | AA    | 1042 | A    | C4-C5-C6   | 5.89  | 119.94      | 117.00   |
| 1   | AA    | 1508 | A    | C4-C5-C6   | 5.89  | 119.94      | 117.00   |
| 26  | B7    | 19   | C    | N3-C4-N4   | 5.89  | 122.12      | 118.00   |
| 27  | B8    | 371  | A    | C5-C6-N1   | -5.89 | 114.76      | 117.70   |
| 27  | B8    | 1366 | A    | C5-C6-N6   | -5.89 | 118.99      | 123.70   |
| 27  | B8    | 2115 | G    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |
| 27  | B8    | 2200 | C    | N3-C4-C5   | -5.89 | 119.55      | 121.90   |
| 27  | B8    | 2250 | G    | C5-C6-O6   | -5.89 | 125.07      | 128.60   |
| 27  | B8    | 2630 | G    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |
| 35  | BG    | 108  | PHE  | CB-CG-CD1  | -5.89 | 116.68      | 120.80   |
| 1   | AA    | 45   | G    | O4'-C1'-N9 | 5.88  | 112.91      | 108.20   |
| 1   | AA    | 694  | A    | C5-C6-N6   | -5.88 | 118.99      | 123.70   |
| 1   | AA    | 736  | C    | N3-C4-N4   | 5.88  | 122.12      | 118.00   |
| 1   | AA    | 815  | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 1   | AA    | 1246 | A    | C5-C6-N1   | -5.88 | 114.76      | 117.70   |
| 1   | AA    | 1358 | U    | O4'-C1'-N1 | 5.88  | 112.91      | 108.20   |
| 1   | AA    | 1377 | A    | C5-C6-N6   | -5.88 | 118.99      | 123.70   |
| 27  | B8    | 410  | G    | N3-C2-N2   | 5.88  | 124.02      | 119.90   |
| 27  | B8    | 691  | C    | N3-C4-N4   | 5.88  | 122.12      | 118.00   |
| 27  | B8    | 2162 | G    | O4'-C1'-N9 | 5.88  | 112.91      | 108.20   |
| 27  | B8    | 2198 | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 27  | B8    | 2820 | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 27  | B8    | 2823 | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 1   | AA    | 1176 | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 27  | B8    | 847  | U    | C2-N1-C1'  | 5.88  | 124.76      | 117.70   |
| 27  | B8    | 982  | C    | C6-N1-C1'  | -5.88 | 113.74      | 120.80   |
| 27  | B8    | 1663 | G    | O4'-C1'-N9 | 5.88  | 112.91      | 108.20   |
| 27  | B8    | 2252 | G    | O4'-C1'-N9 | 5.88  | 112.91      | 108.20   |
| 1   | AA    | 301  | G    | O4'-C1'-N9 | 5.88  | 112.90      | 108.20   |
| 1   | AA    | 1155 | A    | C5-C6-N1   | -5.88 | 114.76      | 117.70   |
| 1   | AA    | 1167 | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 1   | AA    | 1339 | A    | O4'-C1'-N9 | 5.88  | 112.91      | 108.20   |
| 1   | AA    | 1492 | A    | O4'-C1'-N9 | 5.88  | 112.91      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 127  | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 27  | B8    | 961  | C    | O4'-C1'-N1 | 5.88  | 112.91      | 108.20   |
| 27  | B8    | 2000 | C    | N3-C4-N4   | 5.88  | 122.12      | 118.00   |
| 27  | B8    | 2191 | A    | C5-C6-N1   | -5.88 | 114.76      | 117.70   |
| 27  | B8    | 2281 | A    | O4'-C1'-N9 | 5.88  | 112.91      | 108.20   |
| 27  | B8    | 2468 | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 27  | B8    | 2636 | C    | N3-C4-N4   | 5.88  | 122.12      | 118.00   |
| 27  | B8    | 2706 | A    | C5-C6-N6   | -5.88 | 118.99      | 123.70   |
| 27  | B8    | 2882 | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 1   | AA    | 655  | A    | C5-C6-N1   | -5.88 | 114.76      | 117.70   |
| 1   | AA    | 949  | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 1   | AA    | 1340 | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 27  | B8    | 1325 | U    | O4'-C1'-N1 | 5.88  | 112.90      | 108.20   |
| 27  | B8    | 1362 | C    | N3-C4-N4   | 5.88  | 122.12      | 118.00   |
| 27  | B8    | 2169 | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 27  | B8    | 455  | C    | N3-C4-C5   | -5.88 | 119.55      | 121.90   |
| 27  | B8    | 497  | A    | C5-C6-N1   | -5.88 | 114.76      | 117.70   |
| 27  | B8    | 905  | A    | O4'-C1'-N9 | 5.88  | 112.90      | 108.20   |
| 27  | B8    | 1194 | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 27  | B8    | 1768 | C    | N3-C4-N4   | 5.88  | 122.11      | 118.00   |
| 27  | B8    | 2005 | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 27  | B8    | 2090 | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 27  | B8    | 2722 | G    | O4'-C1'-N9 | 5.88  | 112.90      | 108.20   |
| 1   | AA    | 553  | A    | C5-C6-N6   | -5.88 | 119.00      | 123.70   |
| 1   | AA    | 974  | A    | C5-C6-N6   | -5.88 | 119.00      | 123.70   |
| 27  | B8    | 798  | G    | O4'-C1'-N9 | 5.88  | 112.90      | 108.20   |
| 27  | B8    | 1260 | A    | O4'-C1'-N9 | 5.88  | 112.90      | 108.20   |
| 27  | B8    | 1978 | A    | O4'-C1'-N9 | 5.88  | 112.90      | 108.20   |
| 27  | B8    | 2021 | C    | N3-C4-N4   | 5.88  | 122.11      | 118.00   |
| 1   | AA    | 300  | A    | C4-C5-C6   | 5.88  | 119.94      | 117.00   |
| 1   | AA    | 533  | A    | C5-C6-N1   | -5.88 | 114.76      | 117.70   |
| 1   | AA    | 773  | G    | O4'-C1'-N9 | 5.88  | 112.90      | 108.20   |
| 27  | B8    | 2359 | C    | N3-C4-N4   | 5.88  | 122.11      | 118.00   |
| 1   | AA    | 19   | A    | C5-C6-N6   | -5.87 | 119.00      | 123.70   |
| 1   | AA    | 629  | A    | C5-C6-N6   | -5.87 | 119.00      | 123.70   |
| 1   | AA    | 687  | A    | C4-C5-C6   | 5.87  | 119.94      | 117.00   |
| 1   | AA    | 946  | A    | C5-C6-N1   | -5.87 | 114.76      | 117.70   |
| 27  | B8    | 181  | A    | C4-C5-C6   | 5.87  | 119.94      | 117.00   |
| 27  | B8    | 429  | A    | C5-C6-N6   | -5.87 | 119.00      | 123.70   |
| 27  | B8    | 544  | C    | C6-N1-C1'  | -5.87 | 113.75      | 120.80   |
| 27  | B8    | 1757 | A    | C5-C6-N6   | -5.87 | 119.00      | 123.70   |
| 27  | B8    | 1773 | A    | O4'-C1'-N9 | 5.87  | 112.90      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2059 | A    | C4-C5-C6   | 5.87  | 119.94      | 117.00   |
| 1   | AA    | 65   | A    | C4-C5-C6   | 5.87  | 119.94      | 117.00   |
| 1   | AA    | 263  | A    | C5-C6-N6   | -5.87 | 119.00      | 123.70   |
| 1   | AA    | 434  | U    | O4'-C1'-N1 | 5.87  | 112.90      | 108.20   |
| 1   | AA    | 1063 | C    | O4'-C1'-N1 | 5.87  | 112.90      | 108.20   |
| 26  | B7    | 54   | G    | O4'-C1'-N9 | 5.87  | 112.90      | 108.20   |
| 27  | B8    | 746  | U    | O4'-C1'-N1 | 5.87  | 112.90      | 108.20   |
| 1   | AA    | 441  | A    | C4-C5-C6   | 5.87  | 119.94      | 117.00   |
| 1   | AA    | 1058 | G    | O4'-C1'-N9 | 5.87  | 112.90      | 108.20   |
| 27  | B8    | 920  | A    | C5-C6-N1   | -5.87 | 114.77      | 117.70   |
| 1   | AA    | 223  | A    | C5-C6-N1   | -5.87 | 114.77      | 117.70   |
| 27  | B8    | 26   | G    | N3-C2-N2   | 5.87  | 124.01      | 119.90   |
| 27  | B8    | 950  | G    | O4'-C1'-N9 | 5.87  | 112.89      | 108.20   |
| 27  | B8    | 1615 | C    | N3-C4-N4   | 5.87  | 122.11      | 118.00   |
| 27  | B8    | 1618 | A    | C5-C6-N6   | -5.87 | 119.00      | 123.70   |
| 27  | B8    | 1749 | A    | C5-C6-N1   | -5.87 | 114.77      | 117.70   |
| 27  | B8    | 1881 | C    | N3-C4-N4   | 5.87  | 122.11      | 118.00   |
| 27  | B8    | 1969 | A    | C5-C6-N1   | -5.87 | 114.77      | 117.70   |
| 27  | B8    | 2108 | A    | C4-C5-C6   | 5.87  | 119.94      | 117.00   |
| 27  | B8    | 2807 | U    | O4'-C1'-N1 | 5.87  | 112.89      | 108.20   |
| 1   | AA    | 3    | A    | C5-C6-N6   | -5.87 | 119.01      | 123.70   |
| 1   | AA    | 525  | C    | N3-C4-N4   | 5.87  | 122.11      | 118.00   |
| 27  | B8    | 2841 | C    | N3-C4-N4   | 5.87  | 122.11      | 118.00   |
| 1   | AA    | 205  | A    | O4'-C1'-N9 | 5.87  | 112.89      | 108.20   |
| 1   | AA    | 443  | C    | N3-C4-N4   | 5.87  | 122.11      | 118.00   |
| 1   | AA    | 705  | G    | O4'-C1'-N9 | 5.87  | 112.89      | 108.20   |
| 1   | AA    | 1237 | C    | N3-C4-N4   | 5.87  | 122.11      | 118.00   |
| 1   | AA    | 1254 | A    | C4-C5-C6   | 5.87  | 119.93      | 117.00   |
| 1   | AA    | 1513 | A    | C4-C5-C6   | 5.87  | 119.93      | 117.00   |
| 27  | B8    | 395  | U    | O4'-C1'-N1 | 5.87  | 112.89      | 108.20   |
| 27  | B8    | 480  | A    | O4'-C1'-N9 | 5.87  | 112.89      | 108.20   |
| 27  | B8    | 716  | A    | C5-C6-N6   | -5.87 | 119.01      | 123.70   |
| 27  | B8    | 1126 | A    | C4-C5-C6   | 5.87  | 119.93      | 117.00   |
| 27  | B8    | 2311 | A    | C5-C6-N1   | -5.87 | 114.77      | 117.70   |
| 27  | B8    | 2362 | C    | N3-C4-N4   | 5.87  | 122.11      | 118.00   |
| 27  | B8    | 2369 | A    | C4-C5-C6   | 5.87  | 119.93      | 117.00   |
| 27  | B8    | 2753 | A    | O4'-C1'-N9 | 5.87  | 112.89      | 108.20   |
| 27  | B8    | 2756 | U    | P-O3'-C3'  | 5.87  | 126.74      | 119.70   |
| 1   | AA    | 182  | A    | C5-C6-N1   | -5.86 | 114.77      | 117.70   |
| 1   | AA    | 382  | A    | C4-C5-C6   | 5.86  | 119.93      | 117.00   |
| 27  | B8    | 191  | A    | C5-C6-N1   | -5.86 | 114.77      | 117.70   |
| 27  | B8    | 965  | C    | N3-C4-C5   | -5.86 | 119.55      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 977  | G    | O4'-C1'-N9 | 5.86  | 112.89      | 108.20   |
| 27  | B8    | 1771 | C    | N3-C4-N4   | 5.86  | 122.10      | 118.00   |
| 1   | AA    | 453  | G    | O4'-C1'-N9 | 5.86  | 112.89      | 108.20   |
| 27  | B8    | 1496 | A    | C4-C5-C6   | 5.86  | 119.93      | 117.00   |
| 1   | AA    | 199  | A    | C5-C6-N1   | -5.86 | 114.77      | 117.70   |
| 1   | AA    | 346  | G    | O4'-C1'-N9 | 5.86  | 112.89      | 108.20   |
| 1   | AA    | 1054 | C    | N3-C4-N4   | 5.86  | 122.10      | 118.00   |
| 27  | B8    | 53   | A    | C5-C6-N6   | -5.86 | 119.01      | 123.70   |
| 27  | B8    | 2411 | A    | C5-C6-N6   | -5.86 | 119.01      | 123.70   |
| 27  | B8    | 2829 | A    | C5-C6-N1   | -5.86 | 114.77      | 117.70   |
| 1   | AA    | 1280 | A    | C4-C5-C6   | 5.86  | 119.93      | 117.00   |
| 27  | B8    | 1050 | A    | C5-C6-N6   | -5.86 | 119.01      | 123.70   |
| 27  | B8    | 1408 | G    | O4'-C1'-N9 | 5.86  | 112.89      | 108.20   |
| 27  | B8    | 2213 | U    | O4'-C1'-N1 | 5.86  | 112.89      | 108.20   |
| 27  | B8    | 2791 | G    | O4'-C1'-N9 | 5.86  | 112.89      | 108.20   |
| 1   | AA    | 350  | G    | O4'-C1'-N9 | 5.86  | 112.89      | 108.20   |
| 1   | AA    | 441  | A    | O4'-C1'-N9 | 5.86  | 112.89      | 108.20   |
| 1   | AA    | 553  | A    | C4-C5-C6   | 5.86  | 119.93      | 117.00   |
| 1   | AA    | 1021 | A    | C4-C5-C6   | 5.86  | 119.93      | 117.00   |
| 1   | AA    | 1157 | A    | C4-C5-C6   | 5.86  | 119.93      | 117.00   |
| 1   | AA    | 1204 | A    | C5-C6-N1   | -5.86 | 114.77      | 117.70   |
| 1   | AA    | 1388 | C    | N3-C4-N4   | 5.86  | 122.10      | 118.00   |
| 26  | B7    | 73   | A    | C5-C6-N1   | -5.86 | 114.77      | 117.70   |
| 27  | B8    | 382  | A    | C5-C6-N1   | -5.86 | 114.77      | 117.70   |
| 27  | B8    | 421  | C    | N3-C4-N4   | 5.86  | 122.10      | 118.00   |
| 27  | B8    | 1009 | A    | C5-C6-N6   | -5.86 | 119.01      | 123.70   |
| 27  | B8    | 1090 | A    | C4-C5-C6   | 5.86  | 119.93      | 117.00   |
| 27  | B8    | 1244 | A    | C4-C5-C6   | 5.86  | 119.93      | 117.00   |
| 27  | B8    | 1496 | A    | O4'-C1'-N9 | 5.86  | 112.89      | 108.20   |
| 27  | B8    | 1690 | A    | O4'-C1'-N9 | 5.86  | 112.89      | 108.20   |
| 27  | B8    | 2326 | C    | N3-C4-N4   | 5.86  | 122.10      | 118.00   |
| 27  | B8    | 2518 | A    | C4-C5-C6   | 5.86  | 119.93      | 117.00   |
| 27  | B8    | 2670 | A    | C5-C6-N6   | -5.86 | 119.01      | 123.70   |
| 27  | B8    | 2814 | A    | O4'-C1'-N9 | 5.86  | 112.89      | 108.20   |
| 1   | AA    | 647  | C    | N3-C4-N4   | 5.86  | 122.10      | 118.00   |
| 1   | AA    | 949  | A    | C5-C6-N1   | -5.86 | 114.77      | 117.70   |
| 27  | B8    | 945  | A    | C5-C6-N6   | -5.86 | 119.02      | 123.70   |
| 27  | B8    | 1558 | C    | N3-C4-C5   | -5.86 | 119.56      | 121.90   |
| 27  | B8    | 1952 | A    | C5-C6-N6   | -5.86 | 119.02      | 123.70   |
| 27  | B8    | 2206 | C    | N3-C4-N4   | 5.86  | 122.10      | 118.00   |
| 27  | B8    | 2314 | A    | C5-C6-N1   | -5.86 | 114.77      | 117.70   |
| 27  | B8    | 2449 | U    | O4'-C1'-N1 | 5.86  | 112.89      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2570 | G    | O4'-C1'-N9 | 5.86  | 112.89      | 108.20   |
| 27  | B8    | 2676 | C    | N3-C4-N4   | 5.86  | 122.10      | 118.00   |
| 26  | B7    | 70   | C    | N3-C4-N4   | 5.85  | 122.10      | 118.00   |
| 27  | B8    | 1014 | A    | C4-C5-C6   | 5.85  | 119.93      | 117.00   |
| 27  | B8    | 2412 | A    | C5-C6-N6   | -5.85 | 119.02      | 123.70   |
| 1   | AA    | 504  | C    | N3-C4-C5   | -5.85 | 119.56      | 121.90   |
| 1   | AA    | 771  | G    | O4'-C1'-N9 | 5.85  | 112.88      | 108.20   |
| 1   | AA    | 1377 | A    | O4'-C1'-N9 | 5.85  | 112.88      | 108.20   |
| 1   | AA    | 1413 | A    | C5-C6-N1   | -5.85 | 114.77      | 117.70   |
| 27  | B8    | 549  | G    | O4'-C1'-N9 | 5.85  | 112.88      | 108.20   |
| 27  | B8    | 715  | A    | C4-C5-C6   | 5.85  | 119.93      | 117.00   |
| 27  | B8    | 1503 | A    | C5-C6-N1   | -5.85 | 114.77      | 117.70   |
| 1   | AA    | 560  | A    | C5-C6-N6   | -5.85 | 119.02      | 123.70   |
| 1   | AA    | 737  | C    | N3-C4-C5   | -5.85 | 119.56      | 121.90   |
| 1   | AA    | 1196 | A    | C5-C6-N6   | -5.85 | 119.02      | 123.70   |
| 27  | B8    | 429  | A    | C5-C6-N1   | -5.85 | 114.77      | 117.70   |
| 27  | B8    | 557  | C    | N3-C4-N4   | 5.85  | 122.09      | 118.00   |
| 27  | B8    | 1490 | A    | C5-C6-N6   | -5.85 | 119.02      | 123.70   |
| 27  | B8    | 1928 | A    | O4'-C1'-N9 | 5.85  | 112.88      | 108.20   |
| 27  | B8    | 2665 | A    | C5-C6-N6   | -5.85 | 119.02      | 123.70   |
| 1   | AA    | 171  | A    | O4'-C1'-N9 | 5.85  | 112.88      | 108.20   |
| 1   | AA    | 217  | C    | N3-C4-N4   | 5.85  | 122.09      | 118.00   |
| 1   | AA    | 384  | G    | O4'-C1'-N9 | 5.85  | 112.88      | 108.20   |
| 27  | B8    | 1579 | A    | O4'-C1'-N9 | 5.85  | 112.88      | 108.20   |
| 1   | AA    | 236  | A    | C5-C6-N6   | -5.85 | 119.02      | 123.70   |
| 1   | AA    | 341  | C    | N3-C4-N4   | 5.85  | 122.09      | 118.00   |
| 1   | AA    | 414  | A    | O4'-C1'-N9 | 5.85  | 112.88      | 108.20   |
| 3   | AV    | 63   | C    | N3-C4-C5   | -5.85 | 119.56      | 121.90   |
| 27  | B8    | 111  | A    | C5-C6-N6   | -5.85 | 119.02      | 123.70   |
| 27  | B8    | 209  | C    | N3-C4-N4   | 5.85  | 122.09      | 118.00   |
| 27  | B8    | 679  | C    | N3-C4-N4   | 5.85  | 122.09      | 118.00   |
| 27  | B8    | 951  | C    | N3-C4-N4   | 5.85  | 122.09      | 118.00   |
| 27  | B8    | 1502 | A    | C4-C5-C6   | 5.85  | 119.92      | 117.00   |
| 27  | B8    | 2268 | A    | C5-C6-N1   | -5.85 | 114.78      | 117.70   |
| 27  | B8    | 2781 | A    | C4-C5-C6   | 5.85  | 119.92      | 117.00   |
| 1   | AA    | 1352 | C    | N3-C4-N4   | 5.85  | 122.09      | 118.00   |
| 26  | B7    | 94   | A    | C5-C6-N6   | -5.85 | 119.02      | 123.70   |
| 27  | B8    | 1167 | C    | N3-C4-N4   | 5.85  | 122.09      | 118.00   |
| 27  | B8    | 2052 | A    | C4-C5-C6   | 5.85  | 119.92      | 117.00   |
| 27  | B8    | 2733 | A    | O4'-C1'-N9 | 5.85  | 112.88      | 108.20   |
| 27  | B8    | 2740 | A    | C4-C5-C6   | 5.85  | 119.92      | 117.00   |
| 27  | B8    | 2781 | A    | C5-C6-N6   | -5.85 | 119.02      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | B8    | 817  | C    | N3-C4-N4    | 5.84  | 122.09      | 118.00   |
| 27  | B8    | 825  | A    | C4-C5-C6    | 5.84  | 119.92      | 117.00   |
| 27  | B8    | 935  | C    | N3-C4-N4    | 5.84  | 122.09      | 118.00   |
| 27  | B8    | 1609 | A    | C5-C6-N6    | -5.84 | 119.02      | 123.70   |
| 27  | B8    | 1965 | C    | N3-C4-N4    | 5.84  | 122.09      | 118.00   |
| 27  | B8    | 2093 | G    | O4'-C1'-N9  | 5.84  | 112.88      | 108.20   |
| 27  | B8    | 2386 | A    | C4-C5-C6    | 5.84  | 119.92      | 117.00   |
| 1   | AA    | 959  | A    | C5-C6-N1    | -5.84 | 114.78      | 117.70   |
| 27  | B8    | 1764 | C    | N3-C4-N4    | 5.84  | 122.09      | 118.00   |
| 27  | B8    | 2376 | A    | C5-C6-N6    | -5.84 | 119.03      | 123.70   |
| 1   | AA    | 51   | A    | C5-C6-N1    | -5.84 | 114.78      | 117.70   |
| 1   | AA    | 100  | G    | O4'-C1'-N9  | 5.84  | 112.87      | 108.20   |
| 1   | AA    | 825  | A    | O4'-C1'-N9  | 5.84  | 112.87      | 108.20   |
| 26  | B7    | 47   | C    | N3-C4-C5    | -5.84 | 119.56      | 121.90   |
| 27  | B8    | 599  | A    | C4-C5-C6    | 5.84  | 119.92      | 117.00   |
| 27  | B8    | 2156 | G    | C5-C6-O6    | -5.84 | 125.09      | 128.60   |
| 27  | B8    | 2176 | A    | C4-C5-C6    | 5.84  | 119.92      | 117.00   |
| 1   | AA    | 61   | G    | O4'-C1'-N9  | 5.84  | 112.87      | 108.20   |
| 1   | AA    | 257  | G    | O4'-C1'-N9  | 5.84  | 112.87      | 108.20   |
| 1   | AA    | 452  | A    | O4'-C1'-N9  | 5.84  | 112.87      | 108.20   |
| 1   | AA    | 938  | A    | C4-C5-C6    | 5.84  | 119.92      | 117.00   |
| 1   | AA    | 1322 | C    | N3-C4-C5    | -5.84 | 119.56      | 121.90   |
| 27  | B8    | 394  | C    | N3-C4-N4    | 5.84  | 122.09      | 118.00   |
| 27  | B8    | 917  | A    | C5-C6-N1    | -5.84 | 114.78      | 117.70   |
| 27  | B8    | 1416 | G    | O4'-C1'-N9  | 5.84  | 112.87      | 108.20   |
| 27  | B8    | 1595 | C    | N3-C4-N4    | 5.84  | 122.09      | 118.00   |
| 1   | AA    | 32   | A    | C5-C6-N6    | -5.84 | 119.03      | 123.70   |
| 27  | B8    | 1142 | A    | C5'-C4'-O4' | 5.84  | 116.11      | 109.10   |
| 27  | B8    | 1272 | A    | O4'-C1'-N9  | 5.84  | 112.87      | 108.20   |
| 27  | B8    | 1906 | G    | O4'-C1'-N9  | 5.84  | 112.87      | 108.20   |
| 27  | B8    | 2313 | C    | N3-C4-N4    | 5.84  | 122.09      | 118.00   |
| 27  | B8    | 2691 | C    | N3-C4-N4    | 5.84  | 122.09      | 118.00   |
| 1   | AA    | 243  | A    | C4'-C3'-C2' | 5.84  | 108.44      | 102.60   |
| 1   | AA    | 1176 | A    | O4'-C1'-N9  | 5.84  | 112.87      | 108.20   |
| 27  | B8    | 203  | A    | C5-C6-N6    | -5.84 | 119.03      | 123.70   |
| 27  | B8    | 272  | A    | C4-C5-C6    | 5.84  | 119.92      | 117.00   |
| 27  | B8    | 539  | G    | C5-C6-O6    | -5.84 | 125.10      | 128.60   |
| 27  | B8    | 608  | A    | C5-C6-N6    | -5.84 | 119.03      | 123.70   |
| 27  | B8    | 764  | A    | C5-C6-N1    | -5.84 | 114.78      | 117.70   |
| 27  | B8    | 1585 | C    | N3-C4-N4    | 5.84  | 122.09      | 118.00   |
| 27  | B8    | 2060 | A    | C4-C5-C6    | 5.84  | 119.92      | 117.00   |
| 1   | AA    | 435  | A    | C5-C6-N6    | -5.83 | 119.03      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1461 | G    | O4'-C1'-N9 | 5.83  | 112.87      | 108.20   |
| 27  | B8    | 829  | A    | C4-C5-C6   | 5.83  | 119.92      | 117.00   |
| 27  | B8    | 1077 | A    | O4'-C1'-N9 | 5.83  | 112.87      | 108.20   |
| 27  | B8    | 1091 | G    | O4'-C1'-N9 | 5.83  | 112.87      | 108.20   |
| 27  | B8    | 1161 | C    | N3-C4-N4   | 5.83  | 122.08      | 118.00   |
| 27  | B8    | 2183 | A    | C5-C6-N6   | -5.83 | 119.03      | 123.70   |
| 27  | B8    | 2740 | A    | C5-C6-N6   | -5.83 | 119.03      | 123.70   |
| 1   | AA    | 246  | A    | C5-C6-N1   | -5.83 | 114.78      | 117.70   |
| 1   | AA    | 302  | G    | O4'-C1'-N9 | 5.83  | 112.87      | 108.20   |
| 1   | AA    | 497  | G    | O4'-C1'-N9 | 5.83  | 112.87      | 108.20   |
| 1   | AA    | 511  | C    | N3-C4-N4   | 5.83  | 122.08      | 118.00   |
| 1   | AA    | 999  | C    | N3-C4-N4   | 5.83  | 122.08      | 118.00   |
| 1   | AA    | 1155 | A    | C4-C5-C6   | 5.83  | 119.92      | 117.00   |
| 3   | AV    | 52   | A    | C4-C5-C6   | 5.83  | 119.92      | 117.00   |
| 27  | B8    | 146  | A    | C4-C5-C6   | 5.83  | 119.92      | 117.00   |
| 27  | B8    | 203  | A    | C4-C5-C6   | 5.83  | 119.92      | 117.00   |
| 27  | B8    | 949  | G    | O4'-C1'-N9 | 5.83  | 112.87      | 108.20   |
| 27  | B8    | 1079 | C    | N3-C4-N4   | 5.83  | 122.08      | 118.00   |
| 27  | B8    | 1338 | G    | O4'-C1'-N9 | 5.83  | 112.87      | 108.20   |
| 1   | AA    | 819  | A    | C4-C5-C6   | 5.83  | 119.92      | 117.00   |
| 1   | AA    | 1051 | C    | N3-C4-N4   | 5.83  | 122.08      | 118.00   |
| 1   | AA    | 1331 | G    | N3-C2-N2   | 5.83  | 123.98      | 119.90   |
| 3   | AV    | 6    | C    | N3-C4-N4   | 5.83  | 122.08      | 118.00   |
| 26  | B7    | 67   | G    | C5-C6-O6   | -5.83 | 125.10      | 128.60   |
| 27  | B8    | 300  | A    | C5-C6-N6   | -5.83 | 119.03      | 123.70   |
| 27  | B8    | 695  | G    | O4'-C1'-N9 | 5.83  | 112.87      | 108.20   |
| 27  | B8    | 1373 | A    | C5-C6-N1   | -5.83 | 114.78      | 117.70   |
| 27  | B8    | 1654 | A    | C5-C6-N6   | -5.83 | 119.03      | 123.70   |
| 27  | B8    | 1754 | A    | O4'-C1'-N9 | 5.83  | 112.86      | 108.20   |
| 27  | B8    | 2594 | C    | N3-C4-N4   | 5.83  | 122.08      | 118.00   |
| 27  | B8    | 2734 | A    | C4-C5-C6   | 5.83  | 119.92      | 117.00   |
| 1   | AA    | 634  | C    | N3-C4-N4   | 5.83  | 122.08      | 118.00   |
| 1   | AA    | 1107 | C    | N3-C4-N4   | 5.83  | 122.08      | 118.00   |
| 1   | AA    | 1456 | A    | O4'-C1'-N9 | 5.83  | 112.86      | 108.20   |
| 27  | B8    | 666  | A    | C4-C5-C6   | 5.83  | 119.92      | 117.00   |
| 1   | AA    | 522  | C    | N3-C4-N4   | 5.83  | 122.08      | 118.00   |
| 1   | AA    | 1184 | G    | O4'-C1'-N9 | 5.83  | 112.86      | 108.20   |
| 26  | B7    | 39   | A    | O4'-C1'-N9 | 5.83  | 112.86      | 108.20   |
| 27  | B8    | 320  | A    | C5-C6-N6   | -5.83 | 119.04      | 123.70   |
| 27  | B8    | 524  | G    | O4'-C1'-N9 | 5.83  | 112.86      | 108.20   |
| 27  | B8    | 733  | G    | O4'-C1'-N9 | 5.83  | 112.86      | 108.20   |
| 27  | B8    | 1129 | A    | C4-C5-C6   | 5.83  | 119.91      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1239 | G    | O4'-C1'-N9 | 5.83  | 112.86      | 108.20   |
| 27  | B8    | 1499 | C    | N3-C4-N4   | 5.83  | 122.08      | 118.00   |
| 27  | B8    | 1609 | A    | C4-C5-C6   | 5.83  | 119.91      | 117.00   |
| 27  | B8    | 345  | A    | C5-C6-N6   | -5.83 | 119.04      | 123.70   |
| 27  | B8    | 1241 | A    | C5-C6-N6   | -5.83 | 119.04      | 123.70   |
| 27  | B8    | 1986 | C    | N3-C4-N4   | 5.83  | 122.08      | 118.00   |
| 1   | AA    | 303  | A    | C5-C6-N1   | -5.83 | 114.79      | 117.70   |
| 1   | AA    | 487  | A    | C5-C6-N1   | -5.83 | 114.79      | 117.70   |
| 1   | AA    | 780  | A    | C4-C5-C6   | 5.83  | 119.91      | 117.00   |
| 1   | AA    | 781  | A    | C5-C6-N1   | -5.83 | 114.79      | 117.70   |
| 1   | AA    | 787  | A    | C5-C6-N6   | -5.83 | 119.04      | 123.70   |
| 3   | AV    | 12   | G    | O4'-C1'-N9 | 5.83  | 112.86      | 108.20   |
| 27  | B8    | 1009 | A    | C4-C5-C6   | 5.83  | 119.91      | 117.00   |
| 27  | B8    | 1040 | A    | O4'-C1'-N9 | 5.83  | 112.86      | 108.20   |
| 27  | B8    | 1359 | A    | C5-C6-N6   | -5.83 | 119.04      | 123.70   |
| 27  | B8    | 1504 | A    | C5-C6-N1   | -5.83 | 114.79      | 117.70   |
| 27  | B8    | 2091 | C    | N3-C4-N4   | 5.83  | 122.08      | 118.00   |
| 27  | B8    | 2592 | G    | O4'-C1'-N9 | 5.83  | 112.86      | 108.20   |
| 1   | AA    | 8    | A    | C5-C6-N6   | -5.82 | 119.04      | 123.70   |
| 27  | B8    | 655  | A    | C4-C5-C6   | 5.82  | 119.91      | 117.00   |
| 27  | B8    | 1012 | U    | O4'-C1'-N1 | 5.82  | 112.86      | 108.20   |
| 27  | B8    | 1257 | C    | N3-C4-N4   | 5.82  | 122.08      | 118.00   |
| 27  | B8    | 2295 | C    | N3-C4-N4   | 5.82  | 122.08      | 118.00   |
| 27  | B8    | 2642 | G    | O4'-C1'-N9 | 5.82  | 112.86      | 108.20   |
| 27  | B8    | 2671 | G    | O4'-C1'-N9 | 5.82  | 112.86      | 108.20   |
| 1   | AA    | 43   | C    | N3-C4-N4   | 5.82  | 122.08      | 118.00   |
| 1   | AA    | 994  | A    | C5-C6-N6   | -5.82 | 119.04      | 123.70   |
| 26  | B7    | 102  | G    | O4'-C1'-N9 | 5.82  | 112.86      | 108.20   |
| 27  | B8    | 1701 | A    | O4'-C1'-N9 | 5.82  | 112.86      | 108.20   |
| 27  | B8    | 2618 | G    | O4'-C1'-N9 | 5.82  | 112.86      | 108.20   |
| 1   | AA    | 349  | A    | C4-C5-C6   | 5.82  | 119.91      | 117.00   |
| 1   | AA    | 1117 | A    | C4-C5-C6   | 5.82  | 119.91      | 117.00   |
| 26  | B7    | 71   | C    | N3-C4-N4   | 5.82  | 122.07      | 118.00   |
| 27  | B8    | 632  | A    | C5-C6-N6   | -5.82 | 119.04      | 123.70   |
| 27  | B8    | 717  | C    | N3-C4-N4   | 5.82  | 122.08      | 118.00   |
| 27  | B8    | 1701 | A    | C4-C5-C6   | 5.82  | 119.91      | 117.00   |
| 27  | B8    | 2891 | U    | O4'-C1'-N1 | 5.82  | 112.86      | 108.20   |
| 1   | AA    | 1271 | A    | O4'-C1'-N9 | 5.82  | 112.86      | 108.20   |
| 27  | B8    | 634  | C    | N3-C4-N4   | 5.82  | 122.07      | 118.00   |
| 27  | B8    | 996  | A    | C5-C6-N6   | -5.82 | 119.05      | 123.70   |
| 27  | B8    | 1456 | G    | O4'-C1'-N9 | 5.82  | 112.86      | 108.20   |
| 1   | AA    | 338  | A    | C5-C6-N1   | -5.82 | 114.79      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 969  | A    | C4-C5-C6   | 5.82  | 119.91      | 117.00   |
| 27  | B8    | 796  | C    | N3-C4-N4   | 5.82  | 122.07      | 118.00   |
| 27  | B8    | 995  | C    | N3-C4-N4   | 5.82  | 122.07      | 118.00   |
| 27  | B8    | 1028 | A    | C4-C5-C6   | 5.82  | 119.91      | 117.00   |
| 27  | B8    | 1548 | A    | C5-C6-N6   | -5.82 | 119.05      | 123.70   |
| 27  | B8    | 1614 | A    | C4-C5-C6   | 5.82  | 119.91      | 117.00   |
| 27  | B8    | 1711 | A    | C4-C5-C6   | 5.82  | 119.91      | 117.00   |
| 27  | B8    | 1968 | G    | N3-C2-N2   | 5.82  | 123.97      | 119.90   |
| 27  | B8    | 2264 | C    | N3-C4-N4   | 5.82  | 122.07      | 118.00   |
| 27  | B8    | 2340 | A    | C4-C5-C6   | 5.82  | 119.91      | 117.00   |
| 27  | B8    | 2794 | C    | N3-C4-N4   | 5.82  | 122.07      | 118.00   |
| 48  | BT    | 99   | ALA  | N-CA-CB    | 5.82  | 118.24      | 110.10   |
| 1   | AA    | 665  | A    | C4-C5-C6   | 5.82  | 119.91      | 117.00   |
| 1   | AA    | 994  | A    | O4'-C1'-N9 | 5.82  | 112.85      | 108.20   |
| 27  | B8    | 91   | A    | C5-C6-N1   | -5.82 | 114.79      | 117.70   |
| 27  | B8    | 618  | G    | O4'-C1'-N9 | 5.82  | 112.85      | 108.20   |
| 27  | B8    | 1284 | A    | C4-C5-C6   | 5.82  | 119.91      | 117.00   |
| 27  | B8    | 1480 | C    | N3-C4-N4   | 5.82  | 122.07      | 118.00   |
| 27  | B8    | 1495 | A    | C5-C6-N6   | -5.82 | 119.05      | 123.70   |
| 27  | B8    | 2406 | A    | C5-C6-N6   | -5.82 | 119.05      | 123.70   |
| 1   | AA    | 816  | A    | C5-C6-N6   | -5.81 | 119.05      | 123.70   |
| 27  | B8    | 988  | A    | C5-C6-N1   | -5.81 | 114.79      | 117.70   |
| 27  | B8    | 1479 | G    | O4'-C1'-N9 | 5.81  | 112.85      | 108.20   |
| 1   | AA    | 149  | A    | C5-C6-N6   | -5.81 | 119.05      | 123.70   |
| 1   | AA    | 393  | A    | C5-C6-N1   | -5.81 | 114.79      | 117.70   |
| 1   | AA    | 1140 | C    | N3-C4-N4   | 5.81  | 122.07      | 118.00   |
| 1   | AA    | 1311 | A    | C4-C5-C6   | 5.81  | 119.91      | 117.00   |
| 27  | B8    | 1075 | C    | N3-C4-N4   | 5.81  | 122.07      | 118.00   |
| 27  | B8    | 1399 | C    | N3-C4-C5   | -5.81 | 119.58      | 121.90   |
| 27  | B8    | 2021 | C    | N3-C4-C5   | -5.81 | 119.58      | 121.90   |
| 27  | B8    | 2064 | C    | N3-C4-N4   | 5.81  | 122.07      | 118.00   |
| 27  | B8    | 2600 | A    | C4-C5-C6   | 5.81  | 119.91      | 117.00   |
| 27  | B8    | 2651 | C    | N3-C4-N4   | 5.81  | 122.07      | 118.00   |
| 27  | B8    | 2057 | G    | O4'-C1'-N9 | 5.81  | 112.85      | 108.20   |
| 1   | AA    | 124  | C    | N3-C4-N4   | 5.81  | 122.07      | 118.00   |
| 1   | AA    | 411  | A    | C4-C5-C6   | 5.81  | 119.90      | 117.00   |
| 1   | AA    | 1210 | C    | N3-C4-N4   | 5.81  | 122.07      | 118.00   |
| 26  | B7    | 93   | C    | N3-C4-N4   | 5.81  | 122.07      | 118.00   |
| 27  | B8    | 98   | G    | O4'-C1'-N9 | 5.81  | 112.85      | 108.20   |
| 27  | B8    | 1226 | A    | C5-C6-N1   | -5.81 | 114.80      | 117.70   |
| 27  | B8    | 1276 | A    | C4-C5-C6   | 5.81  | 119.91      | 117.00   |
| 27  | B8    | 1549 | A    | C4-C5-C6   | 5.81  | 119.91      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1591 | A    | C4-C5-C6   | 5.81  | 119.90      | 117.00   |
| 27  | B8    | 2063 | C    | N3-C4-N4   | 5.81  | 122.07      | 118.00   |
| 1   | AA    | 44   | A    | C5-C6-N1   | -5.81 | 114.80      | 117.70   |
| 1   | AA    | 76   | G    | P-O5'-C5'  | 5.81  | 130.19      | 120.90   |
| 1   | AA    | 1007 | U    | O4'-C1'-N1 | 5.81  | 112.85      | 108.20   |
| 1   | AA    | 1340 | A    | C5-C6-N1   | -5.81 | 114.80      | 117.70   |
| 27  | B8    | 180  | G    | O4'-C1'-N9 | 5.81  | 112.85      | 108.20   |
| 27  | B8    | 466  | A    | C5-C6-N1   | -5.81 | 114.80      | 117.70   |
| 27  | B8    | 1679 | A    | C4-C5-C6   | 5.81  | 119.90      | 117.00   |
| 27  | B8    | 2097 | A    | C4-C5-C6   | 5.81  | 119.90      | 117.00   |
| 27  | B8    | 2146 | C    | N3-C4-C5   | -5.81 | 119.58      | 121.90   |
| 1   | AA    | 1081 | A    | C4-C5-C6   | 5.81  | 119.90      | 117.00   |
| 1   | AA    | 1437 | A    | C5-C6-N1   | -5.81 | 114.80      | 117.70   |
| 27  | B8    | 608  | A    | O4'-C1'-N9 | 5.81  | 112.84      | 108.20   |
| 27  | B8    | 1260 | A    | C4-C5-C6   | 5.81  | 119.90      | 117.00   |
| 27  | B8    | 2051 | A    | C4-C5-C6   | 5.81  | 119.90      | 117.00   |
| 27  | B8    | 2903 | U    | C6-N1-C1'  | -5.81 | 113.07      | 121.20   |
| 1   | AA    | 576  | C    | N3-C4-N4   | 5.80  | 122.06      | 118.00   |
| 1   | AA    | 1519 | A    | C5-C6-N6   | -5.80 | 119.06      | 123.70   |
| 27  | B8    | 146  | A    | C5-C6-N6   | -5.80 | 119.06      | 123.70   |
| 27  | B8    | 742  | A    | O4'-C1'-N9 | 5.80  | 112.84      | 108.20   |
| 27  | B8    | 1145 | C    | N3-C4-N4   | 5.80  | 122.06      | 118.00   |
| 27  | B8    | 1433 | A    | C5-C6-N6   | -5.80 | 119.06      | 123.70   |
| 26  | B7    | 115  | A    | O4'-C1'-N9 | 5.80  | 112.84      | 108.20   |
| 27  | B8    | 69   | C    | N3-C4-C5   | -5.80 | 119.58      | 121.90   |
| 27  | B8    | 299  | A    | C5-C6-N6   | -5.80 | 119.06      | 123.70   |
| 27  | B8    | 1936 | A    | C5-C6-N1   | -5.80 | 114.80      | 117.70   |
| 1   | AA    | 353  | A    | C4-C5-C6   | 5.80  | 119.90      | 117.00   |
| 1   | AA    | 1350 | A    | C4-C5-C6   | 5.80  | 119.90      | 117.00   |
| 26  | B7    | 115  | A    | C4-C5-C6   | 5.80  | 119.90      | 117.00   |
| 27  | B8    | 144  | A    | O4'-C1'-N9 | 5.80  | 112.84      | 108.20   |
| 27  | B8    | 1048 | A    | C5-C6-N1   | -5.80 | 114.80      | 117.70   |
| 27  | B8    | 1293 | C    | N3-C4-N4   | 5.80  | 122.06      | 118.00   |
| 27  | B8    | 1819 | A    | C5-C6-N6   | -5.80 | 119.06      | 123.70   |
| 27  | B8    | 2158 | A    | C5-C6-N6   | -5.80 | 119.06      | 123.70   |
| 27  | B8    | 2737 | G    | O4'-C1'-N9 | 5.80  | 112.84      | 108.20   |
| 1   | AA    | 26   | A    | C5-C6-N6   | -5.80 | 119.06      | 123.70   |
| 1   | AA    | 44   | A    | C4-C5-C6   | 5.80  | 119.90      | 117.00   |
| 1   | AA    | 579  | A    | C5-C6-N6   | -5.80 | 119.06      | 123.70   |
| 1   | AA    | 749  | A    | C4-C5-C6   | 5.80  | 119.90      | 117.00   |
| 1   | AA    | 784  | A    | C5-C6-N6   | -5.80 | 119.06      | 123.70   |
| 27  | B8    | 845  | A    | C5-C6-N6   | -5.80 | 119.06      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1667 | G    | O4'-C1'-N9 | 5.80  | 112.84      | 108.20   |
| 27  | B8    | 1952 | A    | C4-C5-C6   | 5.80  | 119.90      | 117.00   |
| 27  | B8    | 2247 | A    | C4-C5-C6   | 5.80  | 119.90      | 117.00   |
| 1   | AA    | 342  | C    | N3-C4-N4   | 5.80  | 122.06      | 118.00   |
| 26  | B7    | 12   | C    | N3-C4-N4   | 5.80  | 122.06      | 118.00   |
| 27  | B8    | 940  | G    | O4'-C1'-N9 | 5.80  | 112.84      | 108.20   |
| 27  | B8    | 2020 | A    | C4-C5-C6   | 5.80  | 119.90      | 117.00   |
| 27  | B8    | 2070 | A    | C4-C5-C6   | 5.80  | 119.90      | 117.00   |
| 1   | AA    | 648  | A    | C4-C5-C6   | 5.80  | 119.90      | 117.00   |
| 1   | AA    | 649  | A    | C5-C6-N1   | -5.80 | 114.80      | 117.70   |
| 1   | AA    | 805  | C    | N3-C4-N4   | 5.80  | 122.06      | 118.00   |
| 1   | AA    | 1350 | A    | C5-C6-N6   | -5.80 | 119.06      | 123.70   |
| 27  | B8    | 466  | A    | O4'-C1'-N9 | 5.80  | 112.84      | 108.20   |
| 27  | B8    | 495  | G    | O4'-C1'-N9 | 5.80  | 112.84      | 108.20   |
| 27  | B8    | 638  | G    | O4'-C1'-N9 | 5.80  | 112.84      | 108.20   |
| 27  | B8    | 1616 | A    | C4-C5-C6   | 5.80  | 119.90      | 117.00   |
| 27  | B8    | 2126 | A    | C5-C6-N6   | -5.80 | 119.06      | 123.70   |
| 27  | B8    | 2332 | C    | N3-C4-N4   | 5.80  | 122.06      | 118.00   |
| 27  | B8    | 2700 | A    | C4-C5-C6   | 5.80  | 119.90      | 117.00   |
| 1   | AA    | 752  | G    | O4'-C1'-N9 | 5.79  | 112.84      | 108.20   |
| 1   | AA    | 1375 | A    | C5-C6-N1   | -5.79 | 114.80      | 117.70   |
| 27  | B8    | 226  | A    | O4'-C1'-N9 | 5.79  | 112.84      | 108.20   |
| 27  | B8    | 1949 | G    | O4'-C1'-N9 | 5.79  | 112.84      | 108.20   |
| 27  | B8    | 2328 | A    | C5-C6-N6   | -5.79 | 119.06      | 123.70   |
| 27  | B8    | 2418 | A    | C4-C5-C6   | 5.79  | 119.90      | 117.00   |
| 27  | B8    | 2806 | C    | N3-C4-N4   | 5.79  | 122.06      | 118.00   |
| 1   | AA    | 215  | C    | N3-C4-C5   | -5.79 | 119.58      | 121.90   |
| 1   | AA    | 535  | A    | C4-C5-C6   | 5.79  | 119.90      | 117.00   |
| 1   | AA    | 635  | A    | C4-C5-C6   | 5.79  | 119.90      | 117.00   |
| 1   | AA    | 935  | A    | C5-C6-N6   | -5.79 | 119.06      | 123.70   |
| 27  | B8    | 31   | C    | N3-C4-N4   | 5.79  | 122.06      | 118.00   |
| 27  | B8    | 197  | A    | C5-C6-N6   | -5.79 | 119.07      | 123.70   |
| 27  | B8    | 238  | C    | N3-C4-N4   | 5.79  | 122.06      | 118.00   |
| 27  | B8    | 256  | A    | C5-C6-N1   | -5.79 | 114.80      | 117.70   |
| 27  | B8    | 621  | A    | C4-C5-C6   | 5.79  | 119.90      | 117.00   |
| 27  | B8    | 928  | A    | C4-C5-C6   | 5.79  | 119.90      | 117.00   |
| 27  | B8    | 1150 | C    | N3-C4-C5   | -5.79 | 119.58      | 121.90   |
| 27  | B8    | 1444 | G    | O4'-C1'-N9 | 5.79  | 112.83      | 108.20   |
| 27  | B8    | 1634 | A    | C5-C6-N6   | -5.79 | 119.06      | 123.70   |
| 27  | B8    | 1772 | A    | C4-C5-C6   | 5.79  | 119.90      | 117.00   |
| 27  | B8    | 1903 | G    | O4'-C1'-N9 | 5.79  | 112.83      | 108.20   |
| 27  | B8    | 2462 | C    | N3-C4-N4   | 5.79  | 122.06      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2626 | C    | N3-C4-N4   | 5.79  | 122.06      | 118.00   |
| 27  | B8    | 2628 | C    | N3-C4-N4   | 5.79  | 122.06      | 118.00   |
| 1   | AA    | 546  | A    | C5-C6-N6   | -5.79 | 119.07      | 123.70   |
| 1   | AA    | 825  | A    | C4-C5-C6   | 5.79  | 119.90      | 117.00   |
| 1   | AA    | 1229 | A    | C5-C6-N1   | -5.79 | 114.80      | 117.70   |
| 27  | B8    | 590  | A    | C4-C5-C6   | 5.79  | 119.90      | 117.00   |
| 27  | B8    | 1537 | G    | P-O3'-C3'  | 5.79  | 126.65      | 119.70   |
| 27  | B8    | 1591 | A    | C5-C6-N1   | -5.79 | 114.80      | 117.70   |
| 27  | B8    | 2142 | A    | C4-C5-C6   | 5.79  | 119.90      | 117.00   |
| 27  | B8    | 2456 | C    | N3-C4-N4   | 5.79  | 122.05      | 118.00   |
| 1   | AA    | 33   | A    | O4'-C1'-N9 | 5.79  | 112.83      | 108.20   |
| 1   | AA    | 802  | A    | C4-C5-C6   | 5.79  | 119.89      | 117.00   |
| 26  | B7    | 98   | G    | O4'-C1'-N9 | 5.79  | 112.83      | 108.20   |
| 27  | B8    | 706  | A    | C5-C6-N6   | -5.79 | 119.07      | 123.70   |
| 1   | AA    | 564  | C    | N3-C4-N4   | 5.79  | 122.05      | 118.00   |
| 1   | AA    | 578  | C    | N3-C4-N4   | 5.79  | 122.05      | 118.00   |
| 1   | AA    | 747  | A    | C4-C5-C6   | 5.79  | 119.89      | 117.00   |
| 1   | AA    | 1271 | A    | C4-C5-C6   | 5.79  | 119.89      | 117.00   |
| 1   | AA    | 1280 | A    | C5-C6-N6   | -5.79 | 119.07      | 123.70   |
| 27  | B8    | 473  | G    | O4'-C1'-N9 | 5.79  | 112.83      | 108.20   |
| 27  | B8    | 1172 | C    | N3-C4-N4   | 5.79  | 122.05      | 118.00   |
| 27  | B8    | 1197 | G    | O4'-C1'-N9 | 5.79  | 112.83      | 108.20   |
| 27  | B8    | 1236 | G    | N3-C2-N2   | 5.79  | 123.95      | 119.90   |
| 27  | B8    | 2273 | A    | O4'-C1'-N9 | 5.79  | 112.83      | 108.20   |
| 27  | B8    | 2388 | A    | C5-C6-N1   | -5.79 | 114.81      | 117.70   |
| 1   | AA    | 1161 | C    | N3-C4-N4   | 5.79  | 122.05      | 118.00   |
| 27  | B8    | 64   | A    | C4-C5-C6   | 5.79  | 119.89      | 117.00   |
| 27  | B8    | 2761 | A    | C5-C6-N1   | -5.79 | 114.81      | 117.70   |
| 1   | AA    | 569  | C    | N3-C4-N4   | 5.79  | 122.05      | 118.00   |
| 1   | AA    | 1141 | C    | N3-C4-N4   | 5.79  | 122.05      | 118.00   |
| 26  | B7    | 46   | A    | C4-C5-C6   | 5.79  | 119.89      | 117.00   |
| 1   | AA    | 959  | A    | C4-C5-C6   | 5.78  | 119.89      | 117.00   |
| 1   | AA    | 1373 | G    | O4'-C1'-N9 | 5.78  | 112.83      | 108.20   |
| 27  | B8    | 2296 | U    | O4'-C1'-N1 | 5.78  | 112.83      | 108.20   |
| 27  | B8    | 2482 | A    | C5-C6-N1   | -5.78 | 114.81      | 117.70   |
| 1   | AA    | 1249 | C    | N3-C4-N4   | 5.78  | 122.05      | 118.00   |
| 1   | AA    | 1332 | A    | C4-C5-C6   | 5.78  | 119.89      | 117.00   |
| 27  | B8    | 1276 | A    | O4'-C1'-N9 | 5.78  | 112.83      | 108.20   |
| 27  | B8    | 1367 | A    | C4-C5-C6   | 5.78  | 119.89      | 117.00   |
| 1   | AA    | 600  | A    | C5-C6-N6   | -5.78 | 119.08      | 123.70   |
| 27  | B8    | 462  | C    | N3-C4-N4   | 5.78  | 122.05      | 118.00   |
| 27  | B8    | 590  | A    | C5-C6-N6   | -5.78 | 119.08      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 869  | G    | O4'-C1'-N9 | 5.78  | 112.82      | 108.20   |
| 27  | B8    | 1111 | A    | C4-C5-C6   | 5.78  | 119.89      | 117.00   |
| 27  | B8    | 1134 | A    | C5-C6-N6   | -5.78 | 119.08      | 123.70   |
| 27  | B8    | 1169 | A    | C4-C5-C6   | 5.78  | 119.89      | 117.00   |
| 27  | B8    | 1759 | A    | C4-C5-C6   | 5.78  | 119.89      | 117.00   |
| 27  | B8    | 2107 | G    | O4'-C1'-N9 | 5.78  | 112.82      | 108.20   |
| 27  | B8    | 1028 | A    | O4'-C1'-N9 | 5.78  | 112.82      | 108.20   |
| 27  | B8    | 1503 | A    | C4-C5-C6   | 5.78  | 119.89      | 117.00   |
| 1   | AA    | 325  | A    | O4'-C1'-N9 | 5.78  | 112.82      | 108.20   |
| 1   | AA    | 1275 | A    | O4'-C1'-N9 | 5.78  | 112.82      | 108.20   |
| 1   | AA    | 1507 | A    | C5-C6-N6   | -5.78 | 119.08      | 123.70   |
| 26  | B7    | 90   | C    | N3-C4-N4   | 5.78  | 122.04      | 118.00   |
| 27  | B8    | 689  | A    | C5-C6-N1   | -5.78 | 114.81      | 117.70   |
| 27  | B8    | 844  | A    | C5-C6-N1   | -5.78 | 114.81      | 117.70   |
| 27  | B8    | 982  | C    | N3-C4-N4   | 5.78  | 122.04      | 118.00   |
| 27  | B8    | 1728 | C    | N3-C4-N4   | 5.78  | 122.04      | 118.00   |
| 27  | B8    | 1790 | C    | N3-C4-N4   | 5.78  | 122.05      | 118.00   |
| 27  | B8    | 2088 | A    | C5-C6-N6   | -5.78 | 119.08      | 123.70   |
| 27  | B8    | 2328 | A    | O4'-C1'-N9 | 5.78  | 112.82      | 108.20   |
| 1   | AA    | 50   | A    | C4-C5-C6   | 5.78  | 119.89      | 117.00   |
| 1   | AA    | 407  | U    | O4'-C1'-N1 | 5.78  | 112.82      | 108.20   |
| 1   | AA    | 608  | A    | C4-C5-C6   | 5.78  | 119.89      | 117.00   |
| 1   | AA    | 1106 | G    | O4'-C1'-N9 | 5.78  | 112.82      | 108.20   |
| 1   | AA    | 1128 | C    | N3-C4-N4   | 5.78  | 122.04      | 118.00   |
| 1   | AA    | 1384 | C    | N3-C4-N4   | 5.78  | 122.04      | 118.00   |
| 27  | B8    | 76   | C    | N3-C4-N4   | 5.78  | 122.04      | 118.00   |
| 27  | B8    | 217  | A    | O4'-C1'-N9 | 5.78  | 112.82      | 108.20   |
| 27  | B8    | 783  | A    | C5-C6-N6   | -5.78 | 119.08      | 123.70   |
| 27  | B8    | 948  | C    | N3-C4-N4   | 5.78  | 122.04      | 118.00   |
| 27  | B8    | 1143 | A    | C4-C5-C6   | 5.78  | 119.89      | 117.00   |
| 27  | B8    | 1230 | A    | C4-C5-C6   | 5.78  | 119.89      | 117.00   |
| 27  | B8    | 1383 | A    | C5-C6-N6   | -5.78 | 119.08      | 123.70   |
| 27  | B8    | 2058 | A    | C4-C5-C6   | 5.78  | 119.89      | 117.00   |
| 27  | B8    | 2452 | C    | N3-C4-N4   | 5.78  | 122.04      | 118.00   |
| 27  | B8    | 2727 | A    | C5-C6-N1   | -5.78 | 114.81      | 117.70   |
| 1   | AA    | 1274 | A    | C5-C6-N6   | -5.77 | 119.08      | 123.70   |
| 27  | B8    | 2119 | A    | C5-C6-N1   | -5.77 | 114.81      | 117.70   |
| 1   | AA    | 210  | C    | N3-C4-N4   | 5.77  | 122.04      | 118.00   |
| 1   | AA    | 335  | C    | N3-C4-N4   | 5.77  | 122.04      | 118.00   |
| 1   | AA    | 460  | A    | C4-C5-C6   | 5.77  | 119.89      | 117.00   |
| 1   | AA    | 1171 | A    | C5-C6-N6   | -5.77 | 119.08      | 123.70   |
| 3   | AV    | 5    | A    | C5-C6-N6   | -5.77 | 119.08      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 71   | A    | C5-C6-N1   | -5.77 | 114.81      | 117.70   |
| 27  | B8    | 532  | A    | C4-C5-C6   | 5.77  | 119.89      | 117.00   |
| 27  | B8    | 1670 | C    | N3-C4-C5   | -5.77 | 119.59      | 121.90   |
| 27  | B8    | 66   | C    | N3-C4-C5   | -5.77 | 119.59      | 121.90   |
| 27  | B8    | 352  | A    | C5-C6-N6   | -5.77 | 119.08      | 123.70   |
| 27  | B8    | 582  | A    | O4'-C1'-N9 | 5.77  | 112.82      | 108.20   |
| 27  | B8    | 783  | A    | C4-C5-C6   | 5.77  | 119.89      | 117.00   |
| 27  | B8    | 1437 | C    | N3-C4-N4   | 5.77  | 122.04      | 118.00   |
| 1   | AA    | 496  | A    | O4'-C1'-N9 | 5.77  | 112.81      | 108.20   |
| 1   | AA    | 573  | A    | C5-C6-N6   | -5.77 | 119.08      | 123.70   |
| 1   | AA    | 1113 | C    | N3-C4-N4   | 5.77  | 122.04      | 118.00   |
| 1   | AA    | 1277 | C    | N3-C4-N4   | 5.77  | 122.04      | 118.00   |
| 27  | B8    | 269  | C    | N3-C4-N4   | 5.77  | 122.04      | 118.00   |
| 27  | B8    | 721  | A    | C4-C5-C6   | 5.77  | 119.89      | 117.00   |
| 27  | B8    | 1927 | A    | C5-C6-N6   | -5.77 | 119.08      | 123.70   |
| 27  | B8    | 1933 | G    | O4'-C1'-N9 | 5.77  | 112.81      | 108.20   |
| 27  | B8    | 2325 | G    | O4'-C1'-N9 | 5.77  | 112.81      | 108.20   |
| 27  | B8    | 2422 | C    | N3-C4-N4   | 5.77  | 122.04      | 118.00   |
| 27  | B8    | 2542 | A    | C4-C5-C6   | 5.77  | 119.89      | 117.00   |
| 27  | B8    | 2657 | A    | C4-C5-C6   | 5.77  | 119.89      | 117.00   |
| 1   | AA    | 974  | A    | C5-C6-N1   | -5.77 | 114.82      | 117.70   |
| 1   | AA    | 1343 | G    | O4'-C1'-N9 | 5.77  | 112.81      | 108.20   |
| 27  | B8    | 75   | G    | O4'-C1'-N9 | 5.77  | 112.81      | 108.20   |
| 27  | B8    | 604  | G    | O4'-C1'-N9 | 5.77  | 112.81      | 108.20   |
| 27  | B8    | 1077 | A    | C5-C6-N6   | -5.77 | 119.09      | 123.70   |
| 27  | B8    | 1585 | C    | N3-C4-C5   | -5.77 | 119.59      | 121.90   |
| 27  | B8    | 2365 | G    | O4'-C1'-N9 | 5.77  | 112.81      | 108.20   |
| 27  | B8    | 2521 | C    | N3-C4-N4   | 5.77  | 122.04      | 118.00   |
| 27  | B8    | 2726 | A    | O4'-C1'-N9 | 5.77  | 112.81      | 108.20   |
| 1   | AA    | 228  | A    | O4'-C1'-N9 | 5.77  | 112.81      | 108.20   |
| 26  | B7    | 50   | A    | C4-C5-C6   | 5.77  | 119.88      | 117.00   |
| 27  | B8    | 475  | C    | N3-C4-N4   | 5.77  | 122.04      | 118.00   |
| 27  | B8    | 1040 | A    | C4-C5-C6   | 5.77  | 119.88      | 117.00   |
| 27  | B8    | 1211 | C    | N3-C4-C5   | -5.77 | 119.59      | 121.90   |
| 27  | B8    | 1246 | A    | C4-C5-C6   | 5.77  | 119.88      | 117.00   |
| 27  | B8    | 2868 | A    | O4'-C1'-N9 | 5.77  | 112.81      | 108.20   |
| 1   | AA    | 728  | A    | C5-C6-N6   | -5.76 | 119.09      | 123.70   |
| 1   | AA    | 1214 | C    | N3-C4-N4   | 5.76  | 122.03      | 118.00   |
| 1   | AA    | 1507 | A    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 27  | B8    | 233  | A    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 27  | B8    | 1749 | A    | C4-C5-C6   | 5.76  | 119.88      | 117.00   |
| 27  | B8    | 2179 | C    | N3-C4-N4   | 5.76  | 122.04      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2850 | A    | C5-C6-N6   | -5.76 | 119.09      | 123.70   |
| 1   | AA    | 1008 | U    | O4'-C1'-N1 | 5.76  | 112.81      | 108.20   |
| 27  | B8    | 155  | A    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 27  | B8    | 362  | A    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 27  | B8    | 539  | G    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 27  | B8    | 749  | A    | C4-C5-C6   | 5.76  | 119.88      | 117.00   |
| 27  | B8    | 1413 | A    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 27  | B8    | 1837 | C    | N3-C4-N4   | 5.76  | 122.03      | 118.00   |
| 27  | B8    | 2200 | C    | N3-C4-N4   | 5.76  | 122.03      | 118.00   |
| 27  | B8    | 2556 | C    | N3-C4-N4   | 5.76  | 122.03      | 118.00   |
| 27  | B8    | 2741 | A    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 27  | B8    | 2748 | A    | C5-C6-N1   | -5.76 | 114.82      | 117.70   |
| 1   | AA    | 572  | A    | C5-C6-N1   | -5.76 | 114.82      | 117.70   |
| 1   | AA    | 699  | C    | N3-C4-N4   | 5.76  | 122.03      | 118.00   |
| 1   | AA    | 792  | A    | C4-C5-C6   | 5.76  | 119.88      | 117.00   |
| 1   | AA    | 1041 | G    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 1   | AA    | 1238 | A    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 1   | AA    | 1323 | G    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 27  | B8    | 223  | A    | C4-C5-C6   | 5.76  | 119.88      | 117.00   |
| 27  | B8    | 553  | G    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 27  | B8    | 782  | A    | C5-C6-N1   | -5.76 | 114.82      | 117.70   |
| 27  | B8    | 2309 | A    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 27  | B8    | 2311 | A    | C5-C6-N6   | -5.76 | 119.09      | 123.70   |
| 1   | AA    | 706  | A    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 1   | AA    | 760  | G    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 27  | B8    | 227  | A    | C5-C6-N6   | -5.76 | 119.09      | 123.70   |
| 27  | B8    | 1525 | A    | C5-C6-N1   | -5.76 | 114.82      | 117.70   |
| 1   | AA    | 431  | A    | C4-C5-C6   | 5.76  | 119.88      | 117.00   |
| 1   | AA    | 508  | U    | O4'-C1'-N1 | 5.76  | 112.81      | 108.20   |
| 1   | AA    | 679  | C    | N3-C4-N4   | 5.76  | 122.03      | 118.00   |
| 1   | AA    | 1201 | A    | C5-C6-N6   | -5.76 | 119.09      | 123.70   |
| 1   | AA    | 1366 | C    | N3-C4-N4   | 5.76  | 122.03      | 118.00   |
| 27  | B8    | 142  | A    | C4-C5-C6   | 5.76  | 119.88      | 117.00   |
| 27  | B8    | 176  | A    | C4-C5-C6   | 5.76  | 119.88      | 117.00   |
| 27  | B8    | 515  | A    | C4-C5-C6   | 5.76  | 119.88      | 117.00   |
| 27  | B8    | 1162 | G    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 27  | B8    | 1353 | A    | C5-C6-N1   | -5.76 | 114.82      | 117.70   |
| 27  | B8    | 1472 | C    | N3-C4-N4   | 5.76  | 122.03      | 118.00   |
| 27  | B8    | 1678 | A    | C5-C6-N6   | -5.76 | 119.09      | 123.70   |
| 27  | B8    | 1879 | C    | N3-C4-N4   | 5.76  | 122.03      | 118.00   |
| 27  | B8    | 2116 | G    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 27  | B8    | 2317 | A    | C4-C5-C6   | 5.76  | 119.88      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2808 | G    | O4'-C1'-N9 | 5.76  | 112.81      | 108.20   |
| 26  | B7    | 11   | C    | N3-C4-C5   | -5.75 | 119.60      | 121.90   |
| 27  | B8    | 10   | A    | C5-C6-N1   | -5.75 | 114.82      | 117.70   |
| 27  | B8    | 944  | C    | N3-C4-N4   | 5.75  | 122.03      | 118.00   |
| 27  | B8    | 1794 | A    | C5-C6-N6   | -5.75 | 119.10      | 123.70   |
| 27  | B8    | 1913 | A    | C5-C6-N6   | -5.75 | 119.10      | 123.70   |
| 1   | AA    | 783  | C    | N3-C4-N4   | 5.75  | 122.03      | 118.00   |
| 27  | B8    | 742  | A    | C4-C5-C6   | 5.75  | 119.88      | 117.00   |
| 27  | B8    | 1887 | C    | N3-C4-N4   | 5.75  | 122.03      | 118.00   |
| 27  | B8    | 2451 | A    | C5-C6-N6   | -5.75 | 119.10      | 123.70   |
| 1   | AA    | 719  | C    | N3-C4-N4   | 5.75  | 122.03      | 118.00   |
| 1   | AA    | 1367 | C    | N3-C4-N4   | 5.75  | 122.03      | 118.00   |
| 27  | B8    | 423  | A    | O4'-C1'-N9 | 5.75  | 112.80      | 108.20   |
| 27  | B8    | 557  | C    | N3-C4-C5   | -5.75 | 119.60      | 121.90   |
| 27  | B8    | 1445 | G    | O4'-C1'-N9 | 5.75  | 112.80      | 108.20   |
| 27  | B8    | 1637 | A    | O4'-C1'-N9 | 5.75  | 112.80      | 108.20   |
| 27  | B8    | 2682 | A    | C5-C6-N6   | -5.75 | 119.10      | 123.70   |
| 27  | B8    | 2809 | A    | C5-C6-N6   | -5.75 | 119.10      | 123.70   |
| 1   | AA    | 513  | C    | N3-C4-N4   | 5.75  | 122.03      | 118.00   |
| 1   | AA    | 1476 | A    | O4'-C1'-N9 | 5.75  | 112.80      | 108.20   |
| 27  | B8    | 601  | C    | N3-C4-N4   | 5.75  | 122.03      | 118.00   |
| 27  | B8    | 2641 | G    | O4'-C1'-N9 | 5.75  | 112.80      | 108.20   |
| 1   | AA    | 274  | A    | C4-C5-C6   | 5.75  | 119.88      | 117.00   |
| 27  | B8    | 223  | A    | C5-C6-N6   | -5.75 | 119.10      | 123.70   |
| 27  | B8    | 376  | G    | O4'-C1'-N9 | 5.75  | 112.80      | 108.20   |
| 27  | B8    | 693  | A    | C4-C5-C6   | 5.75  | 119.87      | 117.00   |
| 27  | B8    | 1007 | C    | N3-C4-N4   | 5.75  | 122.02      | 118.00   |
| 27  | B8    | 1569 | A    | C4-C5-C6   | 5.75  | 119.88      | 117.00   |
| 27  | B8    | 262  | A    | C5-C6-N6   | -5.75 | 119.10      | 123.70   |
| 27  | B8    | 294  | A    | C4-C5-C6   | 5.75  | 119.87      | 117.00   |
| 27  | B8    | 965  | C    | N3-C4-N4   | 5.75  | 122.02      | 118.00   |
| 27  | B8    | 1127 | A    | O4'-C1'-N9 | 5.75  | 112.80      | 108.20   |
| 27  | B8    | 1528 | A    | C5-C6-N1   | -5.75 | 114.83      | 117.70   |
| 27  | B8    | 1590 | A    | C5-C6-N1   | -5.75 | 114.83      | 117.70   |
| 27  | B8    | 1821 | A    | C5-C6-N1   | -5.75 | 114.83      | 117.70   |
| 27  | B8    | 2893 | A    | C5-C6-N1   | -5.75 | 114.83      | 117.70   |
| 28  | BA    | 340  | ARG  | N-CA-CB    | 5.75  | 120.94      | 110.60   |
| 1   | AA    | 919  | A    | O4'-C1'-N9 | 5.75  | 112.80      | 108.20   |
| 27  | B8    | 145  | C    | N3-C4-N4   | 5.75  | 122.02      | 118.00   |
| 27  | B8    | 430  | A    | C4-C5-C6   | 5.75  | 119.87      | 117.00   |
| 1   | AA    | 387  | U    | O4'-C1'-N1 | 5.74  | 112.80      | 108.20   |
| 1   | AA    | 478  | A    | C4-C5-C6   | 5.74  | 119.87      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 499  | A    | C5-C6-N6   | -5.74 | 119.11      | 123.70   |
| 1   | AA    | 902  | G    | O4'-C1'-N9 | 5.74  | 112.79      | 108.20   |
| 1   | AA    | 1181 | G    | O4'-C1'-N9 | 5.74  | 112.80      | 108.20   |
| 1   | AA    | 1293 | C    | N3-C4-N4   | 5.74  | 122.02      | 118.00   |
| 1   | AA    | 1399 | C    | N3-C4-N4   | 5.74  | 122.02      | 118.00   |
| 27  | B8    | 905  | A    | C5-C6-N6   | -5.74 | 119.10      | 123.70   |
| 27  | B8    | 1211 | C    | C6-N1-C1'  | -5.74 | 113.91      | 120.80   |
| 27  | B8    | 1600 | C    | N3-C4-N4   | 5.74  | 122.02      | 118.00   |
| 27  | B8    | 1661 | G    | O4'-C1'-N9 | 5.74  | 112.79      | 108.20   |
| 27  | B8    | 1804 | C    | N3-C4-N4   | 5.74  | 122.02      | 118.00   |
| 27  | B8    | 1821 | A    | C4-C5-C6   | 5.74  | 119.87      | 117.00   |
| 27  | B8    | 2184 | A    | O4'-C1'-N9 | 5.74  | 112.80      | 108.20   |
| 27  | B8    | 2417 | C    | N3-C4-N4   | 5.74  | 122.02      | 118.00   |
| 27  | B8    | 2443 | C    | N3-C4-N4   | 5.74  | 122.02      | 118.00   |
| 27  | B8    | 2530 | A    | C4-C5-C6   | 5.74  | 119.87      | 117.00   |
| 27  | B8    | 2733 | A    | C5-C6-N1   | -5.74 | 114.83      | 117.70   |
| 1   | AA    | 611  | C    | N3-C4-N4   | 5.74  | 122.02      | 118.00   |
| 27  | B8    | 1637 | A    | C4-C5-C6   | 5.74  | 119.87      | 117.00   |
| 27  | B8    | 2792 | A    | C5-C6-N6   | -5.74 | 119.11      | 123.70   |
| 1   | AA    | 478  | A    | C5-C6-N1   | -5.74 | 114.83      | 117.70   |
| 1   | AA    | 663  | A    | C4-C5-C6   | 5.74  | 119.87      | 117.00   |
| 1   | AA    | 790  | A    | C5-C6-N6   | -5.74 | 119.11      | 123.70   |
| 1   | AA    | 807  | A    | O4'-C1'-N9 | 5.74  | 112.79      | 108.20   |
| 1   | AA    | 907  | A    | C5-C6-N6   | -5.74 | 119.11      | 123.70   |
| 1   | AA    | 1227 | A    | C5-C6-N6   | -5.74 | 119.11      | 123.70   |
| 1   | AA    | 1433 | A    | C4-C5-C6   | 5.74  | 119.87      | 117.00   |
| 1   | AA    | 1454 | G    | P-O5'-C5'  | 5.74  | 130.09      | 120.90   |
| 27  | B8    | 933  | A    | C4-C5-C6   | 5.74  | 119.87      | 117.00   |
| 27  | B8    | 1054 | A    | C5-C6-N6   | -5.74 | 119.11      | 123.70   |
| 27  | B8    | 2463 | C    | N3-C4-C5   | -5.74 | 119.60      | 121.90   |
| 27  | B8    | 2727 | A    | C5-C6-N6   | -5.74 | 119.11      | 123.70   |
| 28  | BA    | 217  | PHE  | CB-CG-CD1  | 5.74  | 124.82      | 120.80   |
| 1   | AA    | 510  | A    | C5-C6-N1   | -5.74 | 114.83      | 117.70   |
| 1   | AA    | 583  | A    | C4-C5-C6   | 5.74  | 119.87      | 117.00   |
| 1   | AA    | 669  | G    | O4'-C1'-N9 | 5.74  | 112.79      | 108.20   |
| 1   | AA    | 691  | G    | N3-C2-N2   | 5.74  | 123.92      | 119.90   |
| 1   | AA    | 706  | A    | C5-C6-N6   | -5.74 | 119.11      | 123.70   |
| 1   | AA    | 815  | A    | C5-C6-N6   | -5.74 | 119.11      | 123.70   |
| 1   | AA    | 1004 | A    | C5-C6-N1   | -5.74 | 114.83      | 117.70   |
| 3   | AV    | 67   | C    | N3-C4-N4   | 5.74  | 122.02      | 118.00   |
| 26  | B7    | 50   | A    | C5-C6-N6   | -5.74 | 119.11      | 123.70   |
| 27  | B8    | 1398 | C    | N3-C4-N4   | 5.74  | 122.02      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1974 | C    | N3-C4-N4   | 5.74  | 122.02      | 118.00   |
| 27  | B8    | 2136 | G    | O4'-C1'-N9 | 5.74  | 112.79      | 108.20   |
| 1   | AA    | 526  | C    | N3-C4-N4   | 5.74  | 122.02      | 118.00   |
| 1   | AA    | 753  | A    | C5-C6-N1   | -5.74 | 114.83      | 117.70   |
| 1   | AA    | 1152 | A    | C5-C6-N6   | -5.74 | 119.11      | 123.70   |
| 1   | AA    | 1243 | C    | N3-C4-C5   | -5.74 | 119.61      | 121.90   |
| 27  | B8    | 79   | C    | N3-C4-C5   | -5.74 | 119.61      | 121.90   |
| 27  | B8    | 1030 | C    | N3-C4-N4   | 5.74  | 122.02      | 118.00   |
| 27  | B8    | 1806 | C    | N3-C4-N4   | 5.74  | 122.02      | 118.00   |
| 27  | B8    | 2857 | G    | N3-C2-N2   | 5.74  | 123.92      | 119.90   |
| 35  | BG    | 108  | PHE  | CB-CG-CD2  | 5.74  | 124.82      | 120.80   |
| 1   | AA    | 1221 | G    | O4'-C1'-N9 | 5.74  | 112.79      | 108.20   |
| 3   | AV    | 63   | C    | N3-C4-N4   | 5.74  | 122.02      | 118.00   |
| 26  | B7    | 104  | A    | C4-C5-C6   | 5.74  | 119.87      | 117.00   |
| 27  | B8    | 44   | A    | O4'-C1'-N9 | 5.74  | 112.79      | 108.20   |
| 27  | B8    | 282  | A    | C4-C5-C6   | 5.74  | 119.87      | 117.00   |
| 27  | B8    | 1914 | C    | N3-C4-N4   | 5.74  | 122.01      | 118.00   |
| 27  | B8    | 1987 | A    | C5-C6-N1   | -5.74 | 114.83      | 117.70   |
| 27  | B8    | 2882 | A    | O4'-C1'-N9 | 5.74  | 112.79      | 108.20   |
| 1   | AA    | 635  | A    | C5-C6-N6   | -5.73 | 119.11      | 123.70   |
| 27  | B8    | 2003 | A    | C5-C6-N6   | -5.73 | 119.11      | 123.70   |
| 27  | B8    | 2234 | G    | O4'-C1'-N9 | 5.73  | 112.79      | 108.20   |
| 27  | B8    | 2453 | A    | C5-C6-N1   | -5.73 | 114.83      | 117.70   |
| 27  | B8    | 2453 | A    | O4'-C1'-N9 | 5.73  | 112.79      | 108.20   |
| 1   | AA    | 931  | C    | N3-C4-N4   | 5.73  | 122.01      | 118.00   |
| 1   | AA    | 1071 | C    | N3-C4-C5   | -5.73 | 119.61      | 121.90   |
| 27  | B8    | 368  | A    | C5-C6-N6   | -5.73 | 119.11      | 123.70   |
| 27  | B8    | 654  | A    | C4-C5-C6   | 5.73  | 119.87      | 117.00   |
| 27  | B8    | 2603 | G    | O4'-C1'-N9 | 5.73  | 112.79      | 108.20   |
| 1   | AA    | 139  | A    | C4-C5-C6   | 5.73  | 119.86      | 117.00   |
| 1   | AA    | 143  | A    | C5-C6-N1   | -5.73 | 114.83      | 117.70   |
| 1   | AA    | 415  | A    | C5-C6-N1   | -5.73 | 114.83      | 117.70   |
| 1   | AA    | 554  | A    | C4-C5-C6   | 5.73  | 119.87      | 117.00   |
| 1   | AA    | 557  | G    | O4'-C1'-N9 | 5.73  | 112.78      | 108.20   |
| 1   | AA    | 1431 | A    | C5-C6-N6   | -5.73 | 119.11      | 123.70   |
| 1   | AA    | 1446 | A    | C5-C6-N6   | -5.73 | 119.12      | 123.70   |
| 27  | B8    | 402  | A    | C5-C6-N1   | -5.73 | 114.83      | 117.70   |
| 27  | B8    | 1420 | A    | C5-C6-N6   | -5.73 | 119.11      | 123.70   |
| 27  | B8    | 2248 | C    | N3-C4-N4   | 5.73  | 122.01      | 118.00   |
| 27  | B8    | 2619 | C    | N3-C4-N4   | 5.73  | 122.01      | 118.00   |
| 27  | B8    | 2883 | A    | C4-C5-C6   | 5.73  | 119.86      | 117.00   |
| 1   | AA    | 1513 | A    | O4'-C1'-N9 | 5.73  | 112.78      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1154 | G    | N3-C2-N2   | 5.73  | 123.91      | 119.90   |
| 27  | B8    | 1794 | A    | C5-C6-N1   | -5.73 | 114.84      | 117.70   |
| 1   | AA    | 523  | A    | C4-C5-C6   | 5.73  | 119.86      | 117.00   |
| 1   | AA    | 1328 | C    | N3-C4-N4   | 5.73  | 122.01      | 118.00   |
| 26  | B7    | 81   | G    | O4'-C1'-N9 | 5.73  | 112.78      | 108.20   |
| 27  | B8    | 53   | A    | O4'-C1'-N9 | 5.73  | 112.78      | 108.20   |
| 27  | B8    | 422  | A    | C5-C6-N6   | -5.73 | 119.12      | 123.70   |
| 27  | B8    | 727  | A    | C4-C5-C6   | 5.73  | 119.86      | 117.00   |
| 27  | B8    | 1165 | A    | C4-C5-C6   | 5.73  | 119.86      | 117.00   |
| 27  | B8    | 1706 | C    | N3-C4-N4   | 5.73  | 122.01      | 118.00   |
| 27  | B8    | 1772 | A    | O4'-C1'-N9 | 5.73  | 112.78      | 108.20   |
| 27  | B8    | 2688 | G    | O4'-C1'-N9 | 5.73  | 112.78      | 108.20   |
| 1   | AA    | 1011 | C    | N3-C4-N4   | 5.73  | 122.01      | 118.00   |
| 27  | B8    | 14   | A    | C5-C6-N1   | -5.73 | 114.84      | 117.70   |
| 27  | B8    | 272  | A    | O4'-C1'-N9 | 5.73  | 112.78      | 108.20   |
| 27  | B8    | 587  | C    | N3-C4-N4   | 5.73  | 122.01      | 118.00   |
| 27  | B8    | 1046 | A    | C5-C6-N6   | -5.73 | 119.12      | 123.70   |
| 27  | B8    | 1339 | G    | O4'-C1'-N9 | 5.73  | 112.78      | 108.20   |
| 27  | B8    | 1477 | A    | C5-C6-N1   | -5.73 | 114.84      | 117.70   |
| 27  | B8    | 2809 | A    | C4-C5-C6   | 5.73  | 119.86      | 117.00   |
| 1   | AA    | 135  | C    | N3-C4-N4   | 5.72  | 122.01      | 118.00   |
| 1   | AA    | 168  | G    | O4'-C1'-N9 | 5.72  | 112.78      | 108.20   |
| 1   | AA    | 189  | A    | O4'-C1'-N9 | 5.72  | 112.78      | 108.20   |
| 1   | AA    | 243  | A    | C5-C6-N6   | -5.72 | 119.12      | 123.70   |
| 1   | AA    | 746  | A    | O4'-C1'-N9 | 5.72  | 112.78      | 108.20   |
| 1   | AA    | 807  | A    | C5-C6-N1   | -5.72 | 114.84      | 117.70   |
| 1   | AA    | 1171 | A    | C5-C6-N1   | -5.72 | 114.84      | 117.70   |
| 27  | B8    | 155  | A    | C5-C6-N6   | -5.72 | 119.12      | 123.70   |
| 27  | B8    | 2077 | A    | C5-C6-N1   | -5.72 | 114.84      | 117.70   |
| 27  | B8    | 2358 | A    | C5-C6-N6   | -5.72 | 119.12      | 123.70   |
| 27  | B8    | 2412 | A    | C5-C6-N1   | -5.72 | 114.84      | 117.70   |
| 27  | B8    | 2806 | C    | N3-C4-C5   | -5.72 | 119.61      | 121.90   |
| 27  | B8    | 2824 | C    | N3-C4-N4   | 5.72  | 122.01      | 118.00   |
| 1   | AA    | 66   | A    | C5-C6-N1   | -5.72 | 114.84      | 117.70   |
| 1   | AA    | 78   | A    | C4-C5-C6   | 5.72  | 119.86      | 117.00   |
| 1   | AA    | 1324 | A    | C5-C6-N6   | -5.72 | 119.12      | 123.70   |
| 1   | AA    | 1456 | A    | C5-C6-N6   | -5.72 | 119.12      | 123.70   |
| 27  | B8    | 622  | G    | O4'-C1'-N9 | 5.72  | 112.78      | 108.20   |
| 27  | B8    | 677  | A    | C4-C5-C6   | 5.72  | 119.86      | 117.00   |
| 27  | B8    | 1354 | A    | O4'-C1'-N9 | 5.72  | 112.78      | 108.20   |
| 27  | B8    | 2005 | A    | C5-C6-N6   | -5.72 | 119.12      | 123.70   |
| 27  | B8    | 2065 | C    | N3-C4-C5   | -5.72 | 119.61      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2475 | C    | O4'-C1'-N1 | 5.72  | 112.78      | 108.20   |
| 1   | AA    | 22   | G    | O4'-C1'-N9 | 5.72  | 112.78      | 108.20   |
| 1   | AA    | 602  | A    | C4-C5-C6   | 5.72  | 119.86      | 117.00   |
| 1   | AA    | 1225 | A    | C5-C6-N1   | -5.72 | 114.84      | 117.70   |
| 3   | AV    | 59   | A    | C5-C6-N6   | -5.72 | 119.12      | 123.70   |
| 27  | B8    | 497  | A    | C5-C6-N6   | -5.72 | 119.12      | 123.70   |
| 27  | B8    | 980  | A    | C5-C6-N6   | -5.72 | 119.12      | 123.70   |
| 1   | AA    | 482  | A    | C4-C5-C6   | 5.72  | 119.86      | 117.00   |
| 1   | AA    | 640  | A    | C4-C5-C6   | 5.72  | 119.86      | 117.00   |
| 1   | AA    | 1346 | A    | C4-C5-C6   | 5.72  | 119.86      | 117.00   |
| 3   | AV    | 37   | G    | O4'-C1'-N9 | 5.72  | 112.78      | 108.20   |
| 27  | B8    | 485  | C    | N3-C4-N4   | 5.72  | 122.00      | 118.00   |
| 27  | B8    | 943  | A    | C5-C6-N1   | -5.72 | 114.84      | 117.70   |
| 27  | B8    | 1107 | G    | O4'-C1'-N9 | 5.72  | 112.78      | 108.20   |
| 27  | B8    | 1377 | G    | N3-C2-N2   | 5.72  | 123.90      | 119.90   |
| 27  | B8    | 1650 | A    | C4-C5-C6   | 5.72  | 119.86      | 117.00   |
| 27  | B8    | 2761 | A    | C4-C5-C6   | 5.72  | 119.86      | 117.00   |
| 27  | B8    | 2840 | C    | N3-C4-N4   | 5.72  | 122.00      | 118.00   |
| 1   | AA    | 587  | G    | O4'-C1'-N9 | 5.72  | 112.77      | 108.20   |
| 1   | AA    | 1169 | A    | C5-C6-N6   | -5.72 | 119.13      | 123.70   |
| 27  | B8    | 1102 | C    | N3-C4-N4   | 5.72  | 122.00      | 118.00   |
| 27  | B8    | 2298 | A    | O4'-C1'-N9 | 5.72  | 112.77      | 108.20   |
| 1   | AA    | 926  | G    | O4'-C1'-N9 | 5.72  | 112.77      | 108.20   |
| 1   | AA    | 1105 | A    | C4-C5-C6   | 5.72  | 119.86      | 117.00   |
| 1   | AA    | 1216 | A    | C5-C6-N1   | -5.72 | 114.84      | 117.70   |
| 27  | B8    | 46   | G    | O4'-C1'-N9 | 5.72  | 112.77      | 108.20   |
| 27  | B8    | 693  | A    | O4'-C1'-N9 | 5.72  | 112.77      | 108.20   |
| 27  | B8    | 1196 | C    | N3-C4-N4   | 5.72  | 122.00      | 118.00   |
| 27  | B8    | 1502 | A    | C5-C6-N6   | -5.72 | 119.13      | 123.70   |
| 27  | B8    | 2097 | A    | C5-C6-N6   | -5.72 | 119.13      | 123.70   |
| 1   | AA    | 290  | C    | N3-C4-N4   | 5.71  | 122.00      | 118.00   |
| 1   | AA    | 876  | C    | N3-C4-N4   | 5.71  | 122.00      | 118.00   |
| 27  | B8    | 1069 | A    | C5-C6-N6   | -5.71 | 119.13      | 123.70   |
| 27  | B8    | 1140 | C    | N3-C4-N4   | 5.71  | 122.00      | 118.00   |
| 27  | B8    | 2205 | A    | C5-C6-N1   | -5.71 | 114.84      | 117.70   |
| 27  | B8    | 2385 | C    | N3-C4-C5   | -5.71 | 119.61      | 121.90   |
| 27  | B8    | 2572 | A    | C5-C6-N6   | -5.71 | 119.13      | 123.70   |
| 1   | AA    | 631  | C    | N3-C4-N4   | 5.71  | 122.00      | 118.00   |
| 1   | AA    | 963  | G    | O4'-C1'-N9 | 5.71  | 112.77      | 108.20   |
| 27  | B8    | 57   | C    | N3-C4-N4   | 5.71  | 122.00      | 118.00   |
| 27  | B8    | 1551 | A    | C4-C5-C6   | 5.71  | 119.86      | 117.00   |
| 27  | B8    | 1694 | C    | O4'-C1'-N1 | 5.71  | 112.77      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2482 | A    | C5-C6-N6   | -5.71 | 119.13      | 123.70   |
| 27  | B8    | 2515 | C    | N3-C4-N4   | 5.71  | 122.00      | 118.00   |
| 1   | AA    | 389  | A    | C5-C6-N6   | -5.71 | 119.13      | 123.70   |
| 1   | AA    | 607  | A    | O4'-C1'-N9 | 5.71  | 112.77      | 108.20   |
| 27  | B8    | 344  | A    | C4-C5-C6   | 5.71  | 119.86      | 117.00   |
| 27  | B8    | 348  | A    | C4-C5-C6   | 5.71  | 119.86      | 117.00   |
| 27  | B8    | 1493 | C    | N3-C4-N4   | 5.71  | 122.00      | 118.00   |
| 27  | B8    | 1656 | C    | N3-C4-N4   | 5.71  | 122.00      | 118.00   |
| 27  | B8    | 2340 | A    | C5-C6-N6   | -5.71 | 119.13      | 123.70   |
| 27  | B8    | 2377 | A    | C5-C6-N6   | -5.71 | 119.13      | 123.70   |
| 27  | B8    | 2407 | A    | C5-C6-N1   | -5.71 | 114.84      | 117.70   |
| 27  | B8    | 2418 | A    | O4'-C1'-N9 | 5.71  | 112.77      | 108.20   |
| 3   | AV    | 49   | C    | N3-C4-C5   | -5.71 | 119.62      | 121.90   |
| 27  | B8    | 354  | A    | C4-C5-C6   | 5.71  | 119.86      | 117.00   |
| 27  | B8    | 761  | A    | C4-C5-C6   | 5.71  | 119.86      | 117.00   |
| 27  | B8    | 1387 | A    | C4-C5-C6   | 5.71  | 119.86      | 117.00   |
| 1   | AA    | 655  | A    | C5-C6-N6   | -5.71 | 119.13      | 123.70   |
| 1   | AA    | 712  | A    | C4-C5-C6   | 5.71  | 119.86      | 117.00   |
| 1   | AA    | 754  | C    | N3-C4-N4   | 5.71  | 122.00      | 118.00   |
| 1   | AA    | 839  | C    | N3-C4-N4   | 5.71  | 122.00      | 118.00   |
| 1   | AA    | 1103 | C    | N3-C4-C5   | -5.71 | 119.62      | 121.90   |
| 27  | B8    | 79   | C    | N3-C4-N4   | 5.71  | 122.00      | 118.00   |
| 27  | B8    | 626  | A    | C5-C6-N1   | -5.71 | 114.85      | 117.70   |
| 27  | B8    | 851  | C    | N3-C4-N4   | 5.71  | 122.00      | 118.00   |
| 27  | B8    | 1046 | A    | C4-C5-C6   | 5.71  | 119.85      | 117.00   |
| 27  | B8    | 1928 | A    | C5-C6-N1   | -5.71 | 114.85      | 117.70   |
| 27  | B8    | 2602 | A    | C5-C6-N6   | -5.71 | 119.13      | 123.70   |
| 1   | AA    | 336  | A    | C5-C6-N6   | -5.71 | 119.14      | 123.70   |
| 1   | AA    | 759  | A    | C4-C5-C6   | 5.71  | 119.85      | 117.00   |
| 1   | AA    | 1248 | A    | C5-C6-N6   | -5.71 | 119.13      | 123.70   |
| 1   | AA    | 1446 | A    | O4'-C1'-N9 | 5.71  | 112.76      | 108.20   |
| 27  | B8    | 115  | C    | N3-C4-N4   | 5.71  | 122.00      | 118.00   |
| 27  | B8    | 182  | A    | C5-C6-N6   | -5.71 | 119.14      | 123.70   |
| 27  | B8    | 878  | A    | C5-C6-N1   | -5.71 | 114.85      | 117.70   |
| 27  | B8    | 889  | C    | N3-C4-C5   | -5.71 | 119.62      | 121.90   |
| 27  | B8    | 1363 | C    | N3-C4-N4   | 5.71  | 121.99      | 118.00   |
| 27  | B8    | 1735 | A    | C5-C6-N1   | -5.71 | 114.85      | 117.70   |
| 27  | B8    | 1908 | C    | N3-C4-N4   | 5.71  | 122.00      | 118.00   |
| 1   | AA    | 60   | A    | C4-C5-C6   | 5.71  | 119.85      | 117.00   |
| 1   | AA    | 983  | A    | C5-C6-N6   | -5.71 | 119.14      | 123.70   |
| 27  | B8    | 1305 | C    | N3-C4-N4   | 5.71  | 121.99      | 118.00   |
| 1   | AA    | 67   | C    | N3-C4-C5   | -5.70 | 119.62      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 308  | C    | N3-C4-N4   | 5.70  | 121.99      | 118.00   |
| 1   | AA    | 1130 | A    | C4-C5-C6   | 5.70  | 119.85      | 117.00   |
| 27  | B8    | 466  | A    | C4-C5-C6   | 5.70  | 119.85      | 117.00   |
| 27  | B8    | 764  | A    | C4-C5-C6   | 5.70  | 119.85      | 117.00   |
| 27  | B8    | 1426 | G    | N3-C2-N2   | 5.70  | 123.89      | 119.90   |
| 27  | B8    | 2717 | C    | N3-C4-C5   | -5.70 | 119.62      | 121.90   |
| 27  | B8    | 129  | C    | N3-C4-N4   | 5.70  | 121.99      | 118.00   |
| 27  | B8    | 943  | A    | C5-C6-N6   | -5.70 | 119.14      | 123.70   |
| 27  | B8    | 1221 | C    | N3-C4-N4   | 5.70  | 121.99      | 118.00   |
| 27  | B8    | 1637 | A    | C5-C6-N6   | -5.70 | 119.14      | 123.70   |
| 27  | B8    | 2814 | A    | C5-C6-N6   | -5.70 | 119.14      | 123.70   |
| 1   | AA    | 169  | C    | N3-C4-C5   | -5.70 | 119.62      | 121.90   |
| 1   | AA    | 882  | C    | N3-C4-N4   | 5.70  | 121.99      | 118.00   |
| 1   | AA    | 1256 | A    | O4'-C1'-N9 | 5.70  | 112.76      | 108.20   |
| 27  | B8    | 163  | C    | N3-C4-N4   | 5.70  | 121.99      | 118.00   |
| 27  | B8    | 245  | G    | O4'-C1'-N9 | 5.70  | 112.76      | 108.20   |
| 27  | B8    | 1328 | A    | C4-C5-C6   | 5.70  | 119.85      | 117.00   |
| 27  | B8    | 1434 | A    | C4-C5-C6   | 5.70  | 119.85      | 117.00   |
| 27  | B8    | 1564 | C    | N3-C4-C5   | -5.70 | 119.62      | 121.90   |
| 27  | B8    | 1962 | C    | O4'-C1'-N1 | 5.70  | 112.76      | 108.20   |
| 27  | B8    | 1978 | A    | C4-C5-C6   | 5.70  | 119.85      | 117.00   |
| 27  | B8    | 1981 | A    | C4-C5-C6   | 5.70  | 119.85      | 117.00   |
| 27  | B8    | 2624 | G    | O4'-C1'-N9 | 5.70  | 112.76      | 108.20   |
| 1   | AA    | 253  | A    | C4-C5-C6   | 5.70  | 119.85      | 117.00   |
| 1   | AA    | 388  | G    | O4'-C1'-N9 | 5.70  | 112.76      | 108.20   |
| 1   | AA    | 456  | A    | C4-C5-C6   | 5.70  | 119.85      | 117.00   |
| 1   | AA    | 1261 | A    | C5-C6-N1   | -5.70 | 114.85      | 117.70   |
| 27  | B8    | 981  | A    | C5-C6-N6   | -5.70 | 119.14      | 123.70   |
| 27  | B8    | 1142 | A    | C5-C6-N6   | -5.70 | 119.14      | 123.70   |
| 27  | B8    | 1144 | A    | C5-C6-N1   | -5.70 | 114.85      | 117.70   |
| 27  | B8    | 1225 | G    | O4'-C1'-N9 | 5.70  | 112.76      | 108.20   |
| 27  | B8    | 1719 | G    | O4'-C1'-N9 | 5.70  | 112.76      | 108.20   |
| 27  | B8    | 2156 | G    | N3-C2-N2   | 5.70  | 123.89      | 119.90   |
| 27  | B8    | 2688 | G    | N3-C2-N2   | 5.70  | 123.89      | 119.90   |
| 1   | AA    | 559  | A    | C5-C6-N6   | -5.70 | 119.14      | 123.70   |
| 1   | AA    | 1513 | A    | C5-C6-N1   | -5.70 | 114.85      | 117.70   |
| 27  | B8    | 1330 | C    | N3-C4-N4   | 5.70  | 121.99      | 118.00   |
| 27  | B8    | 1901 | A    | O4'-C1'-N9 | 5.70  | 112.76      | 108.20   |
| 27  | B8    | 1971 | U    | C2-N1-C1'  | 5.70  | 124.54      | 117.70   |
| 27  | B8    | 2125 | G    | C5-C6-O6   | -5.70 | 125.18      | 128.60   |
| 1   | AA    | 222  | C    | N3-C4-N4   | 5.70  | 121.99      | 118.00   |
| 1   | AA    | 901  | A    | C5-C6-N1   | -5.70 | 114.85      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 217  | A    | C5-C6-N6   | -5.70 | 119.14      | 123.70   |
| 27  | B8    | 592  | A    | C4-C5-C6   | 5.70  | 119.85      | 117.00   |
| 27  | B8    | 1607 | C    | N3-C4-C5   | -5.70 | 119.62      | 121.90   |
| 27  | B8    | 1784 | A    | C4-C5-C6   | 5.70  | 119.85      | 117.00   |
| 27  | B8    | 2870 | C    | N3-C4-N4   | 5.70  | 121.99      | 118.00   |
| 27  | B8    | 499  | U    | O4'-C1'-N1 | 5.69  | 112.75      | 108.20   |
| 27  | B8    | 627  | A    | C5-C6-N6   | -5.69 | 119.14      | 123.70   |
| 27  | B8    | 1469 | A    | C5-C6-N1   | -5.69 | 114.85      | 117.70   |
| 27  | B8    | 1547 | C    | N3-C4-N4   | 5.69  | 121.99      | 118.00   |
| 1   | AA    | 298  | A    | C4-C5-C6   | 5.69  | 119.85      | 117.00   |
| 1   | AA    | 900  | A    | C5-C6-N6   | -5.69 | 119.15      | 123.70   |
| 27  | B8    | 528  | A    | C5-C6-N1   | -5.69 | 114.85      | 117.70   |
| 27  | B8    | 1675 | C    | N3-C4-N4   | 5.69  | 121.98      | 118.00   |
| 27  | B8    | 1685 | C    | N3-C4-N4   | 5.69  | 121.98      | 118.00   |
| 27  | B8    | 1772 | A    | C5-C6-N6   | -5.69 | 119.15      | 123.70   |
| 27  | B8    | 2288 | A    | C5-C6-N1   | -5.69 | 114.85      | 117.70   |
| 27  | B8    | 2516 | A    | C4-C5-C6   | 5.69  | 119.85      | 117.00   |
| 27  | B8    | 2527 | C    | N3-C4-N4   | 5.69  | 121.98      | 118.00   |
| 1   | AA    | 440  | C    | N3-C4-C5   | -5.69 | 119.62      | 121.90   |
| 1   | AA    | 1179 | A    | O4'-C1'-N9 | 5.69  | 112.75      | 108.20   |
| 1   | AA    | 1250 | A    | C4-C5-C6   | 5.69  | 119.85      | 117.00   |
| 1   | AA    | 1403 | C    | N3-C4-C5   | -5.69 | 119.62      | 121.90   |
| 27  | B8    | 131  | A    | C4-C5-C6   | 5.69  | 119.85      | 117.00   |
| 27  | B8    | 466  | A    | C5-C6-N6   | -5.69 | 119.15      | 123.70   |
| 27  | B8    | 507  | A    | C4-C5-C6   | 5.69  | 119.84      | 117.00   |
| 27  | B8    | 1057 | A    | C5-C6-N6   | -5.69 | 119.15      | 123.70   |
| 27  | B8    | 1502 | A    | C5-C6-N1   | -5.69 | 114.86      | 117.70   |
| 27  | B8    | 1916 | A    | C5-C6-N1   | -5.69 | 114.85      | 117.70   |
| 27  | B8    | 1966 | A    | O4'-C1'-N9 | 5.69  | 112.75      | 108.20   |
| 27  | B8    | 2071 | A    | C5-C6-N6   | -5.69 | 119.15      | 123.70   |
| 1   | AA    | 649  | A    | C4-C5-C6   | 5.69  | 119.84      | 117.00   |
| 27  | B8    | 1327 | A    | C5-C6-N6   | -5.69 | 119.15      | 123.70   |
| 27  | B8    | 1705 | A    | C4-C5-C6   | 5.69  | 119.84      | 117.00   |
| 27  | B8    | 1928 | A    | C5-C6-N6   | -5.69 | 119.15      | 123.70   |
| 1   | AA    | 1055 | A    | C5-C6-N6   | -5.69 | 119.15      | 123.70   |
| 1   | AA    | 1494 | G    | O4'-C1'-N9 | 5.69  | 112.75      | 108.20   |
| 3   | AV    | 26   | C    | N3-C4-N4   | 5.69  | 121.98      | 118.00   |
| 27  | B8    | 482  | A    | C5-C6-N6   | -5.69 | 119.15      | 123.70   |
| 27  | B8    | 1032 | A    | C4-C5-C6   | 5.69  | 119.84      | 117.00   |
| 27  | B8    | 1123 | C    | N3-C4-N4   | 5.69  | 121.98      | 118.00   |
| 27  | B8    | 2013 | A    | C5-C6-N1   | -5.69 | 114.86      | 117.70   |
| 27  | B8    | 2055 | C    | N3-C4-N4   | 5.69  | 121.98      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2309 | A    | C5-C6-N6   | -5.69 | 119.15      | 123.70   |
| 27  | B8    | 2436 | G    | O4'-C1'-N9 | 5.69  | 112.75      | 108.20   |
| 27  | B8    | 339  | U    | O4'-C1'-N1 | 5.69  | 112.75      | 108.20   |
| 27  | B8    | 2434 | A    | C5-C6-N1   | -5.69 | 114.86      | 117.70   |
| 27  | B8    | 2663 | G    | O4'-C1'-N9 | 5.69  | 112.75      | 108.20   |
| 1   | AA    | 153  | C    | N3-C4-N4   | 5.68  | 121.98      | 118.00   |
| 1   | AA    | 321  | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 1   | AA    | 972  | C    | N3-C4-C5   | -5.68 | 119.63      | 121.90   |
| 1   | AA    | 1240 | U    | O4'-C1'-N1 | 5.68  | 112.75      | 108.20   |
| 1   | AA    | 1419 | G    | O4'-C1'-N9 | 5.68  | 112.75      | 108.20   |
| 1   | AA    | 1534 | A    | C5-C6-N1   | -5.68 | 114.86      | 117.70   |
| 3   | AV    | 5    | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 3   | AV    | 77   | A    | C5-C6-N1   | -5.68 | 114.86      | 117.70   |
| 26  | B7    | 109  | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 27  | B8    | 619  | G    | N3-C2-N2   | 5.68  | 123.88      | 119.90   |
| 27  | B8    | 920  | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 27  | B8    | 1508 | A    | C5-C6-N6   | -5.68 | 119.15      | 123.70   |
| 27  | B8    | 1558 | C    | N3-C4-N4   | 5.68  | 121.98      | 118.00   |
| 27  | B8    | 2320 | U    | O4'-C1'-N1 | 5.68  | 112.75      | 108.20   |
| 27  | B8    | 2835 | A    | C5-C6-N6   | -5.68 | 119.15      | 123.70   |
| 1   | AA    | 199  | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 1   | AA    | 914  | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 1   | AA    | 934  | C    | O4'-C1'-N1 | 5.68  | 112.75      | 108.20   |
| 1   | AA    | 1133 | G    | O4'-C1'-N9 | 5.68  | 112.75      | 108.20   |
| 1   | AA    | 1380 | U    | O4'-C1'-N1 | 5.68  | 112.75      | 108.20   |
| 1   | AA    | 1396 | A    | C5-C6-N6   | -5.68 | 119.15      | 123.70   |
| 26  | B7    | 38   | C    | N3-C4-C5   | -5.68 | 119.63      | 121.90   |
| 27  | B8    | 979  | A    | C5-C6-N6   | -5.68 | 119.15      | 123.70   |
| 27  | B8    | 1088 | A    | C5-C6-N1   | -5.68 | 114.86      | 117.70   |
| 27  | B8    | 1262 | A    | C5-C6-N1   | -5.68 | 114.86      | 117.70   |
| 27  | B8    | 1528 | A    | C5-C6-N6   | -5.68 | 119.16      | 123.70   |
| 27  | B8    | 1570 | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 27  | B8    | 1691 | C    | N3-C4-N4   | 5.68  | 121.98      | 118.00   |
| 27  | B8    | 1895 | C    | N3-C4-C5   | -5.68 | 119.63      | 121.90   |
| 27  | B8    | 2015 | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 1   | AA    | 1214 | C    | C2-N1-C1'  | 5.68  | 125.05      | 118.80   |
| 1   | AA    | 1236 | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 27  | B8    | 362  | A    | C5-C6-N6   | -5.68 | 119.16      | 123.70   |
| 27  | B8    | 1711 | A    | C5-C6-N1   | -5.68 | 114.86      | 117.70   |
| 1   | AA    | 87   | C    | N3-C4-C5   | -5.68 | 119.63      | 121.90   |
| 1   | AA    | 122  | G    | O4'-C1'-N9 | 5.68  | 112.74      | 108.20   |
| 1   | AA    | 167  | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 328  | C    | N3-C4-C5   | -5.68 | 119.63      | 121.90   |
| 1   | AA    | 549  | C    | N3-C4-C5   | -5.68 | 119.63      | 121.90   |
| 1   | AA    | 729  | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 1   | AA    | 750  | C    | N3-C4-N4   | 5.68  | 121.98      | 118.00   |
| 1   | AA    | 1082 | A    | O4'-C1'-N9 | 5.68  | 112.74      | 108.20   |
| 1   | AA    | 1281 | C    | N3-C4-N4   | 5.68  | 121.97      | 118.00   |
| 3   | AV    | 74   | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 27  | B8    | 626  | A    | C5-C6-N6   | -5.68 | 119.16      | 123.70   |
| 27  | B8    | 1151 | A    | O4'-C1'-N9 | 5.68  | 112.74      | 108.20   |
| 27  | B8    | 1386 | C    | N3-C4-N4   | 5.68  | 121.98      | 118.00   |
| 27  | B8    | 1895 | C    | N3-C4-N4   | 5.68  | 121.98      | 118.00   |
| 27  | B8    | 1909 | C    | N3-C4-N4   | 5.68  | 121.98      | 118.00   |
| 27  | B8    | 2173 | A    | C5-C6-N1   | -5.68 | 114.86      | 117.70   |
| 27  | B8    | 2434 | A    | C5-C6-N6   | -5.68 | 119.16      | 123.70   |
| 27  | B8    | 2598 | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 1   | AA    | 132  | C    | N3-C4-N4   | 5.68  | 121.97      | 118.00   |
| 1   | AA    | 533  | A    | O4'-C1'-N9 | 5.68  | 112.74      | 108.20   |
| 1   | AA    | 1517 | G    | O4'-C1'-N9 | 5.68  | 112.74      | 108.20   |
| 26  | B7    | 34   | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 27  | B8    | 415  | A    | O4'-C1'-N9 | 5.68  | 112.74      | 108.20   |
| 27  | B8    | 478  | A    | C5-C6-N6   | -5.68 | 119.16      | 123.70   |
| 27  | B8    | 1304 | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 27  | B8    | 1319 | C    | N3-C4-N4   | 5.68  | 121.97      | 118.00   |
| 27  | B8    | 1357 | C    | N3-C4-N4   | 5.68  | 121.97      | 118.00   |
| 27  | B8    | 2088 | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 1   | AA    | 246  | A    | C4-C5-C6   | 5.68  | 119.84      | 117.00   |
| 1   | AA    | 1021 | A    | C5-C6-N6   | -5.68 | 119.16      | 123.70   |
| 1   | AA    | 1257 | A    | C5-C6-N6   | -5.68 | 119.16      | 123.70   |
| 1   | AA    | 1306 | A    | C5-C6-N1   | -5.68 | 114.86      | 117.70   |
| 26  | B7    | 18   | G    | O4'-C1'-N9 | 5.68  | 112.74      | 108.20   |
| 26  | B7    | 52   | A    | C5-C6-N6   | -5.68 | 119.16      | 123.70   |
| 27  | B8    | 722  | A    | C5-C6-N6   | -5.68 | 119.16      | 123.70   |
| 27  | B8    | 1096 | A    | C5-C6-N1   | -5.68 | 114.86      | 117.70   |
| 28  | BA    | 332  | TYR  | CB-CG-CD2  | 5.68  | 124.41      | 121.00   |
| 1   | AA    | 510  | A    | C4-C5-C6   | 5.67  | 119.84      | 117.00   |
| 1   | AA    | 696  | A    | C5-C6-N1   | -5.67 | 114.86      | 117.70   |
| 1   | AA    | 1203 | C    | N3-C4-N4   | 5.67  | 121.97      | 118.00   |
| 1   | AA    | 1251 | A    | C5-C6-N6   | -5.67 | 119.16      | 123.70   |
| 3   | AV    | 2    | G    | O4'-C1'-N9 | 5.67  | 112.74      | 108.20   |
| 3   | AV    | 61   | U    | O4'-C1'-N1 | 5.67  | 112.74      | 108.20   |
| 27  | B8    | 617  | G    | O4'-C1'-N9 | 5.67  | 112.74      | 108.20   |
| 27  | B8    | 946  | C    | N3-C4-N4   | 5.67  | 121.97      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1073 | A    | C4-C5-C6   | 5.67  | 119.84      | 117.00   |
| 27  | B8    | 1762 | A    | C5-C6-N6   | -5.67 | 119.16      | 123.70   |
| 27  | B8    | 1783 | A    | C5-C6-N1   | -5.67 | 114.86      | 117.70   |
| 27  | B8    | 2212 | A    | C5-C6-N1   | -5.67 | 114.86      | 117.70   |
| 27  | B8    | 2258 | C    | N3-C4-N4   | 5.67  | 121.97      | 118.00   |
| 1   | AA    | 648  | A    | C5-C6-N1   | -5.67 | 114.86      | 117.70   |
| 1   | AA    | 721  | G    | O4'-C1'-N9 | 5.67  | 112.74      | 108.20   |
| 27  | B8    | 160  | A    | C5-C6-N6   | -5.67 | 119.16      | 123.70   |
| 27  | B8    | 523  | C    | N3-C4-N4   | 5.67  | 121.97      | 118.00   |
| 27  | B8    | 2110 | G    | P-O3'-C3'  | 5.67  | 126.51      | 119.70   |
| 27  | B8    | 2445 | G    | O4'-C1'-N9 | 5.67  | 112.74      | 108.20   |
| 27  | B8    | 2608 | G    | N3-C2-N2   | 5.67  | 123.87      | 119.90   |
| 1   | AA    | 189  | A    | C5-C6-N6   | -5.67 | 119.16      | 123.70   |
| 1   | AA    | 306  | A    | O4'-C1'-N9 | 5.67  | 112.74      | 108.20   |
| 1   | AA    | 977  | A    | C5-C6-N6   | -5.67 | 119.16      | 123.70   |
| 1   | AA    | 1081 | A    | O4'-C1'-N9 | 5.67  | 112.74      | 108.20   |
| 27  | B8    | 460  | A    | O4'-C1'-N9 | 5.67  | 112.74      | 108.20   |
| 27  | B8    | 541  | A    | C5-C6-N1   | -5.67 | 114.86      | 117.70   |
| 27  | B8    | 631  | A    | C5-C6-N6   | -5.67 | 119.16      | 123.70   |
| 27  | B8    | 1127 | A    | C4-C5-C6   | 5.67  | 119.84      | 117.00   |
| 27  | B8    | 1650 | A    | O4'-C1'-N9 | 5.67  | 112.74      | 108.20   |
| 27  | B8    | 1843 | C    | N3-C4-N4   | 5.67  | 121.97      | 118.00   |
| 27  | B8    | 2009 | A    | C4-C5-C6   | 5.67  | 119.84      | 117.00   |
| 27  | B8    | 2772 | C    | N3-C4-N4   | 5.67  | 121.97      | 118.00   |
| 1   | AA    | 131  | A    | O4'-C1'-N9 | 5.67  | 112.74      | 108.20   |
| 1   | AA    | 408  | A    | C5-C6-N6   | -5.67 | 119.16      | 123.70   |
| 26  | B7    | 93   | C    | N3-C4-C5   | -5.67 | 119.63      | 121.90   |
| 27  | B8    | 479  | A    | P-O3'-C3'  | 5.67  | 126.50      | 119.70   |
| 27  | B8    | 1566 | A    | C5-C6-N6   | -5.67 | 119.16      | 123.70   |
| 27  | B8    | 2080 | A    | C5-C6-N6   | -5.67 | 119.16      | 123.70   |
| 1   | AA    | 272  | C    | N3-C4-N4   | 5.67  | 121.97      | 118.00   |
| 1   | AA    | 542  | G    | O4'-C1'-N9 | 5.67  | 112.73      | 108.20   |
| 1   | AA    | 609  | A    | O4'-C1'-N9 | 5.67  | 112.73      | 108.20   |
| 1   | AA    | 612  | C    | N3-C4-C5   | -5.67 | 119.63      | 121.90   |
| 3   | AV    | 28   | C    | N3-C4-N4   | 5.67  | 121.97      | 118.00   |
| 27  | B8    | 143  | C    | N3-C4-N4   | 5.67  | 121.97      | 118.00   |
| 27  | B8    | 366  | C    | N3-C4-N4   | 5.67  | 121.97      | 118.00   |
| 27  | B8    | 922  | C    | N3-C4-C5   | -5.67 | 119.63      | 121.90   |
| 27  | B8    | 968  | C    | N3-C4-N4   | 5.67  | 121.97      | 118.00   |
| 27  | B8    | 1330 | C    | N3-C4-C5   | -5.67 | 119.63      | 121.90   |
| 27  | B8    | 1678 | A    | O4'-C1'-N9 | 5.67  | 112.73      | 108.20   |
| 27  | B8    | 1773 | A    | C4-C5-C6   | 5.67  | 119.83      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2205 | A    | C4-C5-C6   | 5.67  | 119.83      | 117.00   |
| 27  | B8    | 2547 | A    | C5-C6-N1   | -5.67 | 114.87      | 117.70   |
| 1   | AA    | 101  | A    | C5-C6-N6   | -5.67 | 119.17      | 123.70   |
| 1   | AA    | 261  | U    | O4'-C1'-N1 | 5.67  | 112.73      | 108.20   |
| 1   | AA    | 630  | A    | C5-C6-N6   | -5.67 | 119.17      | 123.70   |
| 1   | AA    | 978  | A    | C4-C5-C6   | 5.67  | 119.83      | 117.00   |
| 1   | AA    | 1019 | A    | C5-C6-N6   | -5.67 | 119.17      | 123.70   |
| 27  | B8    | 781  | A    | C5-C6-N1   | -5.67 | 114.87      | 117.70   |
| 27  | B8    | 833  | A    | O4'-C1'-N9 | 5.67  | 112.73      | 108.20   |
| 27  | B8    | 1307 | A    | C4-C5-C6   | 5.67  | 119.83      | 117.00   |
| 27  | B8    | 1364 | G    | O4'-C1'-N9 | 5.67  | 112.73      | 108.20   |
| 27  | B8    | 2082 | A    | O4'-C1'-N9 | 5.67  | 112.73      | 108.20   |
| 27  | B8    | 2749 | A    | C4-C5-C6   | 5.67  | 119.83      | 117.00   |
| 1   | AA    | 110  | C    | N3-C4-N4   | 5.67  | 121.97      | 118.00   |
| 1   | AA    | 1467 | C    | N3-C4-N4   | 5.67  | 121.97      | 118.00   |
| 27  | B8    | 42   | A    | C4-C5-C6   | 5.67  | 119.83      | 117.00   |
| 27  | B8    | 368  | A    | C5-C6-N1   | -5.67 | 114.87      | 117.70   |
| 27  | B8    | 1385 | A    | C4-C5-C6   | 5.67  | 119.83      | 117.00   |
| 1   | AA    | 518  | C    | N3-C4-N4   | 5.66  | 121.97      | 118.00   |
| 1   | AA    | 580  | C    | N3-C4-N4   | 5.66  | 121.96      | 118.00   |
| 1   | AA    | 1080 | A    | C5-C6-N1   | -5.66 | 114.87      | 117.70   |
| 1   | AA    | 1442 | G    | O4'-C1'-N9 | 5.66  | 112.73      | 108.20   |
| 27  | B8    | 155  | A    | C4-C5-C6   | 5.66  | 119.83      | 117.00   |
| 27  | B8    | 793  | A    | C5-C6-N6   | -5.66 | 119.17      | 123.70   |
| 27  | B8    | 2426 | A    | C5-C6-N6   | -5.66 | 119.17      | 123.70   |
| 27  | B8    | 44   | A    | C5-C6-N1   | -5.66 | 114.87      | 117.70   |
| 27  | B8    | 983  | A    | C5-C6-N6   | -5.66 | 119.17      | 123.70   |
| 27  | B8    | 1384 | A    | C4-C5-C6   | 5.66  | 119.83      | 117.00   |
| 27  | B8    | 1635 | A    | C5-C6-N6   | -5.66 | 119.17      | 123.70   |
| 27  | B8    | 2703 | C    | N3-C4-N4   | 5.66  | 121.96      | 118.00   |
| 1   | AA    | 394  | G    | O4'-C1'-N9 | 5.66  | 112.73      | 108.20   |
| 1   | AA    | 507  | C    | N3-C4-N4   | 5.66  | 121.96      | 118.00   |
| 26  | B7    | 62   | C    | N3-C4-C5   | -5.66 | 119.64      | 121.90   |
| 27  | B8    | 203  | A    | O4'-C1'-N9 | 5.66  | 112.73      | 108.20   |
| 27  | B8    | 382  | A    | C5-C6-N6   | -5.66 | 119.17      | 123.70   |
| 27  | B8    | 483  | A    | O4'-C1'-N9 | 5.66  | 112.73      | 108.20   |
| 27  | B8    | 1246 | A    | C5-C6-N1   | -5.66 | 114.87      | 117.70   |
| 27  | B8    | 1557 | C    | N3-C4-C5   | -5.66 | 119.64      | 121.90   |
| 27  | B8    | 1679 | A    | O4'-C1'-N9 | 5.66  | 112.73      | 108.20   |
| 27  | B8    | 1746 | A    | C4-C5-C6   | 5.66  | 119.83      | 117.00   |
| 27  | B8    | 2036 | C    | N3-C4-N4   | 5.66  | 121.96      | 118.00   |
| 27  | B8    | 2177 | C    | N3-C4-N4   | 5.66  | 121.96      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2182 | U    | O4'-C1'-N1 | 5.66  | 112.73      | 108.20   |
| 27  | B8    | 2765 | A    | C5-C6-N1   | -5.66 | 114.87      | 117.70   |
| 27  | B8    | 2858 | C    | N3-C4-C5   | -5.66 | 119.64      | 121.90   |
| 1   | AA    | 436  | C    | N3-C4-N4   | 5.66  | 121.96      | 118.00   |
| 1   | AA    | 1243 | C    | N3-C4-N4   | 5.66  | 121.96      | 118.00   |
| 1   | AA    | 1302 | C    | O4'-C1'-N1 | 5.66  | 112.73      | 108.20   |
| 26  | B7    | 50   | A    | C5-C6-N1   | -5.66 | 114.87      | 117.70   |
| 27  | B8    | 497  | A    | C4-C5-C6   | 5.66  | 119.83      | 117.00   |
| 27  | B8    | 723  | C    | N3-C4-N4   | 5.66  | 121.96      | 118.00   |
| 27  | B8    | 925  | A    | O4'-C1'-N9 | 5.66  | 112.73      | 108.20   |
| 27  | B8    | 952  | G    | O4'-C1'-N9 | 5.66  | 112.73      | 108.20   |
| 27  | B8    | 1138 | G    | O4'-C1'-N9 | 5.66  | 112.73      | 108.20   |
| 27  | B8    | 1274 | A    | C5-C6-N6   | -5.66 | 119.17      | 123.70   |
| 27  | B8    | 1458 | U    | O4'-C1'-N1 | 5.66  | 112.73      | 108.20   |
| 27  | B8    | 2104 | C    | N3-C4-C5   | -5.66 | 119.64      | 121.90   |
| 27  | B8    | 2439 | A    | C5-C6-N1   | -5.66 | 114.87      | 117.70   |
| 27  | B8    | 2614 | A    | C5-C6-N6   | -5.66 | 119.17      | 123.70   |
| 27  | B8    | 2623 | G    | O4'-C1'-N9 | 5.66  | 112.73      | 108.20   |
| 27  | B8    | 2660 | A    | C5-C6-N6   | -5.66 | 119.17      | 123.70   |
| 1   | AA    | 23   | C    | N3-C4-C5   | -5.66 | 119.64      | 121.90   |
| 1   | AA    | 770  | C    | N3-C4-N4   | 5.66  | 121.96      | 118.00   |
| 1   | AA    | 1411 | C    | N3-C4-N4   | 5.66  | 121.96      | 118.00   |
| 27  | B8    | 1912 | A    | C5-C6-N1   | -5.66 | 114.87      | 117.70   |
| 27  | B8    | 1970 | A    | C5-C6-N6   | -5.66 | 119.17      | 123.70   |
| 27  | B8    | 2298 | A    | C4-C5-C6   | 5.66  | 119.83      | 117.00   |
| 27  | B8    | 2713 | U    | O4'-C1'-N1 | 5.66  | 112.72      | 108.20   |
| 1   | AA    | 106  | C    | N3-C4-C5   | -5.66 | 119.64      | 121.90   |
| 1   | AA    | 124  | C    | N3-C4-C5   | -5.66 | 119.64      | 121.90   |
| 1   | AA    | 174  | A    | C5-C6-N1   | -5.66 | 114.87      | 117.70   |
| 1   | AA    | 488  | C    | N3-C4-N4   | 5.66  | 121.96      | 118.00   |
| 1   | AA    | 908  | A    | C5-C6-N1   | -5.66 | 114.87      | 117.70   |
| 1   | AA    | 1163 | A    | C5-C6-N6   | -5.66 | 119.18      | 123.70   |
| 1   | AA    | 1412 | C    | N3-C4-N4   | 5.66  | 121.96      | 118.00   |
| 26  | B7    | 57   | A    | C4-C5-C6   | 5.66  | 119.83      | 117.00   |
| 27  | B8    | 597  | G    | O4'-C1'-N9 | 5.66  | 112.72      | 108.20   |
| 27  | B8    | 758  | C    | N3-C4-N4   | 5.66  | 121.96      | 118.00   |
| 27  | B8    | 1686 | C    | N3-C4-N4   | 5.66  | 121.96      | 118.00   |
| 27  | B8    | 1721 | G    | N3-C2-N2   | 5.66  | 123.86      | 119.90   |
| 27  | B8    | 1786 | A    | C4-C5-C6   | 5.66  | 119.83      | 117.00   |
| 1   | AA    | 689  | C    | N3-C4-N4   | 5.65  | 121.96      | 118.00   |
| 27  | B8    | 455  | C    | N3-C4-N4   | 5.65  | 121.96      | 118.00   |
| 27  | B8    | 809  | G    | O4'-C1'-N9 | 5.65  | 112.72      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 983  | A    | O4'-C1'-N9 | 5.65  | 112.72      | 108.20   |
| 27  | B8    | 2763 | G    | O4'-C1'-N9 | 5.65  | 112.72      | 108.20   |
| 1   | AA    | 277  | C    | N3-C4-C5   | -5.65 | 119.64      | 121.90   |
| 1   | AA    | 1500 | A    | C5-C6-N1   | -5.65 | 114.87      | 117.70   |
| 1   | AA    | 1518 | A    | C5-C6-N1   | -5.65 | 114.87      | 117.70   |
| 27  | B8    | 270  | A    | C5-C6-N6   | -5.65 | 119.18      | 123.70   |
| 27  | B8    | 1285 | A    | O4'-C1'-N9 | 5.65  | 112.72      | 108.20   |
| 27  | B8    | 2851 | A    | O4'-C1'-N9 | 5.65  | 112.72      | 108.20   |
| 1   | AA    | 823  | C    | N3-C4-C5   | -5.65 | 119.64      | 121.90   |
| 1   | AA    | 1248 | A    | C4-C5-C6   | 5.65  | 119.83      | 117.00   |
| 27  | B8    | 101  | A    | O4'-C1'-N9 | 5.65  | 112.72      | 108.20   |
| 27  | B8    | 250  | G    | C5-C6-O6   | -5.65 | 125.21      | 128.60   |
| 27  | B8    | 2108 | A    | C5-C6-N1   | -5.65 | 114.87      | 117.70   |
| 27  | B8    | 2224 | G    | O4'-C1'-N9 | 5.65  | 112.72      | 108.20   |
| 27  | B8    | 2290 | G    | O4'-C1'-N9 | 5.65  | 112.72      | 108.20   |
| 27  | B8    | 2439 | A    | C5-C6-N6   | -5.65 | 119.18      | 123.70   |
| 27  | B8    | 2716 | C    | N3-C4-N4   | 5.65  | 121.95      | 118.00   |
| 27  | B8    | 151  | C    | N3-C4-N4   | 5.65  | 121.95      | 118.00   |
| 27  | B8    | 343  | C    | N3-C4-N4   | 5.65  | 121.95      | 118.00   |
| 27  | B8    | 602  | A    | O4'-C1'-N9 | 5.65  | 112.72      | 108.20   |
| 27  | B8    | 660  | C    | N3-C4-N4   | 5.65  | 121.95      | 118.00   |
| 27  | B8    | 668  | A    | C5-C6-N1   | -5.65 | 114.88      | 117.70   |
| 27  | B8    | 833  | A    | C5-C6-N1   | -5.65 | 114.88      | 117.70   |
| 1   | AA    | 503  | C    | N3-C4-N4   | 5.65  | 121.95      | 118.00   |
| 27  | B8    | 239  | C    | N3-C4-N4   | 5.65  | 121.95      | 118.00   |
| 27  | B8    | 247  | G    | O4'-C1'-N9 | 5.65  | 112.72      | 108.20   |
| 27  | B8    | 281  | C    | N3-C4-C5   | -5.65 | 119.64      | 121.90   |
| 27  | B8    | 526  | A    | C4-C5-C6   | 5.65  | 119.82      | 117.00   |
| 27  | B8    | 714  | U    | O4'-C1'-N1 | 5.65  | 112.72      | 108.20   |
| 27  | B8    | 890  | C    | N3-C4-N4   | 5.65  | 121.95      | 118.00   |
| 27  | B8    | 901  | C    | P-O5'-C5'  | 5.65  | 129.94      | 120.90   |
| 27  | B8    | 1274 | A    | C5-C6-N1   | -5.65 | 114.88      | 117.70   |
| 27  | B8    | 1304 | A    | C5-C6-N1   | -5.65 | 114.88      | 117.70   |
| 27  | B8    | 2023 | C    | N3-C4-N4   | 5.65  | 121.95      | 118.00   |
| 27  | B8    | 2164 | C    | O4'-C1'-N1 | 5.65  | 112.72      | 108.20   |
| 27  | B8    | 2275 | C    | N3-C4-N4   | 5.65  | 121.95      | 118.00   |
| 27  | B8    | 2856 | A    | C4-C5-C6   | 5.65  | 119.82      | 117.00   |
| 1   | AA    | 58   | C    | N3-C4-C5   | -5.65 | 119.64      | 121.90   |
| 1   | AA    | 223  | A    | C5-C6-N6   | -5.65 | 119.18      | 123.70   |
| 1   | AA    | 885  | G    | O4'-C1'-N9 | 5.65  | 112.72      | 108.20   |
| 3   | AV    | 43   | G    | O4'-C1'-N9 | 5.65  | 112.72      | 108.20   |
| 27  | B8    | 800  | A    | C5-C6-N1   | -5.65 | 114.88      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 866  | A    | C5-C6-N6   | -5.65 | 119.18      | 123.70   |
| 27  | B8    | 960  | A    | C5-C6-N6   | -5.65 | 119.18      | 123.70   |
| 27  | B8    | 2821 | A    | C5-C6-N6   | -5.65 | 119.18      | 123.70   |
| 27  | B8    | 2823 | A    | C5-C6-N6   | -5.65 | 119.18      | 123.70   |
| 1   | AA    | 130  | A    | C5-C6-N6   | -5.64 | 119.19      | 123.70   |
| 1   | AA    | 280  | C    | N3-C4-N4   | 5.64  | 121.95      | 118.00   |
| 1   | AA    | 422  | C    | N3-C4-C5   | -5.64 | 119.64      | 121.90   |
| 1   | AA    | 602  | A    | C5-C6-N1   | -5.64 | 114.88      | 117.70   |
| 1   | AA    | 1204 | A    | C4-C5-C6   | 5.64  | 119.82      | 117.00   |
| 26  | B7    | 108  | A    | C4-C5-C6   | 5.64  | 119.82      | 117.00   |
| 27  | B8    | 1507 | C    | N3-C4-C5   | -5.64 | 119.64      | 121.90   |
| 27  | B8    | 2246 | G    | O4'-C1'-N9 | 5.64  | 112.72      | 108.20   |
| 1   | AA    | 345  | C    | N3-C4-C5   | -5.64 | 119.64      | 121.90   |
| 1   | AA    | 716  | A    | C5-C6-N6   | -5.64 | 119.19      | 123.70   |
| 1   | AA    | 918  | A    | C5-C6-N6   | -5.64 | 119.19      | 123.70   |
| 1   | AA    | 1158 | C    | O4'-C1'-N1 | 5.64  | 112.71      | 108.20   |
| 27  | B8    | 101  | A    | C5-C6-N6   | -5.64 | 119.19      | 123.70   |
| 27  | B8    | 324  | A    | C5-C6-N6   | -5.64 | 119.19      | 123.70   |
| 27  | B8    | 1938 | A    | C5-C6-N6   | -5.64 | 119.19      | 123.70   |
| 27  | B8    | 2423 | U    | O4'-C1'-N1 | 5.64  | 112.71      | 108.20   |
| 27  | B8    | 2448 | A    | C5-C6-N6   | -5.64 | 119.19      | 123.70   |
| 1   | AA    | 315  | A    | C4-C5-C6   | 5.64  | 119.82      | 117.00   |
| 1   | AA    | 676  | A    | C4-C5-C6   | 5.64  | 119.82      | 117.00   |
| 1   | AA    | 1216 | A    | C4-C5-C6   | 5.64  | 119.82      | 117.00   |
| 1   | AA    | 1460 | C    | N3-C4-N4   | 5.64  | 121.95      | 118.00   |
| 27  | B8    | 1164 | C    | N3-C4-N4   | 5.64  | 121.95      | 118.00   |
| 27  | B8    | 1525 | A    | C5-C6-N6   | -5.64 | 119.19      | 123.70   |
| 27  | B8    | 1677 | A    | C5-C6-N1   | -5.64 | 114.88      | 117.70   |
| 27  | B8    | 1744 | A    | C5-C6-N1   | -5.64 | 114.88      | 117.70   |
| 1   | AA    | 348  | G    | O4'-C1'-N9 | 5.64  | 112.71      | 108.20   |
| 1   | AA    | 729  | A    | C5-C6-N6   | -5.64 | 119.19      | 123.70   |
| 1   | AA    | 928  | G    | O4'-C1'-N9 | 5.64  | 112.71      | 108.20   |
| 27  | B8    | 625  | G    | O4'-C1'-N9 | 5.64  | 112.71      | 108.20   |
| 27  | B8    | 739  | A    | C5-C6-N6   | -5.64 | 119.19      | 123.70   |
| 27  | B8    | 834  | G    | O4'-C1'-N9 | 5.64  | 112.71      | 108.20   |
| 27  | B8    | 1211 | C    | P-O3'-C3'  | 5.64  | 126.47      | 119.70   |
| 27  | B8    | 2005 | A    | O4'-C1'-N9 | 5.64  | 112.71      | 108.20   |
| 27  | B8    | 2103 | C    | N3-C4-N4   | 5.64  | 121.95      | 118.00   |
| 27  | B8    | 1699 | G    | O4'-C1'-N9 | 5.64  | 112.71      | 108.20   |
| 1   | AA    | 58   | C    | N3-C4-N4   | 5.64  | 121.95      | 118.00   |
| 1   | AA    | 197  | A    | C4-C5-C6   | 5.64  | 119.82      | 117.00   |
| 1   | AA    | 363  | A    | C5-C6-N6   | -5.64 | 119.19      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 946  | A    | C4-C5-C6   | 5.64  | 119.82      | 117.00   |
| 1   | AA    | 968  | A    | O4'-C1'-N9 | 5.64  | 112.71      | 108.20   |
| 1   | AA    | 1322 | C    | N3-C4-N4   | 5.64  | 121.94      | 118.00   |
| 27  | B8    | 272  | A    | C5-C6-N1   | -5.64 | 114.88      | 117.70   |
| 27  | B8    | 1327 | A    | C4-C5-C6   | 5.64  | 119.82      | 117.00   |
| 27  | B8    | 1672 | A    | C5-C6-N6   | -5.64 | 119.19      | 123.70   |
| 27  | B8    | 1727 | C    | N3-C4-N4   | 5.64  | 121.95      | 118.00   |
| 27  | B8    | 2428 | G    | P-O3'-C3'  | 5.64  | 126.46      | 119.70   |
| 1   | AA    | 238  | A    | O4'-C1'-N9 | 5.63  | 112.71      | 108.20   |
| 1   | AA    | 620  | C    | N3-C4-N4   | 5.63  | 121.94      | 118.00   |
| 1   | AA    | 747  | A    | C5-C6-N6   | -5.63 | 119.19      | 123.70   |
| 1   | AA    | 1155 | A    | C5-C6-N6   | -5.63 | 119.19      | 123.70   |
| 1   | AA    | 1327 | C    | N3-C4-N4   | 5.63  | 121.94      | 118.00   |
| 3   | AV    | 38   | G    | O4'-C1'-N9 | 5.63  | 112.71      | 108.20   |
| 27  | B8    | 88   | G    | C5-C6-O6   | -5.63 | 125.22      | 128.60   |
| 27  | B8    | 299  | A    | C5-C6-N1   | -5.63 | 114.88      | 117.70   |
| 27  | B8    | 430  | A    | C5-C6-N6   | -5.63 | 119.19      | 123.70   |
| 27  | B8    | 1037 | G    | O4'-C1'-N9 | 5.63  | 112.71      | 108.20   |
| 27  | B8    | 1039 | A    | C5-C6-N1   | -5.63 | 114.88      | 117.70   |
| 27  | B8    | 2058 | A    | O4'-C1'-N9 | 5.63  | 112.71      | 108.20   |
| 27  | B8    | 2705 | A    | C4-C5-C6   | 5.63  | 119.82      | 117.00   |
| 27  | B8    | 2757 | A    | C4-C5-C6   | 5.63  | 119.82      | 117.00   |
| 1   | AA    | 195  | A    | C4-C5-C6   | 5.63  | 119.82      | 117.00   |
| 1   | AA    | 1246 | A    | C4-C5-C6   | 5.63  | 119.82      | 117.00   |
| 3   | AV    | 40   | G    | O4'-C1'-N9 | 5.63  | 112.71      | 108.20   |
| 27  | B8    | 2199 | A    | C5-C6-N6   | -5.63 | 119.19      | 123.70   |
| 1   | AA    | 395  | C    | N3-C4-N4   | 5.63  | 121.94      | 118.00   |
| 1   | AA    | 600  | A    | C4-C5-C6   | 5.63  | 119.82      | 117.00   |
| 1   | AA    | 1000 | A    | C4-C5-C6   | 5.63  | 119.81      | 117.00   |
| 3   | AV    | 52   | A    | C5-C6-N1   | -5.63 | 114.88      | 117.70   |
| 3   | AV    | 77   | A    | C5-C6-N6   | -5.63 | 119.19      | 123.70   |
| 27  | B8    | 172  | A    | C5-C6-N6   | -5.63 | 119.19      | 123.70   |
| 27  | B8    | 507  | A    | C5-C6-N6   | -5.63 | 119.19      | 123.70   |
| 27  | B8    | 875  | G    | P-O3'-C3'  | 5.63  | 126.46      | 119.70   |
| 27  | B8    | 1570 | A    | C5-C6-N6   | -5.63 | 119.19      | 123.70   |
| 27  | B8    | 2635 | A    | C5-C6-N6   | -5.63 | 119.19      | 123.70   |
| 27  | B8    | 2675 | A    | C4-C5-C6   | 5.63  | 119.81      | 117.00   |
| 1   | AA    | 633  | G    | C5-C6-O6   | -5.63 | 125.22      | 128.60   |
| 1   | AA    | 913  | A    | C4-C5-C6   | 5.63  | 119.81      | 117.00   |
| 1   | AA    | 959  | A    | C5-C6-N6   | -5.63 | 119.20      | 123.70   |
| 1   | AA    | 1274 | A    | C4-C5-C6   | 5.63  | 119.81      | 117.00   |
| 1   | AA    | 1430 | A    | C5-C6-N1   | -5.63 | 114.89      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1500 | A    | O4'-C1'-N9 | 5.63  | 112.70      | 108.20   |
| 27  | B8    | 736  | C    | N3-C4-C5   | -5.63 | 119.65      | 121.90   |
| 27  | B8    | 819  | A    | C5-C6-N6   | -5.63 | 119.20      | 123.70   |
| 27  | B8    | 1014 | A    | C5-C6-N6   | -5.63 | 119.20      | 123.70   |
| 27  | B8    | 1353 | A    | C4-C5-C6   | 5.63  | 119.81      | 117.00   |
| 27  | B8    | 1870 | C    | N3-C4-N4   | 5.63  | 121.94      | 118.00   |
| 27  | B8    | 2450 | A    | C4-C5-C6   | 5.63  | 119.81      | 117.00   |
| 1   | AA    | 910  | C    | N3-C4-N4   | 5.63  | 121.94      | 118.00   |
| 1   | AA    | 983  | A    | C4-C5-C6   | 5.63  | 119.81      | 117.00   |
| 1   | AA    | 1117 | A    | C5-C6-N6   | -5.63 | 119.20      | 123.70   |
| 1   | AA    | 1430 | A    | C4-C5-C6   | 5.63  | 119.81      | 117.00   |
| 27  | B8    | 22   | C    | N3-C4-N4   | 5.63  | 121.94      | 118.00   |
| 27  | B8    | 672  | C    | N3-C4-N4   | 5.63  | 121.94      | 118.00   |
| 27  | B8    | 765  | C    | N3-C4-N4   | 5.63  | 121.94      | 118.00   |
| 1   | AA    | 210  | C    | N3-C4-C5   | -5.63 | 119.65      | 121.90   |
| 1   | AA    | 978  | A    | C5-C6-N1   | -5.63 | 114.89      | 117.70   |
| 1   | AA    | 1004 | A    | C5-C6-N6   | -5.63 | 119.20      | 123.70   |
| 27  | B8    | 1378 | A    | C5-C6-N1   | -5.63 | 114.89      | 117.70   |
| 27  | B8    | 2104 | C    | N3-C4-N4   | 5.63  | 121.94      | 118.00   |
| 27  | B8    | 2377 | A    | O4'-C1'-N9 | 5.63  | 112.70      | 108.20   |
| 27  | B8    | 2510 | C    | N3-C4-N4   | 5.63  | 121.94      | 118.00   |
| 27  | B8    | 2560 | A    | O4'-C1'-N9 | 5.63  | 112.70      | 108.20   |
| 27  | B8    | 2876 | G    | O4'-C1'-N9 | 5.63  | 112.70      | 108.20   |
| 1   | AA    | 155  | A    | P-O5'-C5'  | 5.62  | 129.90      | 120.90   |
| 1   | AA    | 307  | C    | N3-C4-N4   | 5.62  | 121.94      | 118.00   |
| 1   | AA    | 366  | A    | C5-C6-N1   | -5.62 | 114.89      | 117.70   |
| 1   | AA    | 1112 | C    | N3-C4-N4   | 5.62  | 121.94      | 118.00   |
| 1   | AA    | 1134 | G    | O4'-C1'-N9 | 5.62  | 112.70      | 108.20   |
| 26  | B7    | 31   | C    | N3-C4-N4   | 5.62  | 121.94      | 118.00   |
| 27  | B8    | 1665 | A    | C5-C6-N1   | -5.62 | 114.89      | 117.70   |
| 27  | B8    | 1805 | A    | C5-C6-N1   | -5.62 | 114.89      | 117.70   |
| 27  | B8    | 2059 | A    | C5-C6-N6   | -5.62 | 119.20      | 123.70   |
| 1   | AA    | 1031 | C    | N3-C4-N4   | 5.62  | 121.94      | 118.00   |
| 1   | AA    | 1203 | C    | N3-C4-C5   | -5.62 | 119.65      | 121.90   |
| 3   | AV    | 4    | C    | O4'-C1'-N1 | 5.62  | 112.70      | 108.20   |
| 3   | AV    | 26   | C    | N3-C4-C5   | -5.62 | 119.65      | 121.90   |
| 26  | B7    | 30   | C    | N3-C4-N4   | 5.62  | 121.94      | 118.00   |
| 27  | B8    | 1605 | C    | N3-C4-C5   | -5.62 | 119.65      | 121.90   |
| 27  | B8    | 1618 | A    | O4'-C1'-N9 | 5.62  | 112.70      | 108.20   |
| 27  | B8    | 2010 | G    | O4'-C1'-N9 | 5.62  | 112.70      | 108.20   |
| 27  | B8    | 2270 | A    | C5-C6-N1   | -5.62 | 114.89      | 117.70   |
| 27  | B8    | 2306 | C    | N3-C4-N4   | 5.62  | 121.94      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2432 | A    | C5-C6-N6   | -5.62 | 119.20      | 123.70   |
| 27  | B8    | 2600 | A    | C5-C6-N1   | -5.62 | 114.89      | 117.70   |
| 1   | AA    | 74   | A    | C5-C6-N1   | -5.62 | 114.89      | 117.70   |
| 1   | AA    | 248  | C    | N3-C4-N4   | 5.62  | 121.93      | 118.00   |
| 1   | AA    | 276  | G    | O4'-C1'-N9 | 5.62  | 112.70      | 108.20   |
| 1   | AA    | 1430 | A    | O4'-C1'-N9 | 5.62  | 112.70      | 108.20   |
| 1   | AA    | 1510 | C    | N3-C4-C5   | -5.62 | 119.65      | 121.90   |
| 27  | B8    | 62   | U    | P-O3'-C3'  | 5.62  | 126.45      | 119.70   |
| 27  | B8    | 332  | A    | C5-C6-N1   | -5.62 | 114.89      | 117.70   |
| 27  | B8    | 391  | A    | O4'-C1'-N9 | 5.62  | 112.70      | 108.20   |
| 27  | B8    | 603  | A    | C5-C6-N6   | -5.62 | 119.20      | 123.70   |
| 27  | B8    | 890  | C    | N3-C4-C5   | -5.62 | 119.65      | 121.90   |
| 27  | B8    | 2025 | C    | N3-C4-N4   | 5.62  | 121.94      | 118.00   |
| 27  | B8    | 2483 | C    | N3-C4-N4   | 5.62  | 121.94      | 118.00   |
| 27  | B8    | 2635 | A    | O4'-C1'-N9 | 5.62  | 112.70      | 108.20   |
| 27  | B8    | 2745 | C    | N3-C4-C5   | -5.62 | 119.65      | 121.90   |
| 1   | AA    | 495  | A    | O4'-C1'-N9 | 5.62  | 112.70      | 108.20   |
| 1   | AA    | 651  | C    | N3-C4-C5   | -5.62 | 119.65      | 121.90   |
| 1   | AA    | 983  | A    | C5-C6-N1   | -5.62 | 114.89      | 117.70   |
| 26  | B7    | 11   | C    | N3-C4-N4   | 5.62  | 121.93      | 118.00   |
| 27  | B8    | 226  | A    | C4-C5-C6   | 5.62  | 119.81      | 117.00   |
| 27  | B8    | 1348 | C    | N3-C4-N4   | 5.62  | 121.93      | 118.00   |
| 27  | B8    | 1795 | C    | N3-C4-N4   | 5.62  | 121.93      | 118.00   |
| 27  | B8    | 2178 | C    | N3-C4-C5   | -5.62 | 119.65      | 121.90   |
| 1   | AA    | 518  | C    | N3-C4-C5   | -5.62 | 119.65      | 121.90   |
| 1   | AA    | 532  | A    | C5-C6-N6   | -5.62 | 119.20      | 123.70   |
| 27  | B8    | 131  | A    | C5-C6-N1   | -5.62 | 114.89      | 117.70   |
| 27  | B8    | 244  | A    | C4-C5-C6   | 5.62  | 119.81      | 117.00   |
| 27  | B8    | 470  | A    | C5-C6-N1   | -5.62 | 114.89      | 117.70   |
| 27  | B8    | 542  | C    | N3-C4-N4   | 5.62  | 121.93      | 118.00   |
| 27  | B8    | 941  | A    | C5-C6-N6   | -5.62 | 119.20      | 123.70   |
| 27  | B8    | 1008 | A    | C5-C6-N6   | -5.62 | 119.20      | 123.70   |
| 27  | B8    | 1912 | A    | C4-C5-C6   | 5.62  | 119.81      | 117.00   |
| 27  | B8    | 2088 | A    | C5-C6-N1   | -5.62 | 114.89      | 117.70   |
| 27  | B8    | 2101 | A    | C5-C6-N6   | -5.62 | 119.20      | 123.70   |
| 26  | B7    | 68   | C    | N3-C4-N4   | 5.62  | 121.93      | 118.00   |
| 27  | B8    | 190  | A    | C5-C6-N1   | -5.62 | 114.89      | 117.70   |
| 27  | B8    | 825  | A    | C5-C6-N1   | -5.62 | 114.89      | 117.70   |
| 27  | B8    | 1229 | C    | N3-C4-C5   | -5.62 | 119.65      | 121.90   |
| 27  | B8    | 1395 | A    | C5-C6-N1   | -5.62 | 114.89      | 117.70   |
| 1   | AA    | 105  | G    | O4'-C1'-N9 | 5.62  | 112.69      | 108.20   |
| 1   | AA    | 712  | A    | C5-C6-N6   | -5.62 | 119.21      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1383 | C    | N3-C4-N4   | 5.62  | 121.93      | 118.00   |
| 27  | B8    | 804  | A    | O4'-C1'-N9 | 5.62  | 112.69      | 108.20   |
| 27  | B8    | 900  | A    | C4-C5-C6   | 5.62  | 119.81      | 117.00   |
| 27  | B8    | 1237 | A    | C5-C6-N6   | -5.62 | 119.21      | 123.70   |
| 27  | B8    | 1770 | G    | O4'-C1'-N9 | 5.62  | 112.69      | 108.20   |
| 27  | B8    | 1801 | A    | O4'-C1'-N9 | 5.62  | 112.69      | 108.20   |
| 1   | AA    | 456  | A    | C5-C6-N6   | -5.61 | 119.21      | 123.70   |
| 1   | AA    | 930  | C    | N3-C4-N4   | 5.61  | 121.93      | 118.00   |
| 1   | AA    | 1400 | C    | C6-N1-C1'  | -5.61 | 114.06      | 120.80   |
| 27  | B8    | 792  | A    | C5-C6-N6   | -5.61 | 119.21      | 123.70   |
| 27  | B8    | 823  | C    | N3-C4-N4   | 5.61  | 121.93      | 118.00   |
| 27  | B8    | 1284 | A    | C5-C6-N6   | -5.61 | 119.21      | 123.70   |
| 27  | B8    | 1354 | A    | C5-C6-N1   | -5.61 | 114.89      | 117.70   |
| 27  | B8    | 1689 | A    | O4'-C1'-N9 | 5.61  | 112.69      | 108.20   |
| 27  | B8    | 1735 | A    | C5-C6-N6   | -5.61 | 119.21      | 123.70   |
| 27  | B8    | 2384 | U    | O4'-C1'-N1 | 5.61  | 112.69      | 108.20   |
| 27  | B8    | 2607 | G    | O4'-C1'-N9 | 5.61  | 112.69      | 108.20   |
| 1   | AA    | 66   | A    | C5-C6-N6   | -5.61 | 119.21      | 123.70   |
| 1   | AA    | 325  | A    | C4-C5-C6   | 5.61  | 119.81      | 117.00   |
| 1   | AA    | 897  | C    | N3-C4-N4   | 5.61  | 121.93      | 118.00   |
| 1   | AA    | 1428 | A    | C5-C6-N6   | -5.61 | 119.21      | 123.70   |
| 27  | B8    | 2164 | C    | C2-N1-C1'  | 5.61  | 124.97      | 118.80   |
| 31  | B6    | 189  | ALA  | N-CA-CB    | 5.61  | 117.96      | 110.10   |
| 1   | AA    | 807  | A    | C4-C5-C6   | 5.61  | 119.81      | 117.00   |
| 1   | AA    | 1349 | A    | C4-C5-C6   | 5.61  | 119.81      | 117.00   |
| 27  | B8    | 853  | C    | N3-C4-N4   | 5.61  | 121.93      | 118.00   |
| 27  | B8    | 1172 | C    | N3-C4-C5   | -5.61 | 119.66      | 121.90   |
| 27  | B8    | 1428 | C    | O4'-C1'-N1 | 5.61  | 112.69      | 108.20   |
| 27  | B8    | 2247 | A    | C5-C6-N6   | -5.61 | 119.21      | 123.70   |
| 27  | B8    | 2660 | A    | C5-C6-N1   | -5.61 | 114.89      | 117.70   |
| 2   | AX    | 21   | A    | C5-C6-N6   | -5.61 | 119.21      | 123.70   |
| 3   | AV    | 16   | C    | N3-C4-N4   | 5.61  | 121.93      | 118.00   |
| 27  | B8    | 661  | A    | O4'-C1'-N9 | 5.61  | 112.69      | 108.20   |
| 27  | B8    | 2369 | A    | O4'-C1'-N9 | 5.61  | 112.69      | 108.20   |
| 1   | AA    | 187  | G    | N3-C2-N2   | 5.61  | 123.83      | 119.90   |
| 1   | AA    | 461  | A    | O4'-C1'-N9 | 5.61  | 112.69      | 108.20   |
| 1   | AA    | 728  | A    | C4-C5-C6   | 5.61  | 119.80      | 117.00   |
| 1   | AA    | 1360 | A    | C5-C6-N1   | -5.61 | 114.90      | 117.70   |
| 27  | B8    | 946  | C    | N3-C4-C5   | -5.61 | 119.66      | 121.90   |
| 27  | B8    | 1597 | A    | C5-C6-N6   | -5.61 | 119.21      | 123.70   |
| 27  | B8    | 1833 | C    | N3-C4-C5   | -5.61 | 119.66      | 121.90   |
| 27  | B8    | 2578 | G    | O4'-C1'-N9 | 5.61  | 112.69      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2583 | G    | O4'-C1'-N9 | 5.61  | 112.69      | 108.20   |
| 27  | B8    | 2590 | A    | C5-C6-N1   | -5.61 | 114.90      | 117.70   |
| 27  | B8    | 2785 | C    | N3-C4-N4   | 5.61  | 121.93      | 118.00   |
| 1   | AA    | 438  | U    | O4'-C1'-N1 | 5.61  | 112.68      | 108.20   |
| 1   | AA    | 1251 | A    | C5-C6-N1   | -5.61 | 114.90      | 117.70   |
| 1   | AA    | 1493 | A    | C5-C6-N6   | -5.61 | 119.22      | 123.70   |
| 27  | B8    | 2154 | A    | C5-C6-N1   | -5.61 | 114.90      | 117.70   |
| 27  | B8    | 2241 | A    | C5-C6-N1   | -5.61 | 114.90      | 117.70   |
| 1   | AA    | 1157 | A    | C5-C6-N1   | -5.60 | 114.90      | 117.70   |
| 1   | AA    | 1311 | A    | C5-C6-N6   | -5.60 | 119.22      | 123.70   |
| 1   | AA    | 1519 | A    | O4'-C1'-N9 | 5.60  | 112.68      | 108.20   |
| 1   | AA    | 1542 | A    | C5-C6-N6   | -5.60 | 119.22      | 123.70   |
| 27  | B8    | 814  | C    | N3-C4-C5   | -5.60 | 119.66      | 121.90   |
| 27  | B8    | 1591 | A    | C5-C6-N6   | -5.60 | 119.22      | 123.70   |
| 27  | B8    | 1839 | G    | O4'-C1'-N9 | 5.60  | 112.68      | 108.20   |
| 1   | AA    | 635  | A    | O4'-C1'-N9 | 5.60  | 112.68      | 108.20   |
| 27  | B8    | 1987 | A    | C4-C5-C6   | 5.60  | 119.80      | 117.00   |
| 27  | B8    | 2805 | C    | N3-C4-N4   | 5.60  | 121.92      | 118.00   |
| 1   | AA    | 366  | A    | C5-C6-N6   | -5.60 | 119.22      | 123.70   |
| 1   | AA    | 1151 | A    | C5-C6-N1   | -5.60 | 114.90      | 117.70   |
| 27  | B8    | 173  | A    | C4-C5-C6   | 5.60  | 119.80      | 117.00   |
| 27  | B8    | 227  | A    | C5-C6-N1   | -5.60 | 114.90      | 117.70   |
| 27  | B8    | 1322 | A    | C5-C6-N1   | -5.60 | 114.90      | 117.70   |
| 27  | B8    | 2342 | C    | N3-C4-N4   | 5.60  | 121.92      | 118.00   |
| 1   | AA    | 643  | C    | N3-C4-N4   | 5.60  | 121.92      | 118.00   |
| 1   | AA    | 796  | C    | N3-C4-C5   | -5.60 | 119.66      | 121.90   |
| 1   | AA    | 1480 | A    | C5-C6-N1   | -5.60 | 114.90      | 117.70   |
| 26  | B7    | 6    | G    | O4'-C1'-N9 | 5.60  | 112.68      | 108.20   |
| 27  | B8    | 563  | A    | C5-C6-N1   | -5.60 | 114.90      | 117.70   |
| 27  | B8    | 749  | A    | C5-C6-N1   | -5.60 | 114.90      | 117.70   |
| 27  | B8    | 1462 | C    | N3-C4-N4   | 5.60  | 121.92      | 118.00   |
| 27  | B8    | 1806 | C    | N3-C4-C5   | -5.60 | 119.66      | 121.90   |
| 27  | B8    | 1824 | G    | O4'-C1'-N9 | 5.60  | 112.68      | 108.20   |
| 27  | B8    | 2160 | C    | N3-C4-N4   | 5.60  | 121.92      | 118.00   |
| 27  | B8    | 2317 | A    | C5-C6-N1   | -5.60 | 114.90      | 117.70   |
| 27  | B8    | 2821 | A    | C5-C6-N1   | -5.60 | 114.90      | 117.70   |
| 1   | AA    | 1    | A    | C5-C6-N6   | -5.60 | 119.22      | 123.70   |
| 1   | AA    | 1378 | C    | N3-C4-N4   | 5.60  | 121.92      | 118.00   |
| 1   | AA    | 1461 | G    | C5-C6-O6   | -5.60 | 125.24      | 128.60   |
| 27  | B8    | 63   | A    | C4-C5-C6   | 5.60  | 119.80      | 117.00   |
| 27  | B8    | 128  | C    | N3-C4-C5   | -5.60 | 119.66      | 121.90   |
| 27  | B8    | 144  | A    | C5-C6-N1   | -5.60 | 114.90      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 782  | A    | C5-C6-N6   | -5.60 | 119.22      | 123.70   |
| 27  | B8    | 2012 | G    | O4'-C1'-N9 | 5.60  | 112.68      | 108.20   |
| 1   | AA    | 519  | C    | N3-C4-N4   | 5.60  | 121.92      | 118.00   |
| 3   | AV    | 1    | C    | N3-C4-C5   | -5.60 | 119.66      | 121.90   |
| 27  | B8    | 1001 | A    | C5-C6-N1   | -5.60 | 114.90      | 117.70   |
| 27  | B8    | 1147 | A    | C4-C5-C6   | 5.60  | 119.80      | 117.00   |
| 27  | B8    | 1615 | C    | N3-C4-C5   | -5.60 | 119.66      | 121.90   |
| 27  | B8    | 1989 | G    | O4'-C1'-N9 | 5.60  | 112.68      | 108.20   |
| 1   | AA    | 520  | A    | C5-C6-N1   | -5.59 | 114.90      | 117.70   |
| 1   | AA    | 559  | A    | C5-C6-N1   | -5.59 | 114.90      | 117.70   |
| 1   | AA    | 648  | A    | C5-C6-N6   | -5.59 | 119.22      | 123.70   |
| 1   | AA    | 808  | C    | N3-C4-N4   | 5.59  | 121.92      | 118.00   |
| 1   | AA    | 913  | A    | C5-C6-N1   | -5.59 | 114.90      | 117.70   |
| 1   | AA    | 1413 | A    | C4-C5-C6   | 5.59  | 119.80      | 117.00   |
| 27  | B8    | 83   | A    | C5-C6-N1   | -5.59 | 114.90      | 117.70   |
| 27  | B8    | 199  | A    | O4'-C1'-N9 | 5.59  | 112.68      | 108.20   |
| 27  | B8    | 240  | C    | N3-C4-N4   | 5.59  | 121.92      | 118.00   |
| 27  | B8    | 332  | A    | C5-C6-N6   | -5.59 | 119.22      | 123.70   |
| 27  | B8    | 972  | A    | C5-C6-N6   | -5.59 | 119.22      | 123.70   |
| 27  | B8    | 1095 | A    | C5-C6-N1   | -5.59 | 114.90      | 117.70   |
| 27  | B8    | 1347 | A    | C4-C5-C6   | 5.59  | 119.80      | 117.00   |
| 27  | B8    | 1349 | C    | N3-C4-N4   | 5.59  | 121.92      | 118.00   |
| 27  | B8    | 1847 | A    | C5-C6-N6   | -5.59 | 119.22      | 123.70   |
| 27  | B8    | 2112 | G    | C5-C6-O6   | -5.59 | 125.24      | 128.60   |
| 27  | B8    | 2295 | C    | N3-C4-C5   | -5.59 | 119.66      | 121.90   |
| 1   | AA    | 1476 | A    | C4-C5-C6   | 5.59  | 119.80      | 117.00   |
| 27  | B8    | 1090 | A    | C5-C6-N1   | -5.59 | 114.90      | 117.70   |
| 27  | B8    | 1877 | A    | C5-C6-N6   | -5.59 | 119.23      | 123.70   |
| 27  | B8    | 2178 | C    | N3-C4-N4   | 5.59  | 121.92      | 118.00   |
| 1   | AA    | 372  | C    | N3-C4-C5   | -5.59 | 119.66      | 121.90   |
| 1   | AA    | 1100 | C    | N3-C4-N4   | 5.59  | 121.92      | 118.00   |
| 27  | B8    | 89   | A    | C5-C6-N6   | -5.59 | 119.23      | 123.70   |
| 27  | B8    | 514  | A    | C4-C5-C6   | 5.59  | 119.80      | 117.00   |
| 27  | B8    | 564  | C    | N3-C4-C5   | -5.59 | 119.66      | 121.90   |
| 27  | B8    | 903  | C    | N3-C4-C5   | -5.59 | 119.66      | 121.90   |
| 27  | B8    | 989  | G    | N3-C2-N2   | 5.59  | 123.81      | 119.90   |
| 27  | B8    | 1583 | A    | C5-C6-N6   | -5.59 | 119.23      | 123.70   |
| 27  | B8    | 1858 | A    | C4-C5-C6   | 5.59  | 119.80      | 117.00   |
| 27  | B8    | 1960 | A    | C5-C6-N1   | -5.59 | 114.91      | 117.70   |
| 27  | B8    | 2538 | C    | N3-C4-N4   | 5.59  | 121.91      | 118.00   |
| 27  | B8    | 2758 | A    | C4-C5-C6   | 5.59  | 119.80      | 117.00   |
| 1   | AA    | 206  | C    | N3-C4-C5   | -5.59 | 119.66      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 267  | C    | N3-C4-C5    | -5.59 | 119.66      | 121.90   |
| 1   | AA    | 704  | A    | C5-C6-N6    | -5.59 | 119.23      | 123.70   |
| 1   | AA    | 718  | A    | C5-C6-N1    | -5.59 | 114.91      | 117.70   |
| 1   | AA    | 948  | C    | N3-C4-C5    | -5.59 | 119.66      | 121.90   |
| 1   | AA    | 1538 | C    | N3-C4-N4    | 5.59  | 121.91      | 118.00   |
| 26  | B7    | 47   | C    | N3-C4-N4    | 5.59  | 121.91      | 118.00   |
| 26  | B7    | 83   | G    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 27  | B8    | 278  | A    | C5-C6-N1    | -5.59 | 114.91      | 117.70   |
| 27  | B8    | 541  | A    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 27  | B8    | 753  | A    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 27  | B8    | 962  | G    | N3-C2-N2    | 5.59  | 123.81      | 119.90   |
| 27  | B8    | 1959 | G    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 27  | B8    | 2055 | C    | N3-C4-C5    | -5.59 | 119.67      | 121.90   |
| 27  | B8    | 2314 | A    | C4-C5-C6    | 5.59  | 119.80      | 117.00   |
| 27  | B8    | 2478 | A    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 1   | AA    | 680  | C    | N3-C4-N4    | 5.59  | 121.91      | 118.00   |
| 1   | AA    | 806  | C    | N3-C4-N4    | 5.59  | 121.91      | 118.00   |
| 27  | B8    | 472  | A    | C5-C6-N6    | -5.59 | 119.23      | 123.70   |
| 27  | B8    | 592  | A    | C5-C6-N6    | -5.59 | 119.23      | 123.70   |
| 27  | B8    | 2283 | C    | P-O5'-C5'   | 5.59  | 129.84      | 120.90   |
| 27  | B8    | 2307 | G    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 1   | AA    | 510  | A    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 1   | AA    | 600  | A    | C5-C6-N1    | -5.59 | 114.91      | 117.70   |
| 1   | AA    | 658  | C    | N3-C4-N4    | 5.59  | 121.91      | 118.00   |
| 1   | AA    | 767  | A    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 1   | AA    | 1005 | A    | C5-C6-N1    | -5.59 | 114.91      | 117.70   |
| 1   | AA    | 1192 | C    | N3-C4-N4    | 5.59  | 121.91      | 118.00   |
| 27  | B8    | 300  | A    | C5-C6-N1    | -5.59 | 114.91      | 117.70   |
| 27  | B8    | 341  | C    | N3-C4-C5    | -5.59 | 119.67      | 121.90   |
| 27  | B8    | 382  | A    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 27  | B8    | 693  | A    | C5-C6-N1    | -5.59 | 114.91      | 117.70   |
| 27  | B8    | 1284 | A    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 27  | B8    | 1785 | A    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 1   | AA    | 452  | A    | C4-C5-C6    | 5.58  | 119.79      | 117.00   |
| 1   | AA    | 1524 | C    | N3-C4-C5    | -5.58 | 119.67      | 121.90   |
| 27  | B8    | 430  | A    | C5-C6-N1    | -5.58 | 114.91      | 117.70   |
| 27  | B8    | 1815 | A    | C4-C5-C6    | 5.58  | 119.79      | 117.00   |
| 27  | B8    | 2254 | C    | N3-C4-N4    | 5.58  | 121.91      | 118.00   |
| 27  | B8    | 2685 | G    | O4'-C1'-N9  | 5.58  | 112.67      | 108.20   |
| 27  | B8    | 2813 | A    | C5-C6-N6    | -5.58 | 119.23      | 123.70   |
| 1   | AA    | 172  | A    | C4-C5-C6    | 5.58  | 119.79      | 117.00   |
| 1   | AA    | 243  | A    | C2'-C3'-O3' | 5.58  | 122.64      | 113.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 309  | A    | C5-C6-N6   | -5.58 | 119.23      | 123.70   |
| 27  | B8    | 559  | G    | O4'-C1'-N9 | 5.58  | 112.67      | 108.20   |
| 27  | B8    | 1013 | C    | N3-C4-N4   | 5.58  | 121.91      | 118.00   |
| 27  | B8    | 1913 | A    | C5-C6-N1   | -5.58 | 114.91      | 117.70   |
| 27  | B8    | 2498 | C    | N3-C4-N4   | 5.58  | 121.91      | 118.00   |
| 27  | B8    | 2539 | C    | N3-C4-C5   | -5.58 | 119.67      | 121.90   |
| 27  | B8    | 2665 | A    | O4'-C1'-N9 | 5.58  | 112.67      | 108.20   |
| 1   | AA    | 233  | C    | N3-C4-N4   | 5.58  | 121.91      | 118.00   |
| 1   | AA    | 549  | C    | N3-C4-N4   | 5.58  | 121.91      | 118.00   |
| 27  | B8    | 165  | A    | C5-C6-N1   | -5.58 | 114.91      | 117.70   |
| 27  | B8    | 309  | A    | O4'-C1'-N9 | 5.58  | 112.67      | 108.20   |
| 27  | B8    | 745  | G    | N3-C2-N2   | 5.58  | 123.81      | 119.90   |
| 27  | B8    | 901  | C    | N3-C4-N4   | 5.58  | 121.91      | 118.00   |
| 27  | B8    | 1106 | G    | O4'-C1'-N9 | 5.58  | 112.67      | 108.20   |
| 27  | B8    | 1392 | A    | C5-C6-N6   | -5.58 | 119.23      | 123.70   |
| 27  | B8    | 1418 | G    | N3-C2-N2   | 5.58  | 123.81      | 119.90   |
| 27  | B8    | 1447 | C    | N3-C4-C5   | -5.58 | 119.67      | 121.90   |
| 27  | B8    | 2196 | C    | N3-C4-C5   | -5.58 | 119.67      | 121.90   |
| 27  | B8    | 2255 | G    | O4'-C1'-N9 | 5.58  | 112.66      | 108.20   |
| 27  | B8    | 2310 | C    | N3-C4-C5   | -5.58 | 119.67      | 121.90   |
| 27  | B8    | 2540 | C    | N3-C4-N4   | 5.58  | 121.91      | 118.00   |
| 1   | AA    | 87   | C    | N3-C4-N4   | 5.58  | 121.91      | 118.00   |
| 1   | AA    | 263  | A    | C5-C6-N1   | -5.58 | 114.91      | 117.70   |
| 1   | AA    | 607  | A    | C5-C6-N6   | -5.58 | 119.24      | 123.70   |
| 1   | AA    | 1320 | C    | N3-C4-C5   | -5.58 | 119.67      | 121.90   |
| 3   | AV    | 24   | C    | N3-C4-C5   | -5.58 | 119.67      | 121.90   |
| 27  | B8    | 1033 | U    | O4'-C1'-N1 | 5.58  | 112.66      | 108.20   |
| 27  | B8    | 1043 | C    | N3-C4-N4   | 5.58  | 121.91      | 118.00   |
| 27  | B8    | 1548 | A    | C4-C5-C6   | 5.58  | 119.79      | 117.00   |
| 27  | B8    | 1966 | A    | C5-C6-N6   | -5.58 | 119.24      | 123.70   |
| 27  | B8    | 2346 | A    | C5-C6-N6   | -5.58 | 119.24      | 123.70   |
| 1   | AA    | 80   | A    | C5-C6-N6   | -5.58 | 119.24      | 123.70   |
| 1   | AA    | 1147 | C    | N3-C4-C5   | -5.58 | 119.67      | 121.90   |
| 1   | AA    | 1462 | C    | N3-C4-N4   | 5.58  | 121.91      | 118.00   |
| 3   | AV    | 18   | U    | O4'-C1'-N1 | 5.58  | 112.66      | 108.20   |
| 3   | AV    | 49   | C    | N3-C4-N4   | 5.58  | 121.91      | 118.00   |
| 26  | B7    | 97   | C    | N3-C4-N4   | 5.58  | 121.91      | 118.00   |
| 27  | B8    | 173  | A    | C5-C6-N6   | -5.58 | 119.24      | 123.70   |
| 27  | B8    | 585  | G    | O4'-C1'-N9 | 5.58  | 112.66      | 108.20   |
| 27  | B8    | 804  | A    | C5-C6-N6   | -5.58 | 119.24      | 123.70   |
| 27  | B8    | 1454 | C    | C2-N1-C1'  | 5.58  | 124.94      | 118.80   |
| 27  | B8    | 1551 | A    | C5-C6-N6   | -5.58 | 119.24      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1552 | A    | O4'-C1'-N9 | 5.58  | 112.66      | 108.20   |
| 27  | B8    | 1967 | C    | N3-C4-N4   | 5.58  | 121.90      | 118.00   |
| 27  | B8    | 2577 | A    | C5-C6-N1   | -5.58 | 114.91      | 117.70   |
| 27  | B8    | 2638 | G    | O4'-C1'-N9 | 5.58  | 112.66      | 108.20   |
| 27  | B8    | 2747 | G    | O4'-C1'-N9 | 5.58  | 112.66      | 108.20   |
| 1   | AA    | 1050 | G    | O4'-C1'-N9 | 5.58  | 112.66      | 108.20   |
| 26  | B7    | 57   | A    | O4'-C1'-N9 | 5.58  | 112.66      | 108.20   |
| 27  | B8    | 264  | C    | N3-C4-N4   | 5.58  | 121.90      | 118.00   |
| 27  | B8    | 2335 | A    | C5-C6-N1   | -5.58 | 114.91      | 117.70   |
| 1   | AA    | 7    | A    | O4'-C1'-N9 | 5.58  | 112.66      | 108.20   |
| 1   | AA    | 344  | A    | C5-C6-N6   | -5.58 | 119.24      | 123.70   |
| 1   | AA    | 351  | G    | O4'-C1'-N9 | 5.58  | 112.66      | 108.20   |
| 1   | AA    | 754  | C    | N3-C4-C5   | -5.58 | 119.67      | 121.90   |
| 3   | AV    | 14   | A    | C5-C6-N1   | -5.58 | 114.91      | 117.70   |
| 27  | B8    | 719  | C    | N3-C4-N4   | 5.58  | 121.90      | 118.00   |
| 27  | B8    | 1378 | A    | O4'-C1'-N9 | 5.58  | 112.66      | 108.20   |
| 1   | AA    | 1110 | A    | C5-C6-N1   | -5.57 | 114.91      | 117.70   |
| 1   | AA    | 1198 | G    | O4'-C1'-N9 | 5.57  | 112.66      | 108.20   |
| 27  | B8    | 7    | G    | O4'-C1'-N9 | 5.57  | 112.66      | 108.20   |
| 27  | B8    | 504  | A    | C5-C6-N6   | -5.57 | 119.24      | 123.70   |
| 27  | B8    | 634  | C    | N3-C4-C5   | -5.57 | 119.67      | 121.90   |
| 27  | B8    | 1403 | A    | C5-C6-N1   | -5.57 | 114.91      | 117.70   |
| 27  | B8    | 1494 | A    | C4-C5-C6   | 5.57  | 119.79      | 117.00   |
| 27  | B8    | 1494 | A    | C5-C6-N1   | -5.57 | 114.91      | 117.70   |
| 27  | B8    | 1518 | C    | N3-C4-N4   | 5.57  | 121.90      | 118.00   |
| 27  | B8    | 1552 | A    | P-O5'-C5'  | 5.57  | 129.82      | 120.90   |
| 27  | B8    | 1877 | A    | C5-C6-N1   | -5.57 | 114.91      | 117.70   |
| 27  | B8    | 2433 | A    | C5-C6-N6   | -5.57 | 119.24      | 123.70   |
| 27  | B8    | 795  | C    | N3-C4-C5   | -5.57 | 119.67      | 121.90   |
| 27  | B8    | 865  | C    | N3-C4-N4   | 5.57  | 121.90      | 118.00   |
| 27  | B8    | 2417 | C    | N3-C4-C5   | -5.57 | 119.67      | 121.90   |
| 29  | BB    | 104  | MET  | CG-SD-CE   | -5.57 | 91.28       | 100.20   |
| 1   | AA    | 1382 | C    | N3-C4-N4   | 5.57  | 121.90      | 118.00   |
| 27  | B8    | 163  | C    | N3-C4-C5   | -5.57 | 119.67      | 121.90   |
| 27  | B8    | 272  | A    | C5-C6-N6   | -5.57 | 119.24      | 123.70   |
| 27  | B8    | 351  | C    | N3-C4-N4   | 5.57  | 121.90      | 118.00   |
| 27  | B8    | 1006 | C    | N3-C4-N4   | 5.57  | 121.90      | 118.00   |
| 27  | B8    | 1052 | C    | N3-C4-C5   | -5.57 | 119.67      | 121.90   |
| 27  | B8    | 1218 | G    | O4'-C1'-N9 | 5.57  | 112.66      | 108.20   |
| 27  | B8    | 1308 | A    | C4-C5-C6   | 5.57  | 119.78      | 117.00   |
| 27  | B8    | 1786 | A    | C5-C6-N6   | -5.57 | 119.24      | 123.70   |
| 27  | B8    | 1794 | A    | C4-C5-C6   | 5.57  | 119.79      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2061 | G    | O4'-C1'-N9 | 5.57  | 112.66      | 108.20   |
| 27  | B8    | 2314 | A    | O4'-C1'-N9 | 5.57  | 112.66      | 108.20   |
| 27  | B8    | 2776 | A    | C5-C6-N6   | -5.57 | 119.24      | 123.70   |
| 27  | B8    | 41   | C    | N3-C4-N4   | 5.57  | 121.90      | 118.00   |
| 27  | B8    | 262  | A    | O4'-C1'-N9 | 5.57  | 112.66      | 108.20   |
| 27  | B8    | 344  | A    | C5-C6-N6   | -5.57 | 119.25      | 123.70   |
| 27  | B8    | 433  | C    | N3-C4-N4   | 5.57  | 121.90      | 118.00   |
| 27  | B8    | 1414 | C    | N3-C4-N4   | 5.57  | 121.90      | 118.00   |
| 27  | B8    | 2023 | C    | N3-C4-C5   | -5.57 | 119.67      | 121.90   |
| 27  | B8    | 2164 | C    | N3-C4-N4   | 5.57  | 121.90      | 118.00   |
| 1   | AA    | 996  | A    | O4'-C1'-N9 | 5.57  | 112.66      | 108.20   |
| 3   | AV    | 51   | G    | O4'-C1'-N9 | 5.57  | 112.66      | 108.20   |
| 27  | B8    | 450  | G    | O4'-C1'-N9 | 5.57  | 112.65      | 108.20   |
| 27  | B8    | 637  | A    | C5-C6-N1   | -5.57 | 114.92      | 117.70   |
| 27  | B8    | 1532 | A    | C5-C6-N1   | -5.57 | 114.92      | 117.70   |
| 27  | B8    | 2193 | G    | O4'-C1'-N9 | 5.57  | 112.65      | 108.20   |
| 1   | AA    | 143  | A    | C5-C6-N6   | -5.57 | 119.25      | 123.70   |
| 26  | B7    | 101  | A    | C4-C5-C6   | 5.57  | 119.78      | 117.00   |
| 27  | B8    | 833  | A    | C5-C6-N6   | -5.57 | 119.25      | 123.70   |
| 27  | B8    | 1020 | A    | C5-C6-N6   | -5.57 | 119.25      | 123.70   |
| 27  | B8    | 1169 | A    | C5-C6-N1   | -5.57 | 114.92      | 117.70   |
| 27  | B8    | 1214 | A    | C4-C5-C6   | 5.57  | 119.78      | 117.00   |
| 27  | B8    | 1429 | G    | O4'-C1'-N9 | 5.57  | 112.65      | 108.20   |
| 27  | B8    | 1937 | A    | C4-C5-C6   | 5.57  | 119.78      | 117.00   |
| 27  | B8    | 1969 | A    | C5-C6-N6   | -5.57 | 119.25      | 123.70   |
| 27  | B8    | 2058 | A    | C5-C6-N6   | -5.57 | 119.25      | 123.70   |
| 1   | AA    | 1026 | G    | O4'-C1'-N9 | 5.56  | 112.65      | 108.20   |
| 1   | AA    | 1191 | A    | C5-C6-N1   | -5.56 | 114.92      | 117.70   |
| 27  | B8    | 2114 | A    | C5-C6-N1   | -5.56 | 114.92      | 117.70   |
| 27  | B8    | 2699 | C    | N3-C4-N4   | 5.56  | 121.89      | 118.00   |
| 1   | AA    | 104  | G    | O4'-C1'-N9 | 5.56  | 112.65      | 108.20   |
| 1   | AA    | 503  | C    | N3-C4-C5   | -5.56 | 119.67      | 121.90   |
| 1   | AA    | 980  | C    | N3-C4-N4   | 5.56  | 121.89      | 118.00   |
| 1   | AA    | 1302 | C    | N3-C4-C5   | -5.56 | 119.67      | 121.90   |
| 26  | B7    | 37   | C    | N3-C4-C5   | -5.56 | 119.67      | 121.90   |
| 27  | B8    | 739  | A    | O4'-C1'-N9 | 5.56  | 112.65      | 108.20   |
| 27  | B8    | 908  | C    | N3-C4-C5   | -5.56 | 119.67      | 121.90   |
| 27  | B8    | 1027 | A    | C5-C6-N1   | -5.56 | 114.92      | 117.70   |
| 27  | B8    | 1211 | C    | O4'-C1'-N1 | 5.56  | 112.65      | 108.20   |
| 27  | B8    | 1281 | G    | O4'-C1'-N9 | 5.56  | 112.65      | 108.20   |
| 27  | B8    | 1654 | A    | C5-C6-N1   | -5.56 | 114.92      | 117.70   |
| 27  | B8    | 2047 | C    | N3-C4-C5   | -5.56 | 119.67      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2712 | C    | N3-C4-N4   | 5.56  | 121.89      | 118.00   |
| 27  | B8    | 1632 | A    | C5-C6-N6   | -5.56 | 119.25      | 123.70   |
| 27  | B8    | 2525 | G    | O4'-C1'-N9 | 5.56  | 112.65      | 108.20   |
| 27  | B8    | 2799 | A    | C5-C6-N6   | -5.56 | 119.25      | 123.70   |
| 1   | AA    | 234  | C    | N3-C4-N4   | 5.56  | 121.89      | 118.00   |
| 1   | AA    | 432  | A    | O4'-C1'-N9 | 5.56  | 112.65      | 108.20   |
| 1   | AA    | 642  | A    | C5-C6-N1   | -5.56 | 114.92      | 117.70   |
| 1   | AA    | 924  | C    | N3-C4-C5   | -5.56 | 119.68      | 121.90   |
| 1   | AA    | 1408 | A    | C4-C5-C6   | 5.56  | 119.78      | 117.00   |
| 26  | B7    | 30   | C    | N3-C4-C5   | -5.56 | 119.68      | 121.90   |
| 27  | B8    | 209  | C    | N3-C4-C5   | -5.56 | 119.68      | 121.90   |
| 27  | B8    | 334  | C    | N3-C4-N4   | 5.56  | 121.89      | 118.00   |
| 27  | B8    | 643  | A    | C5-C6-N6   | -5.56 | 119.25      | 123.70   |
| 27  | B8    | 1291 | C    | N3-C4-N4   | 5.56  | 121.89      | 118.00   |
| 27  | B8    | 1295 | C    | N3-C4-N4   | 5.56  | 121.89      | 118.00   |
| 27  | B8    | 1403 | A    | C5-C6-N6   | -5.56 | 119.25      | 123.70   |
| 27  | B8    | 1431 | A    | O4'-C1'-N9 | 5.56  | 112.65      | 108.20   |
| 27  | B8    | 1625 | C    | N3-C4-N4   | 5.56  | 121.89      | 118.00   |
| 1   | AA    | 178  | C    | N3-C4-N4   | 5.56  | 121.89      | 118.00   |
| 1   | AA    | 306  | A    | C5-C6-N6   | -5.56 | 119.25      | 123.70   |
| 1   | AA    | 573  | A    | C5-C6-N1   | -5.56 | 114.92      | 117.70   |
| 27  | B8    | 480  | A    | C5-C6-N6   | -5.56 | 119.25      | 123.70   |
| 27  | B8    | 882  | G    | O4'-C1'-N9 | 5.56  | 112.65      | 108.20   |
| 27  | B8    | 1313 | U    | O4'-C1'-N1 | 5.56  | 112.65      | 108.20   |
| 27  | B8    | 1323 | C    | N3-C4-N4   | 5.56  | 121.89      | 118.00   |
| 27  | B8    | 1761 | C    | N3-C4-N4   | 5.56  | 121.89      | 118.00   |
| 27  | B8    | 1890 | A    | O4'-C1'-N9 | 5.56  | 112.64      | 108.20   |
| 1   | AA    | 749  | A    | C5-C6-N1   | -5.56 | 114.92      | 117.70   |
| 1   | AA    | 1516 | G    | O4'-C1'-N9 | 5.56  | 112.64      | 108.20   |
| 3   | AV    | 14   | A    | C5-C6-N6   | -5.56 | 119.25      | 123.70   |
| 27  | B8    | 156  | A    | C5-C6-N6   | -5.56 | 119.25      | 123.70   |
| 27  | B8    | 610  | C    | N3-C4-N4   | 5.56  | 121.89      | 118.00   |
| 1   | AA    | 392  | C    | N3-C4-N4   | 5.55  | 121.89      | 118.00   |
| 1   | AA    | 767  | A    | C5-C6-N6   | -5.55 | 119.26      | 123.70   |
| 1   | AA    | 1389 | C    | N3-C4-N4   | 5.55  | 121.89      | 118.00   |
| 27  | B8    | 788  | A    | C5-C6-N6   | -5.55 | 119.26      | 123.70   |
| 27  | B8    | 1349 | C    | N3-C4-C5   | -5.55 | 119.68      | 121.90   |
| 27  | B8    | 2029 | G    | N3-C2-N2   | 5.55  | 123.79      | 119.90   |
| 27  | B8    | 2705 | A    | C5-C6-N6   | -5.55 | 119.26      | 123.70   |
| 27  | B8    | 2764 | A    | C5-C6-N1   | -5.55 | 114.92      | 117.70   |
| 1   | AA    | 78   | A    | C5-C6-N1   | -5.55 | 114.92      | 117.70   |
| 27  | B8    | 348  | A    | C5-C6-N1   | -5.55 | 114.92      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 621  | A    | C5-C6-N6   | -5.55 | 119.26      | 123.70   |
| 1   | AA    | 965  | U    | O4'-C1'-N1 | 5.55  | 112.64      | 108.20   |
| 1   | AA    | 1394 | A    | C5-C6-N1   | -5.55 | 114.92      | 117.70   |
| 1   | AA    | 1402 | C    | N3-C4-C5   | -5.55 | 119.68      | 121.90   |
| 3   | AV    | 10   | G    | O4'-C1'-N9 | 5.55  | 112.64      | 108.20   |
| 27  | B8    | 218  | A    | C5-C6-N6   | -5.55 | 119.26      | 123.70   |
| 27  | B8    | 731  | C    | N3-C4-C5   | -5.55 | 119.68      | 121.90   |
| 27  | B8    | 889  | C    | N3-C4-N4   | 5.55  | 121.89      | 118.00   |
| 27  | B8    | 899  | A    | C4-C5-C6   | 5.55  | 119.78      | 117.00   |
| 27  | B8    | 1000 | A    | C5-C6-N1   | -5.55 | 114.92      | 117.70   |
| 27  | B8    | 1005 | C    | N3-C4-N4   | 5.55  | 121.89      | 118.00   |
| 27  | B8    | 1226 | A    | C5-C6-N6   | -5.55 | 119.26      | 123.70   |
| 27  | B8    | 1569 | A    | O4'-C1'-N9 | 5.55  | 112.64      | 108.20   |
| 27  | B8    | 1804 | C    | N3-C4-C5   | -5.55 | 119.68      | 121.90   |
| 27  | B8    | 1985 | C    | N3-C4-N4   | 5.55  | 121.89      | 118.00   |
| 27  | B8    | 2171 | A    | C5-C6-N1   | -5.55 | 114.92      | 117.70   |
| 1   | AA    | 1092 | A    | C5-C6-N1   | -5.55 | 114.92      | 117.70   |
| 1   | AA    | 1479 | C    | N3-C4-N4   | 5.55  | 121.89      | 118.00   |
| 27  | B8    | 959  | A    | C4-C5-C6   | 5.55  | 119.77      | 117.00   |
| 27  | B8    | 1871 | A    | C5-C6-N6   | -5.55 | 119.26      | 123.70   |
| 27  | B8    | 2134 | A    | C5-C6-N1   | -5.55 | 114.92      | 117.70   |
| 27  | B8    | 2425 | A    | C5-C6-N1   | -5.55 | 114.92      | 117.70   |
| 27  | B8    | 2480 | C    | N3-C4-N4   | 5.55  | 121.89      | 118.00   |
| 27  | B8    | 2666 | C    | N3-C4-C5   | -5.55 | 119.68      | 121.90   |
| 1   | AA    | 744  | C    | N3-C4-N4   | 5.55  | 121.88      | 118.00   |
| 27  | B8    | 727  | A    | C5-C6-N6   | -5.55 | 119.26      | 123.70   |
| 27  | B8    | 1089 | A    | C5-C6-N1   | -5.55 | 114.93      | 117.70   |
| 27  | B8    | 1090 | A    | C5-C6-N6   | -5.55 | 119.26      | 123.70   |
| 27  | B8    | 1153 | C    | N3-C4-C5   | -5.55 | 119.68      | 121.90   |
| 27  | B8    | 1730 | C    | N3-C4-N4   | 5.55  | 121.88      | 118.00   |
| 27  | B8    | 2019 | A    | C5-C6-N1   | -5.55 | 114.93      | 117.70   |
| 27  | B8    | 2418 | A    | C5-C6-N1   | -5.55 | 114.93      | 117.70   |
| 1   | AA    | 466  | A    | C5-C6-N6   | -5.55 | 119.26      | 123.70   |
| 1   | AA    | 622  | A    | C5-C6-N6   | -5.55 | 119.26      | 123.70   |
| 1   | AA    | 1421 | G    | O4'-C1'-N9 | 5.55  | 112.64      | 108.20   |
| 1   | AA    | 1499 | A    | C5-C6-N6   | -5.55 | 119.26      | 123.70   |
| 1   | AA    | 1515 | G    | O4'-C1'-N9 | 5.55  | 112.64      | 108.20   |
| 27  | B8    | 140  | C    | N3-C4-C5   | -5.55 | 119.68      | 121.90   |
| 27  | B8    | 157  | C    | N3-C4-N4   | 5.55  | 121.88      | 118.00   |
| 27  | B8    | 195  | A    | O4'-C1'-N9 | 5.55  | 112.64      | 108.20   |
| 27  | B8    | 650  | C    | N3-C4-C5   | -5.55 | 119.68      | 121.90   |
| 27  | B8    | 995  | C    | N3-C4-C5   | -5.55 | 119.68      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | B8    | 1370 | C    | N3-C4-N4    | 5.55  | 121.88      | 118.00   |
| 27  | B8    | 2152 | G    | C5'-C4'-O4' | 5.55  | 115.76      | 109.10   |
| 27  | B8    | 2886 | A    | C5-C6-N6    | -5.55 | 119.26      | 123.70   |
| 1   | AA    | 1186 | G    | O4'-C1'-N9  | 5.54  | 112.64      | 108.20   |
| 27  | B8    | 318  | C    | N3-C4-C5    | -5.54 | 119.68      | 121.90   |
| 27  | B8    | 800  | A    | C4-C5-C6    | 5.54  | 119.77      | 117.00   |
| 27  | B8    | 2241 | A    | C5-C6-N6    | -5.54 | 119.26      | 123.70   |
| 27  | B8    | 2475 | C    | N3-C4-N4    | 5.54  | 121.88      | 118.00   |
| 1   | AA    | 280  | C    | C2-N1-C1'   | 5.54  | 124.90      | 118.80   |
| 1   | AA    | 526  | C    | N3-C4-C5    | -5.54 | 119.68      | 121.90   |
| 1   | AA    | 646  | G    | O4'-C1'-N9  | 5.54  | 112.63      | 108.20   |
| 1   | AA    | 869  | G    | N3-C2-N2    | 5.54  | 123.78      | 119.90   |
| 1   | AA    | 1045 | C    | N3-C4-N4    | 5.54  | 121.88      | 118.00   |
| 1   | AA    | 1136 | C    | N3-C4-N4    | 5.54  | 121.88      | 118.00   |
| 1   | AA    | 1349 | A    | O4'-C1'-N9  | 5.54  | 112.63      | 108.20   |
| 27  | B8    | 821  | A    | C4-C5-C6    | 5.54  | 119.77      | 117.00   |
| 27  | B8    | 1439 | A    | O4'-C1'-N9  | 5.54  | 112.64      | 108.20   |
| 27  | B8    | 2573 | C    | N3-C4-C5    | -5.54 | 119.68      | 121.90   |
| 27  | B8    | 2691 | C    | N3-C4-C5    | -5.54 | 119.68      | 121.90   |
| 1   | AA    | 702  | A    | C5-C6-N1    | -5.54 | 114.93      | 117.70   |
| 26  | B7    | 53   | A    | C5-C6-N1    | -5.54 | 114.93      | 117.70   |
| 27  | B8    | 772  | C    | N3-C4-C5    | -5.54 | 119.68      | 121.90   |
| 27  | B8    | 941  | A    | C4-C5-C6    | 5.54  | 119.77      | 117.00   |
| 27  | B8    | 1205 | A    | C5-C6-N1    | -5.54 | 114.93      | 117.70   |
| 27  | B8    | 2322 | A    | C5-C6-N1    | -5.54 | 114.93      | 117.70   |
| 1   | AA    | 166  | U    | O4'-C1'-N1  | 5.54  | 112.63      | 108.20   |
| 1   | AA    | 459  | A    | C5-C6-N6    | -5.54 | 119.27      | 123.70   |
| 1   | AA    | 1180 | A    | C5-C6-N6    | -5.54 | 119.27      | 123.70   |
| 1   | AA    | 1483 | A    | O4'-C1'-N9  | 5.54  | 112.63      | 108.20   |
| 27  | B8    | 480  | A    | C5-C6-N1    | -5.54 | 114.93      | 117.70   |
| 27  | B8    | 896  | A    | C5-C6-N6    | -5.54 | 119.27      | 123.70   |
| 27  | B8    | 1129 | A    | C5-C6-N6    | -5.54 | 119.27      | 123.70   |
| 27  | B8    | 1151 | A    | C5-C6-N6    | -5.54 | 119.27      | 123.70   |
| 27  | B8    | 2174 | C    | N3-C4-C5    | -5.54 | 119.68      | 121.90   |
| 27  | B8    | 2364 | C    | N3-C4-N4    | 5.54  | 121.88      | 118.00   |
| 27  | B8    | 2889 | C    | N3-C4-N4    | 5.54  | 121.88      | 118.00   |
| 1   | AA    | 1092 | A    | C5-C6-N6    | -5.54 | 119.27      | 123.70   |
| 1   | AA    | 1271 | A    | C5-C6-N1    | -5.54 | 114.93      | 117.70   |
| 1   | AA    | 1395 | C    | N3-C4-N4    | 5.54  | 121.88      | 118.00   |
| 27  | B8    | 380  | G    | O4'-C1'-N9  | 5.54  | 112.63      | 108.20   |
| 27  | B8    | 432  | A    | O4'-C1'-N9  | 5.54  | 112.63      | 108.20   |
| 27  | B8    | 440  | C    | N3-C4-N4    | 5.54  | 121.88      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 849  | A    | C4-C5-C6   | 5.54  | 119.77      | 117.00   |
| 27  | B8    | 861  | A    | C4-C5-C6   | 5.54  | 119.77      | 117.00   |
| 27  | B8    | 2333 | A    | C4-C5-C6   | 5.54  | 119.77      | 117.00   |
| 27  | B8    | 2670 | A    | C5-C6-N1   | -5.54 | 114.93      | 117.70   |
| 1   | AA    | 1046 | A    | C4-C5-C6   | 5.54  | 119.77      | 117.00   |
| 27  | B8    | 311  | A    | C5-C6-N6   | -5.54 | 119.27      | 123.70   |
| 27  | B8    | 1919 | A    | C5-C6-N6   | -5.54 | 119.27      | 123.70   |
| 1   | AA    | 213  | G    | O4'-C1'-N9 | 5.54  | 112.63      | 108.20   |
| 1   | AA    | 668  | G    | O4'-C1'-N9 | 5.54  | 112.63      | 108.20   |
| 1   | AA    | 936  | C    | N3-C4-N4   | 5.54  | 121.88      | 118.00   |
| 1   | AA    | 1368 | A    | C4-C5-C6   | 5.54  | 119.77      | 117.00   |
| 27  | B8    | 752  | A    | C5-C6-N1   | -5.54 | 114.93      | 117.70   |
| 27  | B8    | 1167 | C    | N3-C4-C5   | -5.54 | 119.69      | 121.90   |
| 27  | B8    | 1302 | A    | C4-C5-C6   | 5.54  | 119.77      | 117.00   |
| 27  | B8    | 1805 | A    | C5-C6-N6   | -5.54 | 119.27      | 123.70   |
| 27  | B8    | 1848 | A    | C5-C6-N1   | -5.54 | 114.93      | 117.70   |
| 27  | B8    | 2215 | C    | N3-C4-C5   | -5.54 | 119.69      | 121.90   |
| 27  | B8    | 2352 | A    | C5-C6-N6   | -5.54 | 119.27      | 123.70   |
| 27  | B8    | 2858 | C    | N3-C4-N4   | 5.54  | 121.88      | 118.00   |
| 27  | B8    | 2883 | A    | C5-C6-N6   | -5.54 | 119.27      | 123.70   |
| 27  | B8    | 2893 | A    | C5-C6-N6   | -5.54 | 119.27      | 123.70   |
| 1   | AA    | 36   | C    | N3-C4-C5   | -5.53 | 119.69      | 121.90   |
| 1   | AA    | 198  | G    | O4'-C1'-N9 | 5.53  | 112.63      | 108.20   |
| 1   | AA    | 306  | A    | C5-C6-N1   | -5.53 | 114.93      | 117.70   |
| 1   | AA    | 811  | C    | N3-C4-C5   | -5.53 | 119.69      | 121.90   |
| 26  | B7    | 114  | C    | N3-C4-N4   | 5.53  | 121.87      | 118.00   |
| 27  | B8    | 194  | G    | O4'-C1'-N9 | 5.53  | 112.63      | 108.20   |
| 27  | B8    | 1028 | A    | C5-C6-N6   | -5.53 | 119.27      | 123.70   |
| 27  | B8    | 1816 | C    | N3-C4-N4   | 5.53  | 121.87      | 118.00   |
| 27  | B8    | 1997 | C    | N3-C4-N4   | 5.53  | 121.87      | 118.00   |
| 27  | B8    | 2082 | A    | C5-C6-N6   | -5.53 | 119.27      | 123.70   |
| 27  | B8    | 2163 | A    | O4'-C1'-N9 | 5.53  | 112.63      | 108.20   |
| 1   | AA    | 298  | A    | C5-C6-N6   | -5.53 | 119.27      | 123.70   |
| 1   | AA    | 629  | A    | C5-C6-N1   | -5.53 | 114.93      | 117.70   |
| 1   | AA    | 1161 | C    | C6-N1-C2   | -5.53 | 118.09      | 120.30   |
| 27  | B8    | 992  | C    | N3-C4-N4   | 5.53  | 121.87      | 118.00   |
| 27  | B8    | 1461 | C    | N3-C4-C5   | -5.53 | 119.69      | 121.90   |
| 27  | B8    | 2589 | A    | C5-C6-N6   | -5.53 | 119.28      | 123.70   |
| 1   | AA    | 74   | A    | C4-C5-C6   | 5.53  | 119.77      | 117.00   |
| 1   | AA    | 490  | C    | N3-C4-N4   | 5.53  | 121.87      | 118.00   |
| 1   | AA    | 909  | A    | C5-C6-N6   | -5.53 | 119.28      | 123.70   |
| 1   | AA    | 1094 | G    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 26  | B7    | 52   | A    | C4-C5-C6   | 5.53  | 119.77      | 117.00   |
| 27  | B8    | 231  | A    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |
| 27  | B8    | 417  | C    | N3-C4-C5   | -5.53 | 119.69      | 121.90   |
| 27  | B8    | 590  | A    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |
| 27  | B8    | 1156 | A    | C5-C6-N6   | -5.53 | 119.28      | 123.70   |
| 27  | B8    | 1535 | A    | C5-C6-N6   | -5.53 | 119.28      | 123.70   |
| 27  | B8    | 1676 | A    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |
| 27  | B8    | 1817 | G    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |
| 1   | AA    | 161  | A    | C5-C6-N6   | -5.53 | 119.28      | 123.70   |
| 1   | AA    | 826  | C    | N3-C4-N4   | 5.53  | 121.87      | 118.00   |
| 27  | B8    | 1869 | G    | N3-C2-N2   | 5.53  | 123.77      | 119.90   |
| 27  | B8    | 2851 | A    | C4-C5-C6   | 5.53  | 119.76      | 117.00   |
| 1   | AA    | 706  | A    | C5-C6-N1   | -5.53 | 114.94      | 117.70   |
| 1   | AA    | 747  | A    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |
| 1   | AA    | 1437 | A    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |
| 1   | AA    | 1523 | G    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |
| 27  | B8    | 14   | A    | C5-C6-N6   | -5.53 | 119.28      | 123.70   |
| 27  | B8    | 1051 | G    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |
| 27  | B8    | 1652 | A    | C4-C5-C6   | 5.53  | 119.76      | 117.00   |
| 27  | B8    | 1732 | C    | N3-C4-C5   | -5.53 | 119.69      | 121.90   |
| 27  | B8    | 1990 | C    | N3-C4-C5   | -5.53 | 119.69      | 121.90   |
| 27  | B8    | 2425 | A    | C5-C6-N6   | -5.53 | 119.28      | 123.70   |
| 27  | B8    | 2634 | A    | C5-C6-N1   | -5.53 | 114.94      | 117.70   |
| 1   | AA    | 131  | A    | C5-C6-N6   | -5.53 | 119.28      | 123.70   |
| 1   | AA    | 182  | A    | C5-C6-N6   | -5.53 | 119.28      | 123.70   |
| 1   | AA    | 951  | G    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |
| 1   | AA    | 1371 | G    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |
| 27  | B8    | 49   | A    | C5-C6-N6   | -5.53 | 119.28      | 123.70   |
| 27  | B8    | 118  | A    | C4-C5-C6   | 5.53  | 119.76      | 117.00   |
| 27  | B8    | 1343 | G    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |
| 27  | B8    | 1604 | C    | N3-C4-C5   | -5.53 | 119.69      | 121.90   |
| 27  | B8    | 1748 | C    | N3-C4-N4   | 5.53  | 121.87      | 118.00   |
| 27  | B8    | 2129 | C    | N3-C4-N4   | 5.53  | 121.87      | 118.00   |
| 27  | B8    | 2340 | A    | C5-C6-N1   | -5.53 | 114.94      | 117.70   |
| 27  | B8    | 2367 | G    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |
| 27  | B8    | 2459 | A    | C5-C6-N1   | -5.53 | 114.94      | 117.70   |
| 1   | AA    | 286  | C    | N3-C4-C5   | -5.52 | 119.69      | 121.90   |
| 1   | AA    | 711  | G    | O4'-C1'-N9 | 5.52  | 112.62      | 108.20   |
| 1   | AA    | 1011 | C    | N3-C4-C5   | -5.52 | 119.69      | 121.90   |
| 3   | AV    | 9    | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |
| 26  | B7    | 15   | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |
| 27  | B8    | 792  | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 906  | A    | C4-C5-C6   | 5.52  | 119.76      | 117.00   |
| 1   | AA    | 1176 | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |
| 26  | B7    | 109  | A    | O4'-C1'-N9 | 5.52  | 112.62      | 108.20   |
| 27  | B8    | 432  | A    | C5-C6-N6   | -5.52 | 119.28      | 123.70   |
| 27  | B8    | 804  | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |
| 27  | B8    | 1265 | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |
| 27  | B8    | 1328 | A    | C5-C6-N6   | -5.52 | 119.28      | 123.70   |
| 27  | B8    | 1376 | C    | N3-C4-C5   | -5.52 | 119.69      | 121.90   |
| 27  | B8    | 1759 | A    | C5-C6-N6   | -5.52 | 119.28      | 123.70   |
| 27  | B8    | 1816 | C    | N3-C4-C5   | -5.52 | 119.69      | 121.90   |
| 27  | B8    | 2469 | A    | C4-C5-C6   | 5.52  | 119.76      | 117.00   |
| 27  | B8    | 2565 | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |
| 27  | B8    | 2646 | C    | N3-C4-C5   | -5.52 | 119.69      | 121.90   |
| 2   | AX    | 13   | C    | N3-C4-C5   | -5.52 | 119.69      | 121.90   |
| 27  | B8    | 125  | A    | C5-C6-N6   | -5.52 | 119.28      | 123.70   |
| 27  | B8    | 547  | A    | C5-C6-N6   | -5.52 | 119.28      | 123.70   |
| 27  | B8    | 1274 | A    | C4-C5-C6   | 5.52  | 119.76      | 117.00   |
| 27  | B8    | 2009 | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |
| 27  | B8    | 2559 | C    | N3-C4-N4   | 5.52  | 121.86      | 118.00   |
| 1   | AA    | 403  | C    | N3-C4-C5   | -5.52 | 119.69      | 121.90   |
| 1   | AA    | 612  | C    | N3-C4-N4   | 5.52  | 121.86      | 118.00   |
| 26  | B7    | 42   | C    | N3-C4-C5   | -5.52 | 119.69      | 121.90   |
| 27  | B8    | 393  | C    | N3-C4-C5   | -5.52 | 119.69      | 121.90   |
| 27  | B8    | 502  | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |
| 27  | B8    | 990  | A    | C4-C5-C6   | 5.52  | 119.76      | 117.00   |
| 27  | B8    | 1013 | C    | N3-C4-C5   | -5.52 | 119.69      | 121.90   |
| 27  | B8    | 1077 | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |
| 27  | B8    | 1899 | A    | C4-C5-C6   | 5.52  | 119.76      | 117.00   |
| 27  | B8    | 2534 | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |
| 27  | B8    | 2812 | G    | O4'-C1'-N9 | 5.52  | 112.62      | 108.20   |
| 1   | AA    | 719  | C    | N3-C4-C5   | -5.52 | 119.69      | 121.90   |
| 1   | AA    | 1069 | C    | N3-C4-N4   | 5.52  | 121.86      | 118.00   |
| 1   | AA    | 1213 | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |
| 2   | AX    | 16   | C    | N3-C4-C5   | -5.52 | 119.69      | 121.90   |
| 27  | B8    | 449  | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |
| 27  | B8    | 601  | C    | N3-C4-C5   | -5.52 | 119.69      | 121.90   |
| 27  | B8    | 984  | A    | C5-C6-N6   | -5.52 | 119.29      | 123.70   |
| 27  | B8    | 1789 | A    | C5-C6-N6   | -5.52 | 119.29      | 123.70   |
| 27  | B8    | 2101 | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |
| 1   | AA    | 117  | G    | O4'-C1'-N9 | 5.52  | 112.61      | 108.20   |
| 1   | AA    | 777  | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |
| 1   | AA    | 1180 | A    | C5-C6-N1   | -5.52 | 114.94      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 201  | C    | N3-C4-C5   | -5.52 | 119.69      | 121.90   |
| 27  | B8    | 2019 | A    | C5-C6-N6   | -5.52 | 119.29      | 123.70   |
| 27  | B8    | 2146 | C    | N3-C4-N4   | 5.52  | 121.86      | 118.00   |
| 27  | B8    | 2609 | U    | O4'-C1'-N1 | 5.52  | 112.61      | 108.20   |
| 1   | AA    | 162  | A    | C5-C6-N6   | -5.51 | 119.29      | 123.70   |
| 1   | AA    | 171  | A    | C5-C6-N1   | -5.51 | 114.94      | 117.70   |
| 1   | AA    | 715  | A    | C5-C6-N6   | -5.51 | 119.29      | 123.70   |
| 1   | AA    | 1368 | A    | C5-C6-N1   | -5.51 | 114.94      | 117.70   |
| 26  | B7    | 46   | A    | O4'-C1'-N9 | 5.51  | 112.61      | 108.20   |
| 27  | B8    | 91   | A    | C5-C6-N6   | -5.51 | 119.29      | 123.70   |
| 27  | B8    | 152  | A    | C5-C6-N1   | -5.51 | 114.94      | 117.70   |
| 27  | B8    | 543  | G    | O4'-C1'-N9 | 5.51  | 112.61      | 108.20   |
| 27  | B8    | 1987 | A    | C5-C6-N6   | -5.51 | 119.29      | 123.70   |
| 27  | B8    | 2033 | A    | C5-C6-N1   | -5.51 | 114.94      | 117.70   |
| 1   | AA    | 1169 | A    | C5-C6-N1   | -5.51 | 114.94      | 117.70   |
| 1   | AA    | 1318 | A    | C5-C6-N6   | -5.51 | 119.29      | 123.70   |
| 2   | AX    | 15   | C    | N3-C4-N4   | 5.51  | 121.86      | 118.00   |
| 27  | B8    | 1096 | A    | C5-C6-N6   | -5.51 | 119.29      | 123.70   |
| 1   | AA    | 217  | C    | N3-C4-C5   | -5.51 | 119.69      | 121.90   |
| 1   | AA    | 620  | C    | N3-C4-C5   | -5.51 | 119.69      | 121.90   |
| 7   | AC    | 36   | PHE  | CB-CG-CD2  | 5.51  | 124.66      | 120.80   |
| 27  | B8    | 635  | C    | N3-C4-C5   | -5.51 | 119.69      | 121.90   |
| 27  | B8    | 661  | A    | C5-C6-N6   | -5.51 | 119.29      | 123.70   |
| 27  | B8    | 673  | C    | N3-C4-N4   | 5.51  | 121.86      | 118.00   |
| 27  | B8    | 1610 | A    | C4-C5-C6   | 5.51  | 119.75      | 117.00   |
| 27  | B8    | 2001 | C    | N3-C4-C5   | -5.51 | 119.70      | 121.90   |
| 27  | B8    | 2094 | A    | O4'-C1'-N9 | 5.51  | 112.61      | 108.20   |
| 27  | B8    | 2287 | A    | C5-C6-N1   | -5.51 | 114.94      | 117.70   |
| 27  | B8    | 2342 | C    | N3-C4-C5   | -5.51 | 119.70      | 121.90   |
| 27  | B8    | 2711 | A    | C4-C5-C6   | 5.51  | 119.75      | 117.00   |
| 1   | AA    | 655  | A    | O4'-C1'-N9 | 5.51  | 112.61      | 108.20   |
| 1   | AA    | 907  | A    | C5-C6-N1   | -5.51 | 114.94      | 117.70   |
| 1   | AA    | 1093 | A    | O4'-C1'-N9 | 5.51  | 112.61      | 108.20   |
| 1   | AA    | 1137 | C    | N3-C4-C5   | -5.51 | 119.70      | 121.90   |
| 1   | AA    | 1158 | C    | N3-C4-C5   | -5.51 | 119.70      | 121.90   |
| 1   | AA    | 1466 | C    | N3-C4-N4   | 5.51  | 121.86      | 118.00   |
| 27  | B8    | 311  | A    | C5-C6-N1   | -5.51 | 114.94      | 117.70   |
| 27  | B8    | 477  | A    | O4'-C1'-N9 | 5.51  | 112.61      | 108.20   |
| 27  | B8    | 645  | C    | N3-C4-C5   | -5.51 | 119.70      | 121.90   |
| 27  | B8    | 668  | A    | C4-C5-C6   | 5.51  | 119.75      | 117.00   |
| 27  | B8    | 1006 | C    | N3-C4-C5   | -5.51 | 119.70      | 121.90   |
| 27  | B8    | 1942 | C    | N3-C4-C5   | -5.51 | 119.70      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2332 | C    | N3-C4-C5   | -5.51 | 119.70      | 121.90   |
| 27  | B8    | 2681 | C    | N3-C4-N4   | 5.51  | 121.86      | 118.00   |
| 26  | B7    | 42   | C    | N3-C4-N4   | 5.51  | 121.86      | 118.00   |
| 27  | B8    | 24   | G    | O4'-C1'-N9 | 5.51  | 112.61      | 108.20   |
| 27  | B8    | 1160 | G    | O4'-C1'-N9 | 5.51  | 112.61      | 108.20   |
| 27  | B8    | 1550 | C    | N3-C4-C5   | -5.51 | 119.70      | 121.90   |
| 27  | B8    | 1610 | A    | O4'-C1'-N9 | 5.51  | 112.61      | 108.20   |
| 27  | B8    | 1758 | U    | O4'-C1'-N1 | 5.51  | 112.61      | 108.20   |
| 27  | B8    | 2870 | C    | N3-C4-C5   | -5.51 | 119.70      | 121.90   |
| 1   | AA    | 915  | A    | O4'-C1'-N9 | 5.51  | 112.61      | 108.20   |
| 1   | AA    | 1303 | C    | N3-C4-N4   | 5.51  | 121.85      | 118.00   |
| 26  | B7    | 36   | C    | N3-C4-N4   | 5.51  | 121.85      | 118.00   |
| 27  | B8    | 301  | G    | O4'-C1'-N9 | 5.51  | 112.61      | 108.20   |
| 27  | B8    | 520  | G    | O4'-C1'-N9 | 5.51  | 112.61      | 108.20   |
| 27  | B8    | 815  | C    | N3-C4-C5   | -5.51 | 119.70      | 121.90   |
| 27  | B8    | 951  | C    | N3-C4-C5   | -5.51 | 119.70      | 121.90   |
| 27  | B8    | 1320 | C    | N3-C4-C5   | -5.51 | 119.70      | 121.90   |
| 27  | B8    | 1854 | A    | C4-C5-C6   | 5.51  | 119.75      | 117.00   |
| 27  | B8    | 2275 | C    | N3-C4-C5   | -5.51 | 119.70      | 121.90   |
| 27  | B8    | 2327 | A    | C5-C6-N1   | -5.51 | 114.95      | 117.70   |
| 27  | B8    | 2839 | G    | O4'-C1'-N9 | 5.51  | 112.61      | 108.20   |
| 1   | AA    | 165  | G    | O4'-C1'-N9 | 5.50  | 112.60      | 108.20   |
| 26  | B7    | 17   | C    | N3-C4-N4   | 5.50  | 121.85      | 118.00   |
| 27  | B8    | 12   | U    | P-O3'-C3'  | 5.50  | 126.31      | 119.70   |
| 1   | AA    | 823  | C    | N3-C4-N4   | 5.50  | 121.85      | 118.00   |
| 1   | AA    | 912  | C    | N3-C4-C5   | -5.50 | 119.70      | 121.90   |
| 1   | AA    | 1093 | A    | C5-C6-N6   | -5.50 | 119.30      | 123.70   |
| 27  | B8    | 318  | C    | N3-C4-N4   | 5.50  | 121.85      | 118.00   |
| 27  | B8    | 453  | A    | O4'-C1'-N9 | 5.50  | 112.60      | 108.20   |
| 27  | B8    | 819  | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 27  | B8    | 889  | C    | C6-N1-C1'  | -5.50 | 114.20      | 120.80   |
| 27  | B8    | 1158 | C    | N3-C4-C5   | -5.50 | 119.70      | 121.90   |
| 27  | B8    | 1169 | A    | C5-C6-N6   | -5.50 | 119.30      | 123.70   |
| 27  | B8    | 1351 | C    | N3-C4-N4   | 5.50  | 121.85      | 118.00   |
| 27  | B8    | 1552 | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 27  | B8    | 1748 | C    | N3-C4-C5   | -5.50 | 119.70      | 121.90   |
| 27  | B8    | 2020 | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 1   | AA    | 2    | A    | C5-C6-N6   | -5.50 | 119.30      | 123.70   |
| 1   | AA    | 10   | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 1   | AA    | 280  | C    | N3-C4-C5   | -5.50 | 119.70      | 121.90   |
| 1   | AA    | 1145 | A    | C4-C5-C6   | 5.50  | 119.75      | 117.00   |
| 1   | AA    | 1195 | C    | N3-C4-C5   | -5.50 | 119.70      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 17   | G    | O4'-C1'-N9 | 5.50  | 112.60      | 108.20   |
| 27  | B8    | 454  | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 27  | B8    | 1020 | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 27  | B8    | 1901 | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 27  | B8    | 2454 | G    | O4'-C1'-N9 | 5.50  | 112.60      | 108.20   |
| 27  | B8    | 2820 | A    | C5-C6-N6   | -5.50 | 119.30      | 123.70   |
| 1   | AA    | 556  | C    | N3-C4-C5   | -5.50 | 119.70      | 121.90   |
| 1   | AA    | 1396 | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 26  | B7    | 94   | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 27  | B8    | 384  | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 27  | B8    | 563  | A    | C5-C6-N6   | -5.50 | 119.30      | 123.70   |
| 27  | B8    | 1230 | A    | O4'-C1'-N9 | 5.50  | 112.60      | 108.20   |
| 1   | AA    | 83   | C    | N3-C4-N4   | 5.50  | 121.85      | 118.00   |
| 1   | AA    | 260  | G    | O4'-C1'-N9 | 5.50  | 112.60      | 108.20   |
| 27  | B8    | 716  | A    | O4'-C1'-N9 | 5.50  | 112.60      | 108.20   |
| 27  | B8    | 772  | C    | N3-C4-N4   | 5.50  | 121.85      | 118.00   |
| 27  | B8    | 1439 | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 27  | B8    | 1548 | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 27  | B8    | 2073 | C    | N3-C4-C5   | -5.50 | 119.70      | 121.90   |
| 27  | B8    | 2432 | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 27  | B8    | 2781 | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 1   | AA    | 196  | A    | C4-C5-C6   | 5.50  | 119.75      | 117.00   |
| 1   | AA    | 430  | A    | O4'-C1'-N9 | 5.50  | 112.60      | 108.20   |
| 1   | AA    | 448  | A    | C4-C5-C6   | 5.50  | 119.75      | 117.00   |
| 1   | AA    | 994  | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 1   | AA    | 1336 | C    | N3-C4-N4   | 5.50  | 121.85      | 118.00   |
| 27  | B8    | 482  | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 27  | B8    | 1630 | A    | C4-C5-C6   | 5.50  | 119.75      | 117.00   |
| 27  | B8    | 2801 | G    | O4'-C1'-N9 | 5.50  | 112.60      | 108.20   |
| 1   | AA    | 336  | A    | O4'-C1'-N9 | 5.50  | 112.60      | 108.20   |
| 1   | AA    | 630  | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 1   | AA    | 995  | C    | N3-C4-C5   | -5.50 | 119.70      | 121.90   |
| 1   | AA    | 1410 | A    | C5-C6-N1   | -5.50 | 114.95      | 117.70   |
| 26  | B7    | 88   | C    | N3-C4-C5   | -5.50 | 119.70      | 121.90   |
| 27  | B8    | 56   | A    | O4'-C1'-N9 | 5.50  | 112.60      | 108.20   |
| 1   | AA    | 57   | G    | O4'-C1'-N9 | 5.49  | 112.59      | 108.20   |
| 1   | AA    | 109  | A    | O4'-C1'-N9 | 5.49  | 112.59      | 108.20   |
| 1   | AA    | 264  | C    | N3-C4-N4   | 5.49  | 121.84      | 118.00   |
| 1   | AA    | 610  | U    | C6-N1-C1'  | -5.49 | 113.51      | 121.20   |
| 1   | AA    | 1013 | G    | N3-C2-N2   | 5.49  | 123.75      | 119.90   |
| 3   | AV    | 58   | A    | C5-C6-N6   | -5.49 | 119.31      | 123.70   |
| 27  | B8    | 486  | C    | N3-C4-N4   | 5.49  | 121.85      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 908  | C    | N3-C4-N4   | 5.49  | 121.85      | 118.00   |
| 27  | B8    | 1050 | A    | C4-C5-C6   | 5.49  | 119.75      | 117.00   |
| 27  | B8    | 1496 | A    | P-O3'-C3'  | 5.49  | 126.29      | 119.70   |
| 27  | B8    | 1833 | C    | N3-C4-N4   | 5.49  | 121.84      | 118.00   |
| 33  | BE    | 85   | PHE  | CB-CG-CD1  | 5.49  | 124.64      | 120.80   |
| 27  | B8    | 666  | A    | O4'-C1'-N9 | 5.49  | 112.59      | 108.20   |
| 27  | B8    | 1626 | A    | C5-C6-N1   | -5.49 | 114.95      | 117.70   |
| 1   | AA    | 197  | A    | C5-C6-N1   | -5.49 | 114.95      | 117.70   |
| 1   | AA    | 925  | G    | O4'-C1'-N9 | 5.49  | 112.59      | 108.20   |
| 1   | AA    | 1120 | C    | N3-C4-N4   | 5.49  | 121.84      | 118.00   |
| 1   | AA    | 1456 | A    | C5-C6-N1   | -5.49 | 114.95      | 117.70   |
| 3   | AV    | 52   | A    | O4'-C1'-N9 | 5.49  | 112.59      | 108.20   |
| 27  | B8    | 491  | G    | O4'-C1'-N9 | 5.49  | 112.59      | 108.20   |
| 27  | B8    | 526  | A    | C5-C6-N6   | -5.49 | 119.31      | 123.70   |
| 27  | B8    | 888  | C    | N3-C4-N4   | 5.49  | 121.84      | 118.00   |
| 27  | B8    | 1556 | C    | N3-C4-N4   | 5.49  | 121.84      | 118.00   |
| 27  | B8    | 2003 | A    | O4'-C1'-N9 | 5.49  | 112.59      | 108.20   |
| 1   | AA    | 322  | C    | N3-C4-N4   | 5.49  | 121.84      | 118.00   |
| 1   | AA    | 510  | A    | C5-C6-N6   | -5.49 | 119.31      | 123.70   |
| 1   | AA    | 611  | C    | N3-C4-C5   | -5.49 | 119.70      | 121.90   |
| 1   | AA    | 784  | A    | C5-C6-N1   | -5.49 | 114.96      | 117.70   |
| 27  | B8    | 659  | G    | O4'-C1'-N9 | 5.49  | 112.59      | 108.20   |
| 27  | B8    | 806  | C    | N3-C4-C5   | -5.49 | 119.70      | 121.90   |
| 27  | B8    | 837  | C    | N3-C4-N4   | 5.49  | 121.84      | 118.00   |
| 27  | B8    | 1072 | C    | N3-C4-C5   | -5.49 | 119.70      | 121.90   |
| 27  | B8    | 1080 | A    | C5-C6-N1   | -5.49 | 114.96      | 117.70   |
| 27  | B8    | 1370 | C    | N3-C4-C5   | -5.49 | 119.70      | 121.90   |
| 27  | B8    | 1449 | G    | O4'-C1'-N9 | 5.49  | 112.59      | 108.20   |
| 27  | B8    | 2407 | A    | C5-C6-N6   | -5.49 | 119.31      | 123.70   |
| 27  | B8    | 685  | A    | C4-C5-C6   | 5.49  | 119.74      | 117.00   |
| 1   | AA    | 449  | G    | O4'-C1'-N9 | 5.49  | 112.59      | 108.20   |
| 1   | AA    | 622  | A    | C4-C5-C6   | 5.49  | 119.74      | 117.00   |
| 1   | AA    | 715  | A    | C5-C6-N1   | -5.49 | 114.96      | 117.70   |
| 1   | AA    | 1250 | A    | O4'-C1'-N9 | 5.49  | 112.59      | 108.20   |
| 26  | B7    | 63   | C    | N3-C4-N4   | 5.49  | 121.84      | 118.00   |
| 27  | B8    | 13   | A    | C5-C6-N1   | -5.49 | 114.96      | 117.70   |
| 27  | B8    | 218  | A    | C5-C6-N1   | -5.49 | 114.96      | 117.70   |
| 27  | B8    | 385  | C    | N3-C4-C5   | -5.49 | 119.71      | 121.90   |
| 27  | B8    | 715  | A    | C5-C6-N6   | -5.49 | 119.31      | 123.70   |
| 27  | B8    | 1286 | A    | C5-C6-N6   | -5.49 | 119.31      | 123.70   |
| 27  | B8    | 1994 | C    | N3-C4-C5   | -5.49 | 119.71      | 121.90   |
| 27  | B8    | 2067 | G    | P-O3'-C3'  | 5.49  | 126.28      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2281 | A    | C5-C6-N1   | -5.49 | 114.96      | 117.70   |
| 27  | B8    | 2346 | A    | C5-C6-N1   | -5.49 | 114.96      | 117.70   |
| 1   | AA    | 716  | A    | C4-C5-C6   | 5.48  | 119.74      | 117.00   |
| 1   | AA    | 1271 | A    | C5-C6-N6   | -5.48 | 119.31      | 123.70   |
| 27  | B8    | 205  | G    | O4'-C1'-N9 | 5.48  | 112.59      | 108.20   |
| 27  | B8    | 1509 | A    | C5-C6-N6   | -5.48 | 119.31      | 123.70   |
| 27  | B8    | 1990 | C    | N3-C4-N4   | 5.48  | 121.84      | 118.00   |
| 27  | B8    | 2539 | C    | N3-C4-N4   | 5.48  | 121.84      | 118.00   |
| 1   | AA    | 50   | A    | C5-C6-N6   | -5.48 | 119.31      | 123.70   |
| 1   | AA    | 1204 | A    | O4'-C1'-N9 | 5.48  | 112.59      | 108.20   |
| 27  | B8    | 348  | A    | C5-C6-N6   | -5.48 | 119.31      | 123.70   |
| 27  | B8    | 420  | C    | N3-C4-C5   | -5.48 | 119.71      | 121.90   |
| 27  | B8    | 848  | C    | N3-C4-N4   | 5.48  | 121.84      | 118.00   |
| 27  | B8    | 1153 | C    | N3-C4-N4   | 5.48  | 121.84      | 118.00   |
| 27  | B8    | 1647 | U    | O4'-C1'-N1 | 5.48  | 112.59      | 108.20   |
| 27  | B8    | 2153 | C    | N3-C4-N4   | 5.48  | 121.84      | 118.00   |
| 27  | B8    | 2232 | C    | N3-C4-N4   | 5.48  | 121.84      | 118.00   |
| 1   | AA    | 623  | C    | N3-C4-C5   | -5.48 | 119.71      | 121.90   |
| 1   | AA    | 923  | A    | O4'-C1'-N9 | 5.48  | 112.58      | 108.20   |
| 1   | AA    | 1146 | A    | O4'-C1'-N9 | 5.48  | 112.58      | 108.20   |
| 3   | AV    | 16   | C    | N3-C4-C5   | -5.48 | 119.71      | 121.90   |
| 26  | B7    | 94   | A    | C4-C5-C6   | 5.48  | 119.74      | 117.00   |
| 26  | B7    | 106  | G    | O4'-C1'-N9 | 5.48  | 112.58      | 108.20   |
| 27  | B8    | 316  | C    | N3-C4-N4   | 5.48  | 121.84      | 118.00   |
| 27  | B8    | 752  | A    | C5-C6-N6   | -5.48 | 119.31      | 123.70   |
| 27  | B8    | 1809 | A    | C4-C5-C6   | 5.48  | 119.74      | 117.00   |
| 27  | B8    | 1925 | C    | N3-C4-N4   | 5.48  | 121.84      | 118.00   |
| 1   | AA    | 411  | A    | C5-C6-N6   | -5.48 | 119.32      | 123.70   |
| 1   | AA    | 441  | A    | C5-C6-N6   | -5.48 | 119.32      | 123.70   |
| 1   | AA    | 1492 | A    | C4-C5-C6   | 5.48  | 119.74      | 117.00   |
| 27  | B8    | 2497 | A    | C5-C6-N1   | -5.48 | 114.96      | 117.70   |
| 27  | B8    | 2823 | A    | C5-C6-N1   | -5.48 | 114.96      | 117.70   |
| 1   | AA    | 77   | A    | O4'-C1'-N9 | 5.48  | 112.58      | 108.20   |
| 1   | AA    | 621  | A    | C5-C6-N1   | -5.48 | 114.96      | 117.70   |
| 1   | AA    | 1081 | A    | C5-C6-N1   | -5.48 | 114.96      | 117.70   |
| 1   | AA    | 1280 | A    | C5-C6-N1   | -5.48 | 114.96      | 117.70   |
| 1   | AA    | 1400 | C    | N3-C4-C5   | -5.48 | 119.71      | 121.90   |
| 27  | B8    | 196  | A    | C5-C6-N6   | -5.48 | 119.32      | 123.70   |
| 27  | B8    | 302  | C    | N3-C4-C5   | -5.48 | 119.71      | 121.90   |
| 27  | B8    | 351  | C    | N3-C4-C5   | -5.48 | 119.71      | 121.90   |
| 27  | B8    | 369  | U    | O4'-C1'-N1 | 5.48  | 112.58      | 108.20   |
| 27  | B8    | 423  | A    | C4-C5-C6   | 5.48  | 119.74      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 730  | A    | O4'-C1'-N9 | 5.48  | 112.58      | 108.20   |
| 27  | B8    | 996  | A    | O4'-C1'-N9 | 5.48  | 112.58      | 108.20   |
| 27  | B8    | 1169 | A    | O4'-C1'-N9 | 5.48  | 112.58      | 108.20   |
| 27  | B8    | 1332 | G    | O4'-C1'-N9 | 5.48  | 112.58      | 108.20   |
| 27  | B8    | 1360 | G    | C5-C6-O6   | -5.48 | 125.31      | 128.60   |
| 27  | B8    | 1800 | C    | N3-C4-C5   | -5.48 | 119.71      | 121.90   |
| 27  | B8    | 2278 | A    | C5-C6-N1   | -5.48 | 114.96      | 117.70   |
| 27  | B8    | 2360 | G    | O4'-C1'-N9 | 5.48  | 112.58      | 108.20   |
| 27  | B8    | 2572 | A    | O4'-C1'-N9 | 5.48  | 112.58      | 108.20   |
| 1   | AA    | 975  | A    | C5-C6-N6   | -5.48 | 119.32      | 123.70   |
| 1   | AA    | 1170 | A    | O4'-C1'-N9 | 5.48  | 112.58      | 108.20   |
| 27  | B8    | 631  | A    | O4'-C1'-N9 | 5.48  | 112.58      | 108.20   |
| 27  | B8    | 1549 | A    | C5-C6-N6   | -5.48 | 119.32      | 123.70   |
| 27  | B8    | 1658 | C    | N3-C4-C5   | -5.48 | 119.71      | 121.90   |
| 27  | B8    | 2063 | C    | N3-C4-C5   | -5.48 | 119.71      | 121.90   |
| 27  | B8    | 2386 | A    | O4'-C1'-N9 | 5.48  | 112.58      | 108.20   |
| 1   | AA    | 303  | A    | C5-C6-N6   | -5.47 | 119.32      | 123.70   |
| 1   | AA    | 547  | A    | C5-C6-N1   | -5.47 | 114.96      | 117.70   |
| 1   | AA    | 1412 | C    | N3-C4-C5   | -5.47 | 119.71      | 121.90   |
| 27  | B8    | 393  | C    | N3-C4-N4   | 5.47  | 121.83      | 118.00   |
| 27  | B8    | 445  | C    | N3-C4-N4   | 5.47  | 121.83      | 118.00   |
| 27  | B8    | 508  | A    | C5-C6-N6   | -5.47 | 119.32      | 123.70   |
| 27  | B8    | 886  | A    | C5-C6-N1   | -5.47 | 114.96      | 117.70   |
| 27  | B8    | 1590 | A    | C4-C5-C6   | 5.47  | 119.74      | 117.00   |
| 27  | B8    | 1774 | C    | N3-C4-C5   | -5.47 | 119.71      | 121.90   |
| 27  | B8    | 1810 | A    | C5-C6-N1   | -5.47 | 114.96      | 117.70   |
| 27  | B8    | 2165 | C    | N3-C4-N4   | 5.47  | 121.83      | 118.00   |
| 27  | B8    | 2314 | A    | C5-C6-N6   | -5.47 | 119.32      | 123.70   |
| 27  | B8    | 2830 | C    | N3-C4-C5   | -5.47 | 119.71      | 121.90   |
| 1   | AA    | 307  | C    | N3-C4-C5   | -5.47 | 119.71      | 121.90   |
| 1   | AA    | 1431 | A    | C4-C5-C6   | 5.47  | 119.74      | 117.00   |
| 27  | B8    | 475  | C    | N3-C4-C5   | -5.47 | 119.71      | 121.90   |
| 27  | B8    | 502  | A    | C4-C5-C6   | 5.47  | 119.74      | 117.00   |
| 27  | B8    | 943  | A    | O4'-C1'-N9 | 5.47  | 112.58      | 108.20   |
| 27  | B8    | 1266 | G    | O4'-C1'-N9 | 5.47  | 112.58      | 108.20   |
| 27  | B8    | 2526 | G    | O4'-C1'-N9 | 5.47  | 112.58      | 108.20   |
| 1   | AA    | 839  | C    | N3-C4-C5   | -5.47 | 119.71      | 121.90   |
| 1   | AA    | 1042 | A    | O4'-C1'-N9 | 5.47  | 112.58      | 108.20   |
| 1   | AA    | 1152 | A    | C5-C6-N1   | -5.47 | 114.97      | 117.70   |
| 27  | B8    | 115  | C    | N3-C4-C5   | -5.47 | 119.71      | 121.90   |
| 27  | B8    | 529  | A    | C5-C6-N1   | -5.47 | 114.97      | 117.70   |
| 27  | B8    | 1694 | C    | N3-C4-C5   | -5.47 | 119.71      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1802 | A    | O4'-C1'-N9 | 5.47  | 112.58      | 108.20   |
| 1   | AA    | 535  | A    | O4'-C1'-N9 | 5.47  | 112.58      | 108.20   |
| 1   | AA    | 845  | A    | C5-C6-N6   | -5.47 | 119.32      | 123.70   |
| 1   | AA    | 1109 | C    | N3-C4-N4   | 5.47  | 121.83      | 118.00   |
| 1   | AA    | 1166 | G    | N3-C2-N2   | 5.47  | 123.73      | 119.90   |
| 3   | AV    | 13   | C    | N3-C4-C5   | -5.47 | 119.71      | 121.90   |
| 27  | B8    | 680  | C    | N3-C4-C5   | -5.47 | 119.71      | 121.90   |
| 27  | B8    | 927  | A    | C5-C6-N6   | -5.47 | 119.33      | 123.70   |
| 27  | B8    | 985  | C    | N3-C4-C5   | -5.47 | 119.71      | 121.90   |
| 27  | B8    | 1093 | G    | O4'-C1'-N9 | 5.47  | 112.58      | 108.20   |
| 27  | B8    | 1981 | A    | C5-C6-N1   | -5.47 | 114.97      | 117.70   |
| 27  | B8    | 2078 | C    | N3-C4-N4   | 5.47  | 121.83      | 118.00   |
| 27  | B8    | 2565 | A    | C5-C6-N6   | -5.47 | 119.32      | 123.70   |
| 27  | B8    | 2718 | G    | O4'-C1'-N9 | 5.47  | 112.58      | 108.20   |
| 27  | B8    | 2874 | C    | N3-C4-C5   | -5.47 | 119.71      | 121.90   |
| 32  | BD    | 127  | PHE  | CB-CG-CD2  | 5.47  | 124.63      | 120.80   |
| 1   | AA    | 935  | A    | O4'-C1'-N9 | 5.47  | 112.58      | 108.20   |
| 1   | AA    | 1093 | A    | C5-C6-N1   | -5.47 | 114.97      | 117.70   |
| 27  | B8    | 111  | A    | C5-C6-N1   | -5.47 | 114.97      | 117.70   |
| 27  | B8    | 961  | C    | N3-C4-N4   | 5.47  | 121.83      | 118.00   |
| 27  | B8    | 1871 | A    | C5-C6-N1   | -5.47 | 114.97      | 117.70   |
| 27  | B8    | 2369 | A    | C5-C6-N1   | -5.47 | 114.97      | 117.70   |
| 27  | B8    | 2422 | C    | N3-C4-C5   | -5.47 | 119.71      | 121.90   |
| 1   | AA    | 163  | C    | N3-C4-N4   | 5.47  | 121.83      | 118.00   |
| 1   | AA    | 640  | A    | C5-C6-N1   | -5.47 | 114.97      | 117.70   |
| 1   | AA    | 654  | G    | O4'-C1'-N9 | 5.47  | 112.57      | 108.20   |
| 26  | B7    | 59   | A    | O4'-C1'-N9 | 5.47  | 112.57      | 108.20   |
| 27  | B8    | 345  | A    | C4-C5-C6   | 5.47  | 119.73      | 117.00   |
| 27  | B8    | 624  | C    | N3-C4-N4   | 5.47  | 121.83      | 118.00   |
| 27  | B8    | 863  | A    | O4'-C1'-N9 | 5.47  | 112.57      | 108.20   |
| 27  | B8    | 981  | A    | C5-C6-N1   | -5.47 | 114.97      | 117.70   |
| 27  | B8    | 1348 | C    | N3-C4-C5   | -5.47 | 119.71      | 121.90   |
| 27  | B8    | 1622 | G    | O4'-C1'-N9 | 5.47  | 112.57      | 108.20   |
| 27  | B8    | 2038 | G    | O4'-C1'-N9 | 5.47  | 112.57      | 108.20   |
| 1   | AA    | 95   | C    | C6-N1-C2   | -5.46 | 118.11      | 120.30   |
| 1   | AA    | 968  | A    | C5-C6-N6   | -5.46 | 119.33      | 123.70   |
| 1   | AA    | 1191 | A    | O4'-C1'-N9 | 5.46  | 112.57      | 108.20   |
| 27  | B8    | 9    | G    | O4'-C1'-N9 | 5.46  | 112.57      | 108.20   |
| 27  | B8    | 1010 | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 27  | B8    | 1544 | A    | C5-C6-N6   | -5.46 | 119.33      | 123.70   |
| 27  | B8    | 1665 | A    | C5-C6-N6   | -5.46 | 119.33      | 123.70   |
| 34  | BF    | 7    | TYR  | CB-CG-CD1  | -5.46 | 117.72      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 364  | A    | C5-C6-N6   | -5.46 | 119.33      | 123.70   |
| 27  | B8    | 142  | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 1   | AA    | 233  | C    | N3-C4-C5   | -5.46 | 119.72      | 121.90   |
| 1   | AA    | 397  | A    | C5-C6-N6   | -5.46 | 119.33      | 123.70   |
| 1   | AA    | 1311 | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 2   | AX    | 18   | C    | N3-C4-C5   | -5.46 | 119.72      | 121.90   |
| 27  | B8    | 964  | C    | N3-C4-C5   | -5.46 | 119.72      | 121.90   |
| 27  | B8    | 1981 | A    | C5-C6-N6   | -5.46 | 119.33      | 123.70   |
| 27  | B8    | 2358 | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 27  | B8    | 2749 | A    | O4'-C1'-N9 | 5.46  | 112.57      | 108.20   |
| 1   | AA    | 821  | G    | O4'-C1'-N9 | 5.46  | 112.57      | 108.20   |
| 2   | AX    | 22   | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 27  | B8    | 443  | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 27  | B8    | 1111 | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 27  | B8    | 1808 | A    | C5-C6-N6   | -5.46 | 119.33      | 123.70   |
| 1   | AA    | 269  | C    | N3-C4-C5   | -5.46 | 119.72      | 121.90   |
| 1   | AA    | 694  | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 1   | AA    | 1257 | A    | O4'-C1'-N9 | 5.46  | 112.57      | 108.20   |
| 1   | AA    | 1395 | C    | N3-C4-C5   | -5.46 | 119.72      | 121.90   |
| 3   | AV    | 76   | C    | N3-C4-C5   | -5.46 | 119.72      | 121.90   |
| 27  | B8    | 1135 | C    | N3-C4-N4   | 5.46  | 121.82      | 118.00   |
| 27  | B8    | 1918 | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 27  | B8    | 2368 | C    | N3-C4-N4   | 5.46  | 121.82      | 118.00   |
| 27  | B8    | 2873 | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 1   | AA    | 452  | A    | C5-C6-N6   | -5.46 | 119.33      | 123.70   |
| 1   | AA    | 461  | A    | C5-C6-N6   | -5.46 | 119.33      | 123.70   |
| 1   | AA    | 490  | C    | N3-C4-C5   | -5.46 | 119.72      | 121.90   |
| 1   | AA    | 935  | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 1   | AA    | 1213 | A    | C5-C6-N6   | -5.46 | 119.33      | 123.70   |
| 1   | AA    | 1317 | C    | N3-C4-N4   | 5.46  | 121.82      | 118.00   |
| 1   | AA    | 1357 | A    | O4'-C1'-N9 | 5.46  | 112.56      | 108.20   |
| 1   | AA    | 1499 | A    | O4'-C1'-N9 | 5.46  | 112.57      | 108.20   |
| 26  | B7    | 12   | C    | N3-C4-C5   | -5.46 | 119.72      | 121.90   |
| 27  | B8    | 255  | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 27  | B8    | 314  | C    | N3-C4-N4   | 5.46  | 121.82      | 118.00   |
| 27  | B8    | 668  | A    | C5-C6-N6   | -5.46 | 119.33      | 123.70   |
| 27  | B8    | 1175 | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 27  | B8    | 1365 | A    | C5-C6-N6   | -5.46 | 119.33      | 123.70   |
| 27  | B8    | 1759 | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 27  | B8    | 1801 | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 27  | B8    | 1878 | G    | O4'-C1'-N9 | 5.46  | 112.56      | 108.20   |
| 27  | B8    | 2798 | U    | C2-N1-C1'  | 5.46  | 124.25      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 28  | BA    | 158  | PHE  | CB-CG-CD1  | 5.46  | 124.62      | 120.80   |
| 3   | AV    | 52   | A    | C5-C6-N6   | -5.46 | 119.34      | 123.70   |
| 27  | B8    | 492  | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 27  | B8    | 1000 | A    | C5-C6-N6   | -5.46 | 119.34      | 123.70   |
| 27  | B8    | 1419 | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 27  | B8    | 1570 | A    | C5-C6-N1   | -5.46 | 114.97      | 117.70   |
| 27  | B8    | 1837 | C    | N3-C4-C5   | -5.46 | 119.72      | 121.90   |
| 1   | AA    | 330  | C    | N3-C4-C5   | -5.45 | 119.72      | 121.90   |
| 1   | AA    | 1218 | C    | N3-C4-N4   | 5.45  | 121.82      | 118.00   |
| 27  | B8    | 176  | A    | C5-C6-N1   | -5.45 | 114.97      | 117.70   |
| 27  | B8    | 1505 | A    | C5-C6-N6   | -5.45 | 119.34      | 123.70   |
| 27  | B8    | 2062 | A    | C5-C6-N6   | -5.45 | 119.34      | 123.70   |
| 27  | B8    | 2872 | A    | C5-C6-N6   | -5.45 | 119.34      | 123.70   |
| 1   | AA    | 279  | A    | C4-C5-C6   | 5.45  | 119.73      | 117.00   |
| 1   | AA    | 325  | A    | C5-C6-N6   | -5.45 | 119.34      | 123.70   |
| 1   | AA    | 1027 | C    | N3-C4-C5   | -5.45 | 119.72      | 121.90   |
| 1   | AA    | 1452 | C    | N3-C4-C5   | -5.45 | 119.72      | 121.90   |
| 27  | B8    | 1024 | G    | O4'-C1'-N9 | 5.45  | 112.56      | 108.20   |
| 27  | B8    | 1251 | C    | N3-C4-C5   | -5.45 | 119.72      | 121.90   |
| 1   | AA    | 66   | A    | O4'-C1'-N9 | 5.45  | 112.56      | 108.20   |
| 1   | AA    | 67   | C    | N3-C4-N4   | 5.45  | 121.81      | 118.00   |
| 1   | AA    | 73   | C    | N3-C4-C5   | -5.45 | 119.72      | 121.90   |
| 1   | AA    | 708  | C    | N3-C4-N4   | 5.45  | 121.82      | 118.00   |
| 1   | AA    | 1267 | C    | N3-C4-C5   | -5.45 | 119.72      | 121.90   |
| 1   | AA    | 1503 | A    | C5-C6-N1   | -5.45 | 114.97      | 117.70   |
| 27  | B8    | 544  | C    | N3-C4-N4   | 5.45  | 121.81      | 118.00   |
| 27  | B8    | 1125 | G    | O4'-C1'-N9 | 5.45  | 112.56      | 108.20   |
| 27  | B8    | 1301 | A    | C5-C6-N6   | -5.45 | 119.34      | 123.70   |
| 27  | B8    | 1614 | A    | C5-C6-N6   | -5.45 | 119.34      | 123.70   |
| 27  | B8    | 2736 | A    | C5-C6-N6   | -5.45 | 119.34      | 123.70   |
| 1   | AA    | 722  | G    | O4'-C1'-N9 | 5.45  | 112.56      | 108.20   |
| 1   | AA    | 1179 | A    | C5-C6-N6   | -5.45 | 119.34      | 123.70   |
| 1   | AA    | 1480 | A    | C5-C6-N6   | -5.45 | 119.34      | 123.70   |
| 3   | AV    | 74   | A    | C5-C6-N6   | -5.45 | 119.34      | 123.70   |
| 27  | B8    | 472  | A    | C5-C6-N1   | -5.45 | 114.98      | 117.70   |
| 27  | B8    | 632  | A    | O4'-C1'-N9 | 5.45  | 112.56      | 108.20   |
| 27  | B8    | 805  | G    | O4'-C1'-N9 | 5.45  | 112.56      | 108.20   |
| 27  | B8    | 857  | G    | O4'-C1'-N9 | 5.45  | 112.56      | 108.20   |
| 27  | B8    | 1951 | U    | O4'-C1'-N1 | 5.45  | 112.56      | 108.20   |
| 27  | B8    | 2411 | A    | C5-C6-N1   | -5.45 | 114.98      | 117.70   |
| 27  | B8    | 2442 | C    | N3-C4-C5   | -5.45 | 119.72      | 121.90   |
| 1   | AA    | 470  | C    | N3-C4-C5   | -5.45 | 119.72      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | AV    | 42   | C    | N3-C4-C5   | -5.45 | 119.72      | 121.90   |
| 27  | B8    | 1549 | A    | C5-C6-N1   | -5.45 | 114.98      | 117.70   |
| 27  | B8    | 1626 | A    | C5-C6-N6   | -5.45 | 119.34      | 123.70   |
| 27  | B8    | 2001 | C    | N3-C4-N4   | 5.45  | 121.81      | 118.00   |
| 27  | B8    | 2322 | A    | C5-C6-N6   | -5.45 | 119.34      | 123.70   |
| 1   | AA    | 113  | G    | O4'-C1'-N9 | 5.45  | 112.56      | 108.20   |
| 1   | AA    | 774  | G    | O4'-C1'-N9 | 5.45  | 112.56      | 108.20   |
| 26  | B7    | 35   | C    | N3-C4-N4   | 5.45  | 121.81      | 118.00   |
| 27  | B8    | 161  | A    | C4-C5-C6   | 5.45  | 119.72      | 117.00   |
| 27  | B8    | 217  | A    | C5-C6-N1   | -5.45 | 114.98      | 117.70   |
| 27  | B8    | 1670 | C    | N3-C4-N4   | 5.45  | 121.81      | 118.00   |
| 27  | B8    | 1808 | A    | C5-C6-N1   | -5.45 | 114.98      | 117.70   |
| 27  | B8    | 2159 | G    | O4'-C1'-N9 | 5.45  | 112.56      | 108.20   |
| 27  | B8    | 2516 | A    | C5-C6-N1   | -5.45 | 114.98      | 117.70   |
| 28  | BA    | 314  | GLN  | CA-C-N     | 5.45  | 132.35      | 117.10   |
| 1   | AA    | 8    | A    | C5-C6-N1   | -5.44 | 114.98      | 117.70   |
| 1   | AA    | 1042 | A    | C5-C6-N6   | -5.44 | 119.34      | 123.70   |
| 1   | AA    | 1362 | A    | C4-C5-C6   | 5.44  | 119.72      | 117.00   |
| 27  | B8    | 1762 | A    | C5-C6-N1   | -5.44 | 114.98      | 117.70   |
| 27  | B8    | 2260 | C    | N3-C4-C5   | -5.44 | 119.72      | 121.90   |
| 27  | B8    | 2776 | A    | C5-C6-N1   | -5.44 | 114.98      | 117.70   |
| 33  | BE    | 85   | PHE  | CB-CG-CD2  | -5.44 | 116.99      | 120.80   |
| 1   | AA    | 385  | C    | N3-C4-C5   | -5.44 | 119.72      | 121.90   |
| 1   | AA    | 775  | G    | O4'-C1'-N9 | 5.44  | 112.55      | 108.20   |
| 1   | AA    | 1024 | G    | N3-C2-N2   | 5.44  | 123.71      | 119.90   |
| 1   | AA    | 1363 | A    | C5-C6-N1   | -5.44 | 114.98      | 117.70   |
| 1   | AA    | 1394 | A    | C5-C6-N6   | -5.44 | 119.35      | 123.70   |
| 2   | AX    | 13   | C    | N3-C4-N4   | 5.44  | 121.81      | 118.00   |
| 27  | B8    | 61   | C    | N3-C4-N4   | 5.44  | 121.81      | 118.00   |
| 27  | B8    | 836  | G    | O4'-C1'-N9 | 5.44  | 112.55      | 108.20   |
| 27  | B8    | 1536 | C    | N3-C4-C5   | -5.44 | 119.72      | 121.90   |
| 1   | AA    | 197  | A    | C5-C6-N6   | -5.44 | 119.35      | 123.70   |
| 1   | AA    | 265  | G    | C5-C6-O6   | -5.44 | 125.33      | 128.60   |
| 1   | AA    | 443  | C    | N3-C4-C5   | -5.44 | 119.72      | 121.90   |
| 1   | AA    | 778  | G    | O4'-C1'-N9 | 5.44  | 112.55      | 108.20   |
| 1   | AA    | 845  | A    | P-O3'-C3'  | 5.44  | 126.23      | 119.70   |
| 1   | AA    | 1137 | C    | C6-N1-C1'  | -5.44 | 114.27      | 120.80   |
| 1   | AA    | 1256 | A    | C5-C6-N6   | -5.44 | 119.35      | 123.70   |
| 1   | AA    | 1483 | A    | C5-C6-N6   | -5.44 | 119.35      | 123.70   |
| 1   | AA    | 1539 | C    | N3-C4-C5   | -5.44 | 119.72      | 121.90   |
| 2   | AX    | 22   | A    | C5-C6-N6   | -5.44 | 119.35      | 123.70   |
| 27  | B8    | 716  | A    | C5-C6-N1   | -5.44 | 114.98      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 749  | A    | O4'-C1'-N9 | 5.44  | 112.55      | 108.20   |
| 27  | B8    | 1246 | A    | C5-C6-N6   | -5.44 | 119.35      | 123.70   |
| 27  | B8    | 1253 | A    | C5-C6-N6   | -5.44 | 119.35      | 123.70   |
| 27  | B8    | 1366 | A    | C5-C6-N1   | -5.44 | 114.98      | 117.70   |
| 27  | B8    | 1893 | C    | N3-C4-N4   | 5.44  | 121.81      | 118.00   |
| 27  | B8    | 2235 | G    | O4'-C1'-N9 | 5.44  | 112.55      | 108.20   |
| 27  | B8    | 2654 | A    | C4-C5-C6   | 5.44  | 119.72      | 117.00   |
| 27  | B8    | 2829 | A    | O4'-C1'-N9 | 5.44  | 112.55      | 108.20   |
| 1   | AA    | 967  | C    | N3-C4-C5   | -5.44 | 119.72      | 121.90   |
| 27  | B8    | 330  | A    | C5-C6-N1   | -5.44 | 114.98      | 117.70   |
| 27  | B8    | 444  | C    | N3-C4-N4   | 5.44  | 121.81      | 118.00   |
| 27  | B8    | 1612 | C    | N3-C4-N4   | 5.44  | 121.81      | 118.00   |
| 27  | B8    | 2158 | A    | C5-C6-N1   | -5.44 | 114.98      | 117.70   |
| 1   | AA    | 7    | A    | C5-C6-N6   | -5.44 | 119.35      | 123.70   |
| 1   | AA    | 665  | A    | C5-C6-N6   | -5.44 | 119.35      | 123.70   |
| 1   | AA    | 1163 | A    | C5-C6-N1   | -5.44 | 114.98      | 117.70   |
| 27  | B8    | 1254 | A    | C5-C6-N1   | -5.44 | 114.98      | 117.70   |
| 27  | B8    | 1321 | A    | O4'-C1'-N9 | 5.44  | 112.55      | 108.20   |
| 27  | B8    | 1597 | A    | O4'-C1'-N9 | 5.44  | 112.55      | 108.20   |
| 27  | B8    | 1914 | C    | N3-C4-C5   | -5.44 | 119.72      | 121.90   |
| 27  | B8    | 1920 | C    | N3-C4-C5   | -5.44 | 119.72      | 121.90   |
| 27  | B8    | 1940 | U    | O4'-C1'-N1 | 5.44  | 112.55      | 108.20   |
| 27  | B8    | 2579 | C    | N3-C4-C5   | -5.44 | 119.72      | 121.90   |
| 27  | B8    | 2675 | A    | O4'-C1'-N9 | 5.44  | 112.55      | 108.20   |
| 27  | B8    | 2753 | A    | C5-C6-N1   | -5.44 | 114.98      | 117.70   |
| 27  | B8    | 2894 | G    | O4'-C1'-N9 | 5.44  | 112.55      | 108.20   |
| 1   | AA    | 430  | A    | C4-C5-C6   | 5.44  | 119.72      | 117.00   |
| 1   | AA    | 1416 | G    | O4'-C1'-N9 | 5.44  | 112.55      | 108.20   |
| 27  | B8    | 1935 | G    | O4'-C1'-N9 | 5.44  | 112.55      | 108.20   |
| 27  | B8    | 2665 | A    | C5-C6-N1   | -5.44 | 114.98      | 117.70   |
| 27  | B8    | 2841 | C    | N3-C4-C5   | -5.44 | 119.73      | 121.90   |
| 1   | AA    | 44   | A    | C5-C6-N6   | -5.43 | 119.35      | 123.70   |
| 1   | AA    | 640  | A    | O4'-C1'-N9 | 5.43  | 112.55      | 108.20   |
| 1   | AA    | 900  | A    | C5-C6-N1   | -5.43 | 114.98      | 117.70   |
| 1   | AA    | 1491 | G    | O4'-C1'-N9 | 5.43  | 112.55      | 108.20   |
| 27  | B8    | 531  | C    | N3-C4-N4   | 5.43  | 121.81      | 118.00   |
| 27  | B8    | 574  | A    | C5-C6-N6   | -5.43 | 119.35      | 123.70   |
| 27  | B8    | 1071 | G    | O4'-C1'-N9 | 5.43  | 112.55      | 108.20   |
| 27  | B8    | 1173 | U    | O4'-C1'-N1 | 5.43  | 112.55      | 108.20   |
| 27  | B8    | 1447 | C    | N3-C4-N4   | 5.43  | 121.81      | 118.00   |
| 27  | B8    | 2070 | A    | C5-C6-N6   | -5.43 | 119.35      | 123.70   |
| 27  | B8    | 2147 | A    | C5-C6-N1   | -5.43 | 114.98      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2170 | A    | O4'-C1'-N9 | 5.43  | 112.55      | 108.20   |
| 27  | B8    | 2288 | A    | C5-C6-N6   | -5.43 | 119.35      | 123.70   |
| 27  | B8    | 2601 | C    | O4'-C1'-N1 | 5.43  | 112.55      | 108.20   |
| 27  | B8    | 2644 | G    | O4'-C1'-N9 | 5.43  | 112.55      | 108.20   |
| 1   | AA    | 90   | C    | N3-C4-C5   | -5.43 | 119.73      | 121.90   |
| 1   | AA    | 749  | A    | C5-C6-N6   | -5.43 | 119.35      | 123.70   |
| 1   | AA    | 840  | C    | N3-C4-N4   | 5.43  | 121.80      | 118.00   |
| 1   | AA    | 1132 | C    | N3-C4-C5   | -5.43 | 119.73      | 121.90   |
| 1   | AA    | 1136 | C    | N3-C4-C5   | -5.43 | 119.73      | 121.90   |
| 1   | AA    | 1137 | C    | N3-C4-N4   | 5.43  | 121.80      | 118.00   |
| 1   | AA    | 1346 | A    | C5-C6-N1   | -5.43 | 114.98      | 117.70   |
| 27  | B8    | 69   | C    | N3-C4-N4   | 5.43  | 121.80      | 118.00   |
| 27  | B8    | 140  | C    | N3-C4-N4   | 5.43  | 121.80      | 118.00   |
| 27  | B8    | 1102 | C    | N3-C4-C5   | -5.43 | 119.73      | 121.90   |
| 27  | B8    | 1109 | C    | N3-C4-C5   | -5.43 | 119.73      | 121.90   |
| 27  | B8    | 1290 | C    | N3-C4-C5   | -5.43 | 119.73      | 121.90   |
| 27  | B8    | 1489 | C    | O4'-C1'-N1 | 5.43  | 112.55      | 108.20   |
| 27  | B8    | 2451 | A    | C4-C5-C6   | 5.43  | 119.72      | 117.00   |
| 27  | B8    | 2634 | A    | C5-C6-N6   | -5.43 | 119.35      | 123.70   |
| 1   | AA    | 167  | A    | C5-C6-N6   | -5.43 | 119.36      | 123.70   |
| 1   | AA    | 339  | C    | N3-C4-N4   | 5.43  | 121.80      | 118.00   |
| 1   | AA    | 392  | C    | N3-C4-C5   | -5.43 | 119.73      | 121.90   |
| 1   | AA    | 468  | A    | C5-C6-N6   | -5.43 | 119.36      | 123.70   |
| 1   | AA    | 810  | C    | N3-C4-N4   | 5.43  | 121.80      | 118.00   |
| 27  | B8    | 478  | A    | C4-C5-C6   | 5.43  | 119.72      | 117.00   |
| 27  | B8    | 1658 | C    | N3-C4-N4   | 5.43  | 121.80      | 118.00   |
| 27  | B8    | 2266 | A    | C5-C6-N6   | -5.43 | 119.36      | 123.70   |
| 1   | AA    | 183  | C    | N3-C4-N4   | 5.43  | 121.80      | 118.00   |
| 1   | AA    | 1217 | C    | N3-C4-N4   | 5.43  | 121.80      | 118.00   |
| 27  | B8    | 10   | A    | C5-C6-N6   | -5.43 | 119.36      | 123.70   |
| 27  | B8    | 384  | A    | C5-C6-N6   | -5.43 | 119.36      | 123.70   |
| 27  | B8    | 733  | G    | N3-C2-N2   | 5.43  | 123.70      | 119.90   |
| 27  | B8    | 903  | C    | N3-C4-N4   | 5.43  | 121.80      | 118.00   |
| 27  | B8    | 1175 | A    | C5-C6-N6   | -5.43 | 119.36      | 123.70   |
| 27  | B8    | 1490 | A    | C5-C6-N1   | -5.43 | 114.98      | 117.70   |
| 27  | B8    | 1690 | A    | C5-C6-N1   | -5.43 | 114.99      | 117.70   |
| 27  | B8    | 2459 | A    | C5-C6-N6   | -5.43 | 119.36      | 123.70   |
| 27  | B8    | 2830 | C    | N3-C4-N4   | 5.43  | 121.80      | 118.00   |
| 1   | AA    | 72   | A    | C5-C6-N1   | -5.43 | 114.99      | 117.70   |
| 1   | AA    | 277  | C    | N3-C4-N4   | 5.43  | 121.80      | 118.00   |
| 27  | B8    | 160  | A    | C5-C6-N1   | -5.43 | 114.99      | 117.70   |
| 27  | B8    | 222  | A    | C5-C6-N6   | -5.43 | 119.36      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | B8    | 1114 | C    | N3-C4-C5    | -5.43 | 119.73      | 121.90   |
| 27  | B8    | 2250 | G    | N3-C2-N2    | 5.43  | 123.70      | 119.90   |
| 27  | B8    | 2381 | A    | C5-C6-N1    | -5.43 | 114.99      | 117.70   |
| 1   | AA    | 546  | A    | O4'-C1'-N9  | 5.43  | 112.54      | 108.20   |
| 1   | AA    | 602  | A    | C5-C6-N6    | -5.43 | 119.36      | 123.70   |
| 1   | AA    | 970  | C    | N3-C4-N4    | 5.43  | 121.80      | 118.00   |
| 1   | AA    | 1228 | C    | N3-C4-N4    | 5.43  | 121.80      | 118.00   |
| 1   | AA    | 1483 | A    | C5-C6-N1    | -5.43 | 114.99      | 117.70   |
| 3   | AV    | 33   | A    | C5-C6-N6    | -5.43 | 119.36      | 123.70   |
| 22  | AR    | 4    | PHE  | CB-CG-CD2   | -5.43 | 117.00      | 120.80   |
| 27  | B8    | 671  | C    | C5'-C4'-C3' | -5.43 | 107.32      | 116.00   |
| 27  | B8    | 1358 | G    | N3-C2-N2    | 5.43  | 123.70      | 119.90   |
| 27  | B8    | 1746 | A    | C5-C6-N6    | -5.43 | 119.36      | 123.70   |
| 27  | B8    | 2005 | A    | C5-C6-N1    | -5.43 | 114.99      | 117.70   |
| 27  | B8    | 2042 | A    | C5-C6-N1    | -5.43 | 114.99      | 117.70   |
| 27  | B8    | 2184 | A    | C5-C6-N1    | -5.43 | 114.99      | 117.70   |
| 27  | B8    | 2201 | G    | O4'-C1'-N9  | 5.43  | 112.54      | 108.20   |
| 27  | B8    | 2573 | C    | N3-C4-N4    | 5.43  | 121.80      | 118.00   |
| 1   | AA    | 110  | C    | N3-C4-C5    | -5.42 | 119.73      | 121.90   |
| 1   | AA    | 616  | G    | O4'-C1'-N9  | 5.42  | 112.54      | 108.20   |
| 1   | AA    | 1285 | A    | C5'-C4'-C3' | -5.42 | 107.32      | 116.00   |
| 1   | AA    | 1484 | C    | N3-C4-N4    | 5.42  | 121.80      | 118.00   |
| 3   | AV    | 24   | C    | N3-C4-N4    | 5.42  | 121.80      | 118.00   |
| 27  | B8    | 979  | A    | O4'-C1'-N9  | 5.42  | 112.54      | 108.20   |
| 27  | B8    | 1708 | C    | N3-C4-C5    | -5.42 | 119.73      | 121.90   |
| 1   | AA    | 984  | C    | N3-C4-C5    | -5.42 | 119.73      | 121.90   |
| 1   | AA    | 1003 | G    | O4'-C1'-N9  | 5.42  | 112.54      | 108.20   |
| 1   | AA    | 1037 | C    | N3-C4-N4    | 5.42  | 121.80      | 118.00   |
| 27  | B8    | 873  | C    | N3-C4-N4    | 5.42  | 121.80      | 118.00   |
| 27  | B8    | 1008 | A    | C5-C6-N1    | -5.42 | 114.99      | 117.70   |
| 27  | B8    | 1801 | A    | C5-C6-N6    | -5.42 | 119.36      | 123.70   |
| 1   | AA    | 236  | A    | C5-C6-N1    | -5.42 | 114.99      | 117.70   |
| 1   | AA    | 330  | C    | N3-C4-N4    | 5.42  | 121.79      | 118.00   |
| 3   | AV    | 5    | A    | C5-C6-N1    | -5.42 | 114.99      | 117.70   |
| 27  | B8    | 845  | A    | C5-C6-N1    | -5.42 | 114.99      | 117.70   |
| 27  | B8    | 1262 | A    | C5-C6-N6    | -5.42 | 119.36      | 123.70   |
| 27  | B8    | 1592 | C    | N3-C4-C5    | -5.42 | 119.73      | 121.90   |
| 27  | B8    | 1819 | A    | C5-C6-N1    | -5.42 | 114.99      | 117.70   |
| 27  | B8    | 2734 | A    | O4'-C1'-N9  | 5.42  | 112.54      | 108.20   |
| 1   | AA    | 492  | C    | N3-C4-N4    | 5.42  | 121.79      | 118.00   |
| 1   | AA    | 1045 | C    | N3-C4-C5    | -5.42 | 119.73      | 121.90   |
| 1   | AA    | 1226 | C    | N3-C4-N4    | 5.42  | 121.79      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1484 | C    | N3-C4-C5   | -5.42 | 119.73      | 121.90   |
| 1   | AA    | 1503 | A    | C5-C6-N6   | -5.42 | 119.36      | 123.70   |
| 27  | B8    | 73   | A    | C5-C6-N1   | -5.42 | 114.99      | 117.70   |
| 27  | B8    | 412  | A    | C5-C6-N1   | -5.42 | 114.99      | 117.70   |
| 27  | B8    | 1505 | A    | C5-C6-N1   | -5.42 | 114.99      | 117.70   |
| 27  | B8    | 1708 | C    | N3-C4-N4   | 5.42  | 121.79      | 118.00   |
| 1   | AA    | 640  | A    | C5-C6-N6   | -5.42 | 119.36      | 123.70   |
| 1   | AA    | 688  | G    | O4'-C1'-N9 | 5.42  | 112.53      | 108.20   |
| 1   | AA    | 1118 | U    | O4'-C1'-N1 | 5.42  | 112.54      | 108.20   |
| 27  | B8    | 517  | C    | N3-C4-N4   | 5.42  | 121.79      | 118.00   |
| 27  | B8    | 865  | C    | N3-C4-C5   | -5.42 | 119.73      | 121.90   |
| 27  | B8    | 1049 | C    | N3-C4-N4   | 5.42  | 121.79      | 118.00   |
| 27  | B8    | 1136 | G    | O4'-C1'-N9 | 5.42  | 112.53      | 108.20   |
| 27  | B8    | 1194 | A    | C5-C6-N1   | -5.42 | 114.99      | 117.70   |
| 27  | B8    | 1780 | A    | C5-C6-N1   | -5.42 | 114.99      | 117.70   |
| 27  | B8    | 1889 | A    | C5-C6-N6   | -5.42 | 119.36      | 123.70   |
| 27  | B8    | 2117 | A    | C5-C6-N6   | -5.42 | 119.36      | 123.70   |
| 27  | B8    | 2467 | C    | N3-C4-C5   | -5.42 | 119.73      | 121.90   |
| 1   | AA    | 32   | A    | C5-C6-N1   | -5.42 | 114.99      | 117.70   |
| 1   | AA    | 225  | C    | N3-C4-C5   | -5.42 | 119.73      | 121.90   |
| 1   | AA    | 250  | A    | C5-C6-N1   | -5.42 | 114.99      | 117.70   |
| 1   | AA    | 660  | C    | N3-C4-N4   | 5.42  | 121.79      | 118.00   |
| 1   | AA    | 1408 | A    | C5-C6-N6   | -5.42 | 119.37      | 123.70   |
| 27  | B8    | 42   | A    | C5-C6-N1   | -5.42 | 114.99      | 117.70   |
| 27  | B8    | 125  | A    | C5-C6-N1   | -5.42 | 114.99      | 117.70   |
| 27  | B8    | 233  | A    | C5-C6-N1   | -5.42 | 114.99      | 117.70   |
| 27  | B8    | 342  | A    | C5-C6-N1   | -5.42 | 114.99      | 117.70   |
| 27  | B8    | 363  | G    | P-O5'-C5'  | 5.42  | 129.56      | 120.90   |
| 27  | B8    | 735  | A    | C4-C5-C6   | 5.42  | 119.71      | 117.00   |
| 27  | B8    | 1313 | U    | C6-N1-C1'  | -5.42 | 113.62      | 121.20   |
| 27  | B8    | 1353 | A    | C5-C6-N6   | -5.42 | 119.37      | 123.70   |
| 27  | B8    | 2530 | A    | C5-C6-N6   | -5.42 | 119.37      | 123.70   |
| 27  | B8    | 2710 | C    | N3-C4-C5   | -5.42 | 119.73      | 121.90   |
| 27  | B8    | 1953 | A    | C5-C6-N6   | -5.42 | 119.37      | 123.70   |
| 1   | AA    | 129  | A    | C5-C6-N1   | -5.41 | 114.99      | 117.70   |
| 1   | AA    | 1410 | A    | C4-C5-C6   | 5.41  | 119.71      | 117.00   |
| 1   | AA    | 1467 | C    | N3-C4-C5   | -5.41 | 119.73      | 121.90   |
| 1   | AA    | 1538 | C    | N3-C4-C5   | -5.41 | 119.73      | 121.90   |
| 27  | B8    | 692  | C    | N3-C4-C5   | -5.41 | 119.73      | 121.90   |
| 27  | B8    | 1269 | A    | O4'-C1'-N9 | 5.41  | 112.53      | 108.20   |
| 27  | B8    | 1665 | A    | O4'-C1'-N9 | 5.41  | 112.53      | 108.20   |
| 27  | B8    | 1739 | A    | C4-C5-C6   | 5.41  | 119.71      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2805 | C    | N3-C4-C5   | -5.41 | 119.73      | 121.90   |
| 1   | AA    | 811  | C    | N3-C4-N4   | 5.41  | 121.79      | 118.00   |
| 27  | B8    | 542  | C    | N3-C4-C5   | -5.41 | 119.73      | 121.90   |
| 27  | B8    | 1161 | C    | N3-C4-C5   | -5.41 | 119.73      | 121.90   |
| 27  | B8    | 1588 | G    | O4'-C1'-N9 | 5.41  | 112.53      | 108.20   |
| 27  | B8    | 2037 | A    | C5-C6-N1   | -5.41 | 114.99      | 117.70   |
| 27  | B8    | 2300 | C    | N3-C4-C5   | -5.41 | 119.73      | 121.90   |
| 3   | AV    | 29   | C    | N3-C4-C5   | -5.41 | 119.74      | 121.90   |
| 27  | B8    | 1569 | A    | C5-C6-N6   | -5.41 | 119.37      | 123.70   |
| 27  | B8    | 817  | C    | N3-C4-C5   | -5.41 | 119.74      | 121.90   |
| 27  | B8    | 984  | A    | C5-C6-N1   | -5.41 | 115.00      | 117.70   |
| 27  | B8    | 1014 | A    | C5-C6-N1   | -5.41 | 115.00      | 117.70   |
| 27  | B8    | 1079 | C    | N3-C4-C5   | -5.41 | 119.74      | 121.90   |
| 27  | B8    | 1493 | C    | N3-C4-C5   | -5.41 | 119.74      | 121.90   |
| 27  | B8    | 2208 | C    | N3-C4-N4   | 5.41  | 121.79      | 118.00   |
| 27  | B8    | 2542 | A    | C5-C6-N6   | -5.41 | 119.37      | 123.70   |
| 27  | B8    | 2721 | A    | C5-C6-N6   | -5.41 | 119.37      | 123.70   |
| 27  | B8    | 509  | C    | N3-C4-N4   | 5.41  | 121.78      | 118.00   |
| 27  | B8    | 1889 | A    | C5-C6-N1   | -5.41 | 115.00      | 117.70   |
| 27  | B8    | 2328 | A    | C5-C6-N1   | -5.41 | 115.00      | 117.70   |
| 1   | AA    | 250  | A    | C5-C6-N6   | -5.41 | 119.38      | 123.70   |
| 1   | AA    | 264  | C    | N3-C4-C5   | -5.41 | 119.74      | 121.90   |
| 1   | AA    | 777  | A    | C5-C6-N6   | -5.41 | 119.38      | 123.70   |
| 1   | AA    | 1362 | A    | C5-C6-N6   | -5.41 | 119.38      | 123.70   |
| 1   | AA    | 1536 | C    | N3-C4-N4   | 5.41  | 121.78      | 118.00   |
| 2   | AX    | 15   | C    | N3-C4-C5   | -5.41 | 119.74      | 121.90   |
| 3   | AV    | 29   | C    | N3-C4-N4   | 5.41  | 121.78      | 118.00   |
| 27  | B8    | 63   | A    | O4'-C1'-N9 | 5.41  | 112.53      | 108.20   |
| 27  | B8    | 207  | A    | C4-C5-C6   | 5.41  | 119.70      | 117.00   |
| 27  | B8    | 323  | C    | N3-C4-C5   | -5.41 | 119.74      | 121.90   |
| 27  | B8    | 456  | C    | N3-C4-N4   | 5.41  | 121.78      | 118.00   |
| 27  | B8    | 888  | C    | N3-C4-C5   | -5.41 | 119.74      | 121.90   |
| 27  | B8    | 1655 | A    | C4-C5-C6   | 5.41  | 119.70      | 117.00   |
| 27  | B8    | 1938 | A    | C5-C6-N1   | -5.41 | 115.00      | 117.70   |
| 27  | B8    | 2064 | C    | N3-C4-C5   | -5.41 | 119.74      | 121.90   |
| 27  | B8    | 2145 | C    | O4'-C1'-N1 | 5.41  | 112.52      | 108.20   |
| 27  | B8    | 2177 | C    | N3-C4-C5   | -5.41 | 119.74      | 121.90   |
| 27  | B8    | 2183 | A    | C5-C6-N1   | -5.41 | 115.00      | 117.70   |
| 27  | B8    | 2226 | C    | N3-C4-N4   | 5.41  | 121.78      | 118.00   |
| 27  | B8    | 2468 | A    | C5-C6-N6   | -5.41 | 119.38      | 123.70   |
| 27  | B8    | 2824 | C    | N3-C4-C5   | -5.41 | 119.74      | 121.90   |
| 1   | AA    | 378  | G    | O4'-C1'-N9 | 5.40  | 112.52      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 878  | A    | C5-C6-N6   | -5.40 | 119.38      | 123.70   |
| 1   | AA    | 1149 | C    | N3-C4-C5   | -5.40 | 119.74      | 121.90   |
| 1   | AA    | 1333 | A    | C5-C6-N6   | -5.40 | 119.38      | 123.70   |
| 1   | AA    | 1441 | A    | C5-C6-N1   | -5.40 | 115.00      | 117.70   |
| 27  | B8    | 307  | G    | O4'-C1'-N9 | 5.40  | 112.52      | 108.20   |
| 27  | B8    | 645  | C    | N3-C4-N4   | 5.40  | 121.78      | 118.00   |
| 27  | B8    | 2285 | C    | N3-C4-C5   | -5.40 | 119.74      | 121.90   |
| 27  | B8    | 2347 | C    | N3-C4-N4   | 5.40  | 121.78      | 118.00   |
| 27  | B8    | 2731 | G    | O4'-C1'-N9 | 5.40  | 112.52      | 108.20   |
| 1   | AA    | 305  | G    | O4'-C1'-N9 | 5.40  | 112.52      | 108.20   |
| 1   | AA    | 582  | C    | N3-C4-N4   | 5.40  | 121.78      | 118.00   |
| 27  | B8    | 236  | C    | N3-C4-C5   | -5.40 | 119.74      | 121.90   |
| 27  | B8    | 632  | A    | C5-C6-N1   | -5.40 | 115.00      | 117.70   |
| 27  | B8    | 1596 | A    | C5-C6-N1   | -5.40 | 115.00      | 117.70   |
| 27  | B8    | 1685 | C    | N3-C4-C5   | -5.40 | 119.74      | 121.90   |
| 27  | B8    | 1733 | G    | O4'-C1'-N9 | 5.40  | 112.52      | 108.20   |
| 27  | B8    | 2073 | C    | N3-C4-N4   | 5.40  | 121.78      | 118.00   |
| 27  | B8    | 2388 | A    | C5-C6-N6   | -5.40 | 119.38      | 123.70   |
| 1   | AA    | 339  | C    | N3-C4-C5   | -5.40 | 119.74      | 121.90   |
| 1   | AA    | 505  | G    | O4'-C1'-N9 | 5.40  | 112.52      | 108.20   |
| 1   | AA    | 509  | A    | C5-C6-N1   | -5.40 | 115.00      | 117.70   |
| 1   | AA    | 548  | G    | O4'-C1'-N9 | 5.40  | 112.52      | 108.20   |
| 1   | AA    | 1141 | C    | N3-C4-C5   | -5.40 | 119.74      | 121.90   |
| 1   | AA    | 1174 | G    | O4'-C1'-N9 | 5.40  | 112.52      | 108.20   |
| 1   | AA    | 1214 | C    | N3-C4-C5   | -5.40 | 119.74      | 121.90   |
| 26  | B7    | 43   | C    | N3-C4-N4   | 5.40  | 121.78      | 118.00   |
| 27  | B8    | 753  | A    | C5-C6-N1   | -5.40 | 115.00      | 117.70   |
| 27  | B8    | 1566 | A    | C5-C6-N1   | -5.40 | 115.00      | 117.70   |
| 27  | B8    | 1597 | A    | C5-C6-N1   | -5.40 | 115.00      | 117.70   |
| 27  | B8    | 2705 | A    | O4'-C1'-N9 | 5.40  | 112.52      | 108.20   |
| 27  | B8    | 2736 | A    | C5-C6-N1   | -5.40 | 115.00      | 117.70   |
| 27  | B8    | 2835 | A    | C4-C5-C6   | 5.40  | 119.70      | 117.00   |
| 1   | AA    | 1430 | A    | C5-C6-N6   | -5.40 | 119.38      | 123.70   |
| 27  | B8    | 84   | A    | C5-C6-N1   | -5.40 | 115.00      | 117.70   |
| 27  | B8    | 2762 | C    | N3-C4-N4   | 5.40  | 121.78      | 118.00   |
| 27  | B8    | 2889 | C    | N3-C4-C5   | -5.40 | 119.74      | 121.90   |
| 1   | AA    | 381  | C    | N3-C4-C5   | -5.40 | 119.74      | 121.90   |
| 1   | AA    | 1114 | C    | N3-C4-C5   | -5.40 | 119.74      | 121.90   |
| 1   | AA    | 1509 | C    | N3-C4-N4   | 5.40  | 121.78      | 118.00   |
| 1   | AA    | 1531 | A    | C5-C6-N1   | -5.40 | 115.00      | 117.70   |
| 26  | B7    | 31   | C    | N3-C4-C5   | -5.40 | 119.74      | 121.90   |
| 26  | B7    | 58   | A    | C5-C6-N1   | -5.40 | 115.00      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 675  | A    | C5-C6-N1   | -5.40 | 115.00      | 117.70   |
| 27  | B8    | 1453 | A    | C5-C6-N6   | -5.40 | 119.38      | 123.70   |
| 27  | B8    | 1586 | A    | C5-C6-N1   | -5.40 | 115.00      | 117.70   |
| 27  | B8    | 2176 | A    | C5-C6-N6   | -5.40 | 119.38      | 123.70   |
| 1   | AA    | 661  | G    | O4'-C1'-N9 | 5.40  | 112.52      | 108.20   |
| 27  | B8    | 21   | A    | C5-C6-N6   | -5.40 | 119.38      | 123.70   |
| 27  | B8    | 893  | C    | N3-C4-C5   | -5.40 | 119.74      | 121.90   |
| 27  | B8    | 2266 | A    | C5-C6-N1   | -5.40 | 115.00      | 117.70   |
| 1   | AA    | 183  | C    | N3-C4-C5   | -5.39 | 119.74      | 121.90   |
| 1   | AA    | 618  | C    | N3-C4-C5   | -5.39 | 119.74      | 121.90   |
| 1   | AA    | 1179 | A    | C5-C6-N1   | -5.39 | 115.00      | 117.70   |
| 1   | AA    | 1542 | A    | C5-C6-N1   | -5.39 | 115.00      | 117.70   |
| 26  | B7    | 59   | A    | C5-C6-N6   | -5.39 | 119.39      | 123.70   |
| 27  | B8    | 255  | A    | O4'-C1'-N9 | 5.39  | 112.52      | 108.20   |
| 27  | B8    | 334  | C    | N3-C4-C5   | -5.39 | 119.74      | 121.90   |
| 27  | B8    | 575  | A    | C5-C6-N6   | -5.39 | 119.38      | 123.70   |
| 27  | B8    | 1274 | A    | O4'-C1'-N9 | 5.39  | 112.52      | 108.20   |
| 27  | B8    | 1418 | G    | O4'-C1'-N9 | 5.39  | 112.52      | 108.20   |
| 27  | B8    | 2209 | G    | O4'-C1'-N9 | 5.39  | 112.52      | 108.20   |
| 27  | B8    | 2251 | G    | O4'-C1'-N9 | 5.39  | 112.52      | 108.20   |
| 1   | AA    | 163  | C    | N3-C4-C5   | -5.39 | 119.74      | 121.90   |
| 1   | AA    | 992  | U    | O4'-C1'-N1 | 5.39  | 112.51      | 108.20   |
| 3   | AV    | 1    | C    | N3-C4-N4   | 5.39  | 121.78      | 118.00   |
| 3   | AV    | 22   | A    | O4'-C1'-N9 | 5.39  | 112.51      | 108.20   |
| 27  | B8    | 196  | A    | C5-C6-N1   | -5.39 | 115.00      | 117.70   |
| 27  | B8    | 627  | A    | C5-C6-N1   | -5.39 | 115.00      | 117.70   |
| 27  | B8    | 1133 | A    | C5-C6-N1   | -5.39 | 115.00      | 117.70   |
| 27  | B8    | 1420 | A    | C5-C6-N1   | -5.39 | 115.00      | 117.70   |
| 27  | B8    | 1565 | C    | N3-C4-N4   | 5.39  | 121.78      | 118.00   |
| 27  | B8    | 1925 | C    | N3-C4-C5   | -5.39 | 119.74      | 121.90   |
| 27  | B8    | 2031 | A    | C5-C6-N1   | -5.39 | 115.00      | 117.70   |
| 27  | B8    | 2496 | C    | N3-C4-N4   | 5.39  | 121.78      | 118.00   |
| 28  | BA    | 158  | PHE  | CB-CG-CD2  | -5.39 | 117.03      | 120.80   |
| 1   | AA    | 107  | G    | O4'-C1'-N9 | 5.39  | 112.51      | 108.20   |
| 1   | AA    | 1097 | C    | N3-C4-C5   | -5.39 | 119.74      | 121.90   |
| 27  | B8    | 404  | A    | C5-C6-N6   | -5.39 | 119.39      | 123.70   |
| 27  | B8    | 761  | A    | C5-C6-N1   | -5.39 | 115.00      | 117.70   |
| 27  | B8    | 2009 | A    | C5-C6-N6   | -5.39 | 119.39      | 123.70   |
| 27  | B8    | 2129 | C    | C6-N1-C1'  | -5.39 | 114.33      | 120.80   |
| 27  | B8    | 2191 | A    | C5-C6-N6   | -5.39 | 119.39      | 123.70   |
| 27  | B8    | 2792 | A    | C5-C6-N1   | -5.39 | 115.00      | 117.70   |
| 1   | AA    | 26   | A    | C4-C5-C6   | 5.39  | 119.69      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 379  | C    | N3-C4-N4   | 5.39  | 121.77      | 118.00   |
| 1   | AA    | 412  | A    | C5-C6-N6   | -5.39 | 119.39      | 123.70   |
| 1   | AA    | 460  | A    | C5-C6-N6   | -5.39 | 119.39      | 123.70   |
| 1   | AA    | 532  | A    | C5-C6-N1   | -5.39 | 115.01      | 117.70   |
| 3   | AV    | 65   | C    | N3-C4-N4   | 5.39  | 121.77      | 118.00   |
| 27  | B8    | 22   | C    | N3-C4-C5   | -5.39 | 119.74      | 121.90   |
| 27  | B8    | 226  | A    | C5-C6-N1   | -5.39 | 115.00      | 117.70   |
| 27  | B8    | 947  | A    | O4'-C1'-N9 | 5.39  | 112.51      | 108.20   |
| 27  | B8    | 1129 | A    | C5-C6-N1   | -5.39 | 115.00      | 117.70   |
| 27  | B8    | 1877 | A    | O4'-C1'-N9 | 5.39  | 112.51      | 108.20   |
| 27  | B8    | 2476 | A    | C5-C6-N1   | -5.39 | 115.01      | 117.70   |
| 27  | B8    | 2541 | A    | C5-C6-N1   | -5.39 | 115.01      | 117.70   |
| 27  | B8    | 537  | G    | O4'-C1'-N9 | 5.39  | 112.51      | 108.20   |
| 27  | B8    | 550  | C    | N3-C4-N4   | 5.39  | 121.77      | 118.00   |
| 27  | B8    | 1044 | C    | N3-C4-N4   | 5.39  | 121.77      | 118.00   |
| 27  | B8    | 2339 | C    | N3-C4-N4   | 5.39  | 121.77      | 118.00   |
| 1   | AA    | 356  | A    | C4-C5-C6   | 5.39  | 119.69      | 117.00   |
| 1   | AA    | 412  | A    | C5-C6-N1   | -5.39 | 115.01      | 117.70   |
| 1   | AA    | 535  | A    | C5-C6-N1   | -5.39 | 115.01      | 117.70   |
| 1   | AA    | 566  | G    | C5-C6-O6   | -5.39 | 125.37      | 128.60   |
| 1   | AA    | 1080 | A    | C4-C5-C6   | 5.39  | 119.69      | 117.00   |
| 1   | AA    | 1226 | C    | N3-C4-C5   | -5.39 | 119.75      | 121.90   |
| 27  | B8    | 453  | A    | C5-C6-N6   | -5.39 | 119.39      | 123.70   |
| 27  | B8    | 915  | C    | N3-C4-C5   | -5.39 | 119.75      | 121.90   |
| 27  | B8    | 1583 | A    | C4-C5-C6   | 5.39  | 119.69      | 117.00   |
| 27  | B8    | 2092 | U    | C2-N1-C1'  | 5.39  | 124.16      | 117.70   |
| 1   | AA    | 568  | G    | O4'-C1'-N9 | 5.38  | 112.51      | 108.20   |
| 1   | AA    | 705  | G    | N1-C6-O6   | 5.38  | 123.13      | 119.90   |
| 1   | AA    | 996  | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 27  | B8    | 483  | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 27  | B8    | 1503 | A    | C5-C6-N6   | -5.38 | 119.39      | 123.70   |
| 27  | B8    | 1521 | G    | N3-C2-N2   | 5.38  | 123.67      | 119.90   |
| 27  | B8    | 2030 | A    | C5-C6-N6   | -5.38 | 119.39      | 123.70   |
| 27  | B8    | 2058 | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 27  | B8    | 2448 | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 27  | B8    | 2572 | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 27  | B8    | 2712 | C    | N3-C4-C5   | -5.38 | 119.75      | 121.90   |
| 1   | AA    | 1509 | C    | N3-C4-C5   | -5.38 | 119.75      | 121.90   |
| 27  | B8    | 914  | G    | O4'-C1'-N9 | 5.38  | 112.51      | 108.20   |
| 27  | B8    | 944  | C    | N3-C4-C5   | -5.38 | 119.75      | 121.90   |
| 27  | B8    | 1595 | C    | N3-C4-C5   | -5.38 | 119.75      | 121.90   |
| 27  | B8    | 1745 | A    | O4'-C1'-N9 | 5.38  | 112.51      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2052 | A    | O4'-C1'-N9 | 5.38  | 112.51      | 108.20   |
| 27  | B8    | 2364 | C    | N3-C4-C5   | -5.38 | 119.75      | 121.90   |
| 1   | AA    | 1192 | C    | N3-C4-C5   | -5.38 | 119.75      | 121.90   |
| 27  | B8    | 972  | A    | C4-C5-C6   | 5.38  | 119.69      | 117.00   |
| 27  | B8    | 979  | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 27  | B8    | 1463 | C    | N3-C4-N4   | 5.38  | 121.77      | 118.00   |
| 27  | B8    | 1847 | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 27  | B8    | 2002 | G    | O4'-C1'-N9 | 5.38  | 112.50      | 108.20   |
| 27  | B8    | 2751 | G    | O4'-C1'-N9 | 5.38  | 112.51      | 108.20   |
| 1   | AA    | 2    | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 1   | AA    | 212  | G    | O4'-C1'-N9 | 5.38  | 112.50      | 108.20   |
| 1   | AA    | 381  | C    | N3-C4-N4   | 5.38  | 121.77      | 118.00   |
| 1   | AA    | 880  | C    | N3-C4-C5   | -5.38 | 119.75      | 121.90   |
| 3   | AV    | 46   | G    | O4'-C1'-N9 | 5.38  | 112.50      | 108.20   |
| 27  | B8    | 1287 | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 27  | B8    | 1488 | C    | N3-C4-N4   | 5.38  | 121.77      | 118.00   |
| 27  | B8    | 1947 | C    | N3-C4-N4   | 5.38  | 121.77      | 118.00   |
| 1   | AA    | 207  | C    | N3-C4-N4   | 5.38  | 121.77      | 118.00   |
| 1   | AA    | 335  | C    | N3-C4-C5   | -5.38 | 119.75      | 121.90   |
| 1   | AA    | 584  | G    | O4'-C1'-N9 | 5.38  | 112.50      | 108.20   |
| 1   | AA    | 969  | A    | C5-C6-N6   | -5.38 | 119.40      | 123.70   |
| 26  | B7    | 66   | A    | C4-C5-C6   | 5.38  | 119.69      | 117.00   |
| 27  | B8    | 302  | C    | N3-C4-N4   | 5.38  | 121.77      | 118.00   |
| 27  | B8    | 442  | G    | O4'-C1'-N9 | 5.38  | 112.50      | 108.20   |
| 27  | B8    | 484  | C    | N3-C4-C5   | -5.38 | 119.75      | 121.90   |
| 27  | B8    | 565  | C    | N3-C4-C5   | -5.38 | 119.75      | 121.90   |
| 27  | B8    | 1048 | A    | C5-C6-N6   | -5.38 | 119.40      | 123.70   |
| 27  | B8    | 1419 | A    | C5-C6-N6   | -5.38 | 119.40      | 123.70   |
| 27  | B8    | 1545 | A    | C4-C5-C6   | 5.38  | 119.69      | 117.00   |
| 27  | B8    | 1763 | G    | O4'-C1'-N9 | 5.38  | 112.50      | 108.20   |
| 27  | B8    | 1966 | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 27  | B8    | 1970 | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 27  | B8    | 2205 | A    | C5-C6-N6   | -5.38 | 119.40      | 123.70   |
| 27  | B8    | 2815 | C    | N3-C4-N4   | 5.38  | 121.77      | 118.00   |
| 27  | B8    | 2868 | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 1   | AA    | 383  | A    | C5-C6-N6   | -5.38 | 119.40      | 123.70   |
| 1   | AA    | 447  | G    | O4'-C1'-N9 | 5.38  | 112.50      | 108.20   |
| 1   | AA    | 566  | G    | O4'-C1'-N9 | 5.38  | 112.50      | 108.20   |
| 1   | AA    | 807  | A    | C5-C6-N6   | -5.38 | 119.40      | 123.70   |
| 1   | AA    | 1324 | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 1   | AA    | 1408 | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 27  | B8    | 176  | A    | C5-C6-N6   | -5.38 | 119.40      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 854  | C    | N3-C4-N4   | 5.38  | 121.76      | 118.00   |
| 27  | B8    | 1307 | A    | C5-C6-N6   | -5.38 | 119.40      | 123.70   |
| 27  | B8    | 1598 | A    | O4'-C1'-N9 | 5.38  | 112.50      | 108.20   |
| 27  | B8    | 1645 | G    | O4'-C1'-N9 | 5.38  | 112.50      | 108.20   |
| 27  | B8    | 1757 | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 27  | B8    | 2276 | G    | O4'-C1'-N9 | 5.38  | 112.50      | 108.20   |
| 27  | B8    | 2501 | C    | O4'-C1'-N1 | 5.38  | 112.50      | 108.20   |
| 1   | AA    | 363  | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 1   | AA    | 663  | A    | O4'-C1'-N9 | 5.38  | 112.50      | 108.20   |
| 1   | AA    | 764  | C    | N3-C4-C5   | -5.38 | 119.75      | 121.90   |
| 1   | AA    | 1539 | C    | N3-C4-N4   | 5.38  | 121.76      | 118.00   |
| 27  | B8    | 49   | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 27  | B8    | 1272 | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 27  | B8    | 1451 | C    | N3-C4-N4   | 5.38  | 121.76      | 118.00   |
| 27  | B8    | 2799 | A    | C5-C6-N1   | -5.38 | 115.01      | 117.70   |
| 1   | AA    | 160  | A    | C5-C6-N1   | -5.37 | 115.01      | 117.70   |
| 1   | AA    | 482  | A    | O4'-C1'-N9 | 5.37  | 112.50      | 108.20   |
| 1   | AA    | 1265 | C    | N3-C4-N4   | 5.37  | 121.76      | 118.00   |
| 27  | B8    | 44   | A    | C5-C6-N6   | -5.37 | 119.40      | 123.70   |
| 27  | B8    | 320  | A    | O4'-C1'-N9 | 5.37  | 112.50      | 108.20   |
| 27  | B8    | 1005 | C    | N3-C4-C5   | -5.37 | 119.75      | 121.90   |
| 27  | B8    | 1134 | A    | C5-C6-N1   | -5.37 | 115.01      | 117.70   |
| 27  | B8    | 1276 | A    | C5-C6-N6   | -5.37 | 119.40      | 123.70   |
| 27  | B8    | 1985 | C    | N3-C4-C5   | -5.37 | 119.75      | 121.90   |
| 1   | AA    | 1493 | A    | C5-C6-N1   | -5.37 | 115.01      | 117.70   |
| 1   | AA    | 1499 | A    | C5-C6-N1   | -5.37 | 115.01      | 117.70   |
| 27  | B8    | 537  | G    | N3-C2-N2   | 5.37  | 123.66      | 119.90   |
| 27  | B8    | 928  | A    | O4'-C1'-N9 | 5.37  | 112.50      | 108.20   |
| 27  | B8    | 1511 | G    | O4'-C1'-N9 | 5.37  | 112.50      | 108.20   |
| 27  | B8    | 1596 | A    | C4-C5-C6   | 5.37  | 119.69      | 117.00   |
| 27  | B8    | 1944 | U    | O4'-C1'-N1 | 5.37  | 112.50      | 108.20   |
| 27  | B8    | 2126 | A    | C5-C6-N1   | -5.37 | 115.01      | 117.70   |
| 27  | B8    | 2307 | G    | C5-C6-O6   | -5.37 | 125.38      | 128.60   |
| 27  | B8    | 2336 | A    | C5-C6-N6   | -5.37 | 119.40      | 123.70   |
| 27  | B8    | 2476 | A    | C5-C6-N6   | -5.37 | 119.40      | 123.70   |
| 1   | AA    | 488  | C    | N3-C4-C5   | -5.37 | 119.75      | 121.90   |
| 1   | AA    | 635  | A    | C5-C6-N1   | -5.37 | 115.02      | 117.70   |
| 1   | AA    | 794  | A    | C5-C6-N6   | -5.37 | 119.40      | 123.70   |
| 3   | AV    | 42   | C    | N3-C4-N4   | 5.37  | 121.76      | 118.00   |
| 27  | B8    | 1126 | A    | C5-C6-N6   | -5.37 | 119.40      | 123.70   |
| 1   | AA    | 1319 | A    | C5-C6-N1   | -5.37 | 115.02      | 117.70   |
| 1   | AA    | 1366 | C    | N3-C4-C5   | -5.37 | 119.75      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1448 | C    | N3-C4-C5   | -5.37 | 119.75      | 121.90   |
| 26  | B7    | 100  | G    | O4'-C1'-N9 | 5.37  | 112.50      | 108.20   |
| 27  | B8    | 73   | A    | C5-C6-N6   | -5.37 | 119.41      | 123.70   |
| 27  | B8    | 470  | A    | C5-C6-N6   | -5.37 | 119.40      | 123.70   |
| 27  | B8    | 692  | C    | N3-C4-N4   | 5.37  | 121.76      | 118.00   |
| 27  | B8    | 909  | A    | C4-C5-C6   | 5.37  | 119.68      | 117.00   |
| 27  | B8    | 1010 | A    | C5-C6-N6   | -5.37 | 119.41      | 123.70   |
| 27  | B8    | 1522 | A    | C5-C6-N6   | -5.37 | 119.41      | 123.70   |
| 27  | B8    | 2462 | C    | N3-C4-C5   | -5.37 | 119.75      | 121.90   |
| 27  | B8    | 2874 | C    | N3-C4-N4   | 5.37  | 121.76      | 118.00   |
| 1   | AA    | 397  | A    | C5-C6-N1   | -5.37 | 115.02      | 117.70   |
| 27  | B8    | 848  | C    | N3-C4-C5   | -5.37 | 119.75      | 121.90   |
| 27  | B8    | 1080 | A    | C5-C6-N6   | -5.37 | 119.41      | 123.70   |
| 27  | B8    | 1538 | G    | O4'-C1'-N9 | 5.37  | 112.49      | 108.20   |
| 27  | B8    | 1787 | A    | C5-C6-N1   | -5.37 | 115.02      | 117.70   |
| 1   | AA    | 298  | A    | O4'-C1'-N9 | 5.37  | 112.49      | 108.20   |
| 1   | AA    | 374  | A    | C5-C6-N1   | -5.37 | 115.02      | 117.70   |
| 1   | AA    | 720  | C    | N3-C4-N4   | 5.37  | 121.76      | 118.00   |
| 1   | AA    | 819  | A    | C5-C6-N6   | -5.37 | 119.41      | 123.70   |
| 1   | AA    | 1536 | C    | N3-C4-C5   | -5.37 | 119.75      | 121.90   |
| 27  | B8    | 1889 | A    | O4'-C1'-N9 | 5.37  | 112.49      | 108.20   |
| 27  | B8    | 2327 | A    | O4'-C1'-N9 | 5.37  | 112.49      | 108.20   |
| 27  | B8    | 2759 | G    | O4'-C1'-N9 | 5.37  | 112.49      | 108.20   |
| 1   | AA    | 186  | C    | N3-C4-C5   | -5.36 | 119.75      | 121.90   |
| 1   | AA    | 189  | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 1   | AA    | 1036 | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 27  | B8    | 147  | C    | N3-C4-C5   | -5.36 | 119.75      | 121.90   |
| 27  | B8    | 404  | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 27  | B8    | 516  | C    | N3-C4-N4   | 5.36  | 121.75      | 118.00   |
| 27  | B8    | 603  | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 27  | B8    | 1040 | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 27  | B8    | 1057 | A    | O4'-C1'-N9 | 5.36  | 112.49      | 108.20   |
| 27  | B8    | 1672 | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 27  | B8    | 2117 | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 27  | B8    | 2468 | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 1   | AA    | 374  | A    | C5-C6-N6   | -5.36 | 119.41      | 123.70   |
| 1   | AA    | 907  | A    | O4'-C1'-N9 | 5.36  | 112.49      | 108.20   |
| 1   | AA    | 1347 | G    | O4'-C1'-N9 | 5.36  | 112.49      | 108.20   |
| 27  | B8    | 840  | C    | N3-C4-C5   | -5.36 | 119.75      | 121.90   |
| 27  | B8    | 1170 | C    | N3-C4-C5   | -5.36 | 119.75      | 121.90   |
| 27  | B8    | 2327 | A    | C5-C6-N6   | -5.36 | 119.41      | 123.70   |
| 1   | AA    | 153  | C    | N3-C4-C5   | -5.36 | 119.76      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 161  | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 1   | AA    | 489  | C    | N3-C4-N4   | 5.36  | 121.75      | 118.00   |
| 1   | AA    | 528  | C    | N3-C4-C5   | -5.36 | 119.75      | 121.90   |
| 1   | AA    | 841  | C    | N3-C4-N4   | 5.36  | 121.75      | 118.00   |
| 1   | AA    | 972  | C    | N3-C4-N4   | 5.36  | 121.75      | 118.00   |
| 1   | AA    | 1227 | A    | C4-C5-C6   | 5.36  | 119.68      | 117.00   |
| 1   | AA    | 1363 | A    | C5-C6-N6   | -5.36 | 119.41      | 123.70   |
| 3   | AV    | 57   | C    | N3-C4-N4   | 5.36  | 121.75      | 118.00   |
| 27  | B8    | 762  | U    | O4'-C1'-N1 | 5.36  | 112.49      | 108.20   |
| 27  | B8    | 922  | C    | N3-C4-N4   | 5.36  | 121.75      | 118.00   |
| 27  | B8    | 1335 | C    | N3-C4-N4   | 5.36  | 121.75      | 118.00   |
| 27  | B8    | 1392 | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 27  | B8    | 2094 | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 27  | B8    | 2788 | C    | N3-C4-C5   | -5.36 | 119.76      | 121.90   |
| 1   | AA    | 815  | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 1   | AA    | 967  | C    | N3-C4-N4   | 5.36  | 121.75      | 118.00   |
| 1   | AA    | 1012 | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 27  | B8    | 1151 | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 1   | AA    | 567  | G    | O4'-C1'-N9 | 5.36  | 112.49      | 108.20   |
| 26  | B7    | 76   | G    | O4'-C1'-N9 | 5.36  | 112.49      | 108.20   |
| 27  | B8    | 729  | G    | O4'-C1'-N9 | 5.36  | 112.49      | 108.20   |
| 27  | B8    | 753  | A    | C5-C6-N6   | -5.36 | 119.41      | 123.70   |
| 27  | B8    | 820  | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 27  | B8    | 1086 | A    | C4-C5-C6   | 5.36  | 119.68      | 117.00   |
| 27  | B8    | 1140 | C    | N3-C4-C5   | -5.36 | 119.76      | 121.90   |
| 27  | B8    | 1451 | C    | N3-C4-C5   | -5.36 | 119.76      | 121.90   |
| 27  | B8    | 1761 | C    | N3-C4-C5   | -5.36 | 119.76      | 121.90   |
| 27  | B8    | 1876 | A    | C4-C5-C6   | 5.36  | 119.68      | 117.00   |
| 27  | B8    | 2066 | C    | N3-C4-C5   | -5.36 | 119.76      | 121.90   |
| 27  | B8    | 2066 | C    | N3-C4-N4   | 5.36  | 121.75      | 118.00   |
| 27  | B8    | 2347 | C    | N3-C4-C5   | -5.36 | 119.76      | 121.90   |
| 1   | AA    | 172  | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 1   | AA    | 889  | A    | C4-C5-C6   | 5.36  | 119.68      | 117.00   |
| 1   | AA    | 1110 | A    | O4'-C1'-N9 | 5.36  | 112.48      | 108.20   |
| 27  | B8    | 742  | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 27  | B8    | 788  | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 27  | B8    | 1537 | G    | O4'-C1'-N9 | 5.36  | 112.48      | 108.20   |
| 27  | B8    | 1952 | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 27  | B8    | 2170 | A    | C5-C6-N1   | -5.36 | 115.02      | 117.70   |
| 27  | B8    | 2730 | C    | N3-C4-C5   | -5.36 | 119.76      | 121.90   |
| 1   | AA    | 779  | C    | N3-C4-C5   | -5.35 | 119.76      | 121.90   |
| 27  | B8    | 764  | A    | C5-C6-N6   | -5.35 | 119.42      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1605 | C    | N3-C4-N4   | 5.35  | 121.75      | 118.00   |
| 27  | B8    | 1958 | C    | N3-C4-C5   | -5.35 | 119.76      | 121.90   |
| 27  | B8    | 2522 | U    | O4'-C1'-N1 | 5.35  | 112.48      | 108.20   |
| 1   | AA    | 167  | A    | O4'-C1'-N9 | 5.35  | 112.48      | 108.20   |
| 1   | AA    | 401  | C    | N3-C4-N4   | 5.35  | 121.75      | 118.00   |
| 1   | AA    | 783  | C    | N3-C4-C5   | -5.35 | 119.76      | 121.90   |
| 1   | AA    | 919  | A    | C5-C6-N6   | -5.35 | 119.42      | 123.70   |
| 1   | AA    | 968  | A    | C5-C6-N1   | -5.35 | 115.02      | 117.70   |
| 1   | AA    | 1089 | G    | O4'-C1'-N9 | 5.35  | 112.48      | 108.20   |
| 1   | AA    | 1111 | A    | C5-C6-N1   | -5.35 | 115.02      | 117.70   |
| 1   | AA    | 1201 | A    | C5-C6-N1   | -5.35 | 115.02      | 117.70   |
| 1   | AA    | 1296 | C    | N3-C4-N4   | 5.35  | 121.75      | 118.00   |
| 1   | AA    | 1389 | C    | N3-C4-C5   | -5.35 | 119.76      | 121.90   |
| 1   | AA    | 1535 | C    | N3-C4-N4   | 5.35  | 121.75      | 118.00   |
| 3   | AV    | 67   | C    | N3-C4-C5   | -5.35 | 119.76      | 121.90   |
| 27  | B8    | 118  | A    | O4'-C1'-N9 | 5.35  | 112.48      | 108.20   |
| 27  | B8    | 446  | G    | N3-C2-N2   | 5.35  | 123.65      | 119.90   |
| 27  | B8    | 636  | G    | O4'-C1'-N9 | 5.35  | 112.48      | 108.20   |
| 27  | B8    | 802  | A    | C5-C6-N6   | -5.35 | 119.42      | 123.70   |
| 27  | B8    | 996  | A    | C5-C6-N1   | -5.35 | 115.02      | 117.70   |
| 27  | B8    | 2284 | A    | C5-C6-N1   | -5.35 | 115.02      | 117.70   |
| 1   | AA    | 188  | C    | N3-C4-N4   | 5.35  | 121.75      | 118.00   |
| 27  | B8    | 1746 | A    | C5-C6-N1   | -5.35 | 115.03      | 117.70   |
| 27  | B8    | 2331 | G    | O4'-C1'-N9 | 5.35  | 112.48      | 108.20   |
| 1   | AA    | 1377 | A    | C5-C6-N1   | -5.35 | 115.03      | 117.70   |
| 3   | AV    | 17   | C    | N3-C4-C5   | -5.35 | 119.76      | 121.90   |
| 27  | B8    | 173  | A    | C5-C6-N1   | -5.35 | 115.03      | 117.70   |
| 27  | B8    | 249  | C    | N3-C4-C5   | -5.35 | 119.76      | 121.90   |
| 27  | B8    | 446  | G    | O4'-C1'-N9 | 5.35  | 112.48      | 108.20   |
| 27  | B8    | 477  | A    | C5-C6-N1   | -5.35 | 115.03      | 117.70   |
| 27  | B8    | 614  | A    | C5-C6-N6   | -5.35 | 119.42      | 123.70   |
| 27  | B8    | 666  | A    | C5-C6-N1   | -5.35 | 115.03      | 117.70   |
| 27  | B8    | 1495 | A    | C5-C6-N1   | -5.35 | 115.03      | 117.70   |
| 27  | B8    | 1522 | A    | O4'-C1'-N9 | 5.35  | 112.48      | 108.20   |
| 1   | AA    | 244  | U    | O4'-C1'-N1 | 5.35  | 112.48      | 108.20   |
| 3   | AV    | 65   | C    | N3-C4-C5   | -5.35 | 119.76      | 121.90   |
| 3   | AV    | 75   | C    | N3-C4-N4   | 5.35  | 121.74      | 118.00   |
| 5   | A0    | 192  | TYR  | CB-CG-CD1  | -5.35 | 117.79      | 121.00   |
| 26  | B7    | 66   | A    | C5-C6-N1   | -5.35 | 115.03      | 117.70   |
| 27  | B8    | 348  | A    | O4'-C1'-N9 | 5.35  | 112.48      | 108.20   |
| 27  | B8    | 761  | A    | O4'-C1'-N9 | 5.35  | 112.48      | 108.20   |
| 27  | B8    | 1235 | G    | N3-C2-N2   | 5.35  | 123.64      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1554 | U    | O4'-C1'-N1 | 5.35  | 112.48      | 108.20   |
| 27  | B8    | 1580 | A    | O4'-C1'-N9 | 5.35  | 112.48      | 108.20   |
| 27  | B8    | 1631 | G    | O4'-C1'-N9 | 5.35  | 112.48      | 108.20   |
| 27  | B8    | 1707 | G    | O4'-C1'-N9 | 5.35  | 112.48      | 108.20   |
| 27  | B8    | 2070 | A    | C5-C6-N1   | -5.35 | 115.03      | 117.70   |
| 27  | B8    | 2377 | A    | C5-C6-N1   | -5.35 | 115.03      | 117.70   |
| 27  | B8    | 2855 | C    | N3-C4-C5   | -5.35 | 119.76      | 121.90   |
| 1   | AA    | 901  | A    | O4'-C1'-N9 | 5.35  | 112.48      | 108.20   |
| 1   | AA    | 792  | A    | C5-C6-N6   | -5.34 | 119.42      | 123.70   |
| 1   | AA    | 1054 | C    | C2-N1-C1'  | 5.34  | 124.68      | 118.80   |
| 26  | B7    | 101  | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 27  | B8    | 608  | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 27  | B8    | 937  | C    | N3-C4-C5   | -5.34 | 119.76      | 121.90   |
| 27  | B8    | 2096 | C    | N3-C4-N4   | 5.34  | 121.74      | 118.00   |
| 27  | B8    | 2108 | A    | O4'-C1'-N9 | 5.34  | 112.48      | 108.20   |
| 27  | B8    | 2771 | C    | N3-C4-C5   | -5.34 | 119.76      | 121.90   |
| 27  | B8    | 19   | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 27  | B8    | 1076 | C    | N3-C4-N4   | 5.34  | 121.74      | 118.00   |
| 27  | B8    | 1357 | C    | N3-C4-C5   | -5.34 | 119.76      | 121.90   |
| 27  | B8    | 1436 | G    | O4'-C1'-N9 | 5.34  | 112.47      | 108.20   |
| 27  | B8    | 1785 | A    | C4-C5-C6   | 5.34  | 119.67      | 117.00   |
| 27  | B8    | 2261 | C    | N3-C4-C5   | -5.34 | 119.76      | 121.90   |
| 1   | AA    | 240  | G    | O4'-C1'-N9 | 5.34  | 112.47      | 108.20   |
| 1   | AA    | 465  | A    | C4-C5-C6   | 5.34  | 119.67      | 117.00   |
| 1   | AA    | 523  | A    | C5-C6-N6   | -5.34 | 119.43      | 123.70   |
| 1   | AA    | 720  | C    | N3-C4-C5   | -5.34 | 119.76      | 121.90   |
| 1   | AA    | 1195 | C    | P-O3'-C3'  | 5.34  | 126.11      | 119.70   |
| 27  | B8    | 38   | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 27  | B8    | 1275 | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 27  | B8    | 1321 | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 27  | B8    | 2247 | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 27  | B8    | 2394 | C    | N3-C4-C5   | -5.34 | 119.76      | 121.90   |
| 27  | B8    | 2727 | A    | O4'-C1'-N9 | 5.34  | 112.47      | 108.20   |
| 1   | AA    | 768  | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 1   | AA    | 1054 | C    | N3-C4-C5   | -5.34 | 119.77      | 121.90   |
| 1   | AA    | 1508 | A    | C5-C6-N6   | -5.34 | 119.43      | 123.70   |
| 27  | B8    | 1053 | C    | N3-C4-C5   | -5.34 | 119.76      | 121.90   |
| 27  | B8    | 1327 | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 27  | B8    | 2080 | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 27  | B8    | 2472 | G    | O4'-C1'-N9 | 5.34  | 112.47      | 108.20   |
| 27  | B8    | 2875 | C    | N3-C4-N4   | 5.34  | 121.74      | 118.00   |
| 1   | AA    | 806  | C    | N3-C4-C5   | -5.34 | 119.77      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1211 | C    | N3-C4-N4   | 5.34  | 121.74      | 118.00   |
| 27  | B8    | 1809 | A    | O4'-C1'-N9 | 5.34  | 112.47      | 108.20   |
| 27  | B8    | 2403 | C    | N3-C4-C5   | -5.34 | 119.77      | 121.90   |
| 1   | AA    | 28   | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 1   | AA    | 609  | A    | C5-C6-N6   | -5.34 | 119.43      | 123.70   |
| 1   | AA    | 853  | C    | N3-C4-N4   | 5.34  | 121.74      | 118.00   |
| 1   | AA    | 892  | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 1   | AA    | 985  | C    | N3-C4-C5   | -5.34 | 119.77      | 121.90   |
| 1   | AA    | 1342 | C    | N3-C4-N4   | 5.34  | 121.73      | 118.00   |
| 1   | AA    | 1369 | C    | N3-C4-C5   | -5.34 | 119.77      | 121.90   |
| 27  | B8    | 161  | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 27  | B8    | 942  | G    | O4'-C1'-N9 | 5.34  | 112.47      | 108.20   |
| 27  | B8    | 1232 | G    | O4'-C1'-N9 | 5.34  | 112.47      | 108.20   |
| 27  | B8    | 1789 | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 27  | B8    | 1870 | C    | N3-C4-C5   | -5.34 | 119.77      | 121.90   |
| 27  | B8    | 2095 | A    | C5-C6-N1   | -5.34 | 115.03      | 117.70   |
| 27  | B8    | 2497 | A    | C5-C6-N6   | -5.34 | 119.43      | 123.70   |
| 27  | B8    | 2507 | C    | N3-C4-C5   | -5.34 | 119.77      | 121.90   |
| 27  | B8    | 2610 | C    | N3-C4-C5   | -5.34 | 119.77      | 121.90   |
| 27  | B8    | 2699 | C    | N3-C4-C5   | -5.34 | 119.77      | 121.90   |
| 1   | AA    | 167  | A    | C5-C6-N1   | -5.33 | 115.03      | 117.70   |
| 1   | AA    | 1329 | A    | C5-C6-N1   | -5.33 | 115.03      | 117.70   |
| 27  | B8    | 340  | A    | C5-C6-N6   | -5.33 | 119.43      | 123.70   |
| 27  | B8    | 2406 | A    | C5-C6-N1   | -5.33 | 115.03      | 117.70   |
| 27  | B8    | 2814 | A    | C5-C6-N1   | -5.33 | 115.03      | 117.70   |
| 1   | AA    | 1396 | A    | C4-C5-C6   | 5.33  | 119.67      | 117.00   |
| 1   | AA    | 1510 | C    | N3-C4-N4   | 5.33  | 121.73      | 118.00   |
| 27  | B8    | 717  | C    | N3-C4-C5   | -5.33 | 119.77      | 121.90   |
| 27  | B8    | 948  | C    | N3-C4-C5   | -5.33 | 119.77      | 121.90   |
| 27  | B8    | 1204 | A    | C5-C6-N1   | -5.33 | 115.03      | 117.70   |
| 27  | B8    | 2124 | G    | O4'-C1'-N9 | 5.33  | 112.47      | 108.20   |
| 27  | B8    | 2469 | A    | C5-C6-N6   | -5.33 | 119.43      | 123.70   |
| 27  | B8    | 2534 | A    | C5-C6-N6   | -5.33 | 119.43      | 123.70   |
| 1   | AA    | 18   | C    | N3-C4-C5   | -5.33 | 119.77      | 121.90   |
| 1   | AA    | 309  | A    | C5-C6-N1   | -5.33 | 115.03      | 117.70   |
| 1   | AA    | 321  | A    | C5-C6-N6   | -5.33 | 119.44      | 123.70   |
| 1   | AA    | 344  | A    | C5-C6-N1   | -5.33 | 115.03      | 117.70   |
| 1   | AA    | 595  | A    | C5-C6-N1   | -5.33 | 115.03      | 117.70   |
| 1   | AA    | 781  | A    | C5-C6-N6   | -5.33 | 119.44      | 123.70   |
| 27  | B8    | 490  | C    | N3-C4-C5   | -5.33 | 119.77      | 121.90   |
| 27  | B8    | 778  | G    | O4'-C1'-N9 | 5.33  | 112.47      | 108.20   |
| 27  | B8    | 1273 | U    | O4'-C1'-N1 | 5.33  | 112.47      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1314 | C    | N3-C4-C5   | -5.33 | 119.77      | 121.90   |
| 27  | B8    | 1518 | C    | N3-C4-C5   | -5.33 | 119.77      | 121.90   |
| 27  | B8    | 2394 | C    | N3-C4-N4   | 5.33  | 121.73      | 118.00   |
| 27  | B8    | 2602 | A    | C5-C6-N1   | -5.33 | 115.03      | 117.70   |
| 3   | AV    | 11   | C    | N3-C4-C5   | -5.33 | 119.77      | 121.90   |
| 27  | B8    | 968  | C    | N3-C4-C5   | -5.33 | 119.77      | 121.90   |
| 27  | B8    | 1040 | A    | C5-C6-N6   | -5.33 | 119.44      | 123.70   |
| 27  | B8    | 1616 | A    | C5-C6-N1   | -5.33 | 115.03      | 117.70   |
| 27  | B8    | 2161 | C    | N3-C4-N4   | 5.33  | 121.73      | 118.00   |
| 1   | AA    | 214  | C    | N3-C4-C5   | -5.33 | 119.77      | 121.90   |
| 1   | AA    | 958  | A    | C5-C6-N6   | -5.33 | 119.44      | 123.70   |
| 27  | B8    | 203  | A    | C5-C6-N1   | -5.33 | 115.04      | 117.70   |
| 27  | B8    | 251  | A    | C5-C6-N6   | -5.33 | 119.44      | 123.70   |
| 27  | B8    | 487  | C    | N3-C4-C5   | -5.33 | 119.77      | 121.90   |
| 27  | B8    | 501  | A    | C5-C6-N1   | -5.33 | 115.04      | 117.70   |
| 27  | B8    | 1103 | A    | C5-C6-N1   | -5.33 | 115.04      | 117.70   |
| 27  | B8    | 1322 | A    | C5-C6-N6   | -5.33 | 119.44      | 123.70   |
| 27  | B8    | 1570 | A    | O4'-C1'-N9 | 5.33  | 112.46      | 108.20   |
| 27  | B8    | 1611 | C    | N3-C4-N4   | 5.33  | 121.73      | 118.00   |
| 27  | B8    | 1679 | A    | C5-C6-N1   | -5.33 | 115.03      | 117.70   |
| 1   | AA    | 787  | A    | C5-C6-N1   | -5.33 | 115.04      | 117.70   |
| 1   | AA    | 1021 | A    | C5-C6-N1   | -5.33 | 115.04      | 117.70   |
| 1   | AA    | 1384 | C    | N3-C4-C5   | -5.33 | 119.77      | 121.90   |
| 27  | B8    | 213  | A    | O4'-C1'-N9 | 5.33  | 112.46      | 108.20   |
| 27  | B8    | 536  | G    | O4'-C1'-N9 | 5.33  | 112.46      | 108.20   |
| 27  | B8    | 1069 | A    | C5-C6-N1   | -5.33 | 115.04      | 117.70   |
| 27  | B8    | 1342 | A    | C5-C6-N1   | -5.33 | 115.04      | 117.70   |
| 27  | B8    | 2478 | A    | C5-C6-N1   | -5.33 | 115.04      | 117.70   |
| 1   | AA    | 228  | A    | C5-C6-N1   | -5.33 | 115.04      | 117.70   |
| 1   | AA    | 1507 | A    | C5-C6-N1   | -5.33 | 115.04      | 117.70   |
| 1   | AA    | 1519 | A    | C5-C6-N1   | -5.33 | 115.04      | 117.70   |
| 3   | AV    | 57   | C    | N3-C4-C5   | -5.33 | 119.77      | 121.90   |
| 27  | B8    | 278  | A    | O4'-C1'-N9 | 5.33  | 112.46      | 108.20   |
| 27  | B8    | 354  | A    | C5-C6-N6   | -5.33 | 119.44      | 123.70   |
| 27  | B8    | 1941 | C    | N3-C4-C5   | -5.33 | 119.77      | 121.90   |
| 27  | B8    | 2513 | A    | O4'-C1'-N9 | 5.33  | 112.46      | 108.20   |
| 27  | B8    | 2547 | A    | C5-C6-N6   | -5.33 | 119.44      | 123.70   |
| 1   | AA    | 382  | A    | C5-C6-N1   | -5.32 | 115.04      | 117.70   |
| 1   | AA    | 624  | C    | N3-C4-C5   | -5.32 | 119.77      | 121.90   |
| 1   | AA    | 627  | G    | O4'-C1'-N9 | 5.32  | 112.46      | 108.20   |
| 1   | AA    | 934  | C    | N3-C4-N4   | 5.32  | 121.73      | 118.00   |
| 1   | AA    | 975  | A    | C5-C6-N1   | -5.32 | 115.04      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 1260 | G    | N3-C2-N2    | 5.32  | 123.63      | 119.90   |
| 27  | B8    | 63   | A    | C5-C6-N6    | -5.32 | 119.44      | 123.70   |
| 27  | B8    | 213  | A    | C5-C6-N1    | -5.32 | 115.04      | 117.70   |
| 27  | B8    | 685  | A    | C5-C6-N1    | -5.32 | 115.04      | 117.70   |
| 27  | B8    | 751  | A    | O4'-C1'-N9  | 5.32  | 112.46      | 108.20   |
| 27  | B8    | 1147 | A    | C5-C6-N6    | -5.32 | 119.44      | 123.70   |
| 27  | B8    | 1553 | A    | O4'-C1'-N9  | 5.32  | 112.46      | 108.20   |
| 27  | B8    | 1629 | U    | O4'-C1'-N1  | 5.32  | 112.46      | 108.20   |
| 27  | B8    | 1998 | A    | C5-C6-N1    | -5.32 | 115.04      | 117.70   |
| 27  | B8    | 2553 | G    | O4'-C1'-N9  | 5.32  | 112.46      | 108.20   |
| 27  | B8    | 1461 | C    | N3-C4-N4    | 5.32  | 121.72      | 118.00   |
| 1   | AA    | 889  | A    | C5-C6-N1    | -5.32 | 115.04      | 117.70   |
| 1   | AA    | 1293 | C    | N3-C4-C5    | -5.32 | 119.77      | 121.90   |
| 27  | B8    | 126  | A    | C5-C6-N6    | -5.32 | 119.44      | 123.70   |
| 27  | B8    | 527  | C    | C2-N1-C1'   | 5.32  | 124.65      | 118.80   |
| 27  | B8    | 1328 | A    | C5-C6-N1    | -5.32 | 115.04      | 117.70   |
| 27  | B8    | 1727 | C    | N3-C4-C5    | -5.32 | 119.77      | 121.90   |
| 27  | B8    | 891  | G    | C5'-C4'-O4' | 5.32  | 115.48      | 109.10   |
| 1   | AA    | 34   | C    | N3-C4-C5    | -5.32 | 119.77      | 121.90   |
| 1   | AA    | 499  | A    | C5-C6-N1    | -5.32 | 115.04      | 117.70   |
| 1   | AA    | 546  | A    | C5-C6-N1    | -5.32 | 115.04      | 117.70   |
| 1   | AA    | 1327 | C    | N3-C4-C5    | -5.32 | 119.77      | 121.90   |
| 27  | B8    | 28   | A    | C5-C6-N1    | -5.32 | 115.04      | 117.70   |
| 27  | B8    | 616  | A    | O4'-C1'-N9  | 5.32  | 112.45      | 108.20   |
| 27  | B8    | 1204 | A    | O4'-C1'-N9  | 5.32  | 112.45      | 108.20   |
| 27  | B8    | 1853 | A    | C5-C6-N6    | -5.32 | 119.45      | 123.70   |
| 27  | B8    | 1947 | C    | N3-C4-C5    | -5.32 | 119.77      | 121.90   |
| 27  | B8    | 2309 | A    | C5-C6-N1    | -5.32 | 115.04      | 117.70   |
| 27  | B8    | 2520 | C    | N3-C4-N4    | 5.32  | 121.72      | 118.00   |
| 1   | AA    | 585  | G    | O4'-C1'-N9  | 5.32  | 112.45      | 108.20   |
| 1   | AA    | 815  | A    | O4'-C1'-N9  | 5.32  | 112.45      | 108.20   |
| 27  | B8    | 11   | C    | N3-C4-N4    | 5.32  | 121.72      | 118.00   |
| 27  | B8    | 104  | A    | C5-C6-N1    | -5.32 | 115.04      | 117.70   |
| 27  | B8    | 613  | A    | C5-C6-N6    | -5.32 | 119.45      | 123.70   |
| 27  | B8    | 1509 | A    | C5-C6-N1    | -5.32 | 115.04      | 117.70   |
| 27  | B8    | 2662 | A    | O4'-C1'-N9  | 5.32  | 112.45      | 108.20   |
| 27  | B8    | 2682 | A    | C5-C6-N1    | -5.32 | 115.04      | 117.70   |
| 1   | AA    | 1274 | A    | C5-C6-N1    | -5.31 | 115.04      | 117.70   |
| 1   | AA    | 1518 | A    | C5-C6-N6    | -5.31 | 119.45      | 123.70   |
| 27  | B8    | 1067 | A    | C5-C6-N1    | -5.31 | 115.04      | 117.70   |
| 27  | B8    | 1514 | G    | O4'-C1'-N9  | 5.31  | 112.45      | 108.20   |
| 27  | B8    | 1853 | A    | C4-C5-C6    | 5.31  | 119.66      | 117.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 338  | A    | C5-C6-N6    | -5.31 | 119.45      | 123.70   |
| 1   | AA    | 702  | A    | O4'-C1'-N9  | 5.31  | 112.45      | 108.20   |
| 1   | AA    | 1288 | A    | C5-C6-N1    | -5.31 | 115.04      | 117.70   |
| 1   | AA    | 1399 | C    | N3-C4-C5    | -5.31 | 119.78      | 121.90   |
| 27  | B8    | 2270 | A    | C5-C6-N6    | -5.31 | 119.45      | 123.70   |
| 27  | B8    | 2651 | C    | N3-C4-C5    | -5.31 | 119.78      | 121.90   |
| 1   | AA    | 54   | C    | N3-C4-N4    | 5.31  | 121.72      | 118.00   |
| 1   | AA    | 1069 | C    | N3-C4-C5    | -5.31 | 119.78      | 121.90   |
| 2   | AX    | 20   | G    | O4'-C1'-N9  | 5.31  | 112.45      | 108.20   |
| 27  | B8    | 252  | G    | O4'-C1'-N9  | 5.31  | 112.45      | 108.20   |
| 27  | B8    | 1156 | A    | C5-C6-N1    | -5.31 | 115.05      | 117.70   |
| 27  | B8    | 1606 | C    | N3-C4-C5    | -5.31 | 119.78      | 121.90   |
| 27  | B8    | 2380 | C    | N3-C4-C5    | -5.31 | 119.78      | 121.90   |
| 27  | B8    | 2427 | C    | N3-C4-N4    | 5.31  | 121.72      | 118.00   |
| 1   | AA    | 395  | C    | N3-C4-C5    | -5.31 | 119.78      | 121.90   |
| 1   | AA    | 844  | G    | C5'-C4'-O4' | 5.31  | 115.47      | 109.10   |
| 1   | AA    | 1117 | A    | C5-C6-N1    | -5.31 | 115.05      | 117.70   |
| 1   | AA    | 1332 | A    | C5-C6-N6    | -5.31 | 119.45      | 123.70   |
| 27  | B8    | 106  | C    | N3-C4-N4    | 5.31  | 121.72      | 118.00   |
| 27  | B8    | 322  | A    | O4'-C1'-N9  | 5.31  | 112.45      | 108.20   |
| 27  | B8    | 1125 | G    | N3-C2-N2    | 5.31  | 123.62      | 119.90   |
| 27  | B8    | 1428 | C    | N3-C4-N4    | 5.31  | 121.72      | 118.00   |
| 27  | B8    | 1792 | G    | O4'-C1'-N9  | 5.31  | 112.45      | 108.20   |
| 1   | AA    | 1238 | A    | C4-C5-C6    | 5.31  | 119.65      | 117.00   |
| 27  | B8    | 74   | A    | C5-C6-N6    | -5.31 | 119.45      | 123.70   |
| 27  | B8    | 238  | C    | N3-C4-C5    | -5.31 | 119.78      | 121.90   |
| 27  | B8    | 1009 | A    | C5-C6-N1    | -5.31 | 115.05      | 117.70   |
| 27  | B8    | 1270 | C    | N3-C4-C5    | -5.31 | 119.78      | 121.90   |
| 27  | B8    | 2239 | G    | O4'-C1'-N9  | 5.31  | 112.45      | 108.20   |
| 27  | B8    | 2273 | A    | C5-C6-N1    | -5.31 | 115.05      | 117.70   |
| 1   | AA    | 135  | C    | N3-C4-C5    | -5.31 | 119.78      | 121.90   |
| 1   | AA    | 1427 | C    | N3-C4-C5    | -5.31 | 119.78      | 121.90   |
| 27  | B8    | 74   | A    | C5-C6-N1    | -5.31 | 115.05      | 117.70   |
| 27  | B8    | 512  | G    | O4'-C1'-N9  | 5.31  | 112.44      | 108.20   |
| 27  | B8    | 713  | G    | N3-C2-N2    | 5.31  | 123.61      | 119.90   |
| 27  | B8    | 715  | A    | C5-C6-N1    | -5.31 | 115.05      | 117.70   |
| 27  | B8    | 748  | G    | O4'-C1'-N9  | 5.31  | 112.44      | 108.20   |
| 27  | B8    | 960  | A    | C5-C6-N1    | -5.31 | 115.05      | 117.70   |
| 27  | B8    | 1822 | C    | N3-C4-C5    | -5.31 | 119.78      | 121.90   |
| 27  | B8    | 2376 | A    | C5-C6-N1    | -5.31 | 115.05      | 117.70   |
| 27  | B8    | 2577 | A    | C5-C6-N6    | -5.31 | 119.45      | 123.70   |
| 1   | AA    | 78   | A    | C5-C6-N6    | -5.30 | 119.46      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | AA    | 99   | C    | N3-C4-N4    | 5.30  | 121.71      | 118.00   |
| 1   | AA    | 637  | C    | N3-C4-C5    | -5.30 | 119.78      | 121.90   |
| 1   | AA    | 701  | U    | O4'-C1'-N1  | 5.30  | 112.44      | 108.20   |
| 1   | AA    | 1429 | A    | C5-C6-N1    | -5.30 | 115.05      | 117.70   |
| 26  | B7    | 88   | C    | N3-C4-N4    | 5.30  | 121.71      | 118.00   |
| 27  | B8    | 361  | G    | N3-C2-N2    | 5.30  | 123.61      | 119.90   |
| 27  | B8    | 445  | C    | N3-C4-C5    | -5.30 | 119.78      | 121.90   |
| 27  | B8    | 829  | A    | C5-C6-N1    | -5.30 | 115.05      | 117.70   |
| 27  | B8    | 961  | C    | N3-C4-C5    | -5.30 | 119.78      | 121.90   |
| 27  | B8    | 1365 | A    | C5-C6-N1    | -5.30 | 115.05      | 117.70   |
| 27  | B8    | 1800 | C    | O4'-C1'-N1  | 5.30  | 112.44      | 108.20   |
| 27  | B8    | 2501 | C    | N3-C4-N4    | 5.30  | 121.71      | 118.00   |
| 27  | B8    | 2763 | G    | N3-C2-N2    | 5.30  | 123.61      | 119.90   |
| 28  | BA    | 217  | PHE  | CB-CG-CD2   | -5.30 | 117.09      | 120.80   |
| 1   | AA    | 422  | C    | N3-C4-N4    | 5.30  | 121.71      | 118.00   |
| 1   | AA    | 845  | A    | C5-C6-N1    | -5.30 | 115.05      | 117.70   |
| 1   | AA    | 55   | A    | C5-C6-N1    | -5.30 | 115.05      | 117.70   |
| 1   | AA    | 136  | C    | N3-C4-C5    | -5.30 | 119.78      | 121.90   |
| 1   | AA    | 242  | G    | O4'-C1'-N9  | 5.30  | 112.44      | 108.20   |
| 3   | AV    | 72   | C    | N3-C4-N4    | 5.30  | 121.71      | 118.00   |
| 27  | B8    | 52   | A    | O4'-C1'-N9  | 5.30  | 112.44      | 108.20   |
| 27  | B8    | 94   | A    | C5-C6-N1    | -5.30 | 115.05      | 117.70   |
| 27  | B8    | 208  | C    | N3-C4-C5    | -5.30 | 119.78      | 121.90   |
| 27  | B8    | 2084 | C    | N3-C4-C5    | -5.30 | 119.78      | 121.90   |
| 27  | B8    | 2129 | C    | N3-C4-C5    | -5.30 | 119.78      | 121.90   |
| 27  | B8    | 2282 | G    | C2'-C3'-O3' | 5.30  | 122.18      | 113.70   |
| 27  | B8    | 2726 | A    | C5-C6-N1    | -5.30 | 115.05      | 117.70   |
| 1   | AA    | 3    | A    | C5-C6-N1    | -5.30 | 115.05      | 117.70   |
| 1   | AA    | 65   | A    | C5-C6-N1    | -5.30 | 115.05      | 117.70   |
| 1   | AA    | 432  | A    | C5-C6-N6    | -5.30 | 119.46      | 123.70   |
| 1   | AA    | 1404 | C    | N3-C4-C5    | -5.30 | 119.78      | 121.90   |
| 3   | AV    | 58   | A    | O4'-C1'-N9  | 5.30  | 112.44      | 108.20   |
| 26  | B7    | 4    | C    | N3-C4-N4    | 5.30  | 121.71      | 118.00   |
| 27  | B8    | 127  | A    | C5'-C4'-C3' | -5.30 | 107.52      | 116.00   |
| 27  | B8    | 191  | A    | C5-C6-N6    | -5.30 | 119.46      | 123.70   |
| 27  | B8    | 398  | C    | N3-C4-N4    | 5.30  | 121.71      | 118.00   |
| 27  | B8    | 614  | A    | C5-C6-N1    | -5.30 | 115.05      | 117.70   |
| 27  | B8    | 1243 | C    | N3-C4-C5    | -5.30 | 119.78      | 121.90   |
| 27  | B8    | 1376 | C    | N3-C4-N4    | 5.30  | 121.71      | 118.00   |
| 27  | B8    | 1744 | A    | C5-C6-N6    | -5.30 | 119.46      | 123.70   |
| 27  | B8    | 1960 | A    | C5-C6-N6    | -5.30 | 119.46      | 123.70   |
| 27  | B8    | 2420 | C    | N3-C4-C5    | -5.30 | 119.78      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 856  | C    | N3-C4-N4   | 5.30  | 121.71      | 118.00   |
| 1   | AA    | 1152 | A    | O4'-C1'-N9 | 5.30  | 112.44      | 108.20   |
| 27  | B8    | 264  | C    | N3-C4-C5   | -5.30 | 119.78      | 121.90   |
| 27  | B8    | 368  | A    | O4'-C1'-N9 | 5.30  | 112.44      | 108.20   |
| 27  | B8    | 527  | C    | N3-C4-N4   | 5.30  | 121.71      | 118.00   |
| 27  | B8    | 1575 | C    | N3-C4-N4   | 5.30  | 121.71      | 118.00   |
| 27  | B8    | 172  | A    | C5-C6-N1   | -5.30 | 115.05      | 117.70   |
| 27  | B8    | 555  | G    | N3-C2-N2   | 5.30  | 123.61      | 119.90   |
| 27  | B8    | 846  | U    | C2-N1-C1'  | 5.30  | 124.06      | 117.70   |
| 27  | B8    | 1133 | A    | C5-C6-N6   | -5.30 | 119.46      | 123.70   |
| 27  | B8    | 1254 | A    | C5-C6-N6   | -5.30 | 119.46      | 123.70   |
| 27  | B8    | 1698 | A    | C5-C6-N1   | -5.30 | 115.05      | 117.70   |
| 27  | B8    | 2095 | A    | C5-C6-N6   | -5.30 | 119.46      | 123.70   |
| 27  | B8    | 2338 | C    | N3-C4-N4   | 5.30  | 121.71      | 118.00   |
| 27  | B8    | 2840 | C    | N3-C4-C5   | -5.30 | 119.78      | 121.90   |
| 1   | AA    | 1102 | A    | O4'-C1'-N9 | 5.29  | 112.44      | 108.20   |
| 1   | AA    | 1188 | A    | C5-C6-N1   | -5.29 | 115.05      | 117.70   |
| 27  | B8    | 11   | C    | N3-C4-C5   | -5.29 | 119.78      | 121.90   |
| 1   | AA    | 40   | C    | N3-C4-C5   | -5.29 | 119.78      | 121.90   |
| 1   | AA    | 160  | A    | C5-C6-N6   | -5.29 | 119.47      | 123.70   |
| 1   | AA    | 685  | G    | O4'-C1'-N9 | 5.29  | 112.44      | 108.20   |
| 3   | AV    | 3    | G    | O4'-C1'-N9 | 5.29  | 112.43      | 108.20   |
| 26  | B7    | 44   | G    | O4'-C1'-N9 | 5.29  | 112.44      | 108.20   |
| 27  | B8    | 546  | U    | O4'-C1'-N1 | 5.29  | 112.44      | 108.20   |
| 27  | B8    | 697  | G    | O4'-C1'-N9 | 5.29  | 112.44      | 108.20   |
| 27  | B8    | 1616 | A    | C5-C6-N6   | -5.29 | 119.47      | 123.70   |
| 27  | B8    | 1760 | C    | N3-C4-C5   | -5.29 | 119.78      | 121.90   |
| 27  | B8    | 1965 | C    | N3-C4-C5   | -5.29 | 119.78      | 121.90   |
| 27  | B8    | 2395 | C    | N3-C4-C5   | -5.29 | 119.78      | 121.90   |
| 27  | B8    | 2440 | C    | N3-C4-N4   | 5.29  | 121.71      | 118.00   |
| 1   | AA    | 72   | A    | C5-C6-N6   | -5.29 | 119.47      | 123.70   |
| 1   | AA    | 101  | A    | C5-C6-N1   | -5.29 | 115.05      | 117.70   |
| 1   | AA    | 158  | G    | O4'-C1'-N9 | 5.29  | 112.43      | 108.20   |
| 1   | AA    | 572  | A    | C5-C6-N6   | -5.29 | 119.47      | 123.70   |
| 1   | AA    | 607  | A    | C5-C6-N1   | -5.29 | 115.05      | 117.70   |
| 1   | AA    | 675  | A    | C5-C6-N1   | -5.29 | 115.05      | 117.70   |
| 1   | AA    | 1167 | A    | C5-C6-N1   | -5.29 | 115.06      | 117.70   |
| 1   | AA    | 1410 | A    | C5-C6-N6   | -5.29 | 119.47      | 123.70   |
| 1   | AA    | 1535 | C    | N3-C4-C5   | -5.29 | 119.78      | 121.90   |
| 27  | B8    | 308  | G    | O4'-C1'-N9 | 5.29  | 112.43      | 108.20   |
| 27  | B8    | 352  | A    | C5-C6-N1   | -5.29 | 115.05      | 117.70   |
| 27  | B8    | 1939 | U    | O4'-C1'-N1 | 5.29  | 112.43      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2078 | C    | N3-C4-C5   | -5.29 | 119.78      | 121.90   |
| 27  | B8    | 2821 | A    | O4'-C1'-N9 | 5.29  | 112.43      | 108.20   |
| 27  | B8    | 2853 | C    | N3-C4-C5   | -5.29 | 119.78      | 121.90   |
| 1   | AA    | 1109 | C    | N3-C4-C5   | -5.29 | 119.78      | 121.90   |
| 1   | AA    | 1531 | A    | C5-C6-N6   | -5.29 | 119.47      | 123.70   |
| 27  | B8    | 137  | U    | P-O5'-C5'  | 5.29  | 129.36      | 120.90   |
| 27  | B8    | 1701 | A    | C5-C6-N6   | -5.29 | 119.47      | 123.70   |
| 1   | AA    | 576  | C    | N3-C4-C5   | -5.29 | 119.78      | 121.90   |
| 1   | AA    | 1270 | G    | O4'-C1'-N9 | 5.29  | 112.43      | 108.20   |
| 1   | AA    | 1342 | C    | N3-C4-C5   | -5.29 | 119.78      | 121.90   |
| 27  | B8    | 342  | A    | O4'-C1'-N9 | 5.29  | 112.43      | 108.20   |
| 27  | B8    | 1057 | A    | C5-C6-N1   | -5.29 | 115.06      | 117.70   |
| 27  | B8    | 1146 | C    | N3-C4-N4   | 5.29  | 121.70      | 118.00   |
| 27  | B8    | 1176 | U    | O4'-C1'-N1 | 5.29  | 112.43      | 108.20   |
| 27  | B8    | 1213 | A    | C5-C6-N6   | -5.29 | 119.47      | 123.70   |
| 27  | B8    | 1489 | C    | N3-C4-N4   | 5.29  | 121.70      | 118.00   |
| 27  | B8    | 2425 | A    | O4'-C1'-N9 | 5.29  | 112.43      | 108.20   |
| 27  | B8    | 2426 | A    | C5-C6-N1   | -5.29 | 115.06      | 117.70   |
| 1   | AA    | 676  | A    | C5-C6-N6   | -5.29 | 119.47      | 123.70   |
| 1   | AA    | 1360 | A    | O4'-C1'-N9 | 5.29  | 112.43      | 108.20   |
| 27  | B8    | 897  | C    | N3-C4-C5   | -5.29 | 119.78      | 121.90   |
| 27  | B8    | 1395 | A    | O4'-C1'-N9 | 5.29  | 112.43      | 108.20   |
| 27  | B8    | 1710 | G    | O4'-C1'-N9 | 5.29  | 112.43      | 108.20   |
| 27  | B8    | 2287 | A    | C5-C6-N6   | -5.29 | 119.47      | 123.70   |
| 1   | AA    | 415  | A    | C5-C6-N6   | -5.29 | 119.47      | 123.70   |
| 3   | AV    | 58   | A    | C5-C6-N1   | -5.29 | 115.06      | 117.70   |
| 27  | B8    | 32   | C    | N3-C4-C5   | -5.29 | 119.79      | 121.90   |
| 27  | B8    | 1303 | G    | O4'-C1'-N9 | 5.29  | 112.43      | 108.20   |
| 27  | B8    | 1504 | A    | C5-C6-N6   | -5.29 | 119.47      | 123.70   |
| 27  | B8    | 1942 | C    | N3-C4-N4   | 5.29  | 121.70      | 118.00   |
| 27  | B8    | 2267 | A    | C5-C6-N1   | -5.29 | 115.06      | 117.70   |
| 27  | B8    | 2628 | C    | N3-C4-C5   | -5.29 | 119.79      | 121.90   |
| 1   | AA    | 523  | A    | C5-C6-N1   | -5.28 | 115.06      | 117.70   |
| 27  | B8    | 751  | A    | C5-C6-N6   | -5.28 | 119.47      | 123.70   |
| 27  | B8    | 1067 | A    | C5-C6-N6   | -5.28 | 119.47      | 123.70   |
| 27  | B8    | 1322 | A    | C4-C5-C6   | 5.28  | 119.64      | 117.00   |
| 27  | B8    | 1803 | A    | O4'-C1'-N9 | 5.28  | 112.43      | 108.20   |
| 27  | B8    | 2090 | A    | C5-C6-N1   | -5.28 | 115.06      | 117.70   |
| 1   | AA    | 461  | A    | C5-C6-N1   | -5.28 | 115.06      | 117.70   |
| 27  | B8    | 579  | G    | O4'-C1'-N9 | 5.28  | 112.43      | 108.20   |
| 1   | AA    | 238  | A    | C5-C6-N1   | -5.28 | 115.06      | 117.70   |
| 1   | AA    | 466  | A    | C5-C6-N1   | -5.28 | 115.06      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 946  | A    | C5-C6-N6   | -5.28 | 119.47      | 123.70   |
| 27  | B8    | 118  | A    | C5-C6-N6   | -5.28 | 119.48      | 123.70   |
| 27  | B8    | 309  | A    | C5-C6-N1   | -5.28 | 115.06      | 117.70   |
| 27  | B8    | 354  | A    | O4'-C1'-N9 | 5.28  | 112.42      | 108.20   |
| 27  | B8    | 750  | A    | O4'-C1'-N9 | 5.28  | 112.42      | 108.20   |
| 27  | B8    | 1271 | G    | O4'-C1'-N9 | 5.28  | 112.42      | 108.20   |
| 27  | B8    | 1381 | G    | O4'-C1'-N9 | 5.28  | 112.42      | 108.20   |
| 27  | B8    | 2468 | A    | O4'-C1'-N9 | 5.28  | 112.42      | 108.20   |
| 27  | B8    | 2619 | C    | N3-C4-C5   | -5.28 | 119.79      | 121.90   |
| 27  | B8    | 2652 | C    | N3-C4-N4   | 5.28  | 121.70      | 118.00   |
| 27  | B8    | 2823 | A    | O4'-C1'-N9 | 5.28  | 112.42      | 108.20   |
| 1   | AA    | 609  | A    | C5-C6-N1   | -5.28 | 115.06      | 117.70   |
| 1   | AA    | 1012 | A    | C4-C5-C6   | 5.28  | 119.64      | 117.00   |
| 1   | AA    | 51   | A    | C5-C6-N6   | -5.28 | 119.48      | 123.70   |
| 1   | AA    | 235  | C    | N3-C4-C5   | -5.28 | 119.79      | 121.90   |
| 1   | AA    | 1216 | A    | C5-C6-N6   | -5.28 | 119.48      | 123.70   |
| 1   | AA    | 1402 | C    | N3-C4-N4   | 5.28  | 121.69      | 118.00   |
| 26  | B7    | 57   | A    | C5-C6-N6   | -5.28 | 119.48      | 123.70   |
| 27  | B8    | 504  | A    | C5-C6-N1   | -5.28 | 115.06      | 117.70   |
| 27  | B8    | 1212 | G    | N3-C2-N2   | 5.28  | 123.59      | 119.90   |
| 27  | B8    | 1602 | U    | O4'-C1'-N1 | 5.28  | 112.42      | 108.20   |
| 27  | B8    | 1730 | C    | N3-C4-C5   | -5.28 | 119.79      | 121.90   |
| 27  | B8    | 2019 | A    | O4'-C1'-N9 | 5.28  | 112.42      | 108.20   |
| 27  | B8    | 2164 | C    | N3-C4-C5   | -5.28 | 119.79      | 121.90   |
| 27  | B8    | 2890 | G    | O4'-C1'-N9 | 5.28  | 112.42      | 108.20   |
| 1   | AA    | 704  | A    | O4'-C1'-N9 | 5.28  | 112.42      | 108.20   |
| 1   | AA    | 1359 | C    | N3-C4-C5   | -5.28 | 119.79      | 121.90   |
| 2   | AX    | 21   | A    | C5-C6-N1   | -5.28 | 115.06      | 117.70   |
| 27  | B8    | 660  | C    | N3-C4-C5   | -5.28 | 119.79      | 121.90   |
| 1   | AA    | 162  | A    | C8-N9-C4   | -5.27 | 103.69      | 105.80   |
| 1   | AA    | 410  | G    | C5-C6-O6   | -5.27 | 125.44      | 128.60   |
| 27  | B8    | 357  | C    | N3-C4-C5   | -5.27 | 119.79      | 121.90   |
| 27  | B8    | 1790 | C    | N3-C4-C5   | -5.27 | 119.79      | 121.90   |
| 27  | B8    | 2849 | U    | O4'-C1'-N1 | 5.27  | 112.42      | 108.20   |
| 1   | AA    | 74   | A    | C5-C6-N6   | -5.27 | 119.48      | 123.70   |
| 1   | AA    | 149  | A    | C5-C6-N1   | -5.27 | 115.06      | 117.70   |
| 1   | AA    | 382  | A    | C5-C6-N6   | -5.27 | 119.48      | 123.70   |
| 1   | AA    | 736  | C    | N3-C4-C5   | -5.27 | 119.79      | 121.90   |
| 1   | AA    | 825  | A    | C5-C6-N1   | -5.27 | 115.06      | 117.70   |
| 1   | AA    | 1101 | A    | C4-C5-C6   | 5.27  | 119.64      | 117.00   |
| 27  | B8    | 383  | C    | N3-C4-C5   | -5.27 | 119.79      | 121.90   |
| 27  | B8    | 436  | C    | N3-C4-C5   | -5.27 | 119.79      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 508  | A    | C5-C6-N1   | -5.27 | 115.06      | 117.70   |
| 27  | B8    | 921  | C    | N3-C4-C5   | -5.27 | 119.79      | 121.90   |
| 27  | B8    | 1272 | A    | C5-C6-N6   | -5.27 | 119.48      | 123.70   |
| 27  | B8    | 1500 | G    | O4'-C1'-N9 | 5.27  | 112.42      | 108.20   |
| 27  | B8    | 1983 | G    | O4'-C1'-N9 | 5.27  | 112.42      | 108.20   |
| 27  | B8    | 2051 | A    | C5-C6-N1   | -5.27 | 115.06      | 117.70   |
| 1   | AA    | 580  | C    | N3-C4-C5   | -5.27 | 119.79      | 121.90   |
| 27  | B8    | 1924 | C    | N3-C4-C5   | -5.27 | 119.79      | 121.90   |
| 1   | AA    | 352  | C    | N3-C4-C5   | -5.27 | 119.79      | 121.90   |
| 1   | AA    | 949  | A    | O4'-C1'-N9 | 5.27  | 112.42      | 108.20   |
| 1   | AA    | 1428 | A    | O4'-C1'-N9 | 5.27  | 112.42      | 108.20   |
| 3   | AV    | 4    | C    | N3-C4-C5   | -5.27 | 119.79      | 121.90   |
| 27  | B8    | 27   | G    | N3-C2-N2   | 5.27  | 123.59      | 119.90   |
| 27  | B8    | 41   | C    | N3-C4-C5   | -5.27 | 119.79      | 121.90   |
| 27  | B8    | 182  | A    | O4'-C1'-N9 | 5.27  | 112.42      | 108.20   |
| 27  | B8    | 793  | A    | O4'-C1'-N9 | 5.27  | 112.42      | 108.20   |
| 27  | B8    | 1103 | A    | C5-C6-N6   | -5.27 | 119.48      | 123.70   |
| 27  | B8    | 1968 | G    | O4'-C1'-N9 | 5.27  | 112.42      | 108.20   |
| 27  | B8    | 2161 | C    | N3-C4-C5   | -5.27 | 119.79      | 121.90   |
| 1   | AA    | 373  | A    | C5-C6-N6   | -5.27 | 119.49      | 123.70   |
| 1   | AA    | 380  | G    | O4'-C1'-N9 | 5.27  | 112.41      | 108.20   |
| 1   | AA    | 861  | G    | O4'-C1'-N9 | 5.27  | 112.41      | 108.20   |
| 26  | B7    | 53   | A    | C5-C6-N6   | -5.27 | 119.49      | 123.70   |
| 27  | B8    | 739  | A    | C5-C6-N1   | -5.27 | 115.07      | 117.70   |
| 27  | B8    | 925  | A    | C5-C6-N6   | -5.27 | 119.49      | 123.70   |
| 27  | B8    | 959  | A    | O4'-C1'-N9 | 5.27  | 112.42      | 108.20   |
| 27  | B8    | 1089 | A    | C5-C6-N6   | -5.27 | 119.49      | 123.70   |
| 27  | B8    | 1254 | A    | O4'-C1'-N9 | 5.27  | 112.41      | 108.20   |
| 27  | B8    | 1498 | C    | N3-C4-C5   | -5.27 | 119.79      | 121.90   |
| 27  | B8    | 1780 | A    | C4-C5-C6   | 5.27  | 119.63      | 117.00   |
| 27  | B8    | 2405 | G    | O4'-C1'-N9 | 5.27  | 112.41      | 108.20   |
| 27  | B8    | 2450 | A    | O4'-C1'-N9 | 5.27  | 112.41      | 108.20   |
| 27  | B8    | 2564 | A    | C5-C6-N6   | -5.27 | 119.49      | 123.70   |
| 17  | AM    | 105  | ALA  | N-CA-CB    | 5.27  | 117.47      | 110.10   |
| 27  | B8    | 279  | A    | C5-C6-N1   | -5.27 | 115.07      | 117.70   |
| 27  | B8    | 2681 | C    | N3-C4-C5   | -5.27 | 119.79      | 121.90   |
| 27  | B8    | 2887 | A    | C5-C6-N1   | -5.27 | 115.07      | 117.70   |
| 1   | AA    | 47   | C    | N3-C4-C5   | -5.26 | 119.80      | 121.90   |
| 1   | AA    | 90   | C    | N3-C4-N4   | 5.26  | 121.69      | 118.00   |
| 1   | AA    | 511  | C    | P-O3'-C3'  | 5.26  | 126.02      | 119.70   |
| 27  | B8    | 270  | A    | O4'-C1'-N9 | 5.26  | 112.41      | 108.20   |
| 27  | B8    | 514  | A    | C5-C6-N6   | -5.26 | 119.49      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1689 | A    | C5-C6-N1   | -5.26 | 115.07      | 117.70   |
| 1   | AA    | 119  | A    | C5-C6-N6   | -5.26 | 119.49      | 123.70   |
| 1   | AA    | 691  | G    | O4'-C1'-N9 | 5.26  | 112.41      | 108.20   |
| 1   | AA    | 1059 | C    | N3-C4-C5   | -5.26 | 119.80      | 121.90   |
| 27  | B8    | 943  | A    | C4-C5-C6   | 5.26  | 119.63      | 117.00   |
| 27  | B8    | 1032 | A    | C5-C6-N1   | -5.26 | 115.07      | 117.70   |
| 27  | B8    | 1810 | A    | O4'-C1'-N9 | 5.26  | 112.41      | 108.20   |
| 1   | AA    | 1004 | A    | O4'-C1'-N9 | 5.26  | 112.41      | 108.20   |
| 1   | AA    | 1311 | A    | O4'-C1'-N9 | 5.26  | 112.41      | 108.20   |
| 27  | B8    | 225  | C    | N3-C4-N4   | 5.26  | 121.68      | 118.00   |
| 27  | B8    | 241  | A    | C5-C6-N1   | -5.26 | 115.07      | 117.70   |
| 1   | AA    | 545  | C    | N3-C4-C5   | -5.26 | 119.80      | 121.90   |
| 1   | AA    | 560  | A    | C5-C6-N1   | -5.26 | 115.07      | 117.70   |
| 1   | AA    | 1383 | C    | N3-C4-C5   | -5.26 | 119.80      | 121.90   |
| 1   | AA    | 1411 | C    | N3-C4-C5   | -5.26 | 119.80      | 121.90   |
| 26  | B7    | 29   | A    | C5-C6-N1   | -5.26 | 115.07      | 117.70   |
| 27  | B8    | 386  | G    | O4'-C1'-N9 | 5.26  | 112.41      | 108.20   |
| 27  | B8    | 631  | A    | C5-C6-N1   | -5.26 | 115.07      | 117.70   |
| 27  | B8    | 785  | G    | O4'-C1'-N9 | 5.26  | 112.41      | 108.20   |
| 27  | B8    | 885  | C    | N3-C4-C5   | -5.26 | 119.80      | 121.90   |
| 27  | B8    | 2050 | C    | N3-C4-N4   | 5.26  | 121.68      | 118.00   |
| 27  | B8    | 2866 | U    | O4'-C1'-N1 | 5.26  | 112.41      | 108.20   |
| 1   | AA    | 71   | A    | C4-C5-C6   | 5.26  | 119.63      | 117.00   |
| 1   | AA    | 1533 | C    | N3-C4-N4   | 5.26  | 121.68      | 118.00   |
| 27  | B8    | 57   | C    | N3-C4-C5   | -5.26 | 119.80      | 121.90   |
| 27  | B8    | 621  | A    | C5-C6-N6   | -5.26 | 119.49      | 123.70   |
| 27  | B8    | 1531 | C    | N3-C4-C5   | -5.26 | 119.80      | 121.90   |
| 27  | B8    | 1894 | C    | N3-C4-C5   | -5.26 | 119.80      | 121.90   |
| 27  | B8    | 2067 | G    | O4'-C1'-N9 | 5.26  | 112.41      | 108.20   |
| 27  | B8    | 2254 | C    | N3-C4-C5   | -5.26 | 119.80      | 121.90   |
| 27  | B8    | 2714 | G    | N3-C2-N2   | 5.26  | 123.58      | 119.90   |
| 1   | AA    | 143  | A    | O4'-C1'-N9 | 5.26  | 112.41      | 108.20   |
| 1   | AA    | 162  | A    | O4'-C1'-N9 | 5.26  | 112.41      | 108.20   |
| 1   | AA    | 178  | C    | N3-C4-C5   | -5.26 | 119.80      | 121.90   |
| 1   | AA    | 274  | A    | C5-C6-N6   | -5.26 | 119.50      | 123.70   |
| 1   | AA    | 1196 | A    | C5-C6-N1   | -5.26 | 115.07      | 117.70   |
| 1   | AA    | 1429 | A    | C5-C6-N6   | -5.26 | 119.49      | 123.70   |
| 26  | B7    | 68   | C    | N3-C4-C5   | -5.26 | 119.80      | 121.90   |
| 27  | B8    | 1025 | G    | O4'-C1'-N9 | 5.26  | 112.41      | 108.20   |
| 27  | B8    | 1276 | A    | C5-C6-N1   | -5.26 | 115.07      | 117.70   |
| 27  | B8    | 1669 | A    | C5-C6-N6   | -5.26 | 119.50      | 123.70   |
| 27  | B8    | 1678 | A    | C5-C6-N1   | -5.26 | 115.07      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 126  | A    | C5-C6-N1   | -5.25 | 115.07      | 117.70   |
| 27  | B8    | 335  | C    | N3-C4-N4   | 5.25  | 121.68      | 118.00   |
| 1   | AA    | 95   | C    | N3-C4-C5   | -5.25 | 119.80      | 121.90   |
| 1   | AA    | 1229 | A    | O4'-C1'-N9 | 5.25  | 112.40      | 108.20   |
| 1   | AA    | 1250 | A    | C5-C6-N1   | -5.25 | 115.07      | 117.70   |
| 26  | B7    | 35   | C    | N3-C4-C5   | -5.25 | 119.80      | 121.90   |
| 27  | B8    | 159  | G    | N3-C2-N2   | 5.25  | 123.58      | 119.90   |
| 27  | B8    | 1525 | A    | O4'-C1'-N9 | 5.25  | 112.40      | 108.20   |
| 27  | B8    | 1598 | A    | C5-C6-N1   | -5.25 | 115.07      | 117.70   |
| 27  | B8    | 2097 | A    | C5-C6-N1   | -5.25 | 115.07      | 117.70   |
| 27  | B8    | 2611 | C    | N3-C4-C5   | -5.25 | 119.80      | 121.90   |
| 27  | B8    | 2726 | A    | C5-C6-N6   | -5.25 | 119.50      | 123.70   |
| 27  | B8    | 2813 | A    | C5-C6-N1   | -5.25 | 115.07      | 117.70   |
| 27  | B8    | 2850 | A    | C5-C6-N1   | -5.25 | 115.07      | 117.70   |
| 1   | AA    | 864  | A    | C5-C6-N6   | -5.25 | 119.50      | 123.70   |
| 1   | AA    | 1054 | C    | C6-N1-C1'  | -5.25 | 114.50      | 120.80   |
| 1   | AA    | 1067 | A    | C5-C6-N6   | -5.25 | 119.50      | 123.70   |
| 1   | AA    | 1392 | G    | O4'-C1'-N9 | 5.25  | 112.40      | 108.20   |
| 27  | B8    | 146  | A    | C5-C6-N1   | -5.25 | 115.07      | 117.70   |
| 27  | B8    | 479  | A    | C5-C6-N6   | -5.25 | 119.50      | 123.70   |
| 27  | B8    | 687  | C    | N3-C4-C5   | -5.25 | 119.80      | 121.90   |
| 27  | B8    | 844  | A    | C5-C6-N6   | -5.25 | 119.50      | 123.70   |
| 27  | B8    | 983  | A    | C5-C6-N1   | -5.25 | 115.08      | 117.70   |
| 27  | B8    | 1321 | A    | C5-C6-N6   | -5.25 | 119.50      | 123.70   |
| 27  | B8    | 2176 | A    | C5-C6-N1   | -5.25 | 115.07      | 117.70   |
| 27  | B8    | 2471 | A    | C4-C5-C6   | 5.25  | 119.62      | 117.00   |
| 27  | B8    | 2660 | A    | O4'-C1'-N9 | 5.25  | 112.40      | 108.20   |
| 27  | B8    | 2820 | A    | C5-C6-N1   | -5.25 | 115.07      | 117.70   |
| 1   | AA    | 1    | A    | C5-C6-N1   | -5.25 | 115.08      | 117.70   |
| 26  | B7    | 45   | A    | C4-C5-C6   | 5.25  | 119.62      | 117.00   |
| 27  | B8    | 1752 | C    | N3-C4-N4   | 5.25  | 121.67      | 118.00   |
| 1   | AA    | 196  | A    | C5-C6-N1   | -5.25 | 115.08      | 117.70   |
| 1   | AA    | 345  | C    | O4'-C1'-N1 | 5.25  | 112.40      | 108.20   |
| 1   | AA    | 554  | A    | C5-C6-N1   | -5.25 | 115.08      | 117.70   |
| 1   | AA    | 808  | C    | N3-C4-C5   | -5.25 | 119.80      | 121.90   |
| 1   | AA    | 1353 | G    | O4'-C1'-N9 | 5.25  | 112.40      | 108.20   |
| 3   | AV    | 38   | G    | C5-C6-O6   | -5.25 | 125.45      | 128.60   |
| 3   | AV    | 60   | A    | C5-C6-N1   | -5.25 | 115.08      | 117.70   |
| 27  | B8    | 86   | G    | O4'-C1'-N9 | 5.25  | 112.40      | 108.20   |
| 27  | B8    | 673  | C    | N3-C4-C5   | -5.25 | 119.80      | 121.90   |
| 27  | B8    | 793  | A    | C5-C6-N1   | -5.25 | 115.08      | 117.70   |
| 27  | B8    | 851  | C    | N3-C4-C5   | -5.25 | 119.80      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | B8    | 895  | U    | O4'-C1'-N1  | 5.25  | 112.40      | 108.20   |
| 27  | B8    | 994  | C    | N3-C4-C5    | -5.25 | 119.80      | 121.90   |
| 27  | B8    | 1265 | A    | C5-C6-N6    | -5.25 | 119.50      | 123.70   |
| 27  | B8    | 1323 | C    | N3-C4-C5    | -5.25 | 119.80      | 121.90   |
| 27  | B8    | 1477 | A    | C5-C6-N6    | -5.25 | 119.50      | 123.70   |
| 27  | B8    | 1700 | A    | C5-C6-N1    | -5.25 | 115.08      | 117.70   |
| 27  | B8    | 1910 | G    | O4'-C1'-N9  | 5.25  | 112.40      | 108.20   |
| 27  | B8    | 2103 | C    | N3-C4-C5    | -5.25 | 119.80      | 121.90   |
| 27  | B8    | 2248 | C    | N3-C4-C5    | -5.25 | 119.80      | 121.90   |
| 27  | B8    | 2345 | G    | O4'-C1'-N9  | 5.25  | 112.40      | 108.20   |
| 27  | B8    | 2416 | C    | N3-C4-C5    | -5.25 | 119.80      | 121.90   |
| 27  | B8    | 2556 | C    | N3-C4-C5    | -5.25 | 119.80      | 121.90   |
| 1   | AA    | 1284 | C    | O4'-C1'-N1  | 5.25  | 112.40      | 108.20   |
| 1   | AA    | 1331 | G    | O4'-C1'-N9  | 5.25  | 112.40      | 108.20   |
| 1   | AA    | 1533 | C    | N3-C4-C5    | -5.25 | 119.80      | 121.90   |
| 27  | B8    | 99   | U    | C6-N1-C1'   | -5.25 | 113.86      | 121.20   |
| 27  | B8    | 704  | G    | N3-C2-N2    | 5.25  | 123.57      | 119.90   |
| 27  | B8    | 1324 | G    | C5'-C4'-C3' | -5.25 | 107.61      | 116.00   |
| 27  | B8    | 1630 | A    | C5-C6-N1    | -5.25 | 115.08      | 117.70   |
| 27  | B8    | 1632 | A    | C5-C6-N1    | -5.25 | 115.08      | 117.70   |
| 27  | B8    | 2590 | A    | O4'-C1'-N9  | 5.25  | 112.40      | 108.20   |
| 27  | B8    | 2721 | A    | C5-C6-N1    | -5.25 | 115.08      | 117.70   |
| 1   | AA    | 53   | A    | C5-C6-N1    | -5.25 | 115.08      | 117.70   |
| 1   | AA    | 328  | C    | C6-N1-C1'   | -5.25 | 114.51      | 120.80   |
| 1   | AA    | 1267 | C    | N3-C4-N4    | 5.25  | 121.67      | 118.00   |
| 27  | B8    | 1555 | G    | O4'-C1'-N9  | 5.25  | 112.40      | 108.20   |
| 27  | B8    | 1580 | A    | C5-C6-N1    | -5.25 | 115.08      | 117.70   |
| 27  | B8    | 2515 | C    | N3-C4-C5    | -5.25 | 119.80      | 121.90   |
| 27  | B8    | 2587 | A    | C5-C6-N1    | -5.25 | 115.08      | 117.70   |
| 1   | AA    | 195  | A    | C5-C6-N6    | -5.24 | 119.50      | 123.70   |
| 1   | AA    | 708  | C    | N3-C4-C5    | -5.24 | 119.80      | 121.90   |
| 1   | AA    | 767  | A    | C5-C6-N1    | -5.24 | 115.08      | 117.70   |
| 1   | AA    | 918  | A    | O4'-C1'-N9  | 5.24  | 112.39      | 108.20   |
| 2   | AX    | 14   | G    | O4'-C1'-N9  | 5.24  | 112.39      | 108.20   |
| 27  | B8    | 418  | C    | N3-C4-C5    | -5.24 | 119.80      | 121.90   |
| 27  | B8    | 609  | A    | C5-C6-N1    | -5.24 | 115.08      | 117.70   |
| 27  | B8    | 610  | C    | N3-C4-C5    | -5.24 | 119.80      | 121.90   |
| 27  | B8    | 1821 | A    | C5-C6-N6    | -5.24 | 119.51      | 123.70   |
| 1   | AA    | 322  | C    | N3-C4-C5    | -5.24 | 119.80      | 121.90   |
| 1   | AA    | 574  | A    | C5-C6-N1    | -5.24 | 115.08      | 117.70   |
| 27  | B8    | 472  | A    | O4'-C1'-N9  | 5.24  | 112.39      | 108.20   |
| 27  | B8    | 743  | A    | C5-C6-N1    | -5.24 | 115.08      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1327 | A    | O4'-C1'-N9 | 5.24  | 112.39      | 108.20   |
| 27  | B8    | 2175 | C    | N3-C4-C5   | -5.24 | 119.80      | 121.90   |
| 27  | B8    | 2321 | U    | O4'-C1'-N1 | 5.24  | 112.39      | 108.20   |
| 1   | AA    | 852  | G    | O4'-C1'-N9 | 5.24  | 112.39      | 108.20   |
| 1   | AA    | 1320 | C    | N3-C4-N4   | 5.24  | 121.67      | 118.00   |
| 27  | B8    | 47   | C    | N3-C4-C5   | -5.24 | 119.80      | 121.90   |
| 27  | B8    | 149  | A    | C5-C6-N1   | -5.24 | 115.08      | 117.70   |
| 27  | B8    | 444  | C    | N3-C4-C5   | -5.24 | 119.80      | 121.90   |
| 27  | B8    | 1256 | G    | O4'-C1'-N9 | 5.24  | 112.39      | 108.20   |
| 27  | B8    | 1384 | A    | C5-C6-N1   | -5.24 | 115.08      | 117.70   |
| 27  | B8    | 1908 | C    | N3-C4-C5   | -5.24 | 119.80      | 121.90   |
| 27  | B8    | 2674 | G    | O4'-C1'-N9 | 5.24  | 112.39      | 108.20   |
| 27  | B8    | 2837 | A    | C5-C6-N1   | -5.24 | 115.08      | 117.70   |
| 1   | AA    | 535  | A    | C5-C6-N6   | -5.24 | 119.51      | 123.70   |
| 1   | AA    | 680  | C    | N3-C4-C5   | -5.24 | 119.81      | 121.90   |
| 1   | AA    | 770  | C    | N3-C4-C5   | -5.24 | 119.81      | 121.90   |
| 1   | AA    | 1019 | A    | C5-C6-N1   | -5.24 | 115.08      | 117.70   |
| 1   | AA    | 1033 | G    | O4'-C1'-N9 | 5.24  | 112.39      | 108.20   |
| 1   | AA    | 1105 | A    | C5-C6-N1   | -5.24 | 115.08      | 117.70   |
| 1   | AA    | 1257 | A    | C5-C6-N1   | -5.24 | 115.08      | 117.70   |
| 2   | AX    | 17   | C    | N3-C4-N4   | 5.24  | 121.67      | 118.00   |
| 27  | B8    | 31   | C    | N3-C4-C5   | -5.24 | 119.80      | 121.90   |
| 27  | B8    | 1029 | A    | C5-C6-N6   | -5.24 | 119.51      | 123.70   |
| 27  | B8    | 1068 | G    | O4'-C1'-N9 | 5.24  | 112.39      | 108.20   |
| 27  | B8    | 1189 | A    | C5-C6-N1   | -5.24 | 115.08      | 117.70   |
| 27  | B8    | 2020 | A    | O4'-C1'-N9 | 5.24  | 112.39      | 108.20   |
| 27  | B8    | 2060 | A    | C5-C6-N1   | -5.24 | 115.08      | 117.70   |
| 27  | B8    | 2333 | A    | C5-C6-N1   | -5.24 | 115.08      | 117.70   |
| 27  | B8    | 165  | A    | O4'-C1'-N9 | 5.24  | 112.39      | 108.20   |
| 27  | B8    | 1547 | C    | N3-C4-C5   | -5.24 | 119.81      | 121.90   |
| 27  | B8    | 2616 | C    | N3-C4-C5   | -5.24 | 119.81      | 121.90   |
| 27  | B8    | 2693 | G    | O4'-C1'-N9 | 5.24  | 112.39      | 108.20   |
| 1   | AA    | 587  | G    | P-O3'-C3'  | 5.24  | 125.98      | 119.70   |
| 1   | AA    | 873  | A    | C5-C6-N6   | -5.24 | 119.51      | 123.70   |
| 1   | AA    | 1118 | U    | C2-N1-C1'  | 5.24  | 123.98      | 117.70   |
| 27  | B8    | 640  | C    | N3-C4-C5   | -5.24 | 119.81      | 121.90   |
| 27  | B8    | 1337 | G    | O4'-C1'-N9 | 5.24  | 112.39      | 108.20   |
| 27  | B8    | 1535 | A    | C5-C6-N1   | -5.24 | 115.08      | 117.70   |
| 27  | B8    | 1609 | A    | O4'-C1'-N9 | 5.24  | 112.39      | 108.20   |
| 27  | B8    | 1618 | A    | C5-C6-N1   | -5.24 | 115.08      | 117.70   |
| 27  | B8    | 2062 | A    | C5-C6-N1   | -5.24 | 115.08      | 117.70   |
| 27  | B8    | 2397 | G    | O4'-C1'-N9 | 5.24  | 112.39      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 60   | A    | C5-C6-N6   | -5.23 | 119.51      | 123.70   |
| 1   | AA    | 1172 | C    | N3-C4-C5   | -5.23 | 119.81      | 121.90   |
| 27  | B8    | 274  | C    | N3-C4-C5   | -5.23 | 119.81      | 121.90   |
| 27  | B8    | 1499 | C    | N3-C4-C5   | -5.23 | 119.81      | 121.90   |
| 27  | B8    | 1646 | C    | N3-C4-N4   | 5.23  | 121.66      | 118.00   |
| 28  | BA    | 435  | LYS  | N-CA-CB    | 5.23  | 120.02      | 110.60   |
| 1   | AA    | 415  | A    | O4'-C1'-N9 | 5.23  | 112.39      | 108.20   |
| 1   | AA    | 622  | A    | C5-C6-N1   | -5.23 | 115.08      | 117.70   |
| 1   | AA    | 667  | G    | O4'-C1'-N9 | 5.23  | 112.39      | 108.20   |
| 1   | AA    | 909  | A    | C5-C6-N1   | -5.23 | 115.08      | 117.70   |
| 27  | B8    | 1614 | A    | C5-C6-N1   | -5.23 | 115.08      | 117.70   |
| 27  | B8    | 1626 | A    | O4'-C1'-N9 | 5.23  | 112.39      | 108.20   |
| 27  | B8    | 2114 | A    | C5-C6-N6   | -5.23 | 119.51      | 123.70   |
| 27  | B8    | 2153 | C    | N3-C4-C5   | -5.23 | 119.81      | 121.90   |
| 27  | B8    | 2211 | A    | C5-C6-N1   | -5.23 | 115.08      | 117.70   |
| 27  | B8    | 2391 | G    | O4'-C1'-N9 | 5.23  | 112.39      | 108.20   |
| 1   | AA    | 964  | A    | C5-C6-N1   | -5.23 | 115.08      | 117.70   |
| 1   | AA    | 1217 | C    | N3-C4-C5   | -5.23 | 119.81      | 121.90   |
| 27  | B8    | 751  | A    | C5-C6-N1   | -5.23 | 115.08      | 117.70   |
| 27  | B8    | 1567 | G    | O4'-C1'-N9 | 5.23  | 112.38      | 108.20   |
| 27  | B8    | 2418 | A    | C5-C6-N6   | -5.23 | 119.52      | 123.70   |
| 1   | AA    | 98   | A    | C5-C6-N1   | -5.23 | 115.09      | 117.70   |
| 1   | AA    | 1443 | C    | N3-C4-C5   | -5.23 | 119.81      | 121.90   |
| 27  | B8    | 129  | C    | N3-C4-C5   | -5.23 | 119.81      | 121.90   |
| 27  | B8    | 143  | C    | N3-C4-C5   | -5.23 | 119.81      | 121.90   |
| 27  | B8    | 145  | C    | N3-C4-C5   | -5.23 | 119.81      | 121.90   |
| 27  | B8    | 422  | A    | O4'-C1'-N9 | 5.23  | 112.38      | 108.20   |
| 27  | B8    | 1152 | C    | N3-C4-C5   | -5.23 | 119.81      | 121.90   |
| 27  | B8    | 1536 | C    | N3-C4-N4   | 5.23  | 121.66      | 118.00   |
| 27  | B8    | 2738 | A    | C5-C6-N6   | -5.23 | 119.52      | 123.70   |
| 27  | B8    | 53   | A    | C5-C6-N1   | -5.23 | 115.09      | 117.70   |
| 27  | B8    | 199  | A    | C4-C5-C6   | 5.23  | 119.61      | 117.00   |
| 27  | B8    | 1428 | C    | N3-C4-C5   | -5.23 | 119.81      | 121.90   |
| 27  | B8    | 2563 | U    | O4'-C1'-N1 | 5.23  | 112.38      | 108.20   |
| 27  | B8    | 2639 | A    | C5-C6-N6   | -5.23 | 119.52      | 123.70   |
| 1   | AA    | 800  | G    | O4'-C1'-N9 | 5.22  | 112.38      | 108.20   |
| 1   | AA    | 1254 | A    | C5-C6-N6   | -5.22 | 119.52      | 123.70   |
| 3   | AV    | 22   | A    | C5-C6-N1   | -5.22 | 115.09      | 117.70   |
| 3   | AV    | 28   | C    | N3-C4-C5   | -5.22 | 119.81      | 121.90   |
| 3   | AV    | 60   | A    | C5-C6-N6   | -5.22 | 119.52      | 123.70   |
| 27  | B8    | 655  | A    | C5-C6-N1   | -5.22 | 115.09      | 117.70   |
| 27  | B8    | 896  | A    | C5-C6-N1   | -5.22 | 115.09      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1021 | A    | C5-C6-N6   | -5.22 | 119.52      | 123.70   |
| 27  | B8    | 1463 | C    | N3-C4-C5   | -5.22 | 119.81      | 121.90   |
| 27  | B8    | 1788 | C    | N3-C4-C5   | -5.22 | 119.81      | 121.90   |
| 1   | AA    | 414  | A    | C5-C6-N1   | -5.22 | 115.09      | 117.70   |
| 1   | AA    | 918  | A    | C5-C6-N1   | -5.22 | 115.09      | 117.70   |
| 1   | AA    | 1082 | A    | C5-C6-N6   | -5.22 | 119.52      | 123.70   |
| 1   | AA    | 1150 | A    | C5-C6-N1   | -5.22 | 115.09      | 117.70   |
| 27  | B8    | 241  | A    | O4'-C1'-N9 | 5.22  | 112.38      | 108.20   |
| 27  | B8    | 518  | G    | O4'-C1'-N9 | 5.22  | 112.38      | 108.20   |
| 27  | B8    | 2160 | C    | N3-C4-C5   | -5.22 | 119.81      | 121.90   |
| 1   | AA    | 7    | A    | C5-C6-N1   | -5.22 | 115.09      | 117.70   |
| 1   | AA    | 223  | A    | O4'-C1'-N9 | 5.22  | 112.38      | 108.20   |
| 1   | AA    | 1012 | A    | C5-C6-N6   | -5.22 | 119.52      | 123.70   |
| 1   | AA    | 1154 | G    | O4'-C1'-N9 | 5.22  | 112.38      | 108.20   |
| 27  | B8    | 706  | A    | C5-C6-N1   | -5.22 | 115.09      | 117.70   |
| 27  | B8    | 1118 | C    | N3-C4-C5   | -5.22 | 119.81      | 121.90   |
| 27  | B8    | 1285 | A    | C5-C6-N1   | -5.22 | 115.09      | 117.70   |
| 1   | AA    | 132  | C    | N3-C4-C5   | -5.22 | 119.81      | 121.90   |
| 1   | AA    | 308  | C    | N3-C4-C5   | -5.22 | 119.81      | 121.90   |
| 26  | B7    | 90   | C    | N3-C4-C5   | -5.22 | 119.81      | 121.90   |
| 27  | B8    | 144  | A    | C5-C6-N6   | -5.22 | 119.52      | 123.70   |
| 27  | B8    | 344  | A    | C5-C6-N1   | -5.22 | 115.09      | 117.70   |
| 27  | B8    | 1257 | C    | N3-C4-C5   | -5.22 | 119.81      | 121.90   |
| 27  | B8    | 1315 | C    | N3-C4-C5   | -5.22 | 119.81      | 121.90   |
| 27  | B8    | 1512 | C    | N3-C4-C5   | -5.22 | 119.81      | 121.90   |
| 27  | B8    | 2590 | A    | C5-C6-N6   | -5.22 | 119.53      | 123.70   |
| 27  | B8    | 2675 | A    | C5-C6-N6   | -5.22 | 119.53      | 123.70   |
| 1   | AA    | 1447 | A    | C5-C6-N6   | -5.22 | 119.53      | 123.70   |
| 27  | B8    | 320  | A    | C5-C6-N1   | -5.22 | 115.09      | 117.70   |
| 27  | B8    | 1049 | C    | N3-C4-C5   | -5.22 | 119.81      | 121.90   |
| 1   | AA    | 349  | A    | C5-C6-N6   | -5.22 | 119.53      | 123.70   |
| 1   | AA    | 825  | A    | C5-C6-N6   | -5.22 | 119.53      | 123.70   |
| 1   | AA    | 1269 | A    | C5-C6-N1   | -5.22 | 115.09      | 117.70   |
| 27  | B8    | 219  | A    | C5-C6-N1   | -5.22 | 115.09      | 117.70   |
| 27  | B8    | 270  | A    | C5-C6-N1   | -5.22 | 115.09      | 117.70   |
| 27  | B8    | 278  | A    | C5-C6-N6   | -5.22 | 119.53      | 123.70   |
| 27  | B8    | 609  | A    | O4'-C1'-N9 | 5.22  | 112.37      | 108.20   |
| 27  | B8    | 613  | A    | O4'-C1'-N9 | 5.22  | 112.37      | 108.20   |
| 27  | B8    | 1460 | U    | C2-N1-C1'  | 5.22  | 123.96      | 117.70   |
| 27  | B8    | 2060 | A    | C5-C6-N6   | -5.22 | 119.53      | 123.70   |
| 1   | AA    | 936  | C    | N3-C4-C5   | -5.21 | 119.81      | 121.90   |
| 27  | B8    | 156  | A    | C5-C6-N1   | -5.21 | 115.09      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 590  | A    | C5-C6-N1   | -5.21 | 115.09      | 117.70   |
| 27  | B8    | 721  | A    | C5-C6-N6   | -5.21 | 119.53      | 123.70   |
| 27  | B8    | 854  | C    | N3-C4-C5   | -5.21 | 119.81      | 121.90   |
| 27  | B8    | 1401 | G    | O4'-C1'-N9 | 5.21  | 112.37      | 108.20   |
| 27  | B8    | 1717 | A    | C5-C6-N6   | -5.21 | 119.53      | 123.70   |
| 27  | B8    | 1726 | C    | N3-C4-C5   | -5.21 | 119.81      | 121.90   |
| 32  | BD    | 156  | PHE  | CB-CG-CD1  | 5.21  | 124.45      | 120.80   |
| 1   | AA    | 1409 | C    | N3-C4-N4   | 5.21  | 121.65      | 118.00   |
| 1   | AA    | 215  | C    | N3-C4-N4   | 5.21  | 121.65      | 118.00   |
| 1   | AA    | 498  | A    | C5-C6-N1   | -5.21 | 115.09      | 117.70   |
| 1   | AA    | 569  | C    | N3-C4-C5   | -5.21 | 119.81      | 121.90   |
| 1   | AA    | 702  | A    | C5-C6-N6   | -5.21 | 119.53      | 123.70   |
| 1   | AA    | 1132 | C    | N3-C4-N4   | 5.21  | 121.65      | 118.00   |
| 1   | AA    | 1286 | U    | O4'-C1'-N1 | 5.21  | 112.37      | 108.20   |
| 1   | AA    | 1350 | A    | O4'-C1'-N9 | 5.21  | 112.37      | 108.20   |
| 27  | B8    | 275  | C    | N3-C4-N4   | 5.21  | 121.65      | 118.00   |
| 27  | B8    | 547  | A    | C5-C6-N1   | -5.21 | 115.09      | 117.70   |
| 27  | B8    | 990  | A    | C5-C6-N6   | -5.21 | 119.53      | 123.70   |
| 27  | B8    | 1085 | A    | O4'-C1'-N9 | 5.21  | 112.37      | 108.20   |
| 27  | B8    | 1544 | A    | C5-C6-N1   | -5.21 | 115.09      | 117.70   |
| 27  | B8    | 1609 | A    | C5-C6-N1   | -5.21 | 115.09      | 117.70   |
| 27  | B8    | 2198 | A    | C5-C6-N1   | -5.21 | 115.09      | 117.70   |
| 1   | AA    | 1344 | C    | N3-C4-C5   | -5.21 | 119.82      | 121.90   |
| 26  | B7    | 78   | A    | C4-C5-C6   | 5.21  | 119.61      | 117.00   |
| 27  | B8    | 223  | A    | C5-C6-N1   | -5.21 | 115.09      | 117.70   |
| 27  | B8    | 497  | A    | O4'-C1'-N9 | 5.21  | 112.37      | 108.20   |
| 27  | B8    | 917  | A    | C5-C6-N6   | -5.21 | 119.53      | 123.70   |
| 1   | AA    | 288  | A    | O4'-C1'-N9 | 5.21  | 112.37      | 108.20   |
| 1   | AA    | 631  | C    | N3-C4-C5   | -5.21 | 119.82      | 121.90   |
| 1   | AA    | 998  | C    | N3-C4-N4   | 5.21  | 121.64      | 118.00   |
| 1   | AA    | 1336 | C    | N3-C4-C5   | -5.21 | 119.82      | 121.90   |
| 27  | B8    | 1070 | A    | C5-C6-N1   | -5.21 | 115.09      | 117.70   |
| 27  | B8    | 1145 | C    | N3-C4-C5   | -5.21 | 119.82      | 121.90   |
| 27  | B8    | 1960 | A    | O4'-C1'-N9 | 5.21  | 112.37      | 108.20   |
| 1   | AA    | 48   | C    | N3-C4-C5   | -5.21 | 119.82      | 121.90   |
| 1   | AA    | 1042 | A    | C5-C6-N1   | -5.21 | 115.10      | 117.70   |
| 1   | AA    | 1462 | C    | N3-C4-C5   | -5.21 | 119.82      | 121.90   |
| 27  | B8    | 879  | G    | O4'-C1'-N9 | 5.21  | 112.37      | 108.20   |
| 27  | B8    | 913  | U    | O4'-C1'-N1 | 5.21  | 112.37      | 108.20   |
| 27  | B8    | 945  | A    | C5-C6-N1   | -5.21 | 115.10      | 117.70   |
| 27  | B8    | 957  | C    | N3-C4-C5   | -5.21 | 119.82      | 121.90   |
| 27  | B8    | 1293 | C    | N3-C4-C5   | -5.21 | 119.82      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1650 | A    | C5-C6-N1   | -5.21 | 115.10      | 117.70   |
| 27  | B8    | 2608 | G    | O4'-C1'-N9 | 5.21  | 112.36      | 108.20   |
| 27  | B8    | 2892 | G    | O4'-C1'-N9 | 5.21  | 112.36      | 108.20   |
| 1   | AA    | 858  | G    | O4'-C1'-N9 | 5.21  | 112.36      | 108.20   |
| 1   | AA    | 1482 | G    | N3-C2-N2   | 5.21  | 123.54      | 119.90   |
| 27  | B8    | 1912 | A    | C5-C6-N6   | -5.21 | 119.54      | 123.70   |
| 27  | B8    | 2503 | A    | O4'-C1'-N9 | 5.21  | 112.36      | 108.20   |
| 1   | AA    | 33   | A    | C5-C6-N1   | -5.20 | 115.10      | 117.70   |
| 1   | AA    | 787  | A    | C4-C5-C6   | 5.20  | 119.60      | 117.00   |
| 1   | AA    | 792  | A    | C5-C6-N1   | -5.20 | 115.10      | 117.70   |
| 1   | AA    | 1099 | G    | O4'-C1'-N9 | 5.20  | 112.36      | 108.20   |
| 1   | AA    | 1253 | G    | O4'-C1'-N9 | 5.20  | 112.36      | 108.20   |
| 27  | B8    | 440  | C    | N3-C4-C5   | -5.20 | 119.82      | 121.90   |
| 27  | B8    | 730  | A    | C5-C6-N1   | -5.20 | 115.10      | 117.70   |
| 27  | B8    | 1729 | U    | O4'-C1'-N1 | 5.20  | 112.36      | 108.20   |
| 1   | AA    | 728  | A    | C5-C6-N1   | -5.20 | 115.10      | 117.70   |
| 1   | AA    | 878  | A    | O4'-C1'-N9 | 5.20  | 112.36      | 108.20   |
| 3   | AV    | 72   | C    | N3-C4-C5   | -5.20 | 119.82      | 121.90   |
| 26  | B7    | 43   | C    | N3-C4-C5   | -5.20 | 119.82      | 121.90   |
| 27  | B8    | 165  | A    | C5-C6-N6   | -5.20 | 119.54      | 123.70   |
| 27  | B8    | 332  | A    | P-O3'-C3'  | 5.20  | 125.94      | 119.70   |
| 27  | B8    | 347  | A    | C5-C6-N1   | -5.20 | 115.10      | 117.70   |
| 27  | B8    | 976  | G    | O4'-C1'-N9 | 5.20  | 112.36      | 108.20   |
| 27  | B8    | 1189 | A    | C5-C6-N6   | -5.20 | 119.54      | 123.70   |
| 27  | B8    | 1850 | G    | O4'-C1'-N9 | 5.20  | 112.36      | 108.20   |
| 27  | B8    | 2532 | G    | O4'-C1'-N9 | 5.20  | 112.36      | 108.20   |
| 27  | B8    | 2856 | A    | C5-C6-N1   | -5.20 | 115.10      | 117.70   |
| 1   | AA    | 553  | A    | O4'-C1'-N9 | 5.20  | 112.36      | 108.20   |
| 1   | AA    | 864  | A    | C5-C6-N1   | -5.20 | 115.10      | 117.70   |
| 1   | AA    | 1158 | C    | N3-C4-N4   | 5.20  | 121.64      | 118.00   |
| 1   | AA    | 1338 | G    | C4-N9-C1'  | 5.20  | 133.26      | 126.50   |
| 27  | B8    | 1362 | C    | N3-C4-C5   | -5.20 | 119.82      | 121.90   |
| 27  | B8    | 1569 | A    | C5-C6-N1   | -5.20 | 115.10      | 117.70   |
| 27  | B8    | 2480 | C    | N3-C4-C5   | -5.20 | 119.82      | 121.90   |
| 1   | AA    | 1314 | C    | N3-C4-C5   | -5.20 | 119.82      | 121.90   |
| 26  | B7    | 23   | G    | O4'-C1'-N9 | 5.20  | 112.36      | 108.20   |
| 27  | B8    | 331  | C    | N3-C4-C5   | -5.20 | 119.82      | 121.90   |
| 27  | B8    | 600  | G    | O4'-C1'-N9 | 5.20  | 112.36      | 108.20   |
| 27  | B8    | 1244 | A    | C5-C6-N1   | -5.20 | 115.10      | 117.70   |
| 27  | B8    | 2163 | A    | C5-C6-N1   | -5.20 | 115.10      | 117.70   |
| 1   | AA    | 320  | A    | C5-C6-N1   | -5.20 | 115.10      | 117.70   |
| 1   | AA    | 643  | C    | N3-C4-C5   | -5.20 | 119.82      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 860  | A    | C5-C6-N1   | -5.20 | 115.10      | 117.70   |
| 27  | B8    | 1652 | A    | O4'-C1'-N9 | 5.20  | 112.36      | 108.20   |
| 27  | B8    | 1854 | A    | C5-C6-N1   | -5.20 | 115.10      | 117.70   |
| 1   | AA    | 520  | A    | O4'-C1'-N9 | 5.20  | 112.36      | 108.20   |
| 1   | AA    | 521  | G    | O4'-C1'-N9 | 5.20  | 112.36      | 108.20   |
| 1   | AA    | 1375 | A    | C5-C6-N6   | -5.20 | 119.54      | 123.70   |
| 3   | AV    | 32   | C    | N3-C4-N4   | 5.20  | 121.64      | 118.00   |
| 27  | B8    | 131  | A    | C5-C6-N6   | -5.20 | 119.54      | 123.70   |
| 27  | B8    | 531  | C    | N3-C4-C5   | -5.20 | 119.82      | 121.90   |
| 27  | B8    | 705  | A    | C5-C6-N1   | -5.20 | 115.10      | 117.70   |
| 27  | B8    | 2414 | G    | O4'-C1'-N9 | 5.20  | 112.36      | 108.20   |
| 27  | B8    | 2639 | A    | C4-C5-C6   | 5.20  | 119.60      | 117.00   |
| 27  | B8    | 2755 | C    | N3-C4-C5   | -5.20 | 119.82      | 121.90   |
| 32  | BD    | 156  | PHE  | CB-CG-CD2  | -5.20 | 117.16      | 120.80   |
| 27  | B8    | 401  | A    | C5-C6-N1   | -5.19 | 115.10      | 117.70   |
| 27  | B8    | 1034 | G    | O4'-C1'-N9 | 5.19  | 112.36      | 108.20   |
| 1   | AA    | 687  | A    | P-O3'-C3'  | 5.19  | 125.93      | 119.70   |
| 1   | AA    | 819  | A    | C5-C6-N1   | -5.19 | 115.10      | 117.70   |
| 1   | AA    | 1378 | C    | N3-C4-C5   | -5.19 | 119.82      | 121.90   |
| 3   | AV    | 76   | C    | P-O5'-C5'  | 5.19  | 129.21      | 120.90   |
| 27  | B8    | 457  | A    | C5-C6-N1   | -5.19 | 115.10      | 117.70   |
| 27  | B8    | 661  | A    | C5-C6-N1   | -5.19 | 115.10      | 117.70   |
| 27  | B8    | 1147 | A    | C5-C6-N1   | -5.19 | 115.10      | 117.70   |
| 27  | B8    | 2350 | C    | N3-C4-C5   | -5.19 | 119.82      | 121.90   |
| 27  | B8    | 2815 | C    | N3-C4-C5   | -5.19 | 119.82      | 121.90   |
| 1   | AA    | 272  | C    | N3-C4-C5   | -5.19 | 119.82      | 121.90   |
| 1   | AA    | 608  | A    | C5-C6-N6   | -5.19 | 119.55      | 123.70   |
| 1   | AA    | 884  | U    | O4'-C1'-N1 | 5.19  | 112.35      | 108.20   |
| 27  | B8    | 32   | C    | N3-C4-N4   | 5.19  | 121.63      | 118.00   |
| 27  | B8    | 527  | C    | N3-C4-C5   | -5.19 | 119.82      | 121.90   |
| 27  | B8    | 980  | A    | C5-C6-N1   | -5.19 | 115.10      | 117.70   |
| 27  | B8    | 1749 | A    | O4'-C1'-N9 | 5.19  | 112.35      | 108.20   |
| 27  | B8    | 1865 | U    | P-O3'-C3'  | 5.19  | 125.93      | 119.70   |
| 27  | B8    | 2071 | A    | C5-C6-N1   | -5.19 | 115.11      | 117.70   |
| 27  | B8    | 2456 | C    | N3-C4-C5   | -5.19 | 119.82      | 121.90   |
| 27  | B8    | 2510 | C    | N3-C4-C5   | -5.19 | 119.82      | 121.90   |
| 1   | AA    | 990  | C    | N3-C4-C5   | -5.19 | 119.82      | 121.90   |
| 27  | B8    | 613  | A    | C5-C6-N1   | -5.19 | 115.11      | 117.70   |
| 27  | B8    | 1070 | A    | C5-C6-N6   | -5.19 | 119.55      | 123.70   |
| 27  | B8    | 1732 | C    | O4'-C1'-N1 | 5.19  | 112.35      | 108.20   |
| 27  | B8    | 338  | G    | N3-C2-N2   | 5.19  | 123.53      | 119.90   |
| 27  | B8    | 432  | A    | C5-C6-N1   | -5.19 | 115.11      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 595  | C    | N3-C4-C5   | -5.19 | 119.83      | 121.90   |
| 27  | B8    | 640  | C    | N3-C4-N4   | 5.19  | 121.63      | 118.00   |
| 27  | B8    | 935  | C    | N3-C4-C5   | -5.19 | 119.83      | 121.90   |
| 27  | B8    | 1295 | C    | N3-C4-C5   | -5.19 | 119.83      | 121.90   |
| 27  | B8    | 1385 | A    | C5-C6-N6   | -5.19 | 119.55      | 123.70   |
| 27  | B8    | 2498 | C    | N3-C4-C5   | -5.19 | 119.83      | 121.90   |
| 27  | B8    | 2856 | A    | C5-C6-N6   | -5.19 | 119.55      | 123.70   |
| 1   | AA    | 84   | U    | C2-N1-C1'  | 5.19  | 123.92      | 117.70   |
| 1   | AA    | 1100 | C    | N3-C4-C5   | -5.19 | 119.83      | 121.90   |
| 1   | AA    | 1193 | G    | O4'-C1'-N9 | 5.19  | 112.35      | 108.20   |
| 27  | B8    | 1718 | G    | O4'-C1'-N9 | 5.19  | 112.35      | 108.20   |
| 27  | B8    | 1892 | C    | N3-C4-C5   | -5.19 | 119.83      | 121.90   |
| 27  | B8    | 2750 | A    | C5-C6-N6   | -5.19 | 119.55      | 123.70   |
| 1   | AA    | 253  | A    | C5-C6-N1   | -5.18 | 115.11      | 117.70   |
| 27  | B8    | 20   | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 27  | B8    | 1155 | A    | C5-C6-N1   | -5.18 | 115.11      | 117.70   |
| 27  | B8    | 2030 | A    | C5-C6-N1   | -5.18 | 115.11      | 117.70   |
| 27  | B8    | 2179 | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 27  | B8    | 2558 | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 1   | AA    | 315  | A    | C5-C6-N6   | -5.18 | 119.56      | 123.70   |
| 1   | AA    | 431  | A    | C5-C6-N6   | -5.18 | 119.55      | 123.70   |
| 1   | AA    | 913  | A    | C5-C6-N6   | -5.18 | 119.56      | 123.70   |
| 1   | AA    | 1016 | A    | C5-C6-N6   | -5.18 | 119.55      | 123.70   |
| 1   | AA    | 1346 | A    | C5-C6-N6   | -5.18 | 119.55      | 123.70   |
| 1   | AA    | 1486 | G    | O4'-C1'-N9 | 5.18  | 112.35      | 108.20   |
| 1   | AA    | 1508 | A    | C5-C6-N1   | -5.18 | 115.11      | 117.70   |
| 27  | B8    | 453  | A    | C5-C6-N1   | -5.18 | 115.11      | 117.70   |
| 27  | B8    | 775  | G    | P-O3'-C3'  | 5.18  | 125.92      | 119.70   |
| 27  | B8    | 796  | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 27  | B8    | 972  | A    | C5-C6-N1   | -5.18 | 115.11      | 117.70   |
| 27  | B8    | 1580 | A    | C5-C6-N6   | -5.18 | 119.56      | 123.70   |
| 27  | B8    | 1962 | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 27  | B8    | 2044 | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 1   | AA    | 1394 | A    | O4'-C1'-N9 | 5.18  | 112.34      | 108.20   |
| 27  | B8    | 821  | A    | C5-C6-N1   | -5.18 | 115.11      | 117.70   |
| 27  | B8    | 1393 | A    | C5-C6-N1   | -5.18 | 115.11      | 117.70   |
| 27  | B8    | 1803 | A    | C5-C6-N1   | -5.18 | 115.11      | 117.70   |
| 27  | B8    | 2301 | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 27  | B8    | 162  | U    | O4'-C1'-N1 | 5.18  | 112.34      | 108.20   |
| 27  | B8    | 1489 | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 27  | B8    | 1768 | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 27  | B8    | 1891 | G    | O4'-C1'-N9 | 5.18  | 112.34      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 1916 | A    | C5-C6-N6   | -5.18 | 119.56      | 123.70   |
| 27  | B8    | 2326 | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 1   | AA    | 759  | A    | N1-C6-N6   | 5.18  | 121.71      | 118.60   |
| 1   | AA    | 1534 | A    | C5-C6-N6   | -5.18 | 119.56      | 123.70   |
| 27  | B8    | 366  | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 27  | B8    | 2359 | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 3   | AV    | 45   | G    | O4'-C1'-N9 | 5.18  | 112.34      | 108.20   |
| 27  | B8    | 37   | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 27  | B8    | 276  | U    | C6-N1-C1'  | -5.18 | 113.95      | 121.20   |
| 27  | B8    | 990  | A    | O4'-C1'-N9 | 5.18  | 112.34      | 108.20   |
| 27  | B8    | 1164 | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 27  | B8    | 1195 | G    | O4'-C1'-N9 | 5.18  | 112.34      | 108.20   |
| 27  | B8    | 1297 | C    | N3-C4-C5   | -5.18 | 119.83      | 121.90   |
| 27  | B8    | 1858 | A    | O4'-C1'-N9 | 5.18  | 112.34      | 108.20   |
| 27  | B8    | 2083 | G    | O4'-C1'-N9 | 5.18  | 112.34      | 108.20   |
| 1   | AA    | 188  | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 1   | AA    | 406  | G    | O4'-C1'-N9 | 5.17  | 112.34      | 108.20   |
| 1   | AA    | 1279 | G    | C4-N9-C1'  | 5.17  | 133.23      | 126.50   |
| 26  | B7    | 119  | A    | C5-C6-N1   | -5.17 | 115.11      | 117.70   |
| 27  | B8    | 181  | A    | C5-C6-N1   | -5.17 | 115.11      | 117.70   |
| 27  | B8    | 239  | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 27  | B8    | 897  | C    | N3-C4-N4   | 5.17  | 121.62      | 118.00   |
| 27  | B8    | 995  | C    | C6-N1-C1'  | -5.17 | 114.59      | 120.80   |
| 27  | B8    | 1488 | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 27  | B8    | 2135 | A    | C5-C6-N6   | -5.17 | 119.56      | 123.70   |
| 27  | B8    | 2227 | A    | C5-C6-N1   | -5.17 | 115.11      | 117.70   |
| 27  | B8    | 2433 | A    | C5-C6-N1   | -5.17 | 115.11      | 117.70   |
| 27  | B8    | 2443 | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 1   | AA    | 298  | A    | C5-C6-N1   | -5.17 | 115.11      | 117.70   |
| 1   | AA    | 1521 | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 27  | B8    | 1289 | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 27  | B8    | 2512 | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 27  | B8    | 2636 | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 1   | AA    | 1101 | A    | C5-C6-N6   | -5.17 | 119.56      | 123.70   |
| 27  | B8    | 61   | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 27  | B8    | 648  | G    | O4'-C1'-N9 | 5.17  | 112.34      | 108.20   |
| 27  | B8    | 910  | A    | O4'-C1'-N9 | 5.17  | 112.34      | 108.20   |
| 27  | B8    | 1345 | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 27  | B8    | 1527 | G    | O4'-C1'-N9 | 5.17  | 112.34      | 108.20   |
| 27  | B8    | 1652 | A    | C5-C6-N1   | -5.17 | 115.11      | 117.70   |
| 27  | B8    | 2141 | G    | O4'-C1'-N9 | 5.17  | 112.34      | 108.20   |
| 27  | B8    | 2310 | C    | N3-C4-N4   | 5.17  | 121.62      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1234 | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 26  | B7    | 60   | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 27  | B8    | 42   | A    | C5-C6-N6   | -5.17 | 119.56      | 123.70   |
| 27  | B8    | 66   | C    | N3-C4-N4   | 5.17  | 121.62      | 118.00   |
| 27  | B8    | 106  | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 27  | B8    | 2809 | A    | C5-C6-N1   | -5.17 | 115.11      | 117.70   |
| 1   | AA    | 201  | G    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 1   | AA    | 203  | G    | N3-C2-N2   | 5.17  | 123.52      | 119.90   |
| 1   | AA    | 450  | G    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 1   | AA    | 715  | A    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 1   | AA    | 805  | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 27  | B8    | 691  | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 27  | B8    | 1596 | A    | C5-C6-N6   | -5.17 | 119.56      | 123.70   |
| 27  | B8    | 1617 | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 27  | B8    | 2355 | G    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 1   | AA    | 55   | A    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 1   | AA    | 372  | C    | N3-C4-N4   | 5.17  | 121.62      | 118.00   |
| 1   | AA    | 547  | A    | C5-C6-N6   | -5.17 | 119.57      | 123.70   |
| 1   | AA    | 606  | G    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 1   | AA    | 614  | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 1   | AA    | 676  | A    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 1   | AA    | 831  | A    | C5-C6-N1   | -5.17 | 115.12      | 117.70   |
| 1   | AA    | 836  | G    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 1   | AA    | 1225 | A    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 1   | AA    | 1405 | G    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 27  | B8    | 715  | A    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 27  | B8    | 765  | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 27  | B8    | 898  | C    | N3-C4-N4   | 5.17  | 121.62      | 118.00   |
| 27  | B8    | 973  | A    | C5-C6-N1   | -5.17 | 115.12      | 117.70   |
| 27  | B8    | 1046 | A    | C5-C6-N1   | -5.17 | 115.12      | 117.70   |
| 27  | B8    | 1366 | A    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 27  | B8    | 2150 | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 27  | B8    | 2774 | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 1   | AA    | 933  | G    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 1   | AA    | 1005 | A    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 1   | AA    | 1035 | A    | C5-C6-N1   | -5.17 | 115.12      | 117.70   |
| 1   | AA    | 1449 | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |
| 26  | B7    | 14   | U    | O4'-C1'-N1 | 5.17  | 112.33      | 108.20   |
| 27  | B8    | 101  | A    | C5-C6-N1   | -5.17 | 115.12      | 117.70   |
| 27  | B8    | 340  | A    | C5-C6-N1   | -5.17 | 115.12      | 117.70   |
| 27  | B8    | 856  | G    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 27  | B8    | 1881 | C    | N3-C4-C5   | -5.17 | 119.83      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2015 | A    | C5-C6-N6   | -5.17 | 119.57      | 123.70   |
| 1   | AA    | 79   | G    | O4'-C1'-N9 | 5.16  | 112.33      | 108.20   |
| 1   | AA    | 998  | C    | N3-C4-C5   | -5.16 | 119.83      | 121.90   |
| 1   | AA    | 1400 | C    | N3-C4-N4   | 5.16  | 121.61      | 118.00   |
| 27  | B8    | 21   | A    | C5-C6-N1   | -5.16 | 115.12      | 117.70   |
| 27  | B8    | 701  | G    | O4'-C1'-N9 | 5.16  | 112.33      | 108.20   |
| 27  | B8    | 1974 | C    | N3-C4-C5   | -5.16 | 119.83      | 121.90   |
| 1   | AA    | 50   | A    | C5-C6-N1   | -5.16 | 115.12      | 117.70   |
| 1   | AA    | 199  | A    | O4'-C1'-N9 | 5.16  | 112.33      | 108.20   |
| 1   | AA    | 888  | G    | N3-C2-N2   | 5.16  | 123.51      | 119.90   |
| 3   | AV    | 27   | A    | C5-C6-N1   | -5.16 | 115.12      | 117.70   |
| 27  | B8    | 555  | G    | O4'-C1'-N9 | 5.16  | 112.33      | 108.20   |
| 27  | B8    | 611  | C    | N3-C4-C5   | -5.16 | 119.83      | 121.90   |
| 27  | B8    | 1304 | A    | C5-C6-N6   | -5.16 | 119.57      | 123.70   |
| 37  | BI    | 87   | SER  | N-CA-CB    | 5.16  | 118.24      | 110.50   |
| 1   | AA    | 364  | A    | O4'-C1'-N9 | 5.16  | 112.33      | 108.20   |
| 27  | B8    | 479  | A    | C5-C6-N1   | -5.16 | 115.12      | 117.70   |
| 27  | B8    | 507  | A    | C5-C6-N1   | -5.16 | 115.12      | 117.70   |
| 27  | B8    | 900  | A    | C5-C6-N6   | -5.16 | 119.57      | 123.70   |
| 27  | B8    | 1085 | A    | C4-C5-C6   | 5.16  | 119.58      | 117.00   |
| 27  | B8    | 1644 | C    | N3-C4-C5   | -5.16 | 119.84      | 121.90   |
| 27  | B8    | 1836 | C    | N3-C4-C5   | -5.16 | 119.84      | 121.90   |
| 27  | B8    | 2336 | A    | C5-C6-N1   | -5.16 | 115.12      | 117.70   |
| 27  | B8    | 2649 | C    | N3-C4-C5   | -5.16 | 119.83      | 121.90   |
| 1   | AA    | 1150 | A    | C5-C6-N6   | -5.16 | 119.57      | 123.70   |
| 3   | AV    | 17   | C    | N3-C4-N4   | 5.16  | 121.61      | 118.00   |
| 26  | B7    | 70   | C    | N3-C4-C5   | -5.16 | 119.84      | 121.90   |
| 27  | B8    | 305  | C    | N3-C4-C5   | -5.16 | 119.84      | 121.90   |
| 27  | B8    | 1527 | G    | N3-C2-N2   | 5.16  | 123.51      | 119.90   |
| 27  | B8    | 1600 | C    | N3-C4-C5   | -5.16 | 119.84      | 121.90   |
| 27  | B8    | 1638 | C    | N3-C4-C5   | -5.16 | 119.84      | 121.90   |
| 26  | B7    | 61   | G    | O4'-C1'-N9 | 5.16  | 112.33      | 108.20   |
| 27  | B8    | 643  | A    | C5-C6-N1   | -5.16 | 115.12      | 117.70   |
| 27  | B8    | 1078 | U    | C2-N1-C1'  | 5.16  | 123.89      | 117.70   |
| 27  | B8    | 1296 | G    | O4'-C1'-N9 | 5.16  | 112.33      | 108.20   |
| 1   | AA    | 160  | A    | O4'-C1'-N9 | 5.16  | 112.32      | 108.20   |
| 1   | AA    | 383  | A    | O4'-C1'-N9 | 5.16  | 112.33      | 108.20   |
| 27  | B8    | 85   | G    | O4'-C1'-N9 | 5.16  | 112.32      | 108.20   |
| 27  | B8    | 1872 | A    | C5-C6-N6   | -5.16 | 119.58      | 123.70   |
| 1   | AA    | 177  | G    | C5-C6-O6   | -5.15 | 125.51      | 128.60   |
| 1   | AA    | 1431 | A    | C5-C6-N1   | -5.15 | 115.12      | 117.70   |
| 1   | AA    | 695  | A    | C5-C6-N1   | -5.15 | 115.12      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1287 | A    | C5-C6-N1   | -5.15 | 115.12      | 117.70   |
| 27  | B8    | 127  | A    | C5-C6-N1   | -5.15 | 115.12      | 117.70   |
| 27  | B8    | 670  | A    | C5-C6-N1   | -5.15 | 115.12      | 117.70   |
| 27  | B8    | 911  | A    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 27  | B8    | 2012 | G    | N3-C2-N2   | 5.15  | 123.51      | 119.90   |
| 27  | B8    | 2145 | C    | C2-N1-C1'  | 5.15  | 124.47      | 118.80   |
| 1   | AA    | 369  | G    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 1   | AA    | 558  | G    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 1   | AA    | 613  | C    | N3-C4-C5   | -5.15 | 119.84      | 121.90   |
| 1   | AA    | 969  | A    | C5-C6-N1   | -5.15 | 115.12      | 117.70   |
| 1   | AA    | 1285 | A    | C5-C6-N1   | -5.15 | 115.12      | 117.70   |
| 1   | AA    | 1318 | A    | C5-C6-N1   | -5.15 | 115.12      | 117.70   |
| 1   | AA    | 1332 | A    | C5-C6-N1   | -5.15 | 115.12      | 117.70   |
| 1   | AA    | 1352 | C    | N3-C4-C5   | -5.15 | 119.84      | 121.90   |
| 27  | B8    | 6    | A    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 27  | B8    | 1496 | A    | C5-C6-N1   | -5.15 | 115.12      | 117.70   |
| 27  | B8    | 2082 | A    | C5-C6-N1   | -5.15 | 115.12      | 117.70   |
| 27  | B8    | 2430 | A    | C5-C6-N1   | -5.15 | 115.12      | 117.70   |
| 27  | B8    | 2598 | A    | C5-C6-N1   | -5.15 | 115.12      | 117.70   |
| 27  | B8    | 121  | G    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 27  | B8    | 1495 | A    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 27  | B8    | 1628 | G    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 27  | B8    | 2673 | G    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 27  | B8    | 2682 | A    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 1   | AA    | 59   | A    | C5-C6-N1   | -5.15 | 115.13      | 117.70   |
| 1   | AA    | 630  | A    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 1   | AA    | 833  | G    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 27  | B8    | 314  | C    | N3-C4-C5   | -5.15 | 119.84      | 121.90   |
| 27  | B8    | 477  | A    | C5-C6-N6   | -5.15 | 119.58      | 123.70   |
| 27  | B8    | 570  | G    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 27  | B8    | 789  | A    | C5-C6-N1   | -5.15 | 115.13      | 117.70   |
| 27  | B8    | 1741 | C    | N3-C4-C5   | -5.15 | 119.84      | 121.90   |
| 27  | B8    | 1893 | C    | N3-C4-C5   | -5.15 | 119.84      | 121.90   |
| 27  | B8    | 2664 | G    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 27  | B8    | 2765 | A    | C5-C6-N6   | -5.15 | 119.58      | 123.70   |
| 1   | AA    | 1142 | G    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 2   | AX    | 17   | C    | N3-C4-C5   | -5.15 | 119.84      | 121.90   |
| 3   | AV    | 44   | G    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 27  | B8    | 2595 | G    | O4'-C1'-N9 | 5.15  | 112.32      | 108.20   |
| 1   | AA    | 489  | C    | N3-C4-C5   | -5.14 | 119.84      | 121.90   |
| 1   | AA    | 999  | C    | N3-C4-C5   | -5.14 | 119.84      | 121.90   |
| 1   | AA    | 1022 | A    | C5-C6-N6   | -5.14 | 119.58      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1107 | C    | N3-C4-C5   | -5.14 | 119.84      | 121.90   |
| 1   | AA    | 1111 | A    | O4'-C1'-N9 | 5.14  | 112.32      | 108.20   |
| 27  | B8    | 844  | A    | O4'-C1'-N9 | 5.14  | 112.32      | 108.20   |
| 27  | B8    | 2530 | A    | C5-C6-N1   | -5.14 | 115.13      | 117.70   |
| 1   | AA    | 331  | G    | O4'-C1'-N9 | 5.14  | 112.31      | 108.20   |
| 1   | AA    | 750  | C    | N3-C4-C5   | -5.14 | 119.84      | 121.90   |
| 1   | AA    | 857  | C    | N3-C4-N4   | 5.14  | 121.60      | 118.00   |
| 1   | AA    | 1044 | A    | O4'-C1'-N9 | 5.14  | 112.31      | 108.20   |
| 1   | AA    | 1492 | A    | C5-C6-N1   | -5.14 | 115.13      | 117.70   |
| 27  | B8    | 505  | A    | C5-C6-N1   | -5.14 | 115.13      | 117.70   |
| 27  | B8    | 1587 | G    | O4'-C1'-N9 | 5.14  | 112.31      | 108.20   |
| 27  | B8    | 1753 | G    | O4'-C1'-N9 | 5.14  | 112.31      | 108.20   |
| 27  | B8    | 2750 | A    | C5-C6-N1   | -5.14 | 115.13      | 117.70   |
| 41  | BM    | 122  | ALA  | N-CA-CB    | 5.14  | 117.30      | 110.10   |
| 1   | AA    | 1214 | C    | C6-N1-C1'  | -5.14 | 114.63      | 120.80   |
| 1   | AA    | 1281 | C    | N3-C4-C5   | -5.14 | 119.84      | 121.90   |
| 3   | AV    | 27   | A    | O4'-C1'-N9 | 5.14  | 112.31      | 108.20   |
| 27  | B8    | 616  | A    | C5-C6-N1   | -5.14 | 115.13      | 117.70   |
| 27  | B8    | 873  | C    | N3-C4-C5   | -5.14 | 119.84      | 121.90   |
| 1   | AA    | 236  | A    | O4'-C1'-N9 | 5.14  | 112.31      | 108.20   |
| 1   | AA    | 914  | A    | O4'-C1'-N9 | 5.14  | 112.31      | 108.20   |
| 1   | AA    | 1418 | A    | C5-C6-N1   | -5.14 | 115.13      | 117.70   |
| 27  | B8    | 1048 | A    | O4'-C1'-N9 | 5.14  | 112.31      | 108.20   |
| 27  | B8    | 1722 | A    | C5-C6-N6   | -5.14 | 119.59      | 123.70   |
| 27  | B8    | 2762 | C    | N3-C4-C5   | -5.14 | 119.84      | 121.90   |
| 1   | AA    | 435  | A    | C5-C6-N1   | -5.14 | 115.13      | 117.70   |
| 1   | AA    | 608  | A    | C5-C6-N1   | -5.14 | 115.13      | 117.70   |
| 1   | AA    | 880  | C    | N3-C4-N4   | 5.14  | 121.60      | 118.00   |
| 27  | B8    | 216  | A    | C5-C6-N6   | -5.14 | 119.59      | 123.70   |
| 27  | B8    | 719  | C    | N3-C4-C5   | -5.14 | 119.84      | 121.90   |
| 27  | B8    | 2455 | G    | O4'-C1'-N9 | 5.14  | 112.31      | 108.20   |
| 27  | B8    | 2503 | A    | C5-C6-N1   | -5.14 | 115.13      | 117.70   |
| 1   | AA    | 980  | C    | N3-C4-C5   | -5.14 | 119.84      | 121.90   |
| 1   | AA    | 1368 | A    | C5-C6-N6   | -5.14 | 119.59      | 123.70   |
| 1   | AA    | 1468 | A    | C5-C6-N6   | -5.14 | 119.59      | 123.70   |
| 26  | B7    | 34   | A    | C5-C6-N6   | -5.14 | 119.59      | 123.70   |
| 27  | B8    | 94   | A    | C5-C6-N6   | -5.14 | 119.59      | 123.70   |
| 27  | B8    | 644  | A    | C5-C6-N1   | -5.14 | 115.13      | 117.70   |
| 27  | B8    | 905  | A    | C5-C6-N1   | -5.14 | 115.13      | 117.70   |
| 27  | B8    | 2208 | C    | N3-C4-C5   | -5.14 | 119.85      | 121.90   |
| 1   | AA    | 116  | A    | C5-C6-N6   | -5.13 | 119.59      | 123.70   |
| 1   | AA    | 1120 | C    | N3-C4-C5   | -5.13 | 119.85      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 316  | C    | N3-C4-C5   | -5.13 | 119.85      | 121.90   |
| 27  | B8    | 516  | C    | N3-C4-C5   | -5.13 | 119.85      | 121.90   |
| 27  | B8    | 1454 | C    | N3-C4-N4   | 5.13  | 121.59      | 118.00   |
| 27  | B8    | 2620 | C    | N3-C4-C5   | -5.13 | 119.85      | 121.90   |
| 27  | B8    | 2875 | C    | N3-C4-C5   | -5.13 | 119.85      | 121.90   |
| 27  | B8    | 1879 | C    | N3-C4-C5   | -5.13 | 119.85      | 121.90   |
| 1   | AA    | 727  | G    | N3-C2-N2   | 5.13  | 123.49      | 119.90   |
| 1   | AA    | 1285 | A    | C5-C6-N6   | -5.13 | 119.59      | 123.70   |
| 1   | AA    | 1447 | A    | C4-C5-C6   | 5.13  | 119.56      | 117.00   |
| 27  | B8    | 142  | A    | C5-C6-N6   | -5.13 | 119.59      | 123.70   |
| 27  | B8    | 385  | C    | N3-C4-N4   | 5.13  | 121.59      | 118.00   |
| 27  | B8    | 1075 | C    | N3-C4-C5   | -5.13 | 119.85      | 121.90   |
| 27  | B8    | 1302 | A    | C5-C6-N6   | -5.13 | 119.59      | 123.70   |
| 27  | B8    | 1909 | C    | N3-C4-C5   | -5.13 | 119.85      | 121.90   |
| 1   | AA    | 60   | A    | C5-C6-N1   | -5.13 | 115.14      | 117.70   |
| 1   | AA    | 452  | A    | C5-C6-N1   | -5.13 | 115.14      | 117.70   |
| 1   | AA    | 959  | A    | O4'-C1'-N9 | 5.13  | 112.30      | 108.20   |
| 27  | B8    | 1383 | A    | C5-C6-N1   | -5.13 | 115.14      | 117.70   |
| 27  | B8    | 2509 | G    | O4'-C1'-N9 | 5.13  | 112.30      | 108.20   |
| 27  | B8    | 2832 | U    | O4'-C1'-N1 | 5.13  | 112.30      | 108.20   |
| 1   | AA    | 712  | A    | C5-C6-N1   | -5.13 | 115.14      | 117.70   |
| 26  | B7    | 17   | C    | N3-C4-C5   | -5.13 | 119.85      | 121.90   |
| 27  | B8    | 195  | A    | C5-C6-N1   | -5.13 | 115.14      | 117.70   |
| 27  | B8    | 457  | A    | C4-C5-C6   | 5.13  | 119.56      | 117.00   |
| 27  | B8    | 1298 | C    | N3-C4-C5   | -5.13 | 119.85      | 121.90   |
| 27  | B8    | 2134 | A    | C5-C6-N6   | -5.13 | 119.60      | 123.70   |
| 27  | B8    | 2427 | C    | N3-C4-C5   | -5.13 | 119.85      | 121.90   |
| 27  | B8    | 2833 | U    | O4'-C1'-N1 | 5.13  | 112.30      | 108.20   |
| 27  | B8    | 2883 | A    | C5-C6-N1   | -5.13 | 115.14      | 117.70   |
| 1   | AA    | 1027 | C    | C5-C4-N4   | -5.13 | 116.61      | 120.20   |
| 1   | AA    | 1188 | A    | O4'-C1'-N9 | 5.13  | 112.30      | 108.20   |
| 27  | B8    | 251  | A    | O4'-C1'-N9 | 5.13  | 112.30      | 108.20   |
| 27  | B8    | 849  | A    | C5-C6-N1   | -5.13 | 115.14      | 117.70   |
| 27  | B8    | 2499 | C    | N3-C4-C5   | -5.13 | 119.85      | 121.90   |
| 1   | AA    | 648  | A    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 1   | AA    | 139  | A    | C5-C6-N1   | -5.12 | 115.14      | 117.70   |
| 1   | AA    | 507  | C    | N3-C4-C5   | -5.12 | 119.85      | 121.90   |
| 1   | AA    | 1269 | A    | C4-C5-C6   | 5.12  | 119.56      | 117.00   |
| 1   | AA    | 1350 | A    | C5-C6-N1   | -5.12 | 115.14      | 117.70   |
| 26  | B7    | 26   | C    | N3-C4-N4   | 5.12  | 121.59      | 118.00   |
| 27  | B8    | 34   | U    | C2-N1-C1'  | 5.12  | 123.85      | 117.70   |
| 27  | B8    | 56   | A    | C5-C6-N1   | -5.12 | 115.14      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 513  | A    | C5-C6-N1   | -5.12 | 115.14      | 117.70   |
| 27  | B8    | 599  | A    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 27  | B8    | 1264 | A    | C5-C6-N1   | -5.12 | 115.14      | 117.70   |
| 27  | B8    | 1529 | G    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 27  | B8    | 1572 | A    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 27  | B8    | 1668 | A    | C5-C6-N1   | -5.12 | 115.14      | 117.70   |
| 27  | B8    | 2761 | A    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 1   | AA    | 54   | C    | N3-C4-C5   | -5.12 | 119.85      | 121.90   |
| 26  | B7    | 107  | G    | N3-C2-N2   | 5.12  | 123.49      | 119.90   |
| 27  | B8    | 737  | C    | N3-C4-C5   | -5.12 | 119.85      | 121.90   |
| 27  | B8    | 878  | A    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 27  | B8    | 1996 | C    | O4'-C1'-N1 | 5.12  | 112.30      | 108.20   |
| 27  | B8    | 2706 | A    | C5-C6-N1   | -5.12 | 115.14      | 117.70   |
| 1   | AA    | 177  | G    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 27  | B8    | 1    | G    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 27  | B8    | 218  | A    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 27  | B8    | 250  | G    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 27  | B8    | 387  | U    | O4'-C1'-N1 | 5.12  | 112.30      | 108.20   |
| 27  | B8    | 899  | A    | C5-C6-N1   | -5.12 | 115.14      | 117.70   |
| 1   | AA    | 699  | C    | N3-C4-C5   | -5.12 | 119.85      | 121.90   |
| 1   | AA    | 888  | G    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 27  | B8    | 38   | A    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 27  | B8    | 231  | A    | C5-C6-N6   | -5.12 | 119.60      | 123.70   |
| 27  | B8    | 1117 | C    | N3-C4-C5   | -5.12 | 119.85      | 121.90   |
| 27  | B8    | 1367 | A    | C5-C6-N1   | -5.12 | 115.14      | 117.70   |
| 27  | B8    | 2274 | A    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 1   | AA    | 560  | A    | O4'-C1'-N9 | 5.12  | 112.29      | 108.20   |
| 1   | AA    | 1014 | A    | C5-C6-N1   | -5.12 | 115.14      | 117.70   |
| 27  | B8    | 120  | U    | O4'-C1'-N1 | 5.12  | 112.29      | 108.20   |
| 27  | B8    | 621  | A    | C5-C6-N1   | -5.12 | 115.14      | 117.70   |
| 27  | B8    | 2020 | A    | C5-C6-N6   | -5.12 | 119.61      | 123.70   |
| 27  | B8    | 2467 | C    | N3-C4-N4   | 5.12  | 121.58      | 118.00   |
| 27  | B8    | 2666 | C    | N3-C4-N4   | 5.12  | 121.58      | 118.00   |
| 1   | AA    | 342  | C    | N3-C4-C5   | -5.12 | 119.85      | 121.90   |
| 1   | AA    | 579  | A    | C5-C6-N1   | -5.12 | 115.14      | 117.70   |
| 1   | AA    | 938  | A    | C5-C6-N1   | -5.12 | 115.14      | 117.70   |
| 1   | AA    | 1266 | G    | O4'-C1'-N9 | 5.12  | 112.29      | 108.20   |
| 1   | AA    | 1340 | A    | C5-C6-N6   | -5.12 | 119.61      | 123.70   |
| 1   | AA    | 1434 | A    | C5-C6-N1   | -5.12 | 115.14      | 117.70   |
| 27  | B8    | 70   | G    | O4'-C1'-N9 | 5.12  | 112.29      | 108.20   |
| 27  | B8    | 1074 | G    | O4'-C1'-N9 | 5.12  | 112.29      | 108.20   |
| 27  | B8    | 2365 | G    | N3-C2-N2   | 5.12  | 123.48      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2440 | C    | N3-C4-C5   | -5.12 | 119.85      | 121.90   |
| 1   | AA    | 190  | A    | C5-C6-N6   | -5.11 | 119.61      | 123.70   |
| 1   | AA    | 1047 | G    | O4'-C1'-N9 | 5.11  | 112.29      | 108.20   |
| 1   | AA    | 1096 | C    | N3-C4-C5   | -5.11 | 119.86      | 121.90   |
| 6   | AB    | 212  | TYR  | CB-CG-CD2  | -5.11 | 117.93      | 121.00   |
| 27  | B8    | 330  | A    | O4'-C1'-N9 | 5.11  | 112.29      | 108.20   |
| 27  | B8    | 398  | C    | N3-C4-C5   | -5.11 | 119.86      | 121.90   |
| 27  | B8    | 1308 | A    | O4'-C1'-N9 | 5.11  | 112.29      | 108.20   |
| 27  | B8    | 1428 | C    | P-O3'-C3'  | 5.11  | 125.84      | 119.70   |
| 27  | B8    | 1674 | G    | O4'-C1'-N9 | 5.11  | 112.29      | 108.20   |
| 27  | B8    | 1978 | A    | C5-C6-N1   | -5.11 | 115.14      | 117.70   |
| 27  | B8    | 2164 | C    | C6-N1-C1'  | -5.11 | 114.67      | 120.80   |
| 28  | BA    | 200  | PRO  | CA-C-N     | 5.11  | 131.42      | 117.10   |
| 1   | AA    | 1245 | C    | N3-C4-C5   | -5.11 | 119.86      | 121.90   |
| 27  | B8    | 91   | A    | O4'-C1'-N9 | 5.11  | 112.29      | 108.20   |
| 47  | BS    | 89   | ALA  | N-CA-CB    | 5.11  | 117.26      | 110.10   |
| 1   | AA    | 530  | G    | O4'-C1'-N9 | 5.11  | 112.29      | 108.20   |
| 1   | AA    | 1113 | C    | P-O5'-C5'  | 5.11  | 129.08      | 120.90   |
| 1   | AA    | 1252 | A    | C5-C6-N1   | -5.11 | 115.14      | 117.70   |
| 27  | B8    | 52   | A    | C5-C6-N6   | -5.11 | 119.61      | 123.70   |
| 27  | B8    | 2258 | C    | N3-C4-C5   | -5.11 | 119.86      | 121.90   |
| 27  | B8    | 2531 | A    | C5-C6-N6   | -5.11 | 119.61      | 123.70   |
| 27  | B8    | 2711 | A    | C5-C6-N1   | -5.11 | 115.14      | 117.70   |
| 1   | AA    | 810  | C    | N3-C4-C5   | -5.11 | 119.86      | 121.90   |
| 27  | B8    | 1208 | C    | N3-C4-C5   | -5.11 | 119.86      | 121.90   |
| 27  | B8    | 1711 | A    | C5-C6-N6   | -5.11 | 119.61      | 123.70   |
| 27  | B8    | 910  | A    | C5-C6-N6   | -5.11 | 119.61      | 123.70   |
| 1   | AA    | 285  | C    | N3-C4-C5   | -5.11 | 119.86      | 121.90   |
| 1   | AA    | 475  | C    | N3-C4-C5   | -5.11 | 119.86      | 121.90   |
| 1   | AA    | 639  | G    | O4'-C1'-N9 | 5.11  | 112.28      | 108.20   |
| 27  | B8    | 124  | G    | O4'-C1'-N9 | 5.11  | 112.28      | 108.20   |
| 27  | B8    | 1454 | C    | N3-C4-C5   | -5.11 | 119.86      | 121.90   |
| 27  | B8    | 1494 | A    | O4'-C1'-N9 | 5.11  | 112.28      | 108.20   |
| 27  | B8    | 1553 | A    | C5-C6-N1   | -5.11 | 115.15      | 117.70   |
| 27  | B8    | 2321 | U    | C2-N1-C1'  | 5.11  | 123.83      | 117.70   |
| 27  | B8    | 2704 | C    | N3-C4-C5   | -5.11 | 119.86      | 121.90   |
| 27  | B8    | 2787 | C    | N3-C4-C5   | -5.11 | 119.86      | 121.90   |
| 1   | AA    | 1469 | C    | N3-C4-C5   | -5.10 | 119.86      | 121.90   |
| 27  | B8    | 2810 | A    | C5-C6-N1   | -5.10 | 115.15      | 117.70   |
| 42  | BN    | 21   | PHE  | CB-CG-CD2  | 5.10  | 124.37      | 120.80   |
| 1   | AA    | 528  | C    | N3-C4-N4   | 5.10  | 121.57      | 118.00   |
| 1   | AA    | 966  | G    | O4'-C1'-N9 | 5.10  | 112.28      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 1502 | A    | C5-C6-N6   | -5.10 | 119.62      | 123.70   |
| 3   | AV    | 54   | G    | O4'-C1'-N9 | 5.10  | 112.28      | 108.20   |
| 27  | B8    | 529  | A    | C5-C6-N6   | -5.10 | 119.62      | 123.70   |
| 27  | B8    | 633  | A    | C5-C6-N6   | -5.10 | 119.62      | 123.70   |
| 27  | B8    | 2214 | C    | N3-C4-C5   | -5.10 | 119.86      | 121.90   |
| 1   | AA    | 134  | G    | O4'-C1'-N9 | 5.10  | 112.28      | 108.20   |
| 27  | B8    | 867  | C    | N3-C4-N4   | 5.10  | 121.57      | 118.00   |
| 27  | B8    | 1414 | C    | N3-C4-C5   | -5.10 | 119.86      | 121.90   |
| 27  | B8    | 1789 | A    | O4'-C1'-N9 | 5.10  | 112.28      | 108.20   |
| 1   | AA    | 326  | G    | O4'-C1'-N9 | 5.10  | 112.28      | 108.20   |
| 27  | B8    | 343  | C    | N3-C4-C5   | -5.10 | 119.86      | 121.90   |
| 27  | B8    | 1403 | A    | O4'-C1'-N9 | 5.10  | 112.28      | 108.20   |
| 27  | B8    | 1866 | A    | C5-C6-N1   | -5.10 | 115.15      | 117.70   |
| 27  | B8    | 2035 | G    | O4'-C1'-N9 | 5.10  | 112.28      | 108.20   |
| 27  | B8    | 2678 | C    | N3-C4-C5   | -5.10 | 119.86      | 121.90   |
| 27  | B8    | 2785 | C    | N3-C4-C5   | -5.10 | 119.86      | 121.90   |
| 1   | AA    | 364  | A    | C5-C6-N1   | -5.10 | 115.15      | 117.70   |
| 1   | AA    | 865  | A    | C5-C6-N1   | -5.10 | 115.15      | 117.70   |
| 27  | B8    | 63   | A    | C5-C6-N1   | -5.10 | 115.15      | 117.70   |
| 27  | B8    | 167  | A    | C5-C6-N1   | -5.10 | 115.15      | 117.70   |
| 27  | B8    | 1695 | G    | O4'-C1'-N9 | 5.10  | 112.28      | 108.20   |
| 1   | AA    | 1325 | C    | N3-C4-C5   | -5.10 | 119.86      | 121.90   |
| 27  | B8    | 5    | A    | O4'-C1'-N9 | 5.10  | 112.28      | 108.20   |
| 1   | AA    | 282  | A    | C5-C6-N1   | -5.09 | 115.15      | 117.70   |
| 1   | AA    | 647  | C    | N3-C4-C5   | -5.09 | 119.86      | 121.90   |
| 1   | AA    | 743  | A    | O4'-C1'-N9 | 5.09  | 112.28      | 108.20   |
| 1   | AA    | 1113 | C    | N3-C4-C5   | -5.09 | 119.86      | 121.90   |
| 1   | AA    | 1397 | C    | N3-C4-C5   | -5.09 | 119.86      | 121.90   |
| 26  | B7    | 37   | C    | N3-C4-N4   | 5.09  | 121.57      | 118.00   |
| 27  | B8    | 109  | C    | N3-C4-C5   | -5.09 | 119.86      | 121.90   |
| 27  | B8    | 469  | G    | N3-C2-N2   | 5.09  | 123.47      | 119.90   |
| 27  | B8    | 668  | A    | O4'-C1'-N9 | 5.09  | 112.28      | 108.20   |
| 27  | B8    | 874  | G    | O4'-C1'-N9 | 5.09  | 112.28      | 108.20   |
| 27  | B8    | 1387 | A    | C5-C6-N1   | -5.09 | 115.15      | 117.70   |
| 27  | B8    | 1630 | A    | C5-C6-N6   | -5.09 | 119.62      | 123.70   |
| 27  | B8    | 2368 | C    | N3-C4-C5   | -5.09 | 119.86      | 121.90   |
| 27  | B8    | 2620 | C    | N3-C4-N4   | 5.09  | 121.57      | 118.00   |
| 27  | B8    | 2793 | C    | N3-C4-C5   | -5.09 | 119.86      | 121.90   |
| 27  | B8    | 2857 | G    | O4'-C1'-N9 | 5.09  | 112.28      | 108.20   |
| 27  | B8    | 2879 | A    | C5-C6-N1   | -5.09 | 115.15      | 117.70   |
| 1   | AA    | 910  | C    | N3-C4-C5   | -5.09 | 119.86      | 121.90   |
| 27  | B8    | 626  | A    | O4'-C1'-N9 | 5.09  | 112.28      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | B8    | 973  | A    | C5'-C4'-O4' | 5.09  | 115.21      | 109.10   |
| 27  | B8    | 1640 | A    | C5-C6-N1    | -5.09 | 115.15      | 117.70   |
| 1   | AA    | 52   | C    | N3-C4-C5    | -5.09 | 119.86      | 121.90   |
| 1   | AA    | 411  | A    | C5-C6-N1    | -5.09 | 115.15      | 117.70   |
| 1   | AA    | 1446 | A    | C5-C6-N1    | -5.09 | 115.16      | 117.70   |
| 27  | B8    | 39   | G    | O4'-C1'-N9  | 5.09  | 112.27      | 108.20   |
| 27  | B8    | 1287 | A    | C5-C6-N6    | -5.09 | 119.63      | 123.70   |
| 27  | B8    | 1533 | C    | N3-C4-C5    | -5.09 | 119.86      | 121.90   |
| 27  | B8    | 1902 | C    | N3-C4-N4    | 5.09  | 121.56      | 118.00   |
| 27  | B8    | 2077 | A    | C5-C6-N6    | -5.09 | 119.63      | 123.70   |
| 27  | B8    | 2306 | C    | N3-C4-C5    | -5.09 | 119.86      | 121.90   |
| 1   | AA    | 71   | A    | C5-C6-N1    | -5.09 | 115.16      | 117.70   |
| 1   | AA    | 280  | C    | O4'-C1'-N1  | 5.09  | 112.27      | 108.20   |
| 1   | AA    | 876  | C    | N3-C4-C5    | -5.09 | 119.86      | 121.90   |
| 3   | AV    | 11   | C    | N3-C4-N4    | 5.09  | 121.56      | 118.00   |
| 27  | B8    | 1111 | A    | C5-C6-N6    | -5.09 | 119.63      | 123.70   |
| 27  | B8    | 2386 | A    | C5-C6-N1    | -5.09 | 115.16      | 117.70   |
| 27  | B8    | 2520 | C    | N3-C4-C5    | -5.09 | 119.86      | 121.90   |
| 27  | B8    | 2654 | A    | C5-C6-N1    | -5.09 | 115.16      | 117.70   |
| 1   | AA    | 539  | A    | C5-C6-N1    | -5.09 | 115.16      | 117.70   |
| 27  | B8    | 1050 | A    | C5-C6-N1    | -5.09 | 115.16      | 117.70   |
| 27  | B8    | 1522 | A    | C4-C5-C6    | 5.09  | 119.54      | 117.00   |
| 27  | B8    | 1679 | A    | C5-C6-N6    | -5.09 | 119.63      | 123.70   |
| 1   | AA    | 109  | A    | C5-C6-N6    | -5.09 | 119.63      | 123.70   |
| 1   | AA    | 234  | C    | N3-C4-C5    | -5.09 | 119.87      | 121.90   |
| 1   | AA    | 896  | C    | N3-C4-C5    | -5.09 | 119.87      | 121.90   |
| 27  | B8    | 1233 | C    | N3-C4-C5    | -5.09 | 119.87      | 121.90   |
| 27  | B8    | 2091 | C    | N3-C4-C5    | -5.09 | 119.87      | 121.90   |
| 27  | B8    | 2679 | A    | C5-C6-N1    | -5.09 | 115.16      | 117.70   |
| 1   | AA    | 1261 | A    | O4'-C1'-N9  | 5.08  | 112.27      | 108.20   |
| 27  | B8    | 794  | A    | O4'-C1'-N9  | 5.08  | 112.27      | 108.20   |
| 27  | B8    | 2486 | C    | N3-C4-C5    | -5.08 | 119.87      | 121.90   |
| 1   | AA    | 1236 | A    | O4'-C1'-N9  | 5.08  | 112.27      | 108.20   |
| 2   | AX    | 19   | U    | O4'-C1'-N1  | 5.08  | 112.27      | 108.20   |
| 27  | B8    | 1565 | C    | P-O3'-C3'   | 5.08  | 125.80      | 119.70   |
| 27  | B8    | 1854 | A    | C5-C6-N6    | -5.08 | 119.63      | 123.70   |
| 27  | B8    | 1961 | C    | N3-C4-C5    | -5.08 | 119.87      | 121.90   |
| 27  | B8    | 2366 | A    | O4'-C1'-N9  | 5.08  | 112.27      | 108.20   |
| 27  | B8    | 2487 | G    | O4'-C1'-N9  | 5.08  | 112.27      | 108.20   |
| 1   | AA    | 432  | A    | C5-C6-N1    | -5.08 | 115.16      | 117.70   |
| 1   | AA    | 766  | A    | C5-C6-N1    | -5.08 | 115.16      | 117.70   |
| 1   | AA    | 1265 | C    | N3-C4-C5    | -5.08 | 119.87      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 104  | A    | O4'-C1'-N9 | 5.08  | 112.27      | 108.20   |
| 27  | B8    | 586  | A    | O4'-C1'-N9 | 5.08  | 112.27      | 108.20   |
| 27  | B8    | 1044 | C    | N3-C4-C5   | -5.08 | 119.87      | 121.90   |
| 27  | B8    | 2542 | A    | C5-C6-N1   | -5.08 | 115.16      | 117.70   |
| 1   | AA    | 393  | A    | C5-C6-N6   | -5.08 | 119.64      | 123.70   |
| 1   | AA    | 1178 | G    | N3-C2-N2   | 5.08  | 123.46      | 119.90   |
| 27  | B8    | 74   | A    | O4'-C1'-N9 | 5.08  | 112.26      | 108.20   |
| 1   | AA    | 115  | G    | N3-C2-N2   | 5.08  | 123.46      | 119.90   |
| 1   | AA    | 954  | G    | O4'-C1'-N9 | 5.08  | 112.26      | 108.20   |
| 27  | B8    | 71   | A    | C5-C6-N6   | -5.08 | 119.64      | 123.70   |
| 27  | B8    | 1607 | C    | N3-C4-N4   | 5.08  | 121.55      | 118.00   |
| 27  | B8    | 1977 | A    | O4'-C1'-N9 | 5.08  | 112.26      | 108.20   |
| 27  | B8    | 2626 | C    | N3-C4-C5   | -5.08 | 119.87      | 121.90   |
| 1   | AA    | 729  | A    | C5-C6-N1   | -5.08 | 115.16      | 117.70   |
| 1   | AA    | 790  | A    | O4'-C1'-N9 | 5.08  | 112.26      | 108.20   |
| 1   | AA    | 1417 | G    | N3-C2-N2   | 5.08  | 123.45      | 119.90   |
| 27  | B8    | 792  | A    | O4'-C1'-N9 | 5.08  | 112.26      | 108.20   |
| 27  | B8    | 1574 | C    | N3-C4-C5   | -5.08 | 119.87      | 121.90   |
| 1   | AA    | 660  | C    | N3-C4-C5   | -5.08 | 119.87      | 121.90   |
| 1   | AA    | 1208 | C    | N3-C4-C5   | -5.08 | 119.87      | 121.90   |
| 1   | AA    | 1275 | A    | C5-C6-N6   | -5.08 | 119.64      | 123.70   |
| 3   | AV    | 59   | A    | C5-C6-N1   | -5.08 | 115.16      | 117.70   |
| 27  | B8    | 242  | G    | P-O3'-C3'  | 5.08  | 125.79      | 119.70   |
| 27  | B8    | 958  | U    | O4'-C1'-N1 | 5.08  | 112.26      | 108.20   |
| 27  | B8    | 2366 | A    | C5-C6-N6   | -5.08 | 119.64      | 123.70   |
| 27  | B8    | 2822 | G    | O4'-C1'-N9 | 5.08  | 112.26      | 108.20   |
| 1   | AA    | 744  | C    | N3-C4-C5   | -5.07 | 119.87      | 121.90   |
| 1   | AA    | 802  | A    | C5-C6-N1   | -5.07 | 115.16      | 117.70   |
| 1   | AA    | 878  | A    | C5-C6-N1   | -5.07 | 115.16      | 117.70   |
| 1   | AA    | 1218 | C    | N3-C4-C5   | -5.07 | 119.87      | 121.90   |
| 27  | B8    | 581  | C    | N3-C4-C5   | -5.07 | 119.87      | 121.90   |
| 27  | B8    | 1395 | A    | C5-C6-N6   | -5.07 | 119.64      | 123.70   |
| 27  | B8    | 2795 | C    | N3-C4-C5   | -5.07 | 119.87      | 121.90   |
| 1   | AA    | 704  | A    | C5-C6-N1   | -5.07 | 115.16      | 117.70   |
| 1   | AA    | 864  | A    | O4'-C1'-N9 | 5.07  | 112.26      | 108.20   |
| 1   | AA    | 1112 | C    | N3-C4-C5   | -5.07 | 119.87      | 121.90   |
| 27  | B8    | 1515 | A    | C4-C5-C6   | 5.07  | 119.54      | 117.00   |
| 27  | B8    | 2003 | A    | C5-C6-N1   | -5.07 | 115.16      | 117.70   |
| 27  | B8    | 2015 | A    | C5-C6-N1   | -5.07 | 115.16      | 117.70   |
| 27  | B8    | 2705 | A    | C5-C6-N1   | -5.07 | 115.16      | 117.70   |
| 1   | AA    | 389  | A    | C5-C6-N1   | -5.07 | 115.17      | 117.70   |
| 1   | AA    | 685  | G    | N3-C2-N2   | 5.07  | 123.45      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 799  | G    | O4'-C1'-N9 | 5.07  | 112.26      | 108.20   |
| 26  | B7    | 24   | G    | N3-C2-N2   | 5.07  | 123.45      | 119.90   |
| 27  | B8    | 675  | A    | C5-C6-N6   | -5.07 | 119.64      | 123.70   |
| 27  | B8    | 676  | A    | C5-C6-N1   | -5.07 | 115.17      | 117.70   |
| 27  | B8    | 1749 | A    | C5-C6-N6   | -5.07 | 119.64      | 123.70   |
| 27  | B8    | 1791 | A    | C5-C6-N1   | -5.07 | 115.17      | 117.70   |
| 27  | B8    | 2392 | A    | C5-C6-N1   | -5.07 | 115.17      | 117.70   |
| 1   | AA    | 181  | A    | C5-C6-N1   | -5.07 | 115.17      | 117.70   |
| 27  | B8    | 2115 | G    | N3-C2-N2   | 5.07  | 123.45      | 119.90   |
| 1   | AA    | 353  | A    | C5-C6-N1   | -5.07 | 115.17      | 117.70   |
| 1   | AA    | 890  | G    | O4'-C1'-N9 | 5.07  | 112.25      | 108.20   |
| 1   | AA    | 1476 | A    | C5-C6-N6   | -5.07 | 119.65      | 123.70   |
| 27  | B8    | 204  | A    | C4-C5-C6   | 5.07  | 119.53      | 117.00   |
| 27  | B8    | 916  | G    | O4'-C1'-N9 | 5.07  | 112.25      | 108.20   |
| 27  | B8    | 2080 | A    | O4'-C1'-N9 | 5.07  | 112.25      | 108.20   |
| 1   | AA    | 746  | A    | C5-C6-N1   | -5.07 | 115.17      | 117.70   |
| 26  | B7    | 28   | C    | N3-C4-C5   | -5.07 | 119.87      | 121.90   |
| 27  | B8    | 353  | C    | N3-C4-C5   | -5.07 | 119.87      | 121.90   |
| 27  | B8    | 374  | A    | C5-C6-N6   | -5.07 | 119.65      | 123.70   |
| 27  | B8    | 893  | C    | N3-C4-N4   | 5.07  | 121.55      | 118.00   |
| 27  | B8    | 1545 | A    | O4'-C1'-N9 | 5.07  | 112.25      | 108.20   |
| 27  | B8    | 2090 | A    | O4'-C1'-N9 | 5.07  | 112.25      | 108.20   |
| 27  | B8    | 2224 | G    | N3-C2-N2   | 5.07  | 123.45      | 119.90   |
| 1   | AA    | 523  | A    | O4'-C1'-N9 | 5.06  | 112.25      | 108.20   |
| 1   | AA    | 595  | A    | O4'-C1'-N9 | 5.06  | 112.25      | 108.20   |
| 3   | AV    | 25   | G    | O4'-C1'-N9 | 5.06  | 112.25      | 108.20   |
| 27  | B8    | 721  | A    | O4'-C1'-N9 | 5.06  | 112.25      | 108.20   |
| 27  | B8    | 735  | A    | O4'-C1'-N9 | 5.06  | 112.25      | 108.20   |
| 1   | AA    | 187  | G    | O4'-C1'-N9 | 5.06  | 112.25      | 108.20   |
| 1   | AA    | 561  | U    | P-O3'-C3'  | 5.06  | 125.78      | 119.70   |
| 1   | AA    | 1037 | C    | N3-C4-C5   | -5.06 | 119.88      | 121.90   |
| 27  | B8    | 267  | C    | N3-C4-C5   | -5.06 | 119.88      | 121.90   |
| 27  | B8    | 310  | A    | C5-C6-N6   | -5.06 | 119.65      | 123.70   |
| 27  | B8    | 745  | G    | O4'-C1'-N9 | 5.06  | 112.25      | 108.20   |
| 27  | B8    | 1502 | A    | O4'-C1'-N9 | 5.06  | 112.25      | 108.20   |
| 27  | B8    | 1635 | A    | C5-C6-N1   | -5.06 | 115.17      | 117.70   |
| 27  | B8    | 2004 | G    | O4'-C1'-N9 | 5.06  | 112.25      | 108.20   |
| 27  | B8    | 2733 | A    | C5-C6-N6   | -5.06 | 119.65      | 123.70   |
| 1   | AA    | 553  | A    | C5-C6-N1   | -5.06 | 115.17      | 117.70   |
| 1   | AA    | 1388 | C    | N3-C4-C5   | -5.06 | 119.88      | 121.90   |
| 27  | B8    | 644  | A    | O4'-C1'-N9 | 5.06  | 112.25      | 108.20   |
| 27  | B8    | 679  | C    | N3-C4-C5   | -5.06 | 119.88      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | B8    | 1241 | A    | C5-C6-N1    | -5.06 | 115.17      | 117.70   |
| 27  | B8    | 1462 | C    | N3-C4-C5    | -5.06 | 119.88      | 121.90   |
| 27  | B8    | 2354 | C    | N3-C4-C5    | -5.06 | 119.88      | 121.90   |
| 27  | B8    | 2446 | G    | O4'-C1'-N9  | 5.06  | 112.25      | 108.20   |
| 1   | AA    | 334  | C    | N3-C4-C5    | -5.06 | 119.88      | 121.90   |
| 1   | AA    | 525  | C    | N3-C4-C5    | -5.06 | 119.88      | 121.90   |
| 1   | AA    | 1268 | G    | N3-C2-N2    | 5.06  | 123.44      | 119.90   |
| 27  | B8    | 117  | G    | N3-C2-N2    | 5.06  | 123.44      | 119.90   |
| 27  | B8    | 687  | C    | N3-C4-N4    | 5.06  | 121.54      | 118.00   |
| 27  | B8    | 723  | C    | N3-C4-C5    | -5.06 | 119.88      | 121.90   |
| 27  | B8    | 880  | G    | O4'-C1'-N9  | 5.06  | 112.25      | 108.20   |
| 27  | B8    | 1196 | C    | N3-C4-C5    | -5.06 | 119.88      | 121.90   |
| 27  | B8    | 2169 | A    | C5-C6-N1    | -5.06 | 115.17      | 117.70   |
| 27  | B8    | 2729 | G    | C5'-C4'-O4' | 5.06  | 115.17      | 109.10   |
| 1   | AA    | 698  | G    | O4'-C1'-N9  | 5.06  | 112.25      | 108.20   |
| 1   | AA    | 841  | C    | N3-C4-C5    | -5.06 | 119.88      | 121.90   |
| 26  | B7    | 109  | A    | C5-C6-N1    | -5.06 | 115.17      | 117.70   |
| 27  | B8    | 517  | C    | N3-C4-C5    | -5.06 | 119.88      | 121.90   |
| 27  | B8    | 1336 | A    | C5'-C4'-O4' | 5.06  | 115.17      | 109.10   |
| 1   | AA    | 1304 | G    | N3-C2-N2    | 5.06  | 123.44      | 119.90   |
| 27  | B8    | 139  | U    | O4'-C1'-N1  | 5.06  | 112.25      | 108.20   |
| 27  | B8    | 439  | A    | C5-C6-N6    | -5.06 | 119.66      | 123.70   |
| 27  | B8    | 478  | A    | C5-C6-N1    | -5.06 | 115.17      | 117.70   |
| 27  | B8    | 1668 | A    | C5-C6-N6    | -5.06 | 119.66      | 123.70   |
| 1   | AA    | 207  | C    | N3-C4-C5    | -5.05 | 119.88      | 121.90   |
| 1   | AA    | 300  | A    | C5-C6-N1    | -5.05 | 115.17      | 117.70   |
| 1   | AA    | 617  | G    | O4'-C1'-N9  | 5.05  | 112.24      | 108.20   |
| 1   | AA    | 795  | C    | N3-C4-N4    | 5.05  | 121.54      | 118.00   |
| 1   | AA    | 816  | A    | C5-C6-N1    | -5.05 | 115.17      | 117.70   |
| 1   | AA    | 1102 | A    | C5-C6-N6    | -5.05 | 119.66      | 123.70   |
| 1   | AA    | 1124 | G    | N3-C2-N2    | 5.05  | 123.44      | 119.90   |
| 1   | AA    | 1300 | G    | O4'-C1'-N9  | 5.05  | 112.24      | 108.20   |
| 27  | B8    | 791  | C    | N3-C4-N4    | 5.05  | 121.54      | 118.00   |
| 27  | B8    | 1047 | G    | N3-C2-N2    | 5.05  | 123.44      | 119.90   |
| 27  | B8    | 2880 | C    | N3-C4-C5    | -5.05 | 119.88      | 121.90   |
| 27  | B8    | 556  | A    | C5-C6-N1    | -5.05 | 115.17      | 117.70   |
| 27  | B8    | 892  | A    | C5-C6-N1    | -5.05 | 115.17      | 117.70   |
| 27  | B8    | 1814 | G    | N3-C2-N2    | 5.05  | 123.44      | 119.90   |
| 27  | B8    | 2452 | C    | N3-C4-C5    | -5.05 | 119.88      | 121.90   |
| 27  | B8    | 1021 | A    | C5-C6-N1    | -5.05 | 115.17      | 117.70   |
| 27  | B8    | 1508 | A    | C5-C6-N1    | -5.05 | 115.17      | 117.70   |
| 27  | B8    | 1848 | A    | C5-C6-N6    | -5.05 | 119.66      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 2379 | G    | O4'-C1'-N9 | 5.05  | 112.24      | 108.20   |
| 1   | AA    | 329  | A    | C5-C6-N6   | -5.05 | 119.66      | 123.70   |
| 1   | AA    | 1447 | A    | O4'-C1'-N9 | 5.05  | 112.24      | 108.20   |
| 27  | B8    | 1030 | C    | N3-C4-C5   | -5.05 | 119.88      | 121.90   |
| 27  | B8    | 2197 | U    | P-O3'-C3'  | 5.05  | 125.76      | 119.70   |
| 27  | B8    | 2676 | C    | N3-C4-C5   | -5.05 | 119.88      | 121.90   |
| 1   | AA    | 120  | A    | C5-C6-N1   | -5.05 | 115.18      | 117.70   |
| 27  | B8    | 654  | A    | C5-C6-N1   | -5.05 | 115.18      | 117.70   |
| 27  | B8    | 1266 | G    | P-O3'-C3'  | 5.05  | 125.76      | 119.70   |
| 27  | B8    | 1575 | C    | N3-C4-C5   | -5.05 | 119.88      | 121.90   |
| 27  | B8    | 1654 | A    | O4'-C1'-N9 | 5.05  | 112.24      | 108.20   |
| 27  | B8    | 2154 | A    | O4'-C1'-N9 | 5.05  | 112.24      | 108.20   |
| 27  | B8    | 2559 | C    | N3-C4-C5   | -5.05 | 119.88      | 121.90   |
| 1   | AA    | 26   | A    | O4'-C1'-N9 | 5.05  | 112.24      | 108.20   |
| 1   | AA    | 43   | C    | N3-C4-C5   | -5.05 | 119.88      | 121.90   |
| 1   | AA    | 169  | C    | N3-C4-N4   | 5.05  | 121.53      | 118.00   |
| 1   | AA    | 345  | C    | N3-C4-N4   | 5.05  | 121.53      | 118.00   |
| 1   | AA    | 554  | A    | C5-C6-N6   | -5.05 | 119.66      | 123.70   |
| 1   | AA    | 738  | C    | N3-C4-C5   | -5.05 | 119.88      | 121.90   |
| 1   | AA    | 1125 | U    | O4'-C1'-N1 | 5.05  | 112.24      | 108.20   |
| 27  | B8    | 127  | A    | O4'-C1'-N9 | 5.05  | 112.24      | 108.20   |
| 27  | B8    | 345  | A    | C5-C6-N1   | -5.05 | 115.18      | 117.70   |
| 27  | B8    | 1612 | C    | N3-C4-C5   | -5.05 | 119.88      | 121.90   |
| 27  | B8    | 2567 | G    | O4'-C1'-N9 | 5.05  | 112.24      | 108.20   |
| 27  | B8    | 2589 | A    | O4'-C1'-N9 | 5.05  | 112.24      | 108.20   |
| 27  | B8    | 1282 | U    | P-O3'-C3'  | 5.04  | 125.75      | 119.70   |
| 27  | B8    | 1919 | A    | O4'-C1'-N9 | 5.04  | 112.24      | 108.20   |
| 27  | B8    | 2199 | A    | O4'-C1'-N9 | 5.04  | 112.24      | 108.20   |
| 1   | AA    | 1012 | A    | O4'-C1'-N9 | 5.04  | 112.23      | 108.20   |
| 1   | AA    | 1289 | A    | C5-C6-N1   | -5.04 | 115.18      | 117.70   |
| 27  | B8    | 933  | A    | C5-C6-N6   | -5.04 | 119.67      | 123.70   |
| 1   | AA    | 1263 | C    | N3-C4-C5   | -5.04 | 119.88      | 121.90   |
| 27  | B8    | 103  | A    | C5-C6-N6   | -5.04 | 119.67      | 123.70   |
| 27  | B8    | 927  | A    | C5-C6-N1   | -5.04 | 115.18      | 117.70   |
| 27  | B8    | 1393 | A    | C5-C6-N6   | -5.04 | 119.67      | 123.70   |
| 27  | B8    | 1494 | A    | C5-C6-N6   | -5.04 | 119.67      | 123.70   |
| 27  | B8    | 1656 | C    | N3-C4-C5   | -5.04 | 119.88      | 121.90   |
| 27  | B8    | 1919 | A    | C5-C6-N1   | -5.04 | 115.18      | 117.70   |
| 27  | B8    | 2054 | A    | C5-C6-N6   | -5.04 | 119.67      | 123.70   |
| 27  | B8    | 2283 | C    | N3-C4-C5   | -5.04 | 119.88      | 121.90   |
| 27  | B8    | 2433 | A    | O4'-C1'-N9 | 5.04  | 112.23      | 108.20   |
| 27  | B8    | 2886 | A    | C5-C6-N1   | -5.04 | 115.18      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | AA    | 251  | G    | O4'-C1'-N9 | 5.04  | 112.23      | 108.20   |
| 1   | AA    | 1124 | G    | O4'-C1'-N9 | 5.04  | 112.23      | 108.20   |
| 1   | AA    | 1166 | G    | O4'-C1'-N9 | 5.04  | 112.23      | 108.20   |
| 27  | B8    | 1177 | G    | O4'-C1'-N9 | 5.04  | 112.23      | 108.20   |
| 27  | B8    | 2366 | A    | C5-C6-N1   | -5.04 | 115.18      | 117.70   |
| 1   | AA    | 129  | A    | C5-C6-N6   | -5.04 | 119.67      | 123.70   |
| 1   | AA    | 690  | G    | N3-C2-N2   | 5.04  | 123.43      | 119.90   |
| 1   | AA    | 1357 | A    | C5-C6-N1   | -5.04 | 115.18      | 117.70   |
| 27  | B8    | 181  | A    | C5-C6-N6   | -5.04 | 119.67      | 123.70   |
| 27  | B8    | 787  | C    | N3-C4-C5   | -5.04 | 119.89      | 121.90   |
| 27  | B8    | 1691 | C    | N3-C4-C5   | -5.04 | 119.89      | 121.90   |
| 27  | B8    | 2006 | C    | N3-C4-C5   | -5.04 | 119.89      | 121.90   |
| 27  | B8    | 2014 | A    | C5-C6-N6   | -5.04 | 119.67      | 123.70   |
| 27  | B8    | 2767 | C    | N3-C4-C5   | -5.04 | 119.89      | 121.90   |
| 27  | B8    | 2879 | A    | O4'-C1'-N9 | 5.04  | 112.23      | 108.20   |
| 40  | BL    | 113  | ALA  | N-CA-CB    | 5.04  | 117.15      | 110.10   |
| 1   | AA    | 687  | A    | C5-C6-N1   | -5.04 | 115.18      | 117.70   |
| 1   | AA    | 766  | A    | C5-C6-N6   | -5.04 | 119.67      | 123.70   |
| 1   | AA    | 1256 | A    | C5-C6-N1   | -5.04 | 115.18      | 117.70   |
| 27  | B8    | 972  | A    | O4'-C1'-N9 | 5.04  | 112.23      | 108.20   |
| 27  | B8    | 1652 | A    | C5-C6-N6   | -5.04 | 119.67      | 123.70   |
| 1   | AA    | 183  | C    | C6-N1-C1'  | -5.04 | 114.76      | 120.80   |
| 1   | AA    | 784  | A    | O4'-C1'-N9 | 5.04  | 112.23      | 108.20   |
| 26  | B7    | 71   | C    | N3-C4-C5   | -5.04 | 119.89      | 121.90   |
| 27  | B8    | 279  | A    | C5-C6-N6   | -5.04 | 119.67      | 123.70   |
| 27  | B8    | 975  | A    | C5-C6-N6   | -5.04 | 119.67      | 123.70   |
| 27  | B8    | 2052 | A    | C5-C6-N6   | -5.04 | 119.67      | 123.70   |
| 1   | AA    | 77   | A    | C5-C6-N1   | -5.03 | 115.18      | 117.70   |
| 1   | AA    | 130  | A    | C5-C6-N1   | -5.03 | 115.18      | 117.70   |
| 1   | AA    | 281  | G    | N3-C2-N2   | 5.03  | 123.42      | 119.90   |
| 1   | AA    | 483  | C    | O4'-C1'-N1 | 5.03  | 112.23      | 108.20   |
| 1   | AA    | 883  | C    | N3-C4-C5   | -5.03 | 119.89      | 121.90   |
| 27  | B8    | 886  | A    | C5-C6-N6   | -5.03 | 119.67      | 123.70   |
| 1   | AA    | 1292 | G    | O4'-C1'-N9 | 5.03  | 112.22      | 108.20   |
| 27  | B8    | 791  | C    | N3-C4-C5   | -5.03 | 119.89      | 121.90   |
| 1   | AA    | 194  | C    | N3-C4-C5   | -5.03 | 119.89      | 121.90   |
| 1   | AA    | 370  | C    | N3-C4-N4   | 5.03  | 121.52      | 118.00   |
| 1   | AA    | 400  | C    | N3-C4-C5   | -5.03 | 119.89      | 121.90   |
| 1   | AA    | 511  | C    | N3-C4-C5   | -5.03 | 119.89      | 121.90   |
| 1   | AA    | 914  | A    | C5-C6-N1   | -5.03 | 115.19      | 117.70   |
| 1   | AA    | 1219 | A    | C5-C6-N1   | -5.03 | 115.18      | 117.70   |
| 26  | B7    | 59   | A    | C5-C6-N1   | -5.03 | 115.19      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | B8    | 394  | C    | N3-C4-C5    | -5.03 | 119.89      | 121.90   |
| 27  | B8    | 1492 | G    | O4'-C1'-N9  | 5.03  | 112.22      | 108.20   |
| 27  | B8    | 1785 | A    | C5-C6-N1    | -5.03 | 115.19      | 117.70   |
| 1   | AA    | 495  | A    | P-O3'-C3'   | 5.03  | 125.73      | 119.70   |
| 1   | AA    | 860  | A    | C5-C6-N6    | -5.03 | 119.68      | 123.70   |
| 1   | AA    | 914  | A    | C5-C6-N6    | -5.03 | 119.68      | 123.70   |
| 27  | B8    | 478  | A    | O4'-C1'-N9  | 5.03  | 112.22      | 108.20   |
| 27  | B8    | 2250 | G    | O4'-C1'-N9  | 5.03  | 112.22      | 108.20   |
| 1   | AA    | 618  | C    | N3-C4-N4    | 5.03  | 121.52      | 118.00   |
| 26  | B7    | 26   | C    | N3-C4-C5    | -5.03 | 119.89      | 121.90   |
| 26  | B7    | 72   | G    | O4'-C1'-N9  | 5.03  | 112.22      | 108.20   |
| 27  | B8    | 5    | A    | C5-C6-N1    | -5.03 | 115.19      | 117.70   |
| 27  | B8    | 1093 | G    | N3-C2-N2    | 5.03  | 123.42      | 119.90   |
| 27  | B8    | 1728 | C    | N3-C4-C5    | -5.03 | 119.89      | 121.90   |
| 27  | B8    | 1771 | C    | N3-C4-C5    | -5.03 | 119.89      | 121.90   |
| 27  | B8    | 1802 | A    | C5-C6-N6    | -5.03 | 119.68      | 123.70   |
| 27  | B8    | 2304 | G    | O4'-C1'-N9  | 5.03  | 112.22      | 108.20   |
| 26  | B7    | 107  | G    | C5'-C4'-O4' | 5.03  | 115.13      | 109.10   |
| 27  | B8    | 422  | A    | C5-C6-N1    | -5.03 | 115.19      | 117.70   |
| 27  | B8    | 858  | G    | N3-C2-N2    | 5.03  | 123.42      | 119.90   |
| 27  | B8    | 1032 | A    | C5-C6-N6    | -5.03 | 119.68      | 123.70   |
| 27  | B8    | 2140 | G    | O4'-C1'-N9  | 5.03  | 112.22      | 108.20   |
| 27  | B8    | 2700 | A    | C5-C6-N1    | -5.03 | 115.19      | 117.70   |
| 1   | AA    | 370  | C    | N3-C4-C5    | -5.02 | 119.89      | 121.90   |
| 27  | B8    | 486  | C    | N3-C4-C5    | -5.02 | 119.89      | 121.90   |
| 27  | B8    | 911  | A    | C5-C6-N1    | -5.02 | 115.19      | 117.70   |
| 27  | B8    | 1230 | A    | C5-C6-N1    | -5.02 | 115.19      | 117.70   |
| 27  | B8    | 2108 | A    | C5-C6-N6    | -5.02 | 119.68      | 123.70   |
| 1   | AA    | 65   | A    | O4'-C1'-N9  | 5.02  | 112.22      | 108.20   |
| 1   | AA    | 393  | A    | O4'-C1'-N9  | 5.02  | 112.22      | 108.20   |
| 1   | AA    | 1225 | A    | C5-C6-N6    | -5.02 | 119.68      | 123.70   |
| 27  | B8    | 335  | C    | N3-C4-C5    | -5.02 | 119.89      | 121.90   |
| 27  | B8    | 602  | A    | C5-C6-N1    | -5.02 | 115.19      | 117.70   |
| 27  | B8    | 1830 | C    | N3-C4-C5    | -5.02 | 119.89      | 121.90   |
| 27  | B8    | 2278 | A    | O4'-C1'-N9  | 5.02  | 112.22      | 108.20   |
| 27  | B8    | 2538 | C    | N3-C4-C5    | -5.02 | 119.89      | 121.90   |
| 1   | AA    | 274  | A    | C5-C6-N1    | -5.02 | 115.19      | 117.70   |
| 1   | AA    | 1246 | A    | C5-C6-N6    | -5.02 | 119.68      | 123.70   |
| 27  | B8    | 157  | C    | N3-C4-C5    | -5.02 | 119.89      | 121.90   |
| 27  | B8    | 247  | G    | N3-C2-N2    | 5.02  | 123.42      | 119.90   |
| 27  | B8    | 2032 | G    | O4'-C1'-N9  | 5.02  | 112.22      | 108.20   |
| 3   | AV    | 23   | G    | O4'-C1'-N9  | 5.02  | 112.22      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | AV    | 33   | A    | C5-C6-N1   | -5.02 | 115.19      | 117.70   |
| 26  | B7    | 97   | C    | N3-C4-C5   | -5.02 | 119.89      | 121.90   |
| 27  | B8    | 244  | A    | C5-C6-N6   | -5.02 | 119.68      | 123.70   |
| 27  | B8    | 435  | C    | N3-C4-N4   | 5.02  | 121.51      | 118.00   |
| 27  | B8    | 781  | A    | C5-C6-N6   | -5.02 | 119.69      | 123.70   |
| 27  | B8    | 816  | C    | N3-C4-C5   | -5.02 | 119.89      | 121.90   |
| 27  | B8    | 1284 | A    | C5-C6-N1   | -5.02 | 115.19      | 117.70   |
| 27  | B8    | 1635 | A    | O4'-C1'-N9 | 5.02  | 112.22      | 108.20   |
| 27  | B8    | 2645 | G    | O4'-C1'-N9 | 5.02  | 112.22      | 108.20   |
| 27  | B8    | 228  | C    | N3-C4-C5   | -5.02 | 119.89      | 121.90   |
| 1   | AA    | 586  | C    | N3-C4-C5   | -5.02 | 119.89      | 121.90   |
| 27  | B8    | 654  | A    | C5-C6-N6   | -5.02 | 119.69      | 123.70   |
| 27  | B8    | 1565 | C    | N3-C4-C5   | -5.02 | 119.89      | 121.90   |
| 27  | B8    | 2349 | G    | C5-C6-O6   | -5.02 | 125.59      | 128.60   |
| 1   | AA    | 221  | C    | N3-C4-C5   | -5.01 | 119.89      | 121.90   |
| 1   | AA    | 316  | C    | N3-C4-C5   | -5.01 | 119.89      | 121.90   |
| 1   | AA    | 583  | A    | C5-C6-N1   | -5.01 | 115.19      | 117.70   |
| 1   | AA    | 1170 | A    | C5-C6-N1   | -5.01 | 115.19      | 117.70   |
| 27  | B8    | 301  | G    | P-O3'-C3'  | 5.01  | 125.72      | 119.70   |
| 27  | B8    | 548  | G    | O4'-C1'-N9 | 5.01  | 112.21      | 108.20   |
| 27  | B8    | 800  | A    | C5-C6-N6   | -5.01 | 119.69      | 123.70   |
| 27  | B8    | 936  | A    | O4'-C1'-N9 | 5.01  | 112.21      | 108.20   |
| 27  | B8    | 1029 | A    | O4'-C1'-N9 | 5.01  | 112.21      | 108.20   |
| 27  | B8    | 1335 | C    | N3-C4-C5   | -5.01 | 119.89      | 121.90   |
| 27  | B8    | 2050 | C    | N3-C4-C5   | -5.01 | 119.89      | 121.90   |
| 1   | AA    | 939  | G    | O4'-C1'-N9 | 5.01  | 112.21      | 108.20   |
| 27  | B8    | 2501 | C    | N3-C4-C5   | -5.01 | 119.89      | 121.90   |
| 1   | AA    | 83   | C    | N3-C4-C5   | -5.01 | 119.89      | 121.90   |
| 1   | AA    | 152  | A    | O4'-C1'-N9 | 5.01  | 112.21      | 108.20   |
| 1   | AA    | 1329 | A    | C5-C6-N6   | -5.01 | 119.69      | 123.70   |
| 27  | B8    | 1526 | C    | N3-C4-C5   | -5.01 | 119.89      | 121.90   |
| 27  | B8    | 1972 | G    | O4'-C1'-N9 | 5.01  | 112.21      | 108.20   |
| 27  | B8    | 240  | C    | N3-C4-C5   | -5.01 | 119.90      | 121.90   |
| 27  | B8    | 722  | A    | C5-C6-N1   | -5.01 | 115.19      | 117.70   |
| 27  | B8    | 1329 | U    | O4'-C1'-N1 | 5.01  | 112.21      | 108.20   |
| 27  | B8    | 2657 | A    | O4'-C1'-N9 | 5.01  | 112.21      | 108.20   |
| 1   | AA    | 232  | G    | N3-C2-N2   | 5.01  | 123.41      | 119.90   |
| 27  | B8    | 1027 | A    | O4'-C1'-N9 | 5.01  | 112.21      | 108.20   |
| 27  | B8    | 1469 | A    | C5-C6-N6   | -5.01 | 119.69      | 123.70   |
| 27  | B8    | 1828 | G    | O4'-C1'-N9 | 5.01  | 112.21      | 108.20   |
| 27  | B8    | 2740 | A    | C5-C6-N1   | -5.01 | 115.20      | 117.70   |
| 27  | B8    | 116  | C    | N3-C4-N4   | 5.01  | 121.50      | 118.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 27  | B8    | 249  | C    | N3-C4-N4   | 5.01  | 121.50      | 118.00   |
| 27  | B8    | 582  | A    | C5-C6-N1   | -5.01 | 115.20      | 117.70   |
| 27  | B8    | 883  | G    | O4'-C1'-N9 | 5.01  | 112.20      | 108.20   |
| 27  | B8    | 912  | C    | N3-C4-C5   | -5.01 | 119.90      | 121.90   |
| 27  | B8    | 1997 | C    | N3-C4-C5   | -5.01 | 119.90      | 121.90   |
| 27  | B8    | 2232 | C    | N3-C4-C5   | -5.01 | 119.90      | 121.90   |
| 27  | B8    | 2782 | G    | O4'-C1'-N9 | 5.01  | 112.21      | 108.20   |
| 27  | B8    | 2860 | A    | O4'-C1'-N9 | 5.01  | 112.20      | 108.20   |
| 1   | AA    | 349  | A    | O4'-C1'-N9 | 5.00  | 112.20      | 108.20   |
| 1   | AA    | 1249 | C    | N3-C4-C5   | -5.00 | 119.90      | 121.90   |
| 27  | B8    | 532  | A    | C5-C6-N1   | -5.00 | 115.20      | 117.70   |
| 27  | B8    | 2338 | C    | N3-C4-C5   | -5.00 | 119.90      | 121.90   |
| 27  | B8    | 2614 | A    | C5-C6-N1   | -5.00 | 115.20      | 117.70   |
| 27  | B8    | 2750 | A    | O4'-C1'-N9 | 5.00  | 112.20      | 108.20   |
| 1   | AA    | 782  | A    | C5-C6-N1   | -5.00 | 115.20      | 117.70   |
| 27  | B8    | 299  | A    | O4'-C1'-N9 | 5.00  | 112.20      | 108.20   |
| 27  | B8    | 1155 | A    | O4'-C1'-N9 | 5.00  | 112.20      | 108.20   |
| 27  | B8    | 1743 | G    | O4'-C1'-N9 | 5.00  | 112.20      | 108.20   |
| 27  | B8    | 2474 | U    | C2-N1-C1'  | 5.00  | 123.70      | 117.70   |
| 27  | B8    | 2901 | C    | N3-C4-C5   | -5.00 | 119.90      | 121.90   |
| 1   | AA    | 386  | C    | N3-C4-C5   | -5.00 | 119.90      | 121.90   |
| 1   | AA    | 578  | C    | N3-C4-C5   | -5.00 | 119.90      | 121.90   |
| 1   | AA    | 1142 | G    | N1-C6-O6   | 5.00  | 122.90      | 119.90   |
| 27  | B8    | 423  | A    | C5-C6-N1   | -5.00 | 115.20      | 117.70   |
| 27  | B8    | 758  | C    | N3-C4-C5   | -5.00 | 119.90      | 121.90   |
| 27  | B8    | 2263 | C    | N3-C4-C5   | -5.00 | 119.90      | 121.90   |
| 27  | B8    | 2298 | A    | C5-C6-N6   | -5.00 | 119.70      | 123.70   |
| 27  | B8    | 2319 | G    | O4'-C1'-N9 | 5.00  | 112.20      | 108.20   |

There are no chirality outliers.

All (189) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 5   | A1    | 237  | THR  | Peptide   |
| 1   | AA    | 102  | G    | Sidechain |
| 1   | AA    | 1024 | G    | Sidechain |
| 1   | AA    | 1027 | C    | Sidechain |
| 1   | AA    | 1044 | A    | Sidechain |
| 1   | AA    | 1094 | G    | Sidechain |
| 1   | AA    | 1095 | U    | Sidechain |
| 1   | AA    | 1101 | A    | Sidechain |
| 1   | AA    | 1125 | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 1129 | C    | Sidechain |
| 1   | AA    | 1131 | G    | Sidechain |
| 1   | AA    | 1139 | G    | Sidechain |
| 1   | AA    | 1144 | G    | Sidechain |
| 1   | AA    | 115  | G    | Sidechain |
| 1   | AA    | 1179 | A    | Sidechain |
| 1   | AA    | 1226 | C    | Sidechain |
| 1   | AA    | 1268 | G    | Sidechain |
| 1   | AA    | 1269 | A    | Sidechain |
| 1   | AA    | 1289 | A    | Sidechain |
| 1   | AA    | 1299 | A    | Sidechain |
| 1   | AA    | 13   | U    | Sidechain |
| 1   | AA    | 130  | A    | Sidechain |
| 1   | AA    | 1323 | G    | Sidechain |
| 1   | AA    | 1346 | A    | Sidechain |
| 1   | AA    | 1347 | G    | Sidechain |
| 1   | AA    | 1417 | G    | Sidechain |
| 1   | AA    | 1418 | A    | Sidechain |
| 1   | AA    | 1465 | A    | Sidechain |
| 1   | AA    | 1502 | A    | Sidechain |
| 1   | AA    | 1516 | G    | Sidechain |
| 1   | AA    | 152  | A    | Sidechain |
| 1   | AA    | 1526 | G    | Sidechain |
| 1   | AA    | 1529 | G    | Sidechain |
| 1   | AA    | 173  | U    | Sidechain |
| 1   | AA    | 180  | U    | Sidechain |
| 1   | AA    | 181  | A    | Sidechain |
| 1   | AA    | 184  | G    | Sidechain |
| 1   | AA    | 185  | U    | Sidechain |
| 1   | AA    | 202  | G    | Sidechain |
| 1   | AA    | 204  | G    | Sidechain |
| 1   | AA    | 244  | U    | Sidechain |
| 1   | AA    | 262  | A    | Sidechain |
| 1   | AA    | 265  | G    | Sidechain |
| 1   | AA    | 298  | A    | Sidechain |
| 1   | AA    | 315  | A    | Sidechain |
| 1   | AA    | 353  | A    | Sidechain |
| 1   | AA    | 378  | G    | Sidechain |
| 1   | AA    | 380  | G    | Sidechain |
| 1   | AA    | 439  | U    | Sidechain |
| 1   | AA    | 450  | G    | Sidechain |
| 1   | AA    | 454  | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | AA    | 496  | A    | Sidechain |
| 1   | AA    | 527  | G    | Sidechain |
| 1   | AA    | 557  | G    | Sidechain |
| 1   | AA    | 565  | U    | Sidechain |
| 1   | AA    | 566  | G    | Sidechain |
| 1   | AA    | 581  | G    | Sidechain |
| 1   | AA    | 587  | G    | Sidechain |
| 1   | AA    | 588  | G    | Sidechain |
| 1   | AA    | 620  | C    | Sidechain |
| 1   | AA    | 622  | A    | Sidechain |
| 1   | AA    | 69   | G    | Sidechain |
| 1   | AA    | 718  | A    | Sidechain |
| 1   | AA    | 728  | A    | Sidechain |
| 1   | AA    | 752  | G    | Sidechain |
| 1   | AA    | 874  | G    | Sidechain |
| 1   | AA    | 883  | C    | Sidechain |
| 1   | AA    | 884  | U    | Sidechain |
| 1   | AA    | 927  | G    | Sidechain |
| 1   | AA    | 95   | C    | Sidechain |
| 1   | AA    | 960  | U    | Sidechain |
| 1   | AA    | 974  | A    | Sidechain |
| 1   | AA    | 978  | A    | Sidechain |
| 7   | AC    | 218  | LYS  | Peptide   |
| 12  | AH    | 14   | ARG  | Sidechain |
| 13  | AI    | 6    | TYR  | Sidechain |
| 3   | AV    | 53   | G    | Sidechain |
| 3   | AV    | 7    | G    | Sidechain |
| 57  | B2    | 12   | ARG  | Sidechain |
| 26  | B7    | 111  | U    | Sidechain |
| 26  | B7    | 5    | U    | Sidechain |
| 27  | B8    | 1025 | G    | Sidechain |
| 27  | B8    | 1027 | A    | Sidechain |
| 27  | B8    | 1070 | A    | Sidechain |
| 27  | B8    | 1084 | A    | Sidechain |
| 27  | B8    | 1095 | A    | Sidechain |
| 27  | B8    | 1099 | G    | Sidechain |
| 27  | B8    | 1130 | U    | Sidechain |
| 27  | B8    | 1138 | G    | Sidechain |
| 27  | B8    | 120  | U    | Sidechain |
| 27  | B8    | 1204 | A    | Sidechain |
| 27  | B8    | 1224 | U    | Sidechain |
| 27  | B8    | 1235 | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 27  | B8    | 1236 | G    | Sidechain |
| 27  | B8    | 1296 | G    | Sidechain |
| 27  | B8    | 1327 | A    | Sidechain |
| 27  | B8    | 1334 | G    | Sidechain |
| 27  | B8    | 1360 | G    | Sidechain |
| 27  | B8    | 1383 | A    | Sidechain |
| 27  | B8    | 1394 | U    | Sidechain |
| 27  | B8    | 1427 | A    | Sidechain |
| 27  | B8    | 1515 | A    | Sidechain |
| 27  | B8    | 1517 | G    | Sidechain |
| 27  | B8    | 1530 | G    | Sidechain |
| 27  | B8    | 1573 | G    | Sidechain |
| 27  | B8    | 161  | A    | Sidechain |
| 27  | B8    | 1672 | A    | Sidechain |
| 27  | B8    | 1680 | U    | Sidechain |
| 27  | B8    | 1682 | G    | Sidechain |
| 27  | B8    | 1699 | G    | Sidechain |
| 27  | B8    | 1738 | G    | Sidechain |
| 27  | B8    | 1743 | G    | Sidechain |
| 27  | B8    | 1784 | A    | Sidechain |
| 27  | B8    | 1813 | G    | Sidechain |
| 27  | B8    | 1846 | G    | Sidechain |
| 27  | B8    | 1904 | G    | Sidechain |
| 27  | B8    | 1920 | C    | Sidechain |
| 27  | B8    | 1927 | A    | Sidechain |
| 27  | B8    | 1952 | A    | Sidechain |
| 27  | B8    | 1954 | G    | Sidechain |
| 27  | B8    | 2005 | A    | Sidechain |
| 27  | B8    | 205  | G    | Sidechain |
| 27  | B8    | 2125 | G    | Sidechain |
| 27  | B8    | 2143 | C    | Sidechain |
| 27  | B8    | 2148 | G    | Sidechain |
| 27  | B8    | 2155 | U    | Sidechain |
| 27  | B8    | 2272 | U    | Sidechain |
| 27  | B8    | 2345 | G    | Sidechain |
| 27  | B8    | 2365 | G    | Sidechain |
| 27  | B8    | 2382 | G    | Sidechain |
| 27  | B8    | 2460 | U    | Sidechain |
| 27  | B8    | 2471 | A    | Sidechain |
| 27  | B8    | 250  | G    | Sidechain |
| 27  | B8    | 2517 | C    | Sidechain |
| 27  | B8    | 2580 | U    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 27  | B8    | 2596 | U    | Sidechain |
| 27  | B8    | 261  | G    | Sidechain |
| 27  | B8    | 2637 | U    | Sidechain |
| 27  | B8    | 265  | A    | Sidechain |
| 27  | B8    | 2689 | U    | Sidechain |
| 27  | B8    | 27   | G    | Sidechain |
| 27  | B8    | 2746 | U    | Sidechain |
| 27  | B8    | 2756 | U    | Sidechain |
| 27  | B8    | 2857 | G    | Sidechain |
| 27  | B8    | 2858 | C    | Sidechain |
| 27  | B8    | 2866 | U    | Sidechain |
| 27  | B8    | 2903 | U    | Sidechain |
| 27  | B8    | 303  | G    | Sidechain |
| 27  | B8    | 346  | A    | Sidechain |
| 27  | B8    | 362  | A    | Sidechain |
| 27  | B8    | 370  | G    | Sidechain |
| 27  | B8    | 395  | U    | Sidechain |
| 27  | B8    | 428  | A    | Sidechain |
| 27  | B8    | 445  | C    | Sidechain |
| 27  | B8    | 446  | G    | Sidechain |
| 27  | B8    | 457  | A    | Sidechain |
| 27  | B8    | 467  | G    | Sidechain |
| 27  | B8    | 480  | A    | Sidechain |
| 27  | B8    | 505  | A    | Sidechain |
| 27  | B8    | 507  | A    | Sidechain |
| 27  | B8    | 532  | A    | Sidechain |
| 27  | B8    | 569  | U    | Sidechain |
| 27  | B8    | 60   | G    | Sidechain |
| 27  | B8    | 630  | G    | Sidechain |
| 27  | B8    | 642  | U    | Sidechain |
| 27  | B8    | 674  | G    | Sidechain |
| 27  | B8    | 675  | A    | Sidechain |
| 27  | B8    | 676  | A    | Sidechain |
| 27  | B8    | 684  | G    | Sidechain |
| 27  | B8    | 705  | A    | Sidechain |
| 27  | B8    | 712  | G    | Sidechain |
| 27  | B8    | 72   | U    | Sidechain |
| 27  | B8    | 728  | G    | Sidechain |
| 27  | B8    | 738  | G    | Sidechain |
| 27  | B8    | 773  | U    | Sidechain |
| 27  | B8    | 821  | A    | Sidechain |
| 27  | B8    | 849  | A    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 27  | B8    | 858 | G    | Sidechain |
| 27  | B8    | 877 | A    | Sidechain |
| 27  | B8    | 899 | A    | Sidechain |
| 27  | B8    | 959 | A    | Sidechain |
| 28  | BA    | 181 | ARG  | Peptide   |
| 28  | BA    | 198 | GLY  | Peptide   |
| 28  | BA    | 293 | TRP  | Peptide   |
| 28  | BA    | 314 | GLN  | Peptide   |
| 28  | BA    | 72  | LEU  | Peptide   |
| 34  | BF    | 137 | PHE  | Peptide   |
| 36  | BH    | 31  | VAL  | Peptide   |
| 49  | BU    | 48  | VAL  | 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    | 33080 | 0        | 16649    | 21      | 0            |
| 2   | AX    | 231   | 0        | 120      | 0       | 0            |
| 3   | AV    | 1649  | 0        | 834      | 1       | 0            |
| 4   | AZ    | 779   | 0        | 798      | 4       | 0            |
| 5   | A0    | 1640  | 0        | 1641     | 0       | 0            |
| 5   | A1    | 1640  | 0        | 1641     | 0       | 0            |
| 6   | AB    | 1872  | 0        | 1885     | 3       | 0            |
| 7   | AC    | 1822  | 0        | 1913     | 2       | 0            |
| 8   | AD    | 1643  | 0        | 1710     | 1       | 0            |
| 9   | AE    | 1225  | 0        | 1273     | 1       | 0            |
| 10  | AF    | 1101  | 0        | 1050     | 1       | 0            |
| 11  | AG    | 1400  | 0        | 1449     | 0       | 0            |
| 12  | AH    | 979   | 0        | 1034     | 1       | 0            |
| 13  | AI    | 1036  | 0        | 1084     | 0       | 0            |
| 14  | AJ    | 825   | 0        | 865      | 2       | 0            |
| 15  | AK    | 965   | 0        | 997      | 0       | 0            |
| 16  | AL    | 955   | 0        | 1019     | 2       | 0            |
| 17  | AM    | 910   | 0        | 981      | 0       | 0            |
| 18  | AN    | 805   | 0        | 847      | 1       | 0            |
| 19  | AO    | 716   | 0        | 742      | 0       | 0            |
| 20  | AP    | 649   | 0        | 666      | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 21  | AQ    | 672   | 0        | 716      | 1       | 0            |
| 22  | AR    | 626   | 0        | 651      | 0       | 0            |
| 23  | AS    | 727   | 0        | 769      | 0       | 0            |
| 24  | AT    | 670   | 0        | 722      | 2       | 0            |
| 25  | AU    | 590   | 0        | 631      | 1       | 0            |
| 26  | B7    | 2570  | 0        | 1301     | 0       | 0            |
| 27  | B8    | 62341 | 0        | 31354    | 41      | 0            |
| 28  | BA    | 3362  | 0        | 3511     | 38      | 0            |
| 29  | BB    | 889   | 0        | 982      | 1       | 0            |
| 30  | B5    | 1733  | 0        | 1824     | 1       | 0            |
| 31  | B6    | 2092  | 0        | 2170     | 2       | 0            |
| 32  | BD    | 1565  | 0        | 1616     | 1       | 0            |
| 33  | BE    | 1552  | 0        | 1619     | 1       | 0            |
| 34  | BF    | 1420  | 0        | 1460     | 1       | 0            |
| 35  | BG    | 1323  | 0        | 1374     | 0       | 0            |
| 36  | BH    | 1111  | 0        | 1148     | 2       | 0            |
| 37  | BI    | 1032  | 0        | 1088     | 0       | 0            |
| 38  | BJ    | 1129  | 0        | 1162     | 0       | 0            |
| 39  | BK    | 947   | 0        | 1023     | 0       | 0            |
| 40  | BL    | 1053  | 0        | 1129     | 1       | 0            |
| 41  | BM    | 1074  | 0        | 1157     | 1       | 0            |
| 42  | BN    | 1008  | 0        | 1045     | 1       | 0            |
| 43  | BO    | 900   | 0        | 935      | 0       | 0            |
| 44  | BP    | 917   | 0        | 965      | 0       | 0            |
| 45  | BQ    | 947   | 0        | 1022     | 0       | 0            |
| 46  | BR    | 816   | 0        | 839      | 1       | 0            |
| 47  | BS    | 857   | 0        | 922      | 0       | 0            |
| 48  | BT    | 787   | 0        | 846      | 0       | 0            |
| 49  | BU    | 789   | 0        | 847      | 0       | 0            |
| 50  | BV    | 753   | 0        | 780      | 0       | 0            |
| 51  | BW    | 634   | 0        | 656      | 0       | 0            |
| 52  | BX    | 625   | 0        | 655      | 0       | 0            |
| 53  | BY    | 509   | 0        | 543      | 0       | 0            |
| 54  | BZ    | 449   | 0        | 491      | 0       | 0            |
| 55  | B0    | 444   | 0        | 461      | 0       | 0            |
| 56  | B1    | 441   | 0        | 485      | 2       | 0            |
| 57  | B2    | 377   | 0        | 418      | 1       | 0            |
| 58  | B3    | 504   | 0        | 574      | 1       | 0            |
| 59  | B4    | 302   | 0        | 343      | 0       | 0            |
| 60  | A0    | 1078  | 0        | 1694     | 1       | 0            |
| 60  | A1    | 1225  | 0        | 1925     | 4       | 0            |
| 60  | AZ    | 245   | 0        | 385      | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 60  | B8    | 294    | 0        | 462      | 2       | 0            |
| 60  | BA    | 1568   | 0        | 2464     | 34      | 0            |
| 60  | BB    | 539    | 0        | 847      | 0       | 0            |
| 61  | A0    | 510    | 0        | 760      | 0       | 0            |
| 61  | A1    | 204    | 0        | 304      | 2       | 0            |
| 61  | AZ    | 102    | 0        | 152      | 0       | 0            |
| 61  | B8    | 51     | 0        | 76       | 0       | 0            |
| 61  | BA    | 408    | 0        | 608      | 1       | 0            |
| 61  | BB    | 357    | 0        | 532      | 0       | 0            |
| All | All   | 163040 | 0        | 119641   | 141     | 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 0.

All (141) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:BA:416:PHE:CE1 | 28:BA:416:PHE:CD1  | 1.92                     | 1.58              |
| 28:BA:416:PHE:CD2 | 28:BA:416:PHE:CE2  | 1.95                     | 1.54              |
| 28:BA:416:PHE:CZ  | 28:BA:416:PHE:CE2  | 1.95                     | 1.53              |
| 28:BA:416:PHE:CE1 | 28:BA:416:PHE:CZ   | 1.95                     | 1.51              |
| 28:BA:416:PHE:CD1 | 28:BA:416:PHE:CG   | 1.98                     | 1.49              |
| 28:BA:416:PHE:CD2 | 28:BA:416:PHE:CG   | 2.01                     | 1.46              |
| 28:BA:416:PHE:CG  | 60:BA:533:PEV:H401 | 1.82                     | 1.13              |
| 28:BA:416:PHE:CD2 | 60:BA:533:PEV:C39  | 2.32                     | 1.12              |
| 28:BA:416:PHE:CE2 | 60:BA:533:PEV:C39  | 2.33                     | 1.12              |
| 28:BA:416:PHE:CD1 | 60:BA:533:PEV:C39  | 2.33                     | 1.12              |
| 28:BA:416:PHE:CD2 | 60:BA:533:PEV:H392 | 1.84                     | 1.12              |
| 28:BA:416:PHE:CE2 | 60:BA:533:PEV:C40  | 2.33                     | 1.12              |
| 28:BA:416:PHE:CG  | 60:BA:533:PEV:C40  | 2.33                     | 1.12              |
| 28:BA:416:PHE:CD2 | 60:BA:533:PEV:H402 | 1.85                     | 1.11              |
| 28:BA:416:PHE:CD1 | 60:BA:533:PEV:C40  | 2.33                     | 1.11              |
| 28:BA:416:PHE:CZ  | 60:BA:533:PEV:C40  | 2.33                     | 1.11              |
| 28:BA:416:PHE:CE1 | 60:BA:533:PEV:C39  | 2.33                     | 1.11              |
| 28:BA:416:PHE:CD2 | 60:BA:533:PEV:C40  | 2.32                     | 1.11              |
| 28:BA:416:PHE:CZ  | 60:BA:533:PEV:C39  | 2.33                     | 1.11              |
| 28:BA:416:PHE:CE1 | 60:BA:533:PEV:C40  | 2.34                     | 1.11              |
| 28:BA:416:PHE:CG  | 60:BA:533:PEV:C39  | 2.33                     | 1.10              |
| 28:BA:416:PHE:CG  | 60:BA:533:PEV:H391 | 1.86                     | 1.10              |
| 28:BA:416:PHE:CE2 | 60:BA:533:PEV:H402 | 1.91                     | 1.04              |
| 28:BA:416:PHE:CD1 | 60:BA:533:PEV:H391 | 1.94                     | 1.03              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 28:BA:416:PHE:CE2   | 60:BA:533:PEV:H392  | 1.96                     | 1.01              |
| 28:BA:416:PHE:CD1   | 60:BA:533:PEV:H401  | 1.97                     | 0.99              |
| 60:BA:533:PEV:C40   | 60:BA:533:PEV:C39   | 2.52                     | 0.87              |
| 4:AZ:81:LEU:HD13    | 4:AZ:82:GLY:H       | 1.53                     | 0.72              |
| 28:BA:324:ALA:HB2   | 60:BA:531:PEV:H402  | 1.73                     | 0.70              |
| 28:BA:416:PHE:CZ    | 60:BA:533:PEV:C38   | 2.77                     | 0.68              |
| 28:BA:416:PHE:CE1   | 60:BA:533:PEV:C38   | 2.79                     | 0.65              |
| 28:BA:416:PHE:CZ    | 60:BA:533:PEV:H381  | 2.33                     | 0.63              |
| 28:BA:416:PHE:CE1   | 60:BA:533:PEV:C41   | 2.82                     | 0.62              |
| 28:BA:416:PHE:CZ    | 60:BA:533:PEV:C41   | 2.85                     | 0.59              |
| 28:BA:416:PHE:CE1   | 60:BA:533:PEV:H381  | 2.39                     | 0.57              |
| 27:B8:2091:C:H3'    | 27:B8:2092:U:H5''   | 1.87                     | 0.56              |
| 27:B8:1021:A:H61    | 27:B8:1142:A:H61    | 1.53                     | 0.56              |
| 3:AV:27:A:H61       | 3:AV:45:G:H1        | 1.52                     | 0.55              |
| 27:B8:1024:G:H3'    | 27:B8:1025:G:H5''   | 1.88                     | 0.55              |
| 1:AA:664:G:H22      | 1:AA:741:G:H1       | 1.54                     | 0.55              |
| 27:B8:500:G:H21     | 27:B8:505:A:H62     | 1.55                     | 0.55              |
| 27:B8:2792:A:H3'    | 27:B8:2793:C:H5''   | 1.90                     | 0.53              |
| 27:B8:871:U:H3      | 27:B8:906:U:H3      | 1.56                     | 0.53              |
| 27:B8:962:G:H21     | 27:B8:2250:G:H1     | 1.57                     | 0.53              |
| 27:B8:870:U:H2'     | 27:B8:871:U:H5''    | 1.90                     | 0.53              |
| 61:BA:512:PGV:H72   | 60:BA:513:PEV:H401  | 1.91                     | 0.53              |
| 27:B8:1083:U:HO2'   | 27:B8:1084:A:H8     | 1.58                     | 0.51              |
| 14:AJ:15:HIS:CD2    | 14:AJ:16:ARG:HE     | 2.29                     | 0.51              |
| 1:AA:507:C:H3'      | 1:AA:508:U:H5''     | 1.92                     | 0.50              |
| 4:AZ:39:LEU:HD13    | 28:BA:286:PHE:HB3   | 1.93                     | 0.50              |
| 60:B8:3001:PEV:H401 | 60:B8:3002:PEV:H401 | 1.92                     | 0.50              |
| 21:AQ:18:LYS:H      | 21:AQ:50:ASN:HD21   | 1.59                     | 0.50              |
| 1:AA:1239:A:H62     | 1:AA:1299:A:H62     | 1.60                     | 0.50              |
| 25:AU:33:ARG:HE     | 25:AU:34:ARG:H      | 1.59                     | 0.50              |
| 1:AA:1305:G:H21     | 1:AA:1332:A:H8      | 1.59                     | 0.49              |
| 27:B8:1065:U:H3     | 27:B8:1069:A:H2'    | 1.76                     | 0.49              |
| 36:BH:126:GLY:H     | 36:BH:128:HIS:CE1   | 2.30                     | 0.49              |
| 1:AA:82:G:H3'       | 1:AA:83:C:H4'       | 1.95                     | 0.49              |
| 27:B8:713:G:H21     | 27:B8:718:A:H2      | 1.60                     | 0.49              |
| 1:AA:632:U:H3'      | 1:AA:633:G:H5'      | 1.95                     | 0.49              |
| 28:BA:416:PHE:CZ    | 60:BA:533:PEV:H411  | 2.48                     | 0.49              |
| 27:B8:870:U:C2'     | 27:B8:871:U:H5''    | 2.43                     | 0.48              |
| 1:AA:243:A:H4'      | 1:AA:244:U:H5'      | 1.94                     | 0.48              |
| 27:B8:1551:A:H3'    | 27:B8:1552:A:H5''   | 1.95                     | 0.48              |
| 9:AE:89:THR:HG22    | 9:AE:90:GLY:H       | 1.77                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:AP:54:LEU:H     | 20:AP:54:LEU:HD12  | 1.78                     | 0.48              |
| 60:BA:503:PEV:H401 | 60:BA:503:PEV:H442 | 1.95                     | 0.48              |
| 1:AA:1122:U:H5''   | 7:AC:222:GLN:H     | 1.78                     | 0.48              |
| 28:BA:416:PHE:CE1  | 60:BA:533:PEV:H411 | 2.48                     | 0.48              |
| 12:AH:60:LEU:H     | 12:AH:60:LEU:HD23  | 1.79                     | 0.48              |
| 20:AP:78:VAL:HG23  | 20:AP:81:ALA:H     | 1.79                     | 0.48              |
| 60:A1:301:PEV:H392 | 61:A1:303:PGV:H02  | 1.96                     | 0.47              |
| 24:AT:67:HIS:CD2   | 24:AT:69:ASN:H     | 2.32                     | 0.47              |
| 27:B8:82:U:H3      | 27:B8:104:A:H61    | 1.63                     | 0.47              |
| 30:B5:165:ASN:HD21 | 30:B5:169:GLY:H    | 1.63                     | 0.47              |
| 1:AA:1223:C:H3'    | 1:AA:1224:U:C5'    | 2.45                     | 0.47              |
| 58:B3:36:ALA:H     | 58:B3:39:ARG:HE    | 1.62                     | 0.47              |
| 60:A0:315:PEV:H391 | 60:A1:302:PEV:H401 | 1.96                     | 0.47              |
| 27:B8:957:C:H42    | 27:B8:2494:G:H21   | 1.61                     | 0.47              |
| 27:B8:2091:C:H3'   | 27:B8:2092:U:C5'   | 2.46                     | 0.46              |
| 36:BH:101:ASP:H    | 36:BH:111:ALA:HB3  | 1.80                     | 0.46              |
| 27:B8:2371:G:H21   | 56:B1:45:HIS:HE1   | 1.63                     | 0.46              |
| 4:AZ:25:LEU:CB     | 28:BA:333:THR:HG23 | 2.46                     | 0.46              |
| 27:B8:63:A:H2'     | 27:B8:64:A:C8      | 2.51                     | 0.46              |
| 60:A1:323:PEV:H392 | 60:A1:323:PEV:H142 | 1.97                     | 0.46              |
| 27:B8:2171:A:H1'   | 27:B8:2172:U:C6    | 2.50                     | 0.45              |
| 27:B8:480:A:H3'    | 27:B8:481:G:H5''   | 1.98                     | 0.45              |
| 1:AA:262:A:H4'     | 24:AT:67:HIS:CD2   | 2.52                     | 0.44              |
| 60:A1:319:PEV:H392 | 60:A1:319:PEV:H361 | 1.91                     | 0.44              |
| 27:B8:2371:G:H21   | 56:B1:45:HIS:CE1   | 2.35                     | 0.44              |
| 1:AA:973:G:H3'     | 1:AA:974:A:H5''    | 1.99                     | 0.44              |
| 6:AB:14:HIS:CE1    | 6:AB:200:PRO:HB3   | 2.53                     | 0.44              |
| 27:B8:890:C:H3'    | 27:B8:891:G:H4'    | 2.00                     | 0.44              |
| 27:B8:1203:U:H3'   | 27:B8:1204:A:H5''  | 1.99                     | 0.44              |
| 10:AF:94:HIS:CG    | 10:AF:95:ALA:H     | 2.37                     | 0.43              |
| 1:AA:404:G:H1      | 1:AA:499:A:H62     | 1.65                     | 0.43              |
| 8:AD:96:ARG:HB2    | 8:AD:99:ASN:HD22   | 1.82                     | 0.43              |
| 32:BD:33:ARG:HH11  | 32:BD:93:GLY:H     | 1.67                     | 0.43              |
| 27:B8:1273:U:H3    | 27:B8:2002:G:H21   | 1.67                     | 0.43              |
| 27:B8:2874:C:H4'   | 42:BN:4:ARG:HH21   | 1.84                     | 0.43              |
| 57:B2:24:THR:HG23  | 57:B2:27:GLY:H     | 1.84                     | 0.43              |
| 27:B8:532:A:H4'    | 27:B8:533:G:C8     | 2.54                     | 0.43              |
| 27:B8:572:A:H5''   | 46:BR:80:ARG:HH21  | 1.84                     | 0.43              |
| 27:B8:1567:G:H5'   | 31:B6:57:HIS:CD2   | 2.54                     | 0.43              |
| 6:AB:103:TRP:HE1   | 6:AB:107:ARG:HH21  | 1.66                     | 0.42              |
| 27:B8:2682:A:C2    | 27:B8:2683:C:C5    | 3.06                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 27:B8:1205:A:C5     | 33:BE:165:HIS:HB3   | 2.54                     | 0.42              |
| 27:B8:880:G:H2'     | 27:B8:881:G:C8      | 2.55                     | 0.42              |
| 27:B8:1391:U:H2'    | 27:B8:1393:A:C2     | 2.53                     | 0.42              |
| 27:B8:877:A:C2      | 27:B8:901:C:C2      | 3.08                     | 0.42              |
| 29:BB:123:THR:HA    | 29:BB:126:ARG:HH12  | 1.84                     | 0.42              |
| 31:B6:264:LYS:H     | 31:B6:264:LYS:HD2   | 1.85                     | 0.42              |
| 34:BF:106:ALA:HA    | 34:BF:111:ARG:HH11  | 1.85                     | 0.42              |
| 1:AA:413:G:H4'      | 1:AA:414:A:H5''     | 2.02                     | 0.42              |
| 6:AB:169:HIS:H      | 6:AB:169:HIS:CD2    | 2.37                     | 0.42              |
| 27:B8:962:G:N2      | 27:B8:2250:G:H1     | 2.17                     | 0.42              |
| 27:B8:2233:U:H2'    | 27:B8:2234:G:C8     | 2.55                     | 0.42              |
| 1:AA:995:C:H2'      | 1:AA:996:A:H5''     | 2.02                     | 0.42              |
| 1:AA:1130:A:H61     | 1:AA:1144:G:H1'     | 1.86                     | 0.41              |
| 1:AA:1144:G:N2      | 1:AA:1146:A:H62     | 2.19                     | 0.41              |
| 1:AA:537:G:H5''     | 16:AL:109:ARG:HH12  | 1.85                     | 0.41              |
| 16:AL:41:PRO:HG2    | 16:AL:45:ASN:H      | 1.85                     | 0.41              |
| 27:B8:900:A:H2'     | 27:B8:901:C:H5'     | 2.02                     | 0.41              |
| 27:B8:1082:U:N3     | 27:B8:1086:A:C2     | 2.88                     | 0.41              |
| 1:AA:412:A:H3'      | 1:AA:413:G:C5'      | 2.51                     | 0.41              |
| 60:BA:514:PEV:H391  | 60:BA:514:PEV:H362  | 1.94                     | 0.41              |
| 27:B8:1283:G:H22    | 27:B8:1286:A:H5'    | 1.85                     | 0.41              |
| 27:B8:2351:G:H2'    | 27:B8:2365:G:H22    | 1.84                     | 0.41              |
| 27:B8:251:A:H4'     | 40:BL:49:GLY:HA2    | 2.02                     | 0.41              |
| 61:A1:315:PGV:H132  | 61:A1:315:PGV:H102  | 1.98                     | 0.41              |
| 4:AZ:25:LEU:HB3     | 28:BA:333:THR:HG23  | 2.03                     | 0.41              |
| 1:AA:781:A:H2'      | 1:AA:782:A:H5'      | 2.02                     | 0.41              |
| 27:B8:2645:G:H3'    | 27:B8:2646:C:H5'    | 2.02                     | 0.41              |
| 60:B8:3002:PEV:H392 | 60:B8:3002:PEV:H362 | 1.94                     | 0.41              |
| 1:AA:1118:U:H1'     | 1:AA:1179:A:C4      | 2.55                     | 0.41              |
| 7:AC:10:ARG:HH21    | 7:AC:175:HIS:HA     | 1.85                     | 0.40              |
| 14:AJ:15:HIS:HA     | 14:AJ:18:ILE:HG22   | 2.01                     | 0.40              |
| 60:BA:520:PEV:H402  | 60:BA:526:PEV:H441  | 2.04                     | 0.40              |
| 1:AA:483:C:H2'      | 1:AA:484:G:C8       | 2.57                     | 0.40              |
| 18:AN:60:ARG:HE     | 18:AN:60:ARG:HA     | 1.86                     | 0.40              |
| 41:BM:78:LEU:HD23   | 41:BM:78:LEU:H      | 1.86                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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 |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 4   | AZ    | 96/98 (98%)    | 74 (77%)  | 13 (14%) | 9 (9%)   | 1           | 14  |
| 5   | A0    | 198/200 (99%)  | 174 (88%) | 20 (10%) | 4 (2%)   | 9           | 46  |
| 5   | A1    | 198/200 (99%)  | 169 (85%) | 23 (12%) | 6 (3%)   | 5           | 37  |
| 6   | AB    | 238/240 (99%)  | 190 (80%) | 42 (18%) | 6 (2%)   | 6           | 41  |
| 7   | AC    | 230/232 (99%)  | 184 (80%) | 31 (14%) | 15 (6%)  | 1           | 22  |
| 8   | AD    | 203/205 (99%)  | 163 (80%) | 28 (14%) | 12 (6%)  | 2           | 23  |
| 9   | AE    | 164/166 (99%)  | 137 (84%) | 21 (13%) | 6 (4%)   | 4           | 33  |
| 10  | AF    | 133/135 (98%)  | 109 (82%) | 22 (16%) | 2 (2%)   | 12          | 53  |
| 11  | AG    | 176/178 (99%)  | 142 (81%) | 29 (16%) | 5 (3%)   | 6           | 39  |
| 12  | AH    | 127/129 (98%)  | 102 (80%) | 23 (18%) | 2 (2%)   | 11          | 51  |
| 13  | AI    | 127/129 (98%)  | 108 (85%) | 11 (9%)  | 8 (6%)   | 1           | 22  |
| 14  | AJ    | 101/103 (98%)  | 85 (84%)  | 9 (9%)   | 7 (7%)   | 1           | 20  |
| 15  | AK    | 126/128 (98%)  | 106 (84%) | 15 (12%) | 5 (4%)   | 3           | 31  |
| 16  | AL    | 121/123 (98%)  | 108 (89%) | 12 (10%) | 1 (1%)   | 22          | 67  |
| 17  | AM    | 115/117 (98%)  | 96 (84%)  | 13 (11%) | 6 (5%)   | 2           | 26  |
| 18  | AN    | 98/100 (98%)   | 81 (83%)  | 9 (9%)   | 8 (8%)   | 1           | 16  |
| 19  | AO    | 86/88 (98%)    | 79 (92%)  | 5 (6%)   | 2 (2%)   | 7           | 43  |
| 20  | AP    | 80/82 (98%)    | 73 (91%)  | 5 (6%)   | 2 (2%)   | 6           | 41  |
| 21  | AQ    | 81/83 (98%)    | 67 (83%)  | 8 (10%)  | 6 (7%)   | 1           | 18  |
| 22  | AR    | 72/74 (97%)    | 59 (82%)  | 9 (12%)  | 4 (6%)   | 2           | 25  |
| 23  | AS    | 89/91 (98%)    | 73 (82%)  | 12 (14%) | 4 (4%)   | 3           | 29  |
| 24  | AT    | 84/86 (98%)    | 76 (90%)  | 7 (8%)   | 1 (1%)   | 15          | 57  |
| 25  | AU    | 68/70 (97%)    | 64 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 28  | BA    | 433/435 (100%) | 313 (72%) | 66 (15%) | 54 (12%) | 0           | 7   |
| 29  | BB    | 114/116 (98%)  | 96 (84%)  | 12 (10%) | 6 (5%)   | 2           | 26  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 30  | B5    | 232/234 (99%)   | 211 (91%)  | 15 (6%)   | 6 (3%)   | 6           | 40 |
| 31  | B6    | 270/272 (99%)   | 227 (84%)  | 31 (12%)  | 12 (4%)  | 3           | 29 |
| 32  | BD    | 207/209 (99%)   | 172 (83%)  | 24 (12%)  | 11 (5%)  | 2           | 26 |
| 33  | BE    | 199/201 (99%)   | 169 (85%)  | 20 (10%)  | 10 (5%)  | 2           | 27 |
| 34  | BF    | 176/178 (99%)   | 137 (78%)  | 27 (15%)  | 12 (7%)  | 1           | 20 |
| 35  | BG    | 174/176 (99%)   | 137 (79%)  | 28 (16%)  | 9 (5%)   | 2           | 26 |
| 36  | BH    | 147/149 (99%)   | 108 (74%)  | 31 (21%)  | 8 (5%)   | 2           | 25 |
| 37  | BI    | 139/141 (99%)   | 125 (90%)  | 11 (8%)   | 3 (2%)   | 8           | 44 |
| 38  | BJ    | 140/142 (99%)   | 117 (84%)  | 19 (14%)  | 4 (3%)   | 5           | 38 |
| 39  | BK    | 121/123 (98%)   | 99 (82%)   | 16 (13%)  | 6 (5%)   | 2           | 27 |
| 40  | BL    | 142/144 (99%)   | 129 (91%)  | 10 (7%)   | 3 (2%)   | 8           | 45 |
| 41  | BM    | 134/136 (98%)   | 107 (80%)  | 17 (13%)  | 10 (8%)  | 1           | 18 |
| 42  | BN    | 125/127 (98%)   | 104 (83%)  | 12 (10%)  | 9 (7%)   | 1           | 19 |
| 43  | BO    | 115/117 (98%)   | 97 (84%)   | 15 (13%)  | 3 (3%)   | 6           | 40 |
| 44  | BP    | 112/114 (98%)   | 94 (84%)   | 11 (10%)  | 7 (6%)   | 1           | 22 |
| 45  | BQ    | 115/117 (98%)   | 94 (82%)   | 15 (13%)  | 6 (5%)   | 2           | 26 |
| 46  | BR    | 101/103 (98%)   | 83 (82%)   | 13 (13%)  | 5 (5%)   | 2           | 27 |
| 47  | BS    | 108/110 (98%)   | 81 (75%)   | 18 (17%)  | 9 (8%)   | 1           | 16 |
| 48  | BT    | 98/100 (98%)    | 71 (72%)   | 20 (20%)  | 7 (7%)   | 1           | 19 |
| 49  | BU    | 101/103 (98%)   | 84 (83%)   | 14 (14%)  | 3 (3%)   | 5           | 37 |
| 50  | BV    | 92/94 (98%)     | 82 (89%)   | 9 (10%)   | 1 (1%)   | 17          | 60 |
| 51  | BW    | 82/84 (98%)     | 59 (72%)   | 19 (23%)  | 4 (5%)   | 2           | 27 |
| 52  | BX    | 75/77 (97%)     | 57 (76%)   | 12 (16%)  | 6 (8%)   | 1           | 17 |
| 53  | BY    | 61/63 (97%)     | 48 (79%)   | 11 (18%)  | 2 (3%)   | 4           | 35 |
| 54  | BZ    | 56/58 (97%)     | 49 (88%)   | 4 (7%)    | 3 (5%)   | 2           | 25 |
| 55  | B0    | 54/56 (96%)     | 47 (87%)   | 6 (11%)   | 1 (2%)   | 9           | 47 |
| 56  | B1    | 52/54 (96%)     | 46 (88%)   | 5 (10%)   | 1 (2%)   | 9           | 47 |
| 57  | B2    | 44/46 (96%)     | 31 (70%)   | 10 (23%)  | 3 (7%)   | 1           | 20 |
| 58  | B3    | 62/64 (97%)     | 52 (84%)   | 9 (14%)   | 1 (2%)   | 11          | 51 |
| 59  | B4    | 36/38 (95%)     | 32 (89%)   | 3 (8%)    | 1 (3%)   | 6           | 39 |
| All | All   | 7128/7238 (98%) | 5877 (82%) | 904 (13%) | 347 (5%) | 5           | 27 |



All (347) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AZ    | 48  | TRP  |
| 4   | AZ    | 61  | VAL  |
| 4   | AZ    | 81  | LEU  |
| 5   | A1    | 177 | ARG  |
| 7   | AC    | 206 | ILE  |
| 7   | AC    | 219 | PRO  |
| 9   | AE    | 17  | VAL  |
| 13  | AI    | 127 | SER  |
| 14  | AJ    | 57  | VAL  |
| 14  | AJ    | 67  | ILE  |
| 17  | AM    | 3   | ILE  |
| 18  | AN    | 80  | ARG  |
| 28  | BA    | 48  | VAL  |
| 28  | BA    | 56  | GLN  |
| 28  | BA    | 68  | SER  |
| 28  | BA    | 72  | LEU  |
| 28  | BA    | 79  | ALA  |
| 28  | BA    | 148 | LEU  |
| 28  | BA    | 200 | PRO  |
| 28  | BA    | 237 | VAL  |
| 28  | BA    | 249 | ALA  |
| 28  | BA    | 275 | ILE  |
| 28  | BA    | 314 | GLN  |
| 28  | BA    | 319 | LEU  |
| 28  | BA    | 332 | TYR  |
| 28  | BA    | 353 | VAL  |
| 28  | BA    | 358 | PRO  |
| 28  | BA    | 373 | LEU  |
| 29  | BB    | 67  | ALA  |
| 31  | B6    | 132 | ARG  |
| 31  | B6    | 197 | ALA  |
| 31  | B6    | 231 | HIS  |
| 31  | B6    | 261 | ARG  |
| 33  | BE    | 4   | VAL  |
| 34  | BF    | 82  | TYR  |
| 34  | BF    | 136 | ILE  |
| 35  | BG    | 2   | ARG  |
| 35  | BG    | 94  | ARG  |
| 36  | BH    | 32  | PRO  |
| 36  | BH    | 115 | VAL  |
| 38  | BJ    | 40  | HIS  |
| 39  | BK    | 71  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | BM    | 43  | ALA  |
| 41  | BM    | 56  | ALA  |
| 41  | BM    | 122 | ALA  |
| 44  | BP    | 25  | VAL  |
| 45  | BQ    | 71  | ASN  |
| 46  | BR    | 3   | ALA  |
| 46  | BR    | 48  | LYS  |
| 46  | BR    | 101 | ILE  |
| 47  | BS    | 76  | VAL  |
| 48  | BT    | 35  | ALA  |
| 48  | BT    | 36  | LYS  |
| 48  | BT    | 99  | ALA  |
| 49  | BU    | 49  | PRO  |
| 4   | AZ    | 49  | MET  |
| 6   | AB    | 95  | TRP  |
| 6   | AB    | 224 | ARG  |
| 7   | AC    | 190 | THR  |
| 8   | AD    | 7   | LYS  |
| 10  | AF    | 85  | ILE  |
| 11  | AG    | 77  | ARG  |
| 12  | AH    | 73  | SER  |
| 14  | AJ    | 85  | ASP  |
| 15  | AK    | 11  | VAL  |
| 16  | AL    | 54  | VAL  |
| 17  | AM    | 29  | SER  |
| 17  | AM    | 87  | GLY  |
| 18  | AN    | 21  | ALA  |
| 21  | AQ    | 12  | VAL  |
| 21  | AQ    | 13  | SER  |
| 21  | AQ    | 81  | ALA  |
| 22  | AR    | 24  | ASP  |
| 23  | AS    | 28  | LYS  |
| 28  | BA    | 235 | VAL  |
| 28  | BA    | 256 | ARG  |
| 28  | BA    | 267 | LEU  |
| 28  | BA    | 308 | LEU  |
| 28  | BA    | 320 | LEU  |
| 28  | BA    | 333 | THR  |
| 28  | BA    | 340 | ARG  |
| 28  | BA    | 351 | ALA  |
| 28  | BA    | 362 | THR  |
| 28  | BA    | 363 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | BA    | 369 | VAL  |
| 28  | BA    | 371 | THR  |
| 28  | BA    | 401 | PHE  |
| 28  | BA    | 431 | SER  |
| 29  | BB    | 19  | TRP  |
| 29  | BB    | 71  | PHE  |
| 31  | B6    | 142 | ASN  |
| 32  | BD    | 31  | ALA  |
| 32  | BD    | 46  | ARG  |
| 32  | BD    | 107 | VAL  |
| 33  | BE    | 12  | LEU  |
| 33  | BE    | 30  | GLN  |
| 34  | BF    | 74  | ALA  |
| 34  | BF    | 84  | ILE  |
| 34  | BF    | 103 | ILE  |
| 34  | BF    | 138 | PRO  |
| 37  | BI    | 87  | SER  |
| 40  | BL    | 113 | ALA  |
| 41  | BM    | 55  | ARG  |
| 41  | BM    | 72  | PRO  |
| 41  | BM    | 73  | ILE  |
| 41  | BM    | 135 | VAL  |
| 42  | BN    | 63  | ARG  |
| 44  | BP    | 106 | ALA  |
| 45  | BQ    | 101 | ASP  |
| 46  | BR    | 65  | ALA  |
| 47  | BS    | 12  | SER  |
| 47  | BS    | 53  | SER  |
| 47  | BS    | 89  | ALA  |
| 48  | BT    | 72  | GLN  |
| 53  | BY    | 2   | LYS  |
| 53  | BY    | 37  | LEU  |
| 4   | AZ    | 109 | ASP  |
| 5   | A0    | 170 | LEU  |
| 5   | A1    | 228 | SER  |
| 7   | AC    | 53  | ARG  |
| 7   | AC    | 106 | ARG  |
| 7   | AC    | 116 | ALA  |
| 8   | AD    | 6   | PRO  |
| 8   | AD    | 21  | LYS  |
| 8   | AD    | 146 | GLU  |
| 8   | AD    | 176 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | AE    | 120 | HIS  |
| 11  | AG    | 80  | GLY  |
| 11  | AG    | 138 | GLU  |
| 12  | AH    | 116 | ARG  |
| 13  | AI    | 35  | GLU  |
| 13  | AI    | 59  | LYS  |
| 14  | AJ    | 17  | LEU  |
| 17  | AM    | 105 | ALA  |
| 19  | AO    | 87  | ARG  |
| 20  | AP    | 54  | LEU  |
| 23  | AS    | 86  | LYS  |
| 28  | BA    | 57  | ARG  |
| 28  | BA    | 71  | ALA  |
| 28  | BA    | 78  | PHE  |
| 28  | BA    | 145 | MET  |
| 28  | BA    | 236 | PHE  |
| 28  | BA    | 254 | GLY  |
| 28  | BA    | 260 | ALA  |
| 28  | BA    | 278 | ILE  |
| 28  | BA    | 356 | ILE  |
| 28  | BA    | 391 | MET  |
| 28  | BA    | 432 | ALA  |
| 29  | BB    | 45  | ALA  |
| 29  | BB    | 69  | VAL  |
| 30  | B5    | 87  | ALA  |
| 30  | B5    | 159 | GLY  |
| 31  | B6    | 112 | GLY  |
| 31  | B6    | 152 | GLN  |
| 31  | B6    | 189 | ALA  |
| 31  | B6    | 205 | GLY  |
| 32  | BD    | 65  | ALA  |
| 32  | BD    | 140 | HIS  |
| 32  | BD    | 175 | LEU  |
| 33  | BE    | 16  | GLU  |
| 33  | BE    | 130 | LYS  |
| 33  | BE    | 154 | ASP  |
| 34  | BF    | 42  | ALA  |
| 34  | BF    | 77  | LYS  |
| 34  | BF    | 123 | GLY  |
| 34  | BF    | 124 | ARG  |
| 35  | BG    | 21  | GLN  |
| 36  | BH    | 14  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | BH    | 75  | LEU  |
| 36  | BH    | 84  | ALA  |
| 38  | BJ    | 111 | LYS  |
| 39  | BK    | 36  | GLY  |
| 40  | BL    | 53  | GLY  |
| 42  | BN    | 13  | ASN  |
| 42  | BN    | 122 | ALA  |
| 43  | BO    | 89  | ASP  |
| 43  | BO    | 113 | ALA  |
| 44  | BP    | 54  | LEU  |
| 44  | BP    | 113 | LEU  |
| 48  | BT    | 97  | GLY  |
| 50  | BV    | 44  | HIS  |
| 51  | BW    | 27  | GLY  |
| 51  | BW    | 41  | GLY  |
| 51  | BW    | 52  | CYS  |
| 52  | BX    | 27  | ARG  |
| 52  | BX    | 32  | LEU  |
| 54  | BZ    | 8   | GLN  |
| 54  | BZ    | 10  | ARG  |
| 57  | B2    | 23  | ALA  |
| 57  | B2    | 35  | ARG  |
| 4   | AZ    | 55  | LEU  |
| 4   | AZ    | 101 | GLN  |
| 5   | A0    | 154 | ALA  |
| 5   | A1    | 71  | PHE  |
| 5   | A1    | 164 | ALA  |
| 6   | AB    | 74  | ALA  |
| 7   | AC    | 82  | ASP  |
| 8   | AD    | 20  | LEU  |
| 8   | AD    | 28  | ASP  |
| 8   | AD    | 35  | GLN  |
| 8   | AD    | 36  | ALA  |
| 8   | AD    | 174 | ALA  |
| 9   | AE    | 9   | GLU  |
| 10  | AF    | 114 | ASP  |
| 13  | AI    | 121 | ARG  |
| 14  | AJ    | 78  | GLU  |
| 15  | AK    | 2   | LYS  |
| 17  | AM    | 16  | ILE  |
| 18  | AN    | 38  | GLU  |
| 18  | AN    | 68  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AQ    | 15  | LYS  |
| 21  | AQ    | 51  | GLU  |
| 22  | AR    | 2   | ARG  |
| 22  | AR    | 26  | ALA  |
| 23  | AS    | 55  | GLN  |
| 23  | AS    | 87  | LYS  |
| 28  | BA    | 39  | ILE  |
| 28  | BA    | 42  | PRO  |
| 28  | BA    | 151 | ASN  |
| 28  | BA    | 214 | ASP  |
| 28  | BA    | 346 | LEU  |
| 28  | BA    | 352 | PHE  |
| 28  | BA    | 435 | LYS  |
| 30  | B5    | 52  | ALA  |
| 30  | B5    | 82  | ALA  |
| 30  | B5    | 89  | ALA  |
| 30  | B5    | 147 | PRO  |
| 31  | B6    | 214 | GLY  |
| 31  | B6    | 240 | GLY  |
| 32  | BD    | 122 | VAL  |
| 32  | BD    | 203 | VAL  |
| 33  | BE    | 106 | LYS  |
| 35  | BG    | 31  | GLU  |
| 35  | BG    | 47  | ASN  |
| 37  | BI    | 97  | VAL  |
| 38  | BJ    | 68  | LYS  |
| 39  | BK    | 113 | MET  |
| 40  | BL    | 66  | PHE  |
| 41  | BM    | 134 | THR  |
| 42  | BN    | 10  | LEU  |
| 42  | BN    | 32  | GLU  |
| 42  | BN    | 80  | PHE  |
| 42  | BN    | 121 | LYS  |
| 43  | BO    | 16  | ARG  |
| 44  | BP    | 35  | SER  |
| 44  | BP    | 81  | ASP  |
| 45  | BQ    | 9   | ALA  |
| 46  | BR    | 27  | ILE  |
| 47  | BS    | 31  | GLN  |
| 47  | BS    | 64  | ALA  |
| 49  | BU    | 12  | VAL  |
| 49  | BU    | 75  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | BX    | 15  | ASN  |
| 54  | BZ    | 29  | ARG  |
| 57  | B2    | 8   | SER  |
| 4   | AZ    | 72  | ASP  |
| 4   | AZ    | 94  | ILE  |
| 5   | A1    | 157 | ASP  |
| 6   | AB    | 28  | PRO  |
| 6   | AB    | 33  | ALA  |
| 7   | AC    | 9   | ILE  |
| 7   | AC    | 47  | ALA  |
| 7   | AC    | 61  | LYS  |
| 7   | AC    | 128 | MET  |
| 7   | AC    | 218 | LYS  |
| 8   | AD    | 47  | LEU  |
| 8   | AD    | 147 | LYS  |
| 9   | AE    | 44  | ARG  |
| 11  | AG    | 2   | ARG  |
| 11  | AG    | 4   | ARG  |
| 14  | AJ    | 59  | LYS  |
| 15  | AK    | 101 | ALA  |
| 17  | AM    | 116 | LYS  |
| 18  | AN    | 28  | ALA  |
| 18  | AN    | 43  | ALA  |
| 18  | AN    | 66  | THR  |
| 19  | AO    | 73  | ASP  |
| 24  | AT    | 47  | GLN  |
| 28  | BA    | 61  | ILE  |
| 28  | BA    | 330 | PHE  |
| 29  | BB    | 65  | GLY  |
| 32  | BD    | 9   | VAL  |
| 32  | BD    | 109 | VAL  |
| 33  | BE    | 2   | GLU  |
| 33  | BE    | 83  | VAL  |
| 33  | BE    | 96  | VAL  |
| 34  | BF    | 148 | VAL  |
| 35  | BG    | 100 | ASN  |
| 35  | BG    | 136 | ASP  |
| 35  | BG    | 155 | PRO  |
| 36  | BH    | 55  | GLU  |
| 36  | BH    | 87  | GLU  |
| 39  | BK    | 92  | GLU  |
| 39  | BK    | 122 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | BM    | 67  | VAL  |
| 42  | BN    | 72  | ASP  |
| 44  | BP    | 76  | HIS  |
| 45  | BQ    | 27  | ARG  |
| 45  | BQ    | 81  | GLY  |
| 47  | BS    | 32  | ALA  |
| 47  | BS    | 40  | ASN  |
| 48  | BT    | 10  | VAL  |
| 52  | BX    | 41  | SER  |
| 56  | B1    | 33  | LEU  |
| 5   | A0    | 47  | LEU  |
| 5   | A0    | 156 | VAL  |
| 6   | AB    | 132 | GLU  |
| 7   | AC    | 111 | ASP  |
| 7   | AC    | 205 | GLU  |
| 7   | AC    | 213 | VAL  |
| 13  | AI    | 58  | GLU  |
| 13  | AI    | 109 | GLN  |
| 13  | AI    | 110 | VAL  |
| 14  | AJ    | 48  | ARG  |
| 15  | AK    | 12  | ARG  |
| 22  | AR    | 14  | ALA  |
| 28  | BA    | 337 | PHE  |
| 31  | B6    | 59  | GLN  |
| 34  | BF    | 111 | ARG  |
| 35  | BG    | 156 | TYR  |
| 36  | BH    | 41  | LYS  |
| 37  | BI    | 30  | GLN  |
| 41  | BM    | 70  | ASP  |
| 42  | BN    | 100 | CYS  |
| 48  | BT    | 29  | THR  |
| 52  | BX    | 3   | VAL  |
| 52  | BX    | 6   | VAL  |
| 55  | B0    | 44  | ALA  |
| 58  | B3    | 53  | ASP  |
| 5   | A1    | 227 | VAL  |
| 13  | AI    | 57  | VAL  |
| 18  | AN    | 33  | VAL  |
| 59  | B4    | 16  | ILE  |
| 9   | AE    | 15  | ILE  |
| 20  | AP    | 36  | VAL  |
| 39  | BK    | 35  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | BQ    | 33  | VAL  |
| 9   | AE    | 105 | ILE  |
| 15  | AK    | 88  | PRO  |
| 21  | AQ    | 11  | VAL  |
| 28  | BA    | 306 | ILE  |
| 28  | BA    | 403 | GLY  |
| 32  | BD    | 152 | PRO  |
| 38  | BJ    | 96  | ARG  |
| 28  | BA    | 318 | VAL  |
| 51  | BW    | 73  | PRO  |
| 47  | BS    | 45  | VAL  |

### 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 |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 4   | AZ    | 85/85 (100%)   | 72 (85%)   | 13 (15%) | 3           | 19  |
| 5   | A0    | 176/176 (100%) | 174 (99%)  | 2 (1%)   | 78          | 89  |
| 5   | A1    | 176/176 (100%) | 173 (98%)  | 3 (2%)   | 66          | 84  |
| 6   | AB    | 198/198 (100%) | 194 (98%)  | 4 (2%)   | 60          | 82  |
| 7   | AC    | 189/189 (100%) | 183 (97%)  | 6 (3%)   | 44          | 70  |
| 8   | AD    | 172/172 (100%) | 166 (96%)  | 6 (4%)   | 41          | 69  |
| 9   | AE    | 125/125 (100%) | 122 (98%)  | 3 (2%)   | 54          | 78  |
| 10  | AF    | 116/116 (100%) | 111 (96%)  | 5 (4%)   | 33          | 64  |
| 11  | AG    | 146/146 (100%) | 146 (100%) | 0        | 100         | 100 |
| 12  | AH    | 104/104 (100%) | 101 (97%)  | 3 (3%)   | 48          | 73  |
| 13  | AI    | 106/106 (100%) | 101 (95%)  | 5 (5%)   | 30          | 62  |
| 14  | AJ    | 90/90 (100%)   | 88 (98%)   | 2 (2%)   | 57          | 79  |
| 15  | AK    | 98/98 (100%)   | 95 (97%)   | 3 (3%)   | 45          | 71  |
| 16  | AL    | 103/103 (100%) | 102 (99%)  | 1 (1%)   | 80          | 90  |
| 17  | AM    | 95/95 (100%)   | 92 (97%)   | 3 (3%)   | 44          | 70  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 18  | AN    | 83/83 (100%)   | 81 (98%)   | 2 (2%)   | 54          | 78  |
| 19  | AO    | 76/76 (100%)   | 74 (97%)   | 2 (3%)   | 51          | 75  |
| 20  | AP    | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 21  | AQ    | 77/77 (100%)   | 74 (96%)   | 3 (4%)   | 37          | 66  |
| 22  | AR    | 64/64 (100%)   | 63 (98%)   | 1 (2%)   | 68          | 85  |
| 23  | AS    | 78/78 (100%)   | 78 (100%)  | 0        | 100         | 100 |
| 24  | AT    | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 25  | AU    | 60/60 (100%)   | 58 (97%)   | 2 (3%)   | 43          | 70  |
| 28  | BA    | 353/353 (100%) | 326 (92%)  | 27 (8%)  | 15          | 47  |
| 29  | BB    | 92/92 (100%)   | 88 (96%)   | 4 (4%)   | 33          | 64  |
| 30  | B5    | 181/181 (100%) | 178 (98%)  | 3 (2%)   | 66          | 84  |
| 31  | B6    | 217/217 (100%) | 212 (98%)  | 5 (2%)   | 56          | 79  |
| 32  | BD    | 164/164 (100%) | 158 (96%)  | 6 (4%)   | 39          | 68  |
| 33  | BE    | 165/165 (100%) | 164 (99%)  | 1 (1%)   | 89          | 94  |
| 34  | BF    | 149/149 (100%) | 145 (97%)  | 4 (3%)   | 50          | 74  |
| 35  | BG    | 137/137 (100%) | 134 (98%)  | 3 (2%)   | 57          | 79  |
| 36  | BH    | 114/114 (100%) | 108 (95%)  | 6 (5%)   | 26          | 59  |
| 37  | BI    | 109/109 (100%) | 106 (97%)  | 3 (3%)   | 49          | 74  |
| 38  | BJ    | 116/116 (100%) | 113 (97%)  | 3 (3%)   | 51          | 75  |
| 39  | BK    | 104/104 (100%) | 99 (95%)   | 5 (5%)   | 30          | 61  |
| 40  | BL    | 103/103 (100%) | 102 (99%)  | 1 (1%)   | 80          | 90  |
| 41  | BM    | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 42  | BN    | 103/103 (100%) | 100 (97%)  | 3 (3%)   | 48          | 73  |
| 43  | BO    | 87/87 (100%)   | 87 (100%)  | 0        | 100         | 100 |
| 44  | BP    | 99/99 (100%)   | 96 (97%)   | 3 (3%)   | 46          | 72  |
| 45  | BQ    | 89/89 (100%)   | 89 (100%)  | 0        | 100         | 100 |
| 46  | BR    | 84/84 (100%)   | 84 (100%)  | 0        | 100         | 100 |
| 47  | BS    | 93/93 (100%)   | 93 (100%)  | 0        | 100         | 100 |
| 48  | BT    | 84/84 (100%)   | 79 (94%)   | 5 (6%)   | 22          | 55  |
| 49  | BU    | 84/84 (100%)   | 82 (98%)   | 2 (2%)   | 54          | 78  |
| 50  | BV    | 78/78 (100%)   | 77 (99%)   | 1 (1%)   | 73          | 87  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 51  | BW    | 62/62 (100%)     | 61 (98%)   | 1 (2%)   | 68          | 85  |
| 52  | BX    | 67/67 (100%)     | 66 (98%)   | 1 (2%)   | 70          | 85  |
| 53  | BY    | 55/55 (100%)     | 54 (98%)   | 1 (2%)   | 64          | 84  |
| 54  | BZ    | 48/48 (100%)     | 47 (98%)   | 1 (2%)   | 59          | 80  |
| 55  | B0    | 47/47 (100%)     | 46 (98%)   | 1 (2%)   | 59          | 80  |
| 56  | B1    | 48/48 (100%)     | 47 (98%)   | 1 (2%)   | 59          | 80  |
| 57  | B2    | 38/38 (100%)     | 37 (97%)   | 1 (3%)   | 51          | 75  |
| 58  | B3    | 51/51 (100%)     | 50 (98%)   | 1 (2%)   | 60          | 82  |
| 59  | B4    | 34/34 (100%)     | 34 (100%)  | 0        | 100         | 100 |
| All | All   | 5911/5911 (100%) | 5749 (97%) | 162 (3%) | 54          | 74  |

All (162) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AZ    | 28  | ILE  |
| 4   | AZ    | 54  | ARG  |
| 4   | AZ    | 60  | LEU  |
| 4   | AZ    | 71  | ASN  |
| 4   | AZ    | 75  | ARG  |
| 4   | AZ    | 78  | ILE  |
| 4   | AZ    | 79  | LEU  |
| 4   | AZ    | 81  | LEU  |
| 4   | AZ    | 95  | ILE  |
| 4   | AZ    | 97  | THR  |
| 4   | AZ    | 99  | ILE  |
| 4   | AZ    | 107 | ARG  |
| 4   | AZ    | 115 | HIS  |
| 5   | A0    | 132 | GLN  |
| 5   | A0    | 133 | LYS  |
| 5   | A1    | 112 | MET  |
| 5   | A1    | 132 | GLN  |
| 5   | A1    | 237 | THR  |
| 6   | AB    | 103 | TRP  |
| 6   | AB    | 164 | ASP  |
| 6   | AB    | 169 | HIS  |
| 6   | AB    | 174 | GLU  |
| 7   | AC    | 106 | ARG  |
| 7   | AC    | 114 | LEU  |
| 7   | AC    | 131 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | AC    | 214 | GLU  |
| 7   | AC    | 219 | PRO  |
| 7   | AC    | 225 | LYS  |
| 8   | AD    | 13  | ARG  |
| 8   | AD    | 20  | LEU  |
| 8   | AD    | 43  | ARG  |
| 8   | AD    | 110 | ARG  |
| 8   | AD    | 170 | LEU  |
| 8   | AD    | 182 | LYS  |
| 9   | AE    | 75  | LEU  |
| 9   | AE    | 89  | THR  |
| 9   | AE    | 150 | GLU  |
| 10  | AF    | 16  | GLU  |
| 10  | AF    | 44  | ARG  |
| 10  | AF    | 47  | LEU  |
| 10  | AF    | 104 | LYS  |
| 10  | AF    | 107 | ASP  |
| 12  | AH    | 2   | MET  |
| 12  | AH    | 26  | MET  |
| 12  | AH    | 123 | GLU  |
| 13  | AI    | 17  | ARG  |
| 13  | AI    | 40  | ARG  |
| 13  | AI    | 44  | ARG  |
| 13  | AI    | 58  | GLU  |
| 13  | AI    | 129 | ARG  |
| 14  | AJ    | 31  | ARG  |
| 14  | AJ    | 81  | GLU  |
| 15  | AK    | 10  | ARG  |
| 15  | AK    | 75  | GLU  |
| 15  | AK    | 79  | LYS  |
| 16  | AL    | 50  | LYS  |
| 17  | AM    | 69  | ARG  |
| 17  | AM    | 91  | ARG  |
| 17  | AM    | 113 | LYS  |
| 18  | AN    | 53  | ASP  |
| 18  | AN    | 64  | ARG  |
| 19  | AO    | 16  | ARG  |
| 19  | AO    | 87  | ARG  |
| 21  | AQ    | 5   | ARG  |
| 21  | AQ    | 17  | GLU  |
| 21  | AQ    | 26  | ARG  |
| 22  | AR    | 11  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | AU    | 18  | PHE  |
| 25  | AU    | 69  | LEU  |
| 28  | BA    | 53  | LEU  |
| 28  | BA    | 55  | GLN  |
| 28  | BA    | 85  | TYR  |
| 28  | BA    | 130 | PHE  |
| 28  | BA    | 180 | GLU  |
| 28  | BA    | 189 | ILE  |
| 28  | BA    | 192 | PHE  |
| 28  | BA    | 195 | ILE  |
| 28  | BA    | 212 | GLN  |
| 28  | BA    | 228 | PHE  |
| 28  | BA    | 237 | VAL  |
| 28  | BA    | 252 | GLN  |
| 28  | BA    | 256 | ARG  |
| 28  | BA    | 290 | ILE  |
| 28  | BA    | 309 | TYR  |
| 28  | BA    | 317 | TYR  |
| 28  | BA    | 336 | VAL  |
| 28  | BA    | 340 | ARG  |
| 28  | BA    | 347 | LYS  |
| 28  | BA    | 352 | PHE  |
| 28  | BA    | 356 | ILE  |
| 28  | BA    | 357 | ARG  |
| 28  | BA    | 361 | GLN  |
| 28  | BA    | 372 | ARG  |
| 28  | BA    | 373 | LEU  |
| 28  | BA    | 374 | THR  |
| 28  | BA    | 441 | TYR  |
| 29  | BB    | 44  | ARG  |
| 29  | BB    | 76  | ARG  |
| 29  | BB    | 77  | THR  |
| 29  | BB    | 104 | MET  |
| 30  | B5    | 7   | ARG  |
| 30  | B5    | 9   | ARG  |
| 30  | B5    | 166 | ASP  |
| 31  | B6    | 129 | LEU  |
| 31  | B6    | 212 | TRP  |
| 31  | B6    | 227 | VAL  |
| 31  | B6    | 264 | LYS  |
| 31  | B6    | 269 | ARG  |
| 32  | BD    | 74  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | BD    | 84  | LEU  |
| 32  | BD    | 86  | GLU  |
| 32  | BD    | 124 | ARG  |
| 32  | BD    | 128 | ARG  |
| 32  | BD    | 201 | LEU  |
| 33  | BE    | 60  | TRP  |
| 34  | BF    | 80  | GLN  |
| 34  | BF    | 119 | LYS  |
| 34  | BF    | 129 | MET  |
| 34  | BF    | 136 | ILE  |
| 35  | BG    | 34  | ARG  |
| 35  | BG    | 61  | TRP  |
| 35  | BG    | 94  | ARG  |
| 36  | BH    | 8   | LYS  |
| 36  | BH    | 21  | VAL  |
| 36  | BH    | 32  | PRO  |
| 36  | BH    | 70  | GLU  |
| 36  | BH    | 109 | GLU  |
| 36  | BH    | 144 | VAL  |
| 37  | BI    | 10  | LEU  |
| 37  | BI    | 35  | MET  |
| 37  | BI    | 95  | ASP  |
| 38  | BJ    | 23  | LYS  |
| 38  | BJ    | 35  | ARG  |
| 38  | BJ    | 129 | GLU  |
| 39  | BK    | 41  | ILE  |
| 39  | BK    | 70  | ARG  |
| 39  | BK    | 89  | ASN  |
| 39  | BK    | 114 | LYS  |
| 39  | BK    | 121 | GLU  |
| 40  | BL    | 126 | ARG  |
| 42  | BN    | 8   | ARG  |
| 42  | BN    | 49  | GLU  |
| 42  | BN    | 64  | ARG  |
| 44  | BP    | 43  | GLU  |
| 44  | BP    | 50  | ARG  |
| 44  | BP    | 87  | ARG  |
| 48  | BT    | 36  | LYS  |
| 48  | BT    | 61  | LEU  |
| 48  | BT    | 66  | LYS  |
| 48  | BT    | 69  | ARG  |
| 48  | BT    | 96  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | BU    | 49  | PRO  |
| 49  | BU    | 91  | LYS  |
| 50  | BV    | 46  | LYS  |
| 51  | BW    | 23  | LYS  |
| 52  | BX    | 26  | ARG  |
| 53  | BY    | 27  | ASN  |
| 54  | BZ    | 55  | LYS  |
| 55  | B0    | 31  | LYS  |
| 56  | B1    | 27  | ARG  |
| 57  | B2    | 12  | ARG  |
| 58  | B3    | 6   | VAL  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | AB    | 14  | HIS  |
| 6   | AB    | 169 | HIS  |
| 6   | AB    | 189 | ASN  |
| 7   | AC    | 175 | HIS  |
| 7   | AC    | 215 | GLN  |
| 8   | AD    | 40  | HIS  |
| 8   | AD    | 99  | ASN  |
| 14  | AJ    | 15  | HIS  |
| 15  | AK    | 108 | ASN  |
| 16  | AL    | 71  | HIS  |
| 18  | AN    | 48  | GLN  |
| 20  | AP    | 9   | HIS  |
| 20  | AP    | 18  | GLN  |
| 21  | AQ    | 50  | ASN  |
| 22  | AR    | 53  | GLN  |
| 23  | AS    | 13  | HIS  |
| 24  | AT    | 60  | GLN  |
| 24  | AT    | 67  | HIS  |
| 28  | BA    | 55  | GLN  |
| 28  | BA    | 212 | GLN  |
| 31  | B6    | 52  | HIS  |
| 31  | B6    | 57  | HIS  |
| 31  | B6    | 229 | HIS  |
| 31  | B6    | 238 | ASN  |
| 33  | BE    | 92  | HIS  |
| 35  | BG    | 100 | ASN  |
| 35  | BG    | 115 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | BH    | 2   | GLN  |
| 36  | BH    | 20  | ASN  |
| 36  | BH    | 128 | HIS  |
| 36  | BH    | 133 | GLN  |
| 38  | BJ    | 80  | HIS  |
| 38  | BJ    | 132 | HIS  |
| 39  | BK    | 5   | GLN  |
| 39  | BK    | 89  | ASN  |
| 42  | BN    | 16  | HIS  |
| 43  | BO    | 34  | HIS  |
| 45  | BQ    | 13  | HIS  |
| 46  | BR    | 82  | HIS  |
| 46  | BR    | 87  | GLN  |
| 50  | BV    | 88  | HIS  |
| 52  | BX    | 35  | HIS  |
| 55  | B0    | 18  | HIS  |
| 58  | B3    | 42  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1541/1542 (99%) | 273 (17%)         | 0               |
| 2   | AX    | 10/11 (90%)     | 5 (50%)           | 0               |
| 26  | B7    | 119/120 (99%)   | 19 (15%)          | 0               |
| 27  | B8    | 2903/2904 (99%) | 442 (15%)         | 0               |
| 3   | AV    | 76/77 (98%)     | 14 (18%)          | 0               |
| All | All   | 4649/4654 (99%) | 753 (16%)         | 0               |

All (753) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 2   | A    |
| 1   | AA    | 5   | U    |
| 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    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 51  | A    |
| 1   | AA    | 52  | C    |
| 1   | AA    | 55  | A    |
| 1   | AA    | 61  | G    |
| 1   | AA    | 66  | A    |
| 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    |
| 1   | AA    | 85  | U    |
| 1   | AA    | 86  | G    |
| 1   | AA    | 88  | U    |
| 1   | AA    | 91  | U    |
| 1   | AA    | 101 | A    |
| 1   | AA    | 121 | U    |
| 1   | AA    | 144 | G    |
| 1   | AA    | 149 | A    |
| 1   | AA    | 155 | A    |
| 1   | AA    | 182 | A    |
| 1   | AA    | 196 | 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    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 280 | C    |
| 1   | AA    | 289 | G    |
| 1   | AA    | 306 | A    |
| 1   | AA    | 308 | C    |
| 1   | AA    | 316 | 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    | 381 | C    |
| 1   | AA    | 382 | A    |
| 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    | 421 | U    |
| 1   | AA    | 424 | G    |
| 1   | AA    | 429 | U    |
| 1   | AA    | 430 | A    |
| 1   | AA    | 435 | A    |
| 1   | AA    | 451 | A    |
| 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    | 482 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 484 | G    |
| 1   | AA    | 485 | U    |
| 1   | AA    | 486 | U    |
| 1   | AA    | 493 | A    |
| 1   | AA    | 494 | G    |
| 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    | 532 | A    |
| 1   | AA    | 533 | A    |
| 1   | AA    | 535 | A    |
| 1   | AA    | 547 | A    |
| 1   | AA    | 561 | U    |
| 1   | AA    | 563 | A    |
| 1   | AA    | 564 | C    |
| 1   | AA    | 572 | A    |
| 1   | AA    | 573 | A    |
| 1   | AA    | 576 | C    |
| 1   | AA    | 577 | G    |
| 1   | AA    | 596 | A    |
| 1   | AA    | 611 | C    |
| 1   | AA    | 633 | G    |
| 1   | AA    | 653 | U    |
| 1   | AA    | 654 | G    |
| 1   | AA    | 665 | A    |
| 1   | AA    | 666 | 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    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 815  | A    |
| 1   | AA    | 817  | C    |
| 1   | AA    | 818  | G    |
| 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    |
| 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    | 966  | G    |
| 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    | 1014 | A    |
| 1   | AA    | 1015 | G    |
| 1   | AA    | 1018 | G    |
| 1   | AA    | 1020 | G    |
| 1   | AA    | 1028 | C    |
| 1   | AA    | 1030 | U    |
| 1   | AA    | 1032 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1034 | G    |
| 1   | AA    | 1036 | A    |
| 1   | AA    | 1043 | G    |
| 1   | AA    | 1050 | G    |
| 1   | AA    | 1053 | G    |
| 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    |
| 1   | AA    | 1124 | G    |
| 1   | AA    | 1125 | U    |
| 1   | AA    | 1130 | A    |
| 1   | AA    | 1133 | G    |
| 1   | AA    | 1135 | U    |
| 1   | AA    | 1136 | C    |
| 1   | AA    | 1139 | G    |
| 1   | AA    | 1140 | C    |
| 1   | AA    | 1141 | C    |
| 1   | AA    | 1143 | G    |
| 1   | AA    | 1145 | A    |
| 1   | AA    | 1146 | A    |
| 1   | AA    | 1152 | A    |
| 1   | AA    | 1154 | G    |
| 1   | AA    | 1159 | U    |
| 1   | AA    | 1160 | G    |
| 1   | AA    | 1167 | 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    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1225 | A    |
| 1   | AA    | 1226 | C    |
| 1   | AA    | 1227 | A    |
| 1   | AA    | 1238 | A    |
| 1   | AA    | 1249 | C    |
| 1   | AA    | 1250 | A    |
| 1   | AA    | 1258 | G    |
| 1   | AA    | 1261 | A    |
| 1   | AA    | 1270 | G    |
| 1   | AA    | 1279 | G    |
| 1   | AA    | 1280 | A    |
| 1   | AA    | 1285 | A    |
| 1   | AA    | 1286 | U    |
| 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    | 1323 | G    |
| 1   | AA    | 1331 | G    |
| 1   | AA    | 1346 | A    |
| 1   | AA    | 1353 | G    |
| 1   | AA    | 1363 | A    |
| 1   | AA    | 1364 | U    |
| 1   | AA    | 1380 | U    |
| 1   | AA    | 1399 | C    |
| 1   | AA    | 1419 | G    |
| 1   | AA    | 1432 | G    |
| 1   | AA    | 1446 | A    |
| 1   | AA    | 1448 | C    |
| 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    | 1507 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1517 | G    |
| 1   | AA    | 1520 | C    |
| 1   | AA    | 1526 | G    |
| 1   | AA    | 1528 | U    |
| 1   | AA    | 1529 | G    |
| 1   | AA    | 1530 | G    |
| 1   | AA    | 1535 | C    |
| 1   | AA    | 1539 | C    |
| 1   | AA    | 1540 | U    |
| 1   | AA    | 1541 | U    |
| 1   | AA    | 1542 | A    |
| 2   | AX    | 13   | C    |
| 2   | AX    | 14   | G    |
| 2   | AX    | 18   | C    |
| 2   | AX    | 19   | U    |
| 2   | AX    | 22   | A    |
| 3   | AV    | 4    | C    |
| 3   | AV    | 5    | A    |
| 3   | AV    | 6    | C    |
| 3   | AV    | 8    | U    |
| 3   | AV    | 20   | G    |
| 3   | AV    | 22   | A    |
| 3   | AV    | 32   | C    |
| 3   | AV    | 44   | G    |
| 3   | AV    | 49   | C    |
| 3   | AV    | 50   | G    |
| 3   | AV    | 54   | G    |
| 3   | AV    | 68   | G    |
| 3   | AV    | 72   | C    |
| 3   | AV    | 77   | A    |
| 26  | B7    | 9    | G    |
| 26  | B7    | 13   | G    |
| 26  | B7    | 14   | U    |
| 26  | B7    | 15   | A    |
| 26  | B7    | 16   | G    |
| 26  | B7    | 26   | C    |
| 26  | B7    | 29   | A    |
| 26  | B7    | 30   | C    |
| 26  | B7    | 42   | C    |
| 26  | B7    | 45   | A    |
| 26  | B7    | 52   | A    |
| 26  | B7    | 53   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | B7    | 66  | A    |
| 26  | B7    | 67  | G    |
| 26  | B7    | 90  | C    |
| 26  | B7    | 91  | C    |
| 26  | B7    | 99  | A    |
| 26  | B7    | 109 | A    |
| 26  | B7    | 120 | U    |
| 27  | B8    | 13  | A    |
| 27  | B8    | 34  | U    |
| 27  | B8    | 35  | G    |
| 27  | B8    | 46  | G    |
| 27  | B8    | 63  | A    |
| 27  | B8    | 64  | A    |
| 27  | B8    | 71  | A    |
| 27  | B8    | 74  | A    |
| 27  | B8    | 75  | G    |
| 27  | B8    | 84  | A    |
| 27  | B8    | 90  | U    |
| 27  | B8    | 91  | A    |
| 27  | B8    | 92  | U    |
| 27  | B8    | 93  | G    |
| 27  | B8    | 95  | A    |
| 27  | B8    | 100 | U    |
| 27  | B8    | 103 | A    |
| 27  | B8    | 118 | A    |
| 27  | B8    | 120 | U    |
| 27  | B8    | 136 | G    |
| 27  | B8    | 137 | U    |
| 27  | B8    | 139 | U    |
| 27  | B8    | 141 | G    |
| 27  | B8    | 143 | C    |
| 27  | B8    | 144 | A    |
| 27  | B8    | 160 | A    |
| 27  | B8    | 181 | A    |
| 27  | B8    | 196 | A    |
| 27  | B8    | 199 | A    |
| 27  | B8    | 216 | A    |
| 27  | B8    | 221 | A    |
| 27  | B8    | 222 | A    |
| 27  | B8    | 228 | C    |
| 27  | B8    | 233 | A    |
| 27  | B8    | 241 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | B8    | 248 | G    |
| 27  | B8    | 252 | G    |
| 27  | B8    | 255 | A    |
| 27  | B8    | 265 | A    |
| 27  | B8    | 266 | G    |
| 27  | B8    | 268 | C    |
| 27  | B8    | 271 | G    |
| 27  | B8    | 273 | G    |
| 27  | B8    | 277 | G    |
| 27  | B8    | 278 | A    |
| 27  | B8    | 281 | C    |
| 27  | B8    | 283 | G    |
| 27  | B8    | 285 | G    |
| 27  | B8    | 286 | U    |
| 27  | B8    | 294 | A    |
| 27  | B8    | 311 | A    |
| 27  | B8    | 321 | U    |
| 27  | B8    | 329 | G    |
| 27  | B8    | 330 | A    |
| 27  | B8    | 333 | G    |
| 27  | B8    | 346 | A    |
| 27  | B8    | 352 | A    |
| 27  | B8    | 353 | C    |
| 27  | B8    | 362 | A    |
| 27  | B8    | 363 | G    |
| 27  | B8    | 364 | C    |
| 27  | B8    | 371 | A    |
| 27  | B8    | 372 | G    |
| 27  | B8    | 386 | G    |
| 27  | B8    | 387 | U    |
| 27  | B8    | 405 | U    |
| 27  | B8    | 406 | G    |
| 27  | B8    | 411 | G    |
| 27  | B8    | 412 | A    |
| 27  | B8    | 424 | G    |
| 27  | B8    | 455 | C    |
| 27  | B8    | 457 | A    |
| 27  | B8    | 479 | A    |
| 27  | B8    | 481 | G    |
| 27  | B8    | 491 | G    |
| 27  | B8    | 505 | A    |
| 27  | B8    | 508 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | B8    | 509 | C    |
| 27  | B8    | 510 | C    |
| 27  | B8    | 512 | G    |
| 27  | B8    | 528 | A    |
| 27  | B8    | 531 | C    |
| 27  | B8    | 533 | G    |
| 27  | B8    | 544 | C    |
| 27  | B8    | 545 | U    |
| 27  | B8    | 546 | U    |
| 27  | B8    | 547 | A    |
| 27  | B8    | 548 | G    |
| 27  | B8    | 549 | G    |
| 27  | B8    | 555 | G    |
| 27  | B8    | 563 | A    |
| 27  | B8    | 573 | U    |
| 27  | B8    | 575 | A    |
| 27  | B8    | 586 | A    |
| 27  | B8    | 588 | U    |
| 27  | B8    | 603 | A    |
| 27  | B8    | 613 | A    |
| 27  | B8    | 637 | A    |
| 27  | B8    | 646 | U    |
| 27  | B8    | 647 | G    |
| 27  | B8    | 654 | A    |
| 27  | B8    | 655 | A    |
| 27  | B8    | 671 | C    |
| 27  | B8    | 686 | U    |
| 27  | B8    | 730 | A    |
| 27  | B8    | 747 | U    |
| 27  | B8    | 757 | G    |
| 27  | B8    | 764 | A    |
| 27  | B8    | 775 | G    |
| 27  | B8    | 776 | G    |
| 27  | B8    | 782 | A    |
| 27  | B8    | 784 | G    |
| 27  | B8    | 785 | G    |
| 27  | B8    | 788 | A    |
| 27  | B8    | 789 | A    |
| 27  | B8    | 793 | A    |
| 27  | B8    | 802 | A    |
| 27  | B8    | 805 | G    |
| 27  | B8    | 812 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | B8    | 819  | A    |
| 27  | B8    | 827  | U    |
| 27  | B8    | 828  | U    |
| 27  | B8    | 830  | G    |
| 27  | B8    | 846  | U    |
| 27  | B8    | 847  | U    |
| 27  | B8    | 859  | G    |
| 27  | B8    | 869  | G    |
| 27  | B8    | 871  | U    |
| 27  | B8    | 875  | G    |
| 27  | B8    | 876  | C    |
| 27  | B8    | 881  | G    |
| 27  | B8    | 887  | U    |
| 27  | B8    | 891  | G    |
| 27  | B8    | 896  | A    |
| 27  | B8    | 897  | C    |
| 27  | B8    | 900  | A    |
| 27  | B8    | 901  | C    |
| 27  | B8    | 910  | A    |
| 27  | B8    | 912  | C    |
| 27  | B8    | 919  | U    |
| 27  | B8    | 931  | U    |
| 27  | B8    | 932  | U    |
| 27  | B8    | 941  | A    |
| 27  | B8    | 945  | A    |
| 27  | B8    | 946  | C    |
| 27  | B8    | 961  | C    |
| 27  | B8    | 973  | A    |
| 27  | B8    | 974  | G    |
| 27  | B8    | 980  | A    |
| 27  | B8    | 982  | C    |
| 27  | B8    | 983  | A    |
| 27  | B8    | 985  | C    |
| 27  | B8    | 991  | C    |
| 27  | B8    | 995  | C    |
| 27  | B8    | 996  | A    |
| 27  | B8    | 1005 | C    |
| 27  | B8    | 1012 | U    |
| 27  | B8    | 1013 | C    |
| 27  | B8    | 1022 | G    |
| 27  | B8    | 1025 | G    |
| 27  | B8    | 1033 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | B8    | 1054 | A    |
| 27  | B8    | 1056 | G    |
| 27  | B8    | 1061 | U    |
| 27  | B8    | 1062 | G    |
| 27  | B8    | 1070 | A    |
| 27  | B8    | 1071 | G    |
| 27  | B8    | 1078 | U    |
| 27  | B8    | 1088 | A    |
| 27  | B8    | 1090 | A    |
| 27  | B8    | 1095 | A    |
| 27  | B8    | 1096 | A    |
| 27  | B8    | 1104 | C    |
| 27  | B8    | 1112 | G    |
| 27  | B8    | 1116 | G    |
| 27  | B8    | 1130 | U    |
| 27  | B8    | 1132 | U    |
| 27  | B8    | 1133 | A    |
| 27  | B8    | 1134 | A    |
| 27  | B8    | 1135 | C    |
| 27  | B8    | 1136 | G    |
| 27  | B8    | 1139 | G    |
| 27  | B8    | 1142 | A    |
| 27  | B8    | 1176 | U    |
| 27  | B8    | 1206 | G    |
| 27  | B8    | 1237 | A    |
| 27  | B8    | 1238 | G    |
| 27  | B8    | 1241 | A    |
| 27  | B8    | 1242 | U    |
| 27  | B8    | 1248 | G    |
| 27  | B8    | 1250 | G    |
| 27  | B8    | 1253 | A    |
| 27  | B8    | 1256 | G    |
| 27  | B8    | 1266 | G    |
| 27  | B8    | 1271 | G    |
| 27  | B8    | 1272 | A    |
| 27  | B8    | 1273 | U    |
| 27  | B8    | 1275 | A    |
| 27  | B8    | 1276 | A    |
| 27  | B8    | 1300 | G    |
| 27  | B8    | 1301 | A    |
| 27  | B8    | 1312 | U    |
| 27  | B8    | 1313 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | B8    | 1316 | U    |
| 27  | B8    | 1325 | U    |
| 27  | B8    | 1326 | U    |
| 27  | B8    | 1334 | G    |
| 27  | B8    | 1336 | A    |
| 27  | B8    | 1337 | G    |
| 27  | B8    | 1352 | U    |
| 27  | B8    | 1365 | A    |
| 27  | B8    | 1374 | G    |
| 27  | B8    | 1379 | U    |
| 27  | B8    | 1386 | C    |
| 27  | B8    | 1394 | U    |
| 27  | B8    | 1396 | U    |
| 27  | B8    | 1416 | G    |
| 27  | B8    | 1419 | A    |
| 27  | B8    | 1420 | A    |
| 27  | B8    | 1421 | G    |
| 27  | B8    | 1427 | A    |
| 27  | B8    | 1428 | C    |
| 27  | B8    | 1451 | C    |
| 27  | B8    | 1454 | C    |
| 27  | B8    | 1459 | G    |
| 27  | B8    | 1460 | U    |
| 27  | B8    | 1461 | C    |
| 27  | B8    | 1469 | A    |
| 27  | B8    | 1476 | U    |
| 27  | B8    | 1477 | A    |
| 27  | B8    | 1478 | G    |
| 27  | B8    | 1482 | G    |
| 27  | B8    | 1490 | A    |
| 27  | B8    | 1497 | U    |
| 27  | B8    | 1504 | A    |
| 27  | B8    | 1505 | A    |
| 27  | B8    | 1507 | C    |
| 27  | B8    | 1508 | A    |
| 27  | B8    | 1509 | A    |
| 27  | B8    | 1523 | U    |
| 27  | B8    | 1524 | G    |
| 27  | B8    | 1532 | A    |
| 27  | B8    | 1535 | A    |
| 27  | B8    | 1538 | G    |
| 27  | B8    | 1552 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | B8    | 1560 | G    |
| 27  | B8    | 1569 | A    |
| 27  | B8    | 1578 | U    |
| 27  | B8    | 1583 | A    |
| 27  | B8    | 1585 | C    |
| 27  | B8    | 1608 | A    |
| 27  | B8    | 1609 | A    |
| 27  | B8    | 1610 | A    |
| 27  | B8    | 1618 | A    |
| 27  | B8    | 1634 | A    |
| 27  | B8    | 1635 | A    |
| 27  | B8    | 1640 | A    |
| 27  | B8    | 1647 | U    |
| 27  | B8    | 1648 | U    |
| 27  | B8    | 1654 | A    |
| 27  | B8    | 1674 | G    |
| 27  | B8    | 1677 | A    |
| 27  | B8    | 1700 | A    |
| 27  | B8    | 1714 | U    |
| 27  | B8    | 1715 | G    |
| 27  | B8    | 1729 | U    |
| 27  | B8    | 1730 | C    |
| 27  | B8    | 1731 | G    |
| 27  | B8    | 1733 | G    |
| 27  | B8    | 1738 | G    |
| 27  | B8    | 1756 | G    |
| 27  | B8    | 1758 | U    |
| 27  | B8    | 1761 | C    |
| 27  | B8    | 1764 | C    |
| 27  | B8    | 1773 | A    |
| 27  | B8    | 1776 | G    |
| 27  | B8    | 1781 | U    |
| 27  | B8    | 1782 | U    |
| 27  | B8    | 1784 | A    |
| 27  | B8    | 1800 | C    |
| 27  | B8    | 1801 | A    |
| 27  | B8    | 1808 | A    |
| 27  | B8    | 1809 | A    |
| 27  | B8    | 1816 | C    |
| 27  | B8    | 1819 | A    |
| 27  | B8    | 1829 | A    |
| 27  | B8    | 1870 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | B8    | 1896 | G    |
| 27  | B8    | 1906 | G    |
| 27  | B8    | 1913 | A    |
| 27  | B8    | 1914 | C    |
| 27  | B8    | 1929 | G    |
| 27  | B8    | 1930 | G    |
| 27  | B8    | 1940 | U    |
| 27  | B8    | 1955 | U    |
| 27  | B8    | 1965 | C    |
| 27  | B8    | 1966 | A    |
| 27  | B8    | 1967 | C    |
| 27  | B8    | 1970 | A    |
| 27  | B8    | 1971 | U    |
| 27  | B8    | 1972 | G    |
| 27  | B8    | 1991 | U    |
| 27  | B8    | 1993 | U    |
| 27  | B8    | 1997 | C    |
| 27  | B8    | 2020 | A    |
| 27  | B8    | 2022 | U    |
| 27  | B8    | 2023 | C    |
| 27  | B8    | 2031 | A    |
| 27  | B8    | 2033 | A    |
| 27  | B8    | 2043 | C    |
| 27  | B8    | 2055 | C    |
| 27  | B8    | 2056 | G    |
| 27  | B8    | 2059 | A    |
| 27  | B8    | 2061 | G    |
| 27  | B8    | 2062 | A    |
| 27  | B8    | 2065 | C    |
| 27  | B8    | 2069 | G    |
| 27  | B8    | 2077 | A    |
| 27  | B8    | 2102 | G    |
| 27  | B8    | 2104 | C    |
| 27  | B8    | 2111 | U    |
| 27  | B8    | 2116 | G    |
| 27  | B8    | 2117 | A    |
| 27  | B8    | 2118 | U    |
| 27  | B8    | 2119 | A    |
| 27  | B8    | 2120 | G    |
| 27  | B8    | 2128 | G    |
| 27  | B8    | 2133 | G    |
| 27  | B8    | 2135 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | B8    | 2136 | G    |
| 27  | B8    | 2137 | U    |
| 27  | B8    | 2138 | G    |
| 27  | B8    | 2145 | C    |
| 27  | B8    | 2146 | C    |
| 27  | B8    | 2147 | A    |
| 27  | B8    | 2148 | G    |
| 27  | B8    | 2149 | U    |
| 27  | B8    | 2153 | C    |
| 27  | B8    | 2155 | U    |
| 27  | B8    | 2158 | A    |
| 27  | B8    | 2164 | C    |
| 27  | B8    | 2165 | C    |
| 27  | B8    | 2166 | U    |
| 27  | B8    | 2167 | U    |
| 27  | B8    | 2176 | A    |
| 27  | B8    | 2179 | C    |
| 27  | B8    | 2181 | U    |
| 27  | B8    | 2192 | U    |
| 27  | B8    | 2198 | A    |
| 27  | B8    | 2199 | A    |
| 27  | B8    | 2204 | G    |
| 27  | B8    | 2212 | A    |
| 27  | B8    | 2213 | U    |
| 27  | B8    | 2214 | C    |
| 27  | B8    | 2225 | A    |
| 27  | B8    | 2238 | G    |
| 27  | B8    | 2239 | G    |
| 27  | B8    | 2250 | G    |
| 27  | B8    | 2251 | G    |
| 27  | B8    | 2266 | A    |
| 27  | B8    | 2271 | G    |
| 27  | B8    | 2278 | A    |
| 27  | B8    | 2279 | G    |
| 27  | B8    | 2283 | C    |
| 27  | B8    | 2286 | G    |
| 27  | B8    | 2287 | A    |
| 27  | B8    | 2297 | A    |
| 27  | B8    | 2305 | U    |
| 27  | B8    | 2307 | G    |
| 27  | B8    | 2308 | G    |
| 27  | B8    | 2311 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | B8    | 2322 | A    |
| 27  | B8    | 2324 | U    |
| 27  | B8    | 2325 | G    |
| 27  | B8    | 2333 | A    |
| 27  | B8    | 2335 | A    |
| 27  | B8    | 2336 | A    |
| 27  | B8    | 2337 | G    |
| 27  | B8    | 2347 | C    |
| 27  | B8    | 2357 | G    |
| 27  | B8    | 2383 | G    |
| 27  | B8    | 2385 | C    |
| 27  | B8    | 2396 | G    |
| 27  | B8    | 2407 | A    |
| 27  | B8    | 2426 | A    |
| 27  | B8    | 2429 | G    |
| 27  | B8    | 2430 | A    |
| 27  | B8    | 2434 | A    |
| 27  | B8    | 2441 | U    |
| 27  | B8    | 2448 | A    |
| 27  | B8    | 2458 | G    |
| 27  | B8    | 2472 | G    |
| 27  | B8    | 2473 | U    |
| 27  | B8    | 2476 | A    |
| 27  | B8    | 2478 | A    |
| 27  | B8    | 2491 | U    |
| 27  | B8    | 2498 | C    |
| 27  | B8    | 2505 | G    |
| 27  | B8    | 2506 | U    |
| 27  | B8    | 2518 | A    |
| 27  | B8    | 2529 | G    |
| 27  | B8    | 2530 | A    |
| 27  | B8    | 2534 | A    |
| 27  | B8    | 2535 | G    |
| 27  | B8    | 2554 | U    |
| 27  | B8    | 2566 | A    |
| 27  | B8    | 2567 | G    |
| 27  | B8    | 2573 | C    |
| 27  | B8    | 2585 | U    |
| 27  | B8    | 2586 | U    |
| 27  | B8    | 2602 | A    |
| 27  | B8    | 2609 | U    |
| 27  | B8    | 2613 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 27  | B8    | 2629 | U    |
| 27  | B8    | 2630 | G    |
| 27  | B8    | 2689 | U    |
| 27  | B8    | 2690 | U    |
| 27  | B8    | 2714 | G    |
| 27  | B8    | 2726 | A    |
| 27  | B8    | 2729 | G    |
| 27  | B8    | 2744 | G    |
| 27  | B8    | 2748 | A    |
| 27  | B8    | 2757 | A    |
| 27  | B8    | 2765 | A    |
| 27  | B8    | 2778 | A    |
| 27  | B8    | 2791 | G    |
| 27  | B8    | 2793 | C    |
| 27  | B8    | 2799 | A    |
| 27  | B8    | 2800 | A    |
| 27  | B8    | 2808 | G    |
| 27  | B8    | 2809 | A    |
| 27  | B8    | 2820 | A    |
| 27  | B8    | 2821 | A    |
| 27  | B8    | 2832 | U    |
| 27  | B8    | 2836 | U    |
| 27  | B8    | 2849 | U    |
| 27  | B8    | 2850 | A    |
| 27  | B8    | 2867 | G    |
| 27  | B8    | 2872 | A    |
| 27  | B8    | 2873 | A    |
| 27  | B8    | 2883 | A    |
| 27  | B8    | 2904 | U    |

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

133 ligands are 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$ |
| 60  | PEV  | A0    | 301 | -    | 48,48,48     | 0.78 | 1 (2%)      | 50,53,53    | 0.69 | 2 (4%)      |
| 60  | PEV  | A0    | 302 | -    | 48,48,48     | 0.78 | 2 (4%)      | 50,53,53    | 0.70 | 2 (4%)      |
| 60  | PEV  | A0    | 303 | -    | 48,48,48     | 0.80 | 2 (4%)      | 50,53,53    | 0.70 | 2 (4%)      |
| 61  | PGV  | A0    | 304 | -    | 50,50,50     | 1.09 | 3 (6%)      | 51,56,56    | 0.87 | 2 (3%)      |
| 61  | PGV  | A0    | 305 | -    | 50,50,50     | 1.07 | 2 (4%)      | 51,56,56    | 0.79 | 2 (3%)      |
| 61  | PGV  | A0    | 306 | -    | 50,50,50     | 1.08 | 2 (4%)      | 51,56,56    | 0.81 | 2 (3%)      |
| 60  | PEV  | A0    | 307 | -    | 48,48,48     | 0.77 | 1 (2%)      | 50,53,53    | 0.65 | 2 (4%)      |
| 60  | PEV  | A0    | 308 | -    | 48,48,48     | 0.79 | 2 (4%)      | 50,53,53    | 0.75 | 2 (4%)      |
| 60  | PEV  | A0    | 309 | -    | 48,48,48     | 0.80 | 2 (4%)      | 50,53,53    | 0.69 | 2 (4%)      |
| 60  | PEV  | A0    | 310 | -    | 48,48,48     | 0.79 | 2 (4%)      | 50,53,53    | 0.84 | 2 (4%)      |
| 60  | PEV  | A0    | 311 | -    | 48,48,48     | 0.78 | 1 (2%)      | 50,53,53    | 0.67 | 2 (4%)      |
| 60  | PEV  | A0    | 312 | -    | 48,48,48     | 0.79 | 1 (2%)      | 50,53,53    | 0.61 | 2 (4%)      |
| 60  | PEV  | A0    | 313 | -    | 48,48,48     | 0.81 | 2 (4%)      | 50,53,53    | 0.74 | 2 (4%)      |
| 60  | PEV  | A0    | 314 | -    | 48,48,48     | 0.80 | 2 (4%)      | 50,53,53    | 0.70 | 2 (4%)      |
| 60  | PEV  | A0    | 315 | -    | 48,48,48     | 0.76 | 1 (2%)      | 50,53,53    | 0.64 | 2 (4%)      |
| 60  | PEV  | A0    | 316 | -    | 48,48,48     | 0.80 | 1 (2%)      | 50,53,53    | 0.84 | 2 (4%)      |
| 61  | PGV  | A0    | 317 | -    | 50,50,50     | 1.08 | 2 (4%)      | 51,56,56    | 0.90 | 2 (3%)      |
| 61  | PGV  | A0    | 318 | -    | 50,50,50     | 1.09 | 2 (4%)      | 51,56,56    | 0.80 | 2 (3%)      |
| 60  | PEV  | A0    | 319 | -    | 48,48,48     | 0.79 | 1 (2%)      | 50,53,53    | 0.74 | 2 (4%)      |
| 60  | PEV  | A0    | 320 | -    | 48,48,48     | 0.80 | 1 (2%)      | 50,53,53    | 0.65 | 2 (4%)      |
| 60  | PEV  | A0    | 321 | -    | 48,48,48     | 0.79 | 1 (2%)      | 50,53,53    | 0.83 | 4 (8%)      |
| 60  | PEV  | A0    | 322 | -    | 48,48,48     | 0.79 | 1 (2%)      | 50,53,53    | 0.75 | 2 (4%)      |
| 60  | PEV  | A0    | 323 | -    | 48,48,48     | 0.77 | 1 (2%)      | 50,53,53    | 0.71 | 2 (4%)      |
| 60  | PEV  | A0    | 324 | -    | 48,48,48     | 0.79 | 2 (4%)      | 50,53,53    | 0.71 | 2 (4%)      |
| 61  | PGV  | A0    | 325 | -    | 50,50,50     | 1.09 | 2 (4%)      | 51,56,56    | 0.92 | 2 (3%)      |
| 60  | PEV  | A0    | 326 | -    | 48,48,48     | 0.76 | 1 (2%)      | 50,53,53    | 0.71 | 2 (4%)      |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 61  | PGV  | A0    | 327 | -    | 50,50,50     | 1.10 | 2 (4%)   | 51,56,56    | 0.77 | 2 (3%)   |
| 61  | PGV  | A0    | 328 | -    | 50,50,50     | 1.08 | 2 (4%)   | 51,56,56    | 0.82 | 2 (3%)   |
| 60  | PEV  | A0    | 329 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.72 | 2 (4%)   |
| 60  | PEV  | A0    | 330 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.66 | 2 (4%)   |
| 61  | PGV  | A0    | 331 | -    | 50,50,50     | 1.07 | 2 (4%)   | 51,56,56    | 0.83 | 2 (3%)   |
| 61  | PGV  | A0    | 332 | -    | 50,50,50     | 1.09 | 2 (4%)   | 51,56,56    | 0.82 | 2 (3%)   |
| 60  | PEV  | A1    | 301 | -    | 48,48,48     | 0.78 | 2 (4%)   | 50,53,53    | 0.72 | 2 (4%)   |
| 60  | PEV  | A1    | 302 | -    | 48,48,48     | 0.79 | 2 (4%)   | 50,53,53    | 0.72 | 2 (4%)   |
| 61  | PGV  | A1    | 303 | -    | 50,50,50     | 1.08 | 2 (4%)   | 51,56,56    | 0.81 | 2 (3%)   |
| 60  | PEV  | A1    | 304 | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.63 | 2 (4%)   |
| 60  | PEV  | A1    | 305 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.69 | 2 (4%)   |
| 60  | PEV  | A1    | 306 | -    | 48,48,48     | 0.79 | 1 (2%)   | 50,53,53    | 0.63 | 2 (4%)   |
| 60  | PEV  | A1    | 307 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.69 | 2 (4%)   |
| 60  | PEV  | A1    | 308 | -    | 48,48,48     | 0.80 | 2 (4%)   | 50,53,53    | 0.65 | 2 (4%)   |
| 60  | PEV  | A1    | 309 | -    | 48,48,48     | 0.78 | 2 (4%)   | 50,53,53    | 0.74 | 2 (4%)   |
| 60  | PEV  | A1    | 310 | -    | 48,48,48     | 0.77 | 2 (4%)   | 50,53,53    | 0.73 | 2 (4%)   |
| 61  | PGV  | A1    | 311 | -    | 50,50,50     | 1.09 | 2 (4%)   | 51,56,56    | 0.87 | 2 (3%)   |
| 60  | PEV  | A1    | 312 | -    | 48,48,48     | 0.78 | 2 (4%)   | 50,53,53    | 0.68 | 2 (4%)   |
| 60  | PEV  | A1    | 313 | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.73 | 2 (4%)   |
| 60  | PEV  | A1    | 314 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.70 | 2 (4%)   |
| 61  | PGV  | A1    | 315 | -    | 50,50,50     | 1.10 | 4 (8%)   | 51,56,56    | 0.86 | 2 (3%)   |
| 60  | PEV  | A1    | 316 | -    | 48,48,48     | 0.78 | 2 (4%)   | 50,53,53    | 0.75 | 2 (4%)   |
| 60  | PEV  | A1    | 317 | -    | 48,48,48     | 0.79 | 2 (4%)   | 50,53,53    | 0.70 | 3 (6%)   |
| 61  | PGV  | A1    | 318 | -    | 50,50,50     | 1.09 | 2 (4%)   | 51,56,56    | 0.85 | 2 (3%)   |
| 60  | PEV  | A1    | 319 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.66 | 1 (2%)   |
| 60  | PEV  | A1    | 320 | -    | 48,48,48     | 0.79 | 2 (4%)   | 50,53,53    | 0.71 | 2 (4%)   |
| 60  | PEV  | A1    | 321 | -    | 48,48,48     | 0.79 | 1 (2%)   | 50,53,53    | 0.68 | 2 (4%)   |
| 60  | PEV  | A1    | 322 | -    | 48,48,48     | 0.76 | 1 (2%)   | 50,53,53    | 0.70 | 2 (4%)   |
| 60  | PEV  | A1    | 323 | -    | 48,48,48     | 0.76 | 1 (2%)   | 50,53,53    | 0.67 | 2 (4%)   |
| 60  | PEV  | A1    | 324 | -    | 48,48,48     | 0.79 | 1 (2%)   | 50,53,53    | 0.65 | 2 (4%)   |
| 60  | PEV  | A1    | 325 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.66 | 2 (4%)   |
| 60  | PEV  | A1    | 326 | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.69 | 2 (4%)   |
| 60  | PEV  | A1    | 327 | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.68 | 2 (4%)   |
| 60  | PEV  | A1    | 328 | -    | 48,48,48     | 0.76 | 1 (2%)   | 50,53,53    | 0.68 | 2 (4%)   |
| 60  | PEV  | A1    | 329 | -    | 48,48,48     | 0.79 | 2 (4%)   | 50,53,53    | 0.72 | 2 (4%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 60  | PEV  | AZ    | 201  | -    | 48,48,48     | 0.75 | 1 (2%)   | 50,53,53    | 0.70 | 2 (4%)   |
| 60  | PEV  | AZ    | 202  | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.72 | 2 (4%)   |
| 60  | PEV  | AZ    | 203  | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.62 | 2 (4%)   |
| 60  | PEV  | AZ    | 204  | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.68 | 2 (4%)   |
| 61  | PGV  | AZ    | 205  | -    | 50,50,50     | 1.08 | 2 (4%)   | 51,56,56    | 0.82 | 2 (3%)   |
| 60  | PEV  | AZ    | 206  | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.62 | 2 (4%)   |
| 61  | PGV  | AZ    | 207  | -    | 50,50,50     | 1.08 | 2 (4%)   | 51,56,56    | 0.81 | 2 (3%)   |
| 60  | PEV  | B8    | 3001 | -    | 48,48,48     | 0.79 | 2 (4%)   | 50,53,53    | 0.72 | 2 (4%)   |
| 60  | PEV  | B8    | 3002 | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.66 | 2 (4%)   |
| 60  | PEV  | B8    | 3003 | -    | 48,48,48     | 0.79 | 1 (2%)   | 50,53,53    | 0.72 | 2 (4%)   |
| 60  | PEV  | B8    | 3004 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.70 | 2 (4%)   |
| 61  | PGV  | B8    | 3005 | -    | 50,50,50     | 1.08 | 2 (4%)   | 51,56,56    | 0.78 | 2 (3%)   |
| 60  | PEV  | B8    | 3006 | -    | 48,48,48     | 0.79 | 1 (2%)   | 50,53,53    | 0.67 | 2 (4%)   |
| 60  | PEV  | B8    | 3007 | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.64 | 2 (4%)   |
| 61  | PGV  | BA    | 501  | -    | 50,50,50     | 1.08 | 2 (4%)   | 51,56,56    | 0.87 | 2 (3%)   |
| 60  | PEV  | BA    | 502  | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.71 | 2 (4%)   |
| 60  | PEV  | BA    | 503  | -    | 48,48,48     | 0.80 | 3 (6%)   | 50,53,53    | 0.74 | 2 (4%)   |
| 60  | PEV  | BA    | 504  | -    | 48,48,48     | 0.79 | 2 (4%)   | 50,53,53    | 0.80 | 2 (4%)   |
| 61  | PGV  | BA    | 505  | -    | 50,50,50     | 1.08 | 2 (4%)   | 51,56,56    | 0.83 | 2 (3%)   |
| 60  | PEV  | BA    | 506  | -    | 48,48,48     | 0.74 | 1 (2%)   | 50,53,53    | 0.70 | 2 (4%)   |
| 60  | PEV  | BA    | 507  | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.69 | 2 (4%)   |
| 60  | PEV  | BA    | 508  | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.68 | 2 (4%)   |
| 60  | PEV  | BA    | 509  | -    | 48,48,48     | 0.80 | 2 (4%)   | 50,53,53    | 0.75 | 2 (4%)   |
| 60  | PEV  | BA    | 510  | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.70 | 2 (4%)   |
| 60  | PEV  | BA    | 511  | -    | 48,48,48     | 0.75 | 1 (2%)   | 50,53,53    | 0.70 | 2 (4%)   |
| 61  | PGV  | BA    | 512  | -    | 50,50,50     | 1.07 | 2 (4%)   | 51,56,56    | 0.81 | 2 (3%)   |
| 60  | PEV  | BA    | 513  | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.69 | 2 (4%)   |
| 60  | PEV  | BA    | 514  | -    | 48,48,48     | 0.80 | 2 (4%)   | 50,53,53    | 0.76 | 2 (4%)   |
| 61  | PGV  | BA    | 515  | -    | 50,50,50     | 1.08 | 2 (4%)   | 51,56,56    | 0.80 | 2 (3%)   |
| 61  | PGV  | BA    | 516  | -    | 50,50,50     | 1.09 | 2 (4%)   | 51,56,56    | 0.75 | 2 (3%)   |
| 60  | PEV  | BA    | 517  | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.69 | 2 (4%)   |
| 60  | PEV  | BA    | 518  | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.67 | 2 (4%)   |
| 60  | PEV  | BA    | 519  | -    | 48,48,48     | 0.79 | 2 (4%)   | 50,53,53    | 0.74 | 2 (4%)   |
| 60  | PEV  | BA    | 520  | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.64 | 2 (4%)   |
| 60  | PEV  | BA    | 521  | -    | 48,48,48     | 0.78 | 2 (4%)   | 50,53,53    | 0.67 | 2 (4%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 61  | PGV  | BA    | 522 | -    | 50,50,50     | 1.09 | 2 (4%)   | 51,56,56    | 0.76 | 2 (3%)   |
| 60  | PEV  | BA    | 523 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.74 | 2 (4%)   |
| 60  | PEV  | BA    | 524 | -    | 48,48,48     | 0.80 | 2 (4%)   | 50,53,53    | 0.71 | 2 (4%)   |
| 60  | PEV  | BA    | 525 | -    | 48,48,48     | 0.79 | 2 (4%)   | 50,53,53    | 0.75 | 2 (4%)   |
| 60  | PEV  | BA    | 526 | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.69 | 2 (4%)   |
| 60  | PEV  | BA    | 527 | -    | 48,48,48     | 0.79 | 1 (2%)   | 50,53,53    | 0.76 | 2 (4%)   |
| 60  | PEV  | BA    | 528 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.72 | 2 (4%)   |
| 60  | PEV  | BA    | 529 | -    | 48,48,48     | 0.80 | 2 (4%)   | 50,53,53    | 0.70 | 2 (4%)   |
| 60  | PEV  | BA    | 530 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.67 | 2 (4%)   |
| 60  | PEV  | BA    | 531 | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.66 | 2 (4%)   |
| 60  | PEV  | BA    | 532 | -    | 48,48,48     | 0.76 | 1 (2%)   | 50,53,53    | 0.75 | 2 (4%)   |
| 60  | PEV  | BA    | 533 | -    | 48,48,48     | 2.66 | 1 (2%)   | 50,53,53    | 1.32 | 2 (4%)   |
| 60  | PEV  | BA    | 534 | -    | 48,48,48     | 0.82 | 3 (6%)   | 50,53,53    | 0.77 | 3 (6%)   |
| 60  | PEV  | BA    | 535 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.67 | 2 (4%)   |
| 61  | PGV  | BA    | 536 | -    | 50,50,50     | 1.08 | 2 (4%)   | 51,56,56    | 0.79 | 2 (3%)   |
| 60  | PEV  | BA    | 537 | -    | 48,48,48     | 0.81 | 2 (4%)   | 50,53,53    | 0.75 | 2 (4%)   |
| 60  | PEV  | BA    | 538 | -    | 48,48,48     | 0.75 | 1 (2%)   | 50,53,53    | 0.65 | 2 (4%)   |
| 60  | PEV  | BA    | 539 | -    | 48,48,48     | 0.79 | 2 (4%)   | 50,53,53    | 0.80 | 2 (4%)   |
| 61  | PGV  | BA    | 540 | -    | 50,50,50     | 1.07 | 2 (4%)   | 51,56,56    | 0.83 | 2 (3%)   |
| 60  | PEV  | BB    | 201 | -    | 48,48,48     | 0.79 | 1 (2%)   | 50,53,53    | 0.70 | 2 (4%)   |
| 60  | PEV  | BB    | 202 | -    | 48,48,48     | 0.78 | 2 (4%)   | 50,53,53    | 0.71 | 2 (4%)   |
| 61  | PGV  | BB    | 203 | -    | 50,50,50     | 1.09 | 2 (4%)   | 51,56,56    | 0.83 | 2 (3%)   |
| 61  | PGV  | BB    | 204 | -    | 50,50,50     | 1.09 | 3 (6%)   | 51,56,56    | 0.87 | 3 (5%)   |
| 61  | PGV  | BB    | 205 | -    | 50,50,50     | 1.07 | 2 (4%)   | 51,56,56    | 0.87 | 2 (3%)   |
| 60  | PEV  | BB    | 206 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.69 | 2 (4%)   |
| 61  | PGV  | BB    | 207 | -    | 50,50,50     | 1.09 | 2 (4%)   | 51,56,56    | 0.83 | 2 (3%)   |
| 61  | PGV  | BB    | 208 | -    | 50,50,50     | 1.09 | 2 (4%)   | 51,56,56    | 0.80 | 2 (3%)   |
| 60  | PEV  | BB    | 209 | -    | 48,48,48     | 0.76 | 1 (2%)   | 50,53,53    | 0.69 | 2 (4%)   |
| 60  | PEV  | BB    | 210 | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.73 | 2 (4%)   |
| 60  | PEV  | BB    | 211 | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.72 | 2 (4%)   |
| 60  | PEV  | BB    | 212 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.66 | 2 (4%)   |
| 61  | PGV  | BB    | 213 | -    | 50,50,50     | 1.09 | 2 (4%)   | 51,56,56    | 0.86 | 2 (3%)   |
| 60  | PEV  | BB    | 214 | -    | 48,48,48     | 0.78 | 1 (2%)   | 50,53,53    | 0.71 | 2 (4%)   |
| 60  | PEV  | BB    | 215 | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.70 | 2 (4%)   |
| 60  | PEV  | BB    | 216 | -    | 48,48,48     | 0.78 | 2 (4%)   | 50,53,53    | 0.78 | 2 (4%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 61  | PGV  | BB    | 217 | -    | 50,50,50     | 1.08 | 2 (4%)   | 51,56,56    | 0.82 | 2 (3%)   |
| 60  | PEV  | BB    | 218 | -    | 48,48,48     | 0.77 | 1 (2%)   | 50,53,53    | 0.71 | 2 (4%)   |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 60  | PEV  | A0    | 301 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 302 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 303 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | A0    | 304 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 61  | PGV  | A0    | 305 | -    | 1/1/5/7 | 0/55/55/55 | 0/0/0/0 |
| 61  | PGV  | A0    | 306 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | A0    | 307 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 308 | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 309 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 310 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 311 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 312 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 313 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 314 | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 315 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 316 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | A0    | 317 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 61  | PGV  | A0    | 318 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | A0    | 319 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 320 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 321 | -    | -       | 2/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 322 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 323 | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 324 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | A0    | 325 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | A0    | 326 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | A0    | 327 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 61  | PGV  | A0    | 328 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | A0    | 329 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A0    | 330 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | A0    | 331 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 61  | PGV  | A0    | 332  | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | A1    | 301  | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 302  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | A1    | 303  | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | A1    | 304  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 305  | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 306  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 307  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 308  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 309  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 310  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | A1    | 311  | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | A1    | 312  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 313  | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 314  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | A1    | 315  | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | A1    | 316  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 317  | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | A1    | 318  | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | A1    | 319  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 320  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 321  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 322  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 323  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 324  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 325  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 326  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 327  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 328  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | A1    | 329  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | AZ    | 201  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | AZ    | 202  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | AZ    | 203  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | AZ    | 204  | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | AZ    | 205  | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | AZ    | 206  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | AZ    | 207  | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | B8    | 3001 | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | B8    | 3002 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | B8    | 3003 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | B8    | 3004 | -    | -       | 0/52/52/52 | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 61  | PGV  | B8    | 3005 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | B8    | 3006 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | B8    | 3007 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | BA    | 501  | -    | 1/1/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | BA    | 502  | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 503  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 504  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | BA    | 505  | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | BA    | 506  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 507  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 508  | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 509  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 510  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 511  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | BA    | 512  | -    | 1/1/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | BA    | 513  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 514  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | BA    | 515  | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 61  | PGV  | BA    | 516  | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | BA    | 517  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 518  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 519  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 520  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 521  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | BA    | 522  | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | BA    | 523  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 524  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 525  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 526  | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 527  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 528  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 529  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 530  | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 531  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 532  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 533  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 534  | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 535  | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | BA    | 536  | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | BA    | 537  | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BA    | 538  | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 60  | PEV  | BA    | 539 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | BA    | 540 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | BB    | 201 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BB    | 202 | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | BB    | 203 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 61  | PGV  | BB    | 204 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 61  | PGV  | BB    | 205 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | BB    | 206 | -    | 1/1/4/4 | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | BB    | 207 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 61  | PGV  | BB    | 208 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | BB    | 209 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BB    | 210 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BB    | 211 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BB    | 212 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | BB    | 213 | -    | 1/1/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | BB    | 214 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BB    | 215 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 60  | PEV  | BB    | 216 | -    | -       | 0/52/52/52 | 0/0/0/0 |
| 61  | PGV  | BB    | 217 | -    | 2/2/5/7 | 0/55/55/55 | 0/0/0/0 |
| 60  | PEV  | BB    | 218 | -    | -       | 0/52/52/52 | 0/0/0/0 |

All (204) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 61  | BA    | 516 | PGV  | C9-C10 | -4.69 | 1.34        | 1.52     |
| 61  | BB    | 213 | PGV  | C9-C10 | -4.67 | 1.34        | 1.52     |
| 61  | BA    | 522 | PGV  | C9-C10 | -4.63 | 1.34        | 1.52     |
| 61  | A1    | 315 | PGV  | C9-C10 | -4.62 | 1.34        | 1.52     |
| 61  | BB    | 204 | PGV  | C9-C10 | -4.62 | 1.34        | 1.52     |
| 61  | BA    | 501 | PGV  | C9-C10 | -4.61 | 1.34        | 1.52     |
| 61  | BB    | 205 | PGV  | C9-C10 | -4.61 | 1.34        | 1.52     |
| 61  | AZ    | 207 | PGV  | C9-C10 | -4.60 | 1.34        | 1.52     |
| 61  | BA    | 515 | PGV  | C9-C10 | -4.60 | 1.34        | 1.52     |
| 61  | A0    | 327 | PGV  | C9-C10 | -4.59 | 1.34        | 1.52     |
| 61  | A0    | 331 | PGV  | C9-C10 | -4.59 | 1.35        | 1.52     |
| 61  | A0    | 318 | PGV  | C9-C10 | -4.59 | 1.35        | 1.52     |
| 61  | BB    | 208 | PGV  | C9-C10 | -4.58 | 1.35        | 1.52     |
| 61  | BA    | 540 | PGV  | C9-C10 | -4.58 | 1.35        | 1.52     |
| 61  | A0    | 305 | PGV  | C9-C10 | -4.58 | 1.35        | 1.52     |
| 61  | AZ    | 205 | PGV  | C9-C10 | -4.57 | 1.35        | 1.52     |
| 61  | BB    | 207 | PGV  | C9-C10 | -4.57 | 1.35        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 61  | A1    | 303  | PGV  | C9-C10  | -4.56 | 1.35        | 1.52     |
| 61  | A1    | 311  | PGV  | C9-C10  | -4.56 | 1.35        | 1.52     |
| 61  | A0    | 317  | PGV  | C9-C10  | -4.56 | 1.35        | 1.52     |
| 61  | BB    | 217  | PGV  | C9-C10  | -4.54 | 1.35        | 1.52     |
| 61  | BA    | 512  | PGV  | C9-C10  | -4.54 | 1.35        | 1.52     |
| 61  | A0    | 328  | PGV  | C9-C10  | -4.54 | 1.35        | 1.52     |
| 61  | BA    | 536  | PGV  | C9-C10  | -4.54 | 1.35        | 1.52     |
| 61  | A0    | 306  | PGV  | C9-C10  | -4.53 | 1.35        | 1.52     |
| 61  | A0    | 304  | PGV  | C9-C10  | -4.53 | 1.35        | 1.52     |
| 61  | B8    | 3005 | PGV  | C9-C10  | -4.53 | 1.35        | 1.52     |
| 61  | A1    | 318  | PGV  | C9-C10  | -4.52 | 1.35        | 1.52     |
| 61  | BA    | 505  | PGV  | C9-C10  | -4.52 | 1.35        | 1.52     |
| 61  | BB    | 203  | PGV  | C9-C10  | -4.52 | 1.35        | 1.52     |
| 61  | A0    | 332  | PGV  | C9-C10  | -4.51 | 1.35        | 1.52     |
| 61  | A0    | 325  | PGV  | C9-C10  | -4.50 | 1.35        | 1.52     |
| 60  | A1    | 319  | PEV  | C39-C40 | -2.95 | 1.34        | 1.51     |
| 60  | B8    | 3004 | PEV  | C39-C40 | -2.95 | 1.34        | 1.51     |
| 60  | A0    | 309  | PEV  | C39-C40 | -2.94 | 1.34        | 1.51     |
| 60  | B8    | 3002 | PEV  | C39-C40 | -2.93 | 1.34        | 1.51     |
| 60  | BA    | 519  | PEV  | C39-C40 | -2.93 | 1.34        | 1.51     |
| 60  | BA    | 531  | PEV  | C39-C40 | -2.93 | 1.34        | 1.51     |
| 60  | A1    | 308  | PEV  | C39-C40 | -2.93 | 1.34        | 1.51     |
| 60  | A1    | 326  | PEV  | C39-C40 | -2.93 | 1.34        | 1.51     |
| 60  | AZ    | 204  | PEV  | C39-C40 | -2.92 | 1.34        | 1.51     |
| 60  | A0    | 314  | PEV  | C39-C40 | -2.92 | 1.34        | 1.51     |
| 60  | A1    | 301  | PEV  | C39-C40 | -2.92 | 1.34        | 1.51     |
| 60  | A0    | 308  | PEV  | C39-C40 | -2.92 | 1.34        | 1.51     |
| 60  | B8    | 3007 | PEV  | C39-C40 | -2.92 | 1.34        | 1.51     |
| 60  | BA    | 518  | PEV  | C39-C40 | -2.92 | 1.34        | 1.51     |
| 60  | BA    | 528  | PEV  | C39-C40 | -2.92 | 1.34        | 1.51     |
| 60  | BA    | 532  | PEV  | C39-C40 | -2.92 | 1.34        | 1.51     |
| 60  | BA    | 514  | PEV  | C39-C40 | -2.92 | 1.34        | 1.51     |
| 60  | BA    | 507  | PEV  | C39-C40 | -2.92 | 1.34        | 1.51     |
| 60  | A0    | 330  | PEV  | C39-C40 | -2.92 | 1.34        | 1.51     |
| 60  | AZ    | 206  | PEV  | C39-C40 | -2.92 | 1.35        | 1.51     |
| 60  | BA    | 530  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |
| 60  | AZ    | 202  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |
| 60  | A1    | 323  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |
| 60  | BA    | 534  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |
| 60  | A1    | 310  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |
| 60  | A1    | 305  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |
| 60  | A1    | 322  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 60  | BA    | 521  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |
| 60  | A0    | 310  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |
| 60  | BA    | 539  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |
| 60  | BB    | 211  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |
| 60  | A0    | 322  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |
| 60  | A1    | 324  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |
| 60  | A1    | 304  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |
| 60  | A0    | 315  | PEV  | C39-C40 | -2.91 | 1.35        | 1.51     |
| 60  | A1    | 306  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | A1    | 329  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | BB    | 201  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | A0    | 319  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | B8    | 3006 | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | A0    | 326  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | A1    | 328  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | BA    | 517  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | BA    | 535  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | BA    | 504  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | A0    | 313  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | A0    | 329  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | AZ    | 201  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | A1    | 327  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | BB    | 212  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | BB    | 218  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | A0    | 302  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | BB    | 216  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | A0    | 324  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | BA    | 538  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | AZ    | 203  | PEV  | C39-C40 | -2.90 | 1.35        | 1.51     |
| 60  | A0    | 312  | PEV  | C39-C40 | -2.89 | 1.35        | 1.51     |
| 60  | BA    | 527  | PEV  | C39-C40 | -2.89 | 1.35        | 1.51     |
| 60  | BB    | 202  | PEV  | C39-C40 | -2.89 | 1.35        | 1.51     |
| 60  | BA    | 508  | PEV  | C39-C40 | -2.89 | 1.35        | 1.51     |
| 60  | BB    | 210  | PEV  | C39-C40 | -2.89 | 1.35        | 1.51     |
| 60  | A1    | 302  | PEV  | C39-C40 | -2.89 | 1.35        | 1.51     |
| 60  | A1    | 314  | PEV  | C39-C40 | -2.89 | 1.35        | 1.51     |
| 60  | BA    | 537  | PEV  | C39-C40 | -2.89 | 1.35        | 1.51     |
| 60  | A0    | 303  | PEV  | C39-C40 | -2.89 | 1.35        | 1.51     |
| 60  | BA    | 509  | PEV  | C39-C40 | -2.89 | 1.35        | 1.51     |
| 60  | BB    | 214  | PEV  | C39-C40 | -2.89 | 1.35        | 1.51     |
| 60  | BA    | 526  | PEV  | C39-C40 | -2.89 | 1.35        | 1.51     |
| 60  | BA    | 520  | PEV  | C39-C40 | -2.89 | 1.35        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 60  | BA    | 506  | PEV  | C39-C40 | -2.89 | 1.35        | 1.51     |
| 60  | B8    | 3003 | PEV  | C39-C40 | -2.88 | 1.35        | 1.51     |
| 60  | BA    | 513  | PEV  | C39-C40 | -2.88 | 1.35        | 1.51     |
| 60  | A0    | 301  | PEV  | C39-C40 | -2.88 | 1.35        | 1.51     |
| 60  | A1    | 321  | PEV  | C39-C40 | -2.88 | 1.35        | 1.51     |
| 60  | BA    | 503  | PEV  | C39-C40 | -2.88 | 1.35        | 1.51     |
| 60  | BA    | 529  | PEV  | C39-C40 | -2.88 | 1.35        | 1.51     |
| 60  | BA    | 502  | PEV  | C39-C40 | -2.88 | 1.35        | 1.51     |
| 60  | A0    | 311  | PEV  | C39-C40 | -2.88 | 1.35        | 1.51     |
| 60  | A0    | 320  | PEV  | C39-C40 | -2.88 | 1.35        | 1.51     |
| 60  | BA    | 510  | PEV  | C39-C40 | -2.88 | 1.35        | 1.51     |
| 60  | BA    | 523  | PEV  | C39-C40 | -2.88 | 1.35        | 1.51     |
| 60  | A1    | 317  | PEV  | C39-C40 | -2.88 | 1.35        | 1.51     |
| 60  | A1    | 309  | PEV  | C39-C40 | -2.88 | 1.35        | 1.51     |
| 60  | A1    | 316  | PEV  | C39-C40 | -2.87 | 1.35        | 1.51     |
| 60  | B8    | 3001 | PEV  | C39-C40 | -2.87 | 1.35        | 1.51     |
| 60  | A0    | 321  | PEV  | C39-C40 | -2.87 | 1.35        | 1.51     |
| 60  | A1    | 320  | PEV  | C39-C40 | -2.87 | 1.35        | 1.51     |
| 60  | A1    | 307  | PEV  | C39-C40 | -2.87 | 1.35        | 1.51     |
| 60  | BB    | 209  | PEV  | C39-C40 | -2.87 | 1.35        | 1.51     |
| 60  | A1    | 312  | PEV  | C39-C40 | -2.87 | 1.35        | 1.51     |
| 60  | BA    | 525  | PEV  | C39-C40 | -2.87 | 1.35        | 1.51     |
| 60  | A0    | 307  | PEV  | C39-C40 | -2.86 | 1.35        | 1.51     |
| 60  | A0    | 323  | PEV  | C39-C40 | -2.86 | 1.35        | 1.51     |
| 60  | A1    | 313  | PEV  | C39-C40 | -2.86 | 1.35        | 1.51     |
| 60  | BA    | 524  | PEV  | C39-C40 | -2.86 | 1.35        | 1.51     |
| 60  | BB    | 206  | PEV  | C39-C40 | -2.86 | 1.35        | 1.51     |
| 60  | BB    | 215  | PEV  | C39-C40 | -2.86 | 1.35        | 1.51     |
| 60  | A1    | 325  | PEV  | C39-C40 | -2.86 | 1.35        | 1.51     |
| 60  | BA    | 511  | PEV  | C39-C40 | -2.83 | 1.35        | 1.51     |
| 60  | A0    | 316  | PEV  | C39-C40 | -2.82 | 1.35        | 1.51     |
| 60  | A0    | 302  | PEV  | C3-C2   | 2.00  | 1.56        | 1.50     |
| 60  | A1    | 309  | PEV  | C3-C2   | 2.00  | 1.56        | 1.50     |
| 60  | A0    | 324  | PEV  | C3-C2   | 2.01  | 1.56        | 1.50     |
| 60  | BA    | 521  | PEV  | C3-C2   | 2.01  | 1.56        | 1.50     |
| 60  | BA    | 525  | PEV  | C3-C2   | 2.02  | 1.56        | 1.50     |
| 61  | A1    | 315  | PGV  | C01-C02 | 2.02  | 1.56        | 1.50     |
| 61  | A1    | 315  | PGV  | C03-C02 | 2.02  | 1.56        | 1.50     |
| 61  | A0    | 304  | PGV  | C01-C02 | 2.02  | 1.56        | 1.50     |
| 60  | B8    | 3001 | PEV  | C3-C2   | 2.02  | 1.56        | 1.50     |
| 60  | A1    | 329  | PEV  | C3-C2   | 2.02  | 1.56        | 1.50     |
| 60  | A1    | 310  | PEV  | C3-C2   | 2.03  | 1.56        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 60  | BA    | 524  | PEV  | C3-C2   | 2.03 | 1.56        | 1.50     |
| 60  | BA    | 539  | PEV  | C3-C2   | 2.04 | 1.56        | 1.50     |
| 60  | A0    | 314  | PEV  | C3-C2   | 2.04 | 1.56        | 1.50     |
| 60  | A1    | 320  | PEV  | C3-C2   | 2.04 | 1.56        | 1.50     |
| 60  | A0    | 313  | PEV  | C3-C2   | 2.04 | 1.56        | 1.50     |
| 60  | A1    | 312  | PEV  | C3-C2   | 2.04 | 1.56        | 1.50     |
| 60  | BA    | 534  | PEV  | C1-C2   | 2.04 | 1.56        | 1.50     |
| 60  | A0    | 310  | PEV  | C3-C2   | 2.04 | 1.56        | 1.50     |
| 60  | A1    | 308  | PEV  | C3-C2   | 2.05 | 1.56        | 1.50     |
| 60  | BA    | 519  | PEV  | C3-C2   | 2.05 | 1.56        | 1.50     |
| 60  | BB    | 216  | PEV  | C3-C2   | 2.05 | 1.56        | 1.50     |
| 60  | A1    | 302  | PEV  | C3-C2   | 2.06 | 1.56        | 1.50     |
| 60  | A1    | 316  | PEV  | C1-C2   | 2.06 | 1.56        | 1.50     |
| 60  | BA    | 503  | PEV  | C1-C2   | 2.06 | 1.56        | 1.50     |
| 60  | BA    | 503  | PEV  | C3-C2   | 2.06 | 1.56        | 1.50     |
| 60  | A0    | 309  | PEV  | C3-C2   | 2.06 | 1.56        | 1.50     |
| 60  | BA    | 529  | PEV  | C3-C2   | 2.06 | 1.56        | 1.50     |
| 60  | BA    | 514  | PEV  | C1-C2   | 2.08 | 1.56        | 1.50     |
| 60  | BB    | 202  | PEV  | C3-C2   | 2.09 | 1.56        | 1.50     |
| 60  | BA    | 509  | PEV  | C1-C2   | 2.10 | 1.56        | 1.50     |
| 60  | BA    | 534  | PEV  | C3-C2   | 2.10 | 1.56        | 1.50     |
| 60  | A0    | 303  | PEV  | C3-C2   | 2.12 | 1.56        | 1.50     |
| 60  | BA    | 504  | PEV  | C3-C2   | 2.13 | 1.56        | 1.50     |
| 61  | BB    | 204  | PGV  | C01-C02 | 2.15 | 1.56        | 1.50     |
| 60  | A0    | 308  | PEV  | C3-C2   | 2.16 | 1.56        | 1.50     |
| 60  | A1    | 301  | PEV  | C3-C2   | 2.20 | 1.57        | 1.50     |
| 60  | BA    | 537  | PEV  | C3-C2   | 2.23 | 1.57        | 1.50     |
| 60  | A1    | 317  | PEV  | C3-C2   | 2.23 | 1.57        | 1.50     |
| 61  | BB    | 205  | PGV  | C12-C11 | 4.02 | 1.54        | 1.31     |
| 61  | BA    | 515  | PGV  | C12-C11 | 4.02 | 1.54        | 1.31     |
| 61  | B8    | 3005 | PGV  | C12-C11 | 4.03 | 1.54        | 1.31     |
| 61  | BA    | 512  | PGV  | C12-C11 | 4.04 | 1.54        | 1.31     |
| 61  | A0    | 305  | PGV  | C12-C11 | 4.05 | 1.54        | 1.31     |
| 61  | BA    | 501  | PGV  | C12-C11 | 4.05 | 1.54        | 1.31     |
| 61  | BB    | 207  | PGV  | C12-C11 | 4.05 | 1.54        | 1.31     |
| 61  | A0    | 331  | PGV  | C12-C11 | 4.05 | 1.54        | 1.31     |
| 61  | AZ    | 207  | PGV  | C12-C11 | 4.06 | 1.54        | 1.31     |
| 61  | AZ    | 205  | PGV  | C12-C11 | 4.06 | 1.54        | 1.31     |
| 61  | A0    | 317  | PGV  | C12-C11 | 4.06 | 1.54        | 1.31     |
| 61  | BB    | 208  | PGV  | C12-C11 | 4.06 | 1.54        | 1.31     |
| 61  | A0    | 328  | PGV  | C12-C11 | 4.07 | 1.54        | 1.31     |
| 61  | A1    | 318  | PGV  | C12-C11 | 4.08 | 1.54        | 1.31     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 61  | BA    | 540 | PGV  | C12-C11 | 4.08  | 1.54        | 1.31     |
| 61  | BB    | 217 | PGV  | C12-C11 | 4.08  | 1.54        | 1.31     |
| 61  | BA    | 536 | PGV  | C12-C11 | 4.08  | 1.54        | 1.31     |
| 61  | A0    | 318 | PGV  | C12-C11 | 4.09  | 1.54        | 1.31     |
| 61  | A0    | 304 | PGV  | C12-C11 | 4.09  | 1.54        | 1.31     |
| 61  | A0    | 332 | PGV  | C12-C11 | 4.09  | 1.54        | 1.31     |
| 61  | A1    | 311 | PGV  | C12-C11 | 4.09  | 1.54        | 1.31     |
| 61  | BB    | 204 | PGV  | C12-C11 | 4.10  | 1.54        | 1.31     |
| 61  | A0    | 306 | PGV  | C12-C11 | 4.10  | 1.54        | 1.31     |
| 61  | A0    | 327 | PGV  | C12-C11 | 4.11  | 1.54        | 1.31     |
| 61  | A1    | 315 | PGV  | C12-C11 | 4.11  | 1.54        | 1.31     |
| 61  | A1    | 303 | PGV  | C12-C11 | 4.12  | 1.54        | 1.31     |
| 61  | BB    | 213 | PGV  | C12-C11 | 4.13  | 1.54        | 1.31     |
| 61  | BA    | 516 | PGV  | C12-C11 | 4.13  | 1.54        | 1.31     |
| 61  | BA    | 505 | PGV  | C12-C11 | 4.13  | 1.54        | 1.31     |
| 61  | BB    | 203 | PGV  | C12-C11 | 4.14  | 1.54        | 1.31     |
| 61  | BA    | 522 | PGV  | C12-C11 | 4.14  | 1.54        | 1.31     |
| 61  | A0    | 325 | PGV  | C12-C11 | 4.15  | 1.55        | 1.31     |
| 60  | BA    | 533 | PEV  | C39-C40 | 17.65 | 2.52        | 1.51     |

All (270) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 61  | BB    | 204 | PGV  | O01-C1-C2   | -2.06 | 107.28      | 111.55   |
| 60  | A1    | 317 | PEV  | O3-C3-C2    | 2.01  | 113.72      | 108.66   |
| 60  | A0    | 321 | PEV  | O2-C31-C32  | 2.02  | 115.75      | 111.55   |
| 60  | A1    | 304 | PEV  | C39-C40-C41 | 2.09  | 125.24      | 114.45   |
| 60  | AZ    | 203 | PEV  | C38-C39-C40 | 2.10  | 125.25      | 114.45   |
| 60  | A0    | 330 | PEV  | C38-C39-C40 | 2.11  | 125.34      | 114.45   |
| 60  | A0    | 312 | PEV  | C39-C40-C41 | 2.12  | 125.38      | 114.45   |
| 60  | AZ    | 203 | PEV  | C39-C40-C41 | 2.15  | 125.55      | 114.45   |
| 60  | AZ    | 206 | PEV  | C38-C39-C40 | 2.16  | 125.57      | 114.45   |
| 60  | BA    | 534 | PEV  | O3-C3-C2    | 2.21  | 114.21      | 108.66   |
| 60  | A0    | 330 | PEV  | C39-C40-C41 | 2.22  | 125.88      | 114.45   |
| 60  | A1    | 304 | PEV  | C38-C39-C40 | 2.24  | 125.99      | 114.45   |
| 60  | BA    | 529 | PEV  | C38-C39-C40 | 2.24  | 126.02      | 114.45   |
| 60  | BA    | 518 | PEV  | C39-C40-C41 | 2.26  | 126.08      | 114.45   |
| 60  | BA    | 537 | PEV  | C39-C40-C41 | 2.26  | 126.11      | 114.45   |
| 60  | A0    | 310 | PEV  | C39-C40-C41 | 2.28  | 126.21      | 114.45   |
| 60  | A0    | 302 | PEV  | C38-C39-C40 | 2.28  | 126.22      | 114.45   |
| 60  | A0    | 312 | PEV  | C38-C39-C40 | 2.29  | 126.24      | 114.45   |
| 60  | AZ    | 204 | PEV  | C38-C39-C40 | 2.29  | 126.24      | 114.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 60  | AZ    | 206  | PEV  | C39-C40-C41 | 2.29 | 126.27      | 114.45   |
| 60  | BA    | 513  | PEV  | C38-C39-C40 | 2.30 | 126.32      | 114.45   |
| 60  | A0    | 302  | PEV  | C39-C40-C41 | 2.31 | 126.35      | 114.45   |
| 60  | B8    | 3007 | PEV  | C38-C39-C40 | 2.31 | 126.35      | 114.45   |
| 60  | BB    | 218  | PEV  | C39-C40-C41 | 2.31 | 126.35      | 114.45   |
| 60  | A1    | 312  | PEV  | C38-C39-C40 | 2.31 | 126.37      | 114.45   |
| 60  | BA    | 519  | PEV  | C38-C39-C40 | 2.31 | 126.38      | 114.45   |
| 60  | BA    | 518  | PEV  | C38-C39-C40 | 2.31 | 126.38      | 114.45   |
| 60  | A1    | 308  | PEV  | C39-C40-C41 | 2.31 | 126.38      | 114.45   |
| 60  | BA    | 529  | PEV  | C39-C40-C41 | 2.32 | 126.40      | 114.45   |
| 60  | A0    | 314  | PEV  | C39-C40-C41 | 2.32 | 126.41      | 114.45   |
| 60  | A1    | 319  | PEV  | C38-C39-C40 | 2.33 | 126.44      | 114.45   |
| 60  | BA    | 537  | PEV  | C38-C39-C40 | 2.33 | 126.47      | 114.45   |
| 60  | BB    | 201  | PEV  | C38-C39-C40 | 2.33 | 126.47      | 114.45   |
| 60  | BB    | 215  | PEV  | C38-C39-C40 | 2.33 | 126.48      | 114.45   |
| 60  | A0    | 303  | PEV  | C39-C40-C41 | 2.33 | 126.49      | 114.45   |
| 60  | A1    | 308  | PEV  | C38-C39-C40 | 2.34 | 126.53      | 114.45   |
| 60  | A1    | 312  | PEV  | C39-C40-C41 | 2.36 | 126.61      | 114.45   |
| 60  | A0    | 315  | PEV  | C38-C39-C40 | 2.36 | 126.61      | 114.45   |
| 60  | A0    | 314  | PEV  | C38-C39-C40 | 2.36 | 126.63      | 114.45   |
| 60  | B8    | 3007 | PEV  | C39-C40-C41 | 2.36 | 126.63      | 114.45   |
| 60  | A1    | 302  | PEV  | C38-C39-C40 | 2.37 | 126.65      | 114.45   |
| 60  | BA    | 531  | PEV  | C38-C39-C40 | 2.37 | 126.67      | 114.45   |
| 60  | A1    | 310  | PEV  | C39-C40-C41 | 2.38 | 126.69      | 114.45   |
| 60  | A1    | 320  | PEV  | C39-C40-C41 | 2.38 | 126.69      | 114.45   |
| 60  | A1    | 320  | PEV  | C38-C39-C40 | 2.38 | 126.71      | 114.45   |
| 60  | A1    | 305  | PEV  | C39-C40-C41 | 2.39 | 126.75      | 114.45   |
| 60  | BA    | 520  | PEV  | C39-C40-C41 | 2.39 | 126.75      | 114.45   |
| 60  | A1    | 326  | PEV  | C38-C39-C40 | 2.39 | 126.75      | 114.45   |
| 60  | BB    | 215  | PEV  | C39-C40-C41 | 2.39 | 126.77      | 114.45   |
| 60  | A1    | 306  | PEV  | C39-C40-C41 | 2.39 | 126.79      | 114.45   |
| 60  | A1    | 327  | PEV  | C38-C39-C40 | 2.40 | 126.80      | 114.45   |
| 60  | A1    | 324  | PEV  | C39-C40-C41 | 2.40 | 126.81      | 114.45   |
| 60  | AZ    | 204  | PEV  | C39-C40-C41 | 2.40 | 126.82      | 114.45   |
| 60  | BA    | 531  | PEV  | C39-C40-C41 | 2.40 | 126.84      | 114.45   |
| 60  | BB    | 209  | PEV  | C38-C39-C40 | 2.40 | 126.85      | 114.45   |
| 60  | B8    | 3002 | PEV  | C38-C39-C40 | 2.40 | 126.85      | 114.45   |
| 61  | BA    | 516  | PGV  | C9-C10-C11  | 2.41 | 125.61      | 112.50   |
| 60  | A0    | 324  | PEV  | C38-C39-C40 | 2.41 | 126.87      | 114.45   |
| 60  | A0    | 303  | PEV  | C38-C39-C40 | 2.41 | 126.88      | 114.45   |
| 60  | A1    | 306  | PEV  | C38-C39-C40 | 2.41 | 126.88      | 114.45   |
| 60  | A1    | 326  | PEV  | C39-C40-C41 | 2.41 | 126.88      | 114.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 60  | A0    | 309  | PEV  | C38-C39-C40 | 2.41 | 126.89      | 114.45   |
| 60  | BA    | 530  | PEV  | C39-C40-C41 | 2.42 | 126.90      | 114.45   |
| 60  | A0    | 321  | PEV  | C38-C39-C40 | 2.42 | 126.92      | 114.45   |
| 60  | A1    | 317  | PEV  | C38-C39-C40 | 2.42 | 126.92      | 114.45   |
| 60  | BB    | 201  | PEV  | C39-C40-C41 | 2.42 | 126.95      | 114.45   |
| 60  | BB    | 209  | PEV  | C39-C40-C41 | 2.43 | 126.95      | 114.45   |
| 60  | A0    | 315  | PEV  | C39-C40-C41 | 2.43 | 126.96      | 114.45   |
| 60  | BA    | 538  | PEV  | C38-C39-C40 | 2.43 | 126.97      | 114.45   |
| 60  | A1    | 317  | PEV  | C39-C40-C41 | 2.43 | 126.97      | 114.45   |
| 60  | BA    | 513  | PEV  | C39-C40-C41 | 2.43 | 126.99      | 114.45   |
| 60  | A1    | 302  | PEV  | C39-C40-C41 | 2.43 | 127.00      | 114.45   |
| 60  | A0    | 313  | PEV  | C39-C40-C41 | 2.44 | 127.00      | 114.45   |
| 60  | BA    | 523  | PEV  | C38-C39-C40 | 2.44 | 127.01      | 114.45   |
| 60  | A1    | 316  | PEV  | C38-C39-C40 | 2.44 | 127.03      | 114.45   |
| 60  | A0    | 321  | PEV  | C39-C40-C41 | 2.44 | 127.03      | 114.45   |
| 60  | A0    | 313  | PEV  | C38-C39-C40 | 2.44 | 127.04      | 114.45   |
| 60  | A1    | 323  | PEV  | C39-C40-C41 | 2.44 | 127.04      | 114.45   |
| 60  | A1    | 310  | PEV  | C38-C39-C40 | 2.44 | 127.04      | 114.45   |
| 60  | BA    | 511  | PEV  | C38-C39-C40 | 2.44 | 127.05      | 114.45   |
| 60  | A0    | 309  | PEV  | C39-C40-C41 | 2.44 | 127.05      | 114.45   |
| 60  | BA    | 519  | PEV  | C39-C40-C41 | 2.45 | 127.06      | 114.45   |
| 60  | A0    | 322  | PEV  | C38-C39-C40 | 2.45 | 127.07      | 114.45   |
| 60  | A0    | 324  | PEV  | C39-C40-C41 | 2.45 | 127.08      | 114.45   |
| 60  | B8    | 3001 | PEV  | C38-C39-C40 | 2.45 | 127.09      | 114.45   |
| 61  | B8    | 3005 | PGV  | C9-C10-C11  | 2.45 | 125.86      | 112.50   |
| 60  | A1    | 316  | PEV  | C39-C40-C41 | 2.46 | 127.12      | 114.45   |
| 60  | BA    | 520  | PEV  | C38-C39-C40 | 2.46 | 127.13      | 114.45   |
| 60  | A1    | 321  | PEV  | C38-C39-C40 | 2.46 | 127.14      | 114.45   |
| 61  | A0    | 305  | PGV  | C9-C10-C11  | 2.46 | 125.90      | 112.50   |
| 60  | B8    | 3003 | PEV  | C38-C39-C40 | 2.46 | 127.14      | 114.45   |
| 60  | BA    | 514  | PEV  | C39-C40-C41 | 2.47 | 127.17      | 114.45   |
| 60  | BA    | 521  | PEV  | C39-C40-C41 | 2.47 | 127.18      | 114.45   |
| 60  | BA    | 504  | PEV  | C38-C39-C40 | 2.47 | 127.19      | 114.45   |
| 60  | B8    | 3006 | PEV  | C38-C39-C40 | 2.47 | 127.19      | 114.45   |
| 60  | BB    | 202  | PEV  | C38-C39-C40 | 2.47 | 127.20      | 114.45   |
| 60  | A0    | 307  | PEV  | C38-C39-C40 | 2.48 | 127.23      | 114.45   |
| 60  | A1    | 301  | PEV  | C39-C40-C41 | 2.48 | 127.24      | 114.45   |
| 60  | A1    | 321  | PEV  | C39-C40-C41 | 2.48 | 127.24      | 114.45   |
| 60  | BA    | 538  | PEV  | C39-C40-C41 | 2.48 | 127.25      | 114.45   |
| 60  | BB    | 202  | PEV  | C39-C40-C41 | 2.48 | 127.25      | 114.45   |
| 60  | BB    | 212  | PEV  | C39-C40-C41 | 2.49 | 127.27      | 114.45   |
| 60  | A1    | 325  | PEV  | C38-C39-C40 | 2.49 | 127.29      | 114.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 60  | BB    | 216  | PEV  | C39-C40-C41 | 2.49 | 127.29      | 114.45   |
| 60  | A0    | 310  | PEV  | C38-C39-C40 | 2.49 | 127.31      | 114.45   |
| 60  | A1    | 329  | PEV  | C39-C40-C41 | 2.50 | 127.33      | 114.45   |
| 60  | BA    | 524  | PEV  | C38-C39-C40 | 2.50 | 127.35      | 114.45   |
| 60  | BA    | 530  | PEV  | C38-C39-C40 | 2.50 | 127.35      | 114.45   |
| 60  | A1    | 327  | PEV  | C39-C40-C41 | 2.50 | 127.35      | 114.45   |
| 60  | A1    | 324  | PEV  | C38-C39-C40 | 2.50 | 127.35      | 114.45   |
| 60  | A1    | 313  | PEV  | C38-C39-C40 | 2.50 | 127.35      | 114.45   |
| 60  | B8    | 3006 | PEV  | C39-C40-C41 | 2.50 | 127.35      | 114.45   |
| 60  | A0    | 322  | PEV  | C39-C40-C41 | 2.51 | 127.37      | 114.45   |
| 60  | BA    | 502  | PEV  | C38-C39-C40 | 2.51 | 127.38      | 114.45   |
| 60  | BA    | 521  | PEV  | C38-C39-C40 | 2.51 | 127.38      | 114.45   |
| 60  | A1    | 328  | PEV  | C38-C39-C40 | 2.51 | 127.39      | 114.45   |
| 60  | A0    | 307  | PEV  | C39-C40-C41 | 2.51 | 127.39      | 114.45   |
| 60  | A0    | 311  | PEV  | C38-C39-C40 | 2.51 | 127.39      | 114.45   |
| 60  | BA    | 539  | PEV  | C39-C40-C41 | 2.51 | 127.40      | 114.45   |
| 61  | BA    | 515  | PGV  | C9-C10-C11  | 2.52 | 126.20      | 112.50   |
| 60  | B8    | 3002 | PEV  | C39-C40-C41 | 2.52 | 127.42      | 114.45   |
| 60  | BA    | 508  | PEV  | C39-C40-C41 | 2.52 | 127.43      | 114.45   |
| 60  | A1    | 328  | PEV  | C39-C40-C41 | 2.52 | 127.43      | 114.45   |
| 60  | A1    | 322  | PEV  | C38-C39-C40 | 2.52 | 127.44      | 114.45   |
| 60  | BA    | 509  | PEV  | C39-C40-C41 | 2.52 | 127.45      | 114.45   |
| 60  | A0    | 320  | PEV  | C38-C39-C40 | 2.53 | 127.47      | 114.45   |
| 60  | A0    | 301  | PEV  | C38-C39-C40 | 2.53 | 127.47      | 114.45   |
| 60  | A1    | 301  | PEV  | C38-C39-C40 | 2.53 | 127.47      | 114.45   |
| 61  | A0    | 318  | PGV  | C9-C10-C11  | 2.53 | 126.26      | 112.50   |
| 60  | A1    | 325  | PEV  | C39-C40-C41 | 2.53 | 127.49      | 114.45   |
| 60  | BA    | 509  | PEV  | C38-C39-C40 | 2.53 | 127.49      | 114.45   |
| 60  | A1    | 313  | PEV  | C39-C40-C41 | 2.53 | 127.50      | 114.45   |
| 60  | BA    | 502  | PEV  | C39-C40-C41 | 2.54 | 127.52      | 114.45   |
| 60  | BB    | 212  | PEV  | C38-C39-C40 | 2.54 | 127.55      | 114.45   |
| 60  | BA    | 507  | PEV  | C38-C39-C40 | 2.54 | 127.55      | 114.45   |
| 60  | BA    | 508  | PEV  | C38-C39-C40 | 2.54 | 127.55      | 114.45   |
| 60  | A1    | 309  | PEV  | C38-C39-C40 | 2.54 | 127.56      | 114.45   |
| 60  | BA    | 523  | PEV  | C39-C40-C41 | 2.55 | 127.57      | 114.45   |
| 60  | A1    | 314  | PEV  | C38-C39-C40 | 2.55 | 127.58      | 114.45   |
| 60  | B8    | 3003 | PEV  | C39-C40-C41 | 2.55 | 127.58      | 114.45   |
| 60  | A0    | 320  | PEV  | C39-C40-C41 | 2.55 | 127.60      | 114.45   |
| 60  | BA    | 510  | PEV  | C38-C39-C40 | 2.55 | 127.60      | 114.45   |
| 60  | BB    | 214  | PEV  | C38-C39-C40 | 2.55 | 127.61      | 114.45   |
| 60  | A0    | 326  | PEV  | C38-C39-C40 | 2.55 | 127.62      | 114.45   |
| 60  | BB    | 206  | PEV  | C39-C40-C41 | 2.55 | 127.62      | 114.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 60  | B8    | 3001 | PEV  | C39-C40-C41 | 2.56 | 127.62      | 114.45   |
| 60  | BA    | 510  | PEV  | C39-C40-C41 | 2.56 | 127.63      | 114.45   |
| 60  | A1    | 309  | PEV  | C39-C40-C41 | 2.56 | 127.63      | 114.45   |
| 60  | BA    | 526  | PEV  | C38-C39-C40 | 2.56 | 127.64      | 114.45   |
| 61  | AZ    | 205  | PGV  | C9-C10-C11  | 2.56 | 126.44      | 112.50   |
| 60  | BB    | 216  | PEV  | C38-C39-C40 | 2.56 | 127.67      | 114.45   |
| 60  | BA    | 535  | PEV  | C38-C39-C40 | 2.57 | 127.68      | 114.45   |
| 60  | BA    | 514  | PEV  | C38-C39-C40 | 2.57 | 127.68      | 114.45   |
| 61  | BB    | 217  | PGV  | C9-C10-C11  | 2.57 | 126.48      | 112.50   |
| 60  | BA    | 504  | PEV  | C39-C40-C41 | 2.57 | 127.69      | 114.45   |
| 60  | BA    | 524  | PEV  | C39-C40-C41 | 2.57 | 127.69      | 114.45   |
| 60  | A0    | 326  | PEV  | C39-C40-C41 | 2.57 | 127.69      | 114.45   |
| 60  | BA    | 511  | PEV  | C39-C40-C41 | 2.57 | 127.69      | 114.45   |
| 60  | BA    | 539  | PEV  | C38-C39-C40 | 2.57 | 127.69      | 114.45   |
| 60  | BA    | 527  | PEV  | C39-C40-C41 | 2.57 | 127.72      | 114.45   |
| 60  | A0    | 311  | PEV  | C39-C40-C41 | 2.57 | 127.72      | 114.45   |
| 60  | A1    | 305  | PEV  | C38-C39-C40 | 2.58 | 127.73      | 114.45   |
| 60  | BA    | 507  | PEV  | C39-C40-C41 | 2.58 | 127.73      | 114.45   |
| 61  | BB    | 204  | PGV  | C9-C10-C11  | 2.58 | 126.52      | 112.50   |
| 60  | A1    | 322  | PEV  | C39-C40-C41 | 2.58 | 127.73      | 114.45   |
| 60  | BA    | 517  | PEV  | C39-C40-C41 | 2.58 | 127.73      | 114.45   |
| 61  | A0    | 327  | PGV  | C9-C10-C11  | 2.58 | 126.54      | 112.50   |
| 60  | BB    | 214  | PEV  | C39-C40-C41 | 2.58 | 127.75      | 114.45   |
| 60  | AZ    | 201  | PEV  | C39-C40-C41 | 2.59 | 127.79      | 114.45   |
| 60  | BA    | 528  | PEV  | C38-C39-C40 | 2.59 | 127.81      | 114.45   |
| 60  | A0    | 308  | PEV  | C39-C40-C41 | 2.59 | 127.81      | 114.45   |
| 60  | A1    | 314  | PEV  | C39-C40-C41 | 2.59 | 127.82      | 114.45   |
| 60  | BA    | 525  | PEV  | C39-C40-C41 | 2.60 | 127.83      | 114.45   |
| 60  | BA    | 535  | PEV  | C39-C40-C41 | 2.60 | 127.84      | 114.45   |
| 60  | BA    | 525  | PEV  | C38-C39-C40 | 2.60 | 127.85      | 114.45   |
| 60  | A0    | 319  | PEV  | C39-C40-C41 | 2.60 | 127.85      | 114.45   |
| 60  | AZ    | 201  | PEV  | C38-C39-C40 | 2.60 | 127.87      | 114.45   |
| 60  | A1    | 323  | PEV  | C38-C39-C40 | 2.60 | 127.87      | 114.45   |
| 61  | A0    | 306  | PGV  | C9-C10-C11  | 2.61 | 126.70      | 112.50   |
| 61  | A1    | 318  | PGV  | C9-C10-C11  | 2.62 | 126.76      | 112.50   |
| 60  | BA    | 506  | PEV  | C38-C39-C40 | 2.62 | 127.95      | 114.45   |
| 60  | A0    | 329  | PEV  | C38-C39-C40 | 2.62 | 127.98      | 114.45   |
| 60  | BA    | 526  | PEV  | C39-C40-C41 | 2.63 | 127.98      | 114.45   |
| 60  | B8    | 3004 | PEV  | C38-C39-C40 | 2.63 | 127.99      | 114.45   |
| 61  | A0    | 304  | PGV  | C9-C10-C11  | 2.63 | 126.80      | 112.50   |
| 60  | BB    | 218  | PEV  | C38-C39-C40 | 2.63 | 128.00      | 114.45   |
| 60  | A0    | 301  | PEV  | C39-C40-C41 | 2.63 | 128.00      | 114.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 60  | A0    | 329  | PEV  | C39-C40-C41 | 2.63 | 128.00      | 114.45   |
| 61  | A1    | 315  | PGV  | C9-C10-C11  | 2.63 | 126.83      | 112.50   |
| 61  | BA    | 536  | PGV  | C9-C10-C11  | 2.63 | 126.84      | 112.50   |
| 60  | AZ    | 202  | PEV  | C38-C39-C40 | 2.64 | 128.05      | 114.45   |
| 60  | BA    | 528  | PEV  | C39-C40-C41 | 2.64 | 128.05      | 114.45   |
| 60  | BB    | 206  | PEV  | C38-C39-C40 | 2.64 | 128.06      | 114.45   |
| 60  | BA    | 534  | PEV  | C38-C39-C40 | 2.64 | 128.06      | 114.45   |
| 60  | AZ    | 202  | PEV  | C39-C40-C41 | 2.64 | 128.07      | 114.45   |
| 60  | BA    | 506  | PEV  | C39-C40-C41 | 2.64 | 128.08      | 114.45   |
| 60  | BA    | 532  | PEV  | C39-C40-C41 | 2.65 | 128.10      | 114.45   |
| 60  | B8    | 3004 | PEV  | C39-C40-C41 | 2.65 | 128.11      | 114.45   |
| 60  | BB    | 210  | PEV  | C38-C39-C40 | 2.66 | 128.16      | 114.45   |
| 60  | A0    | 319  | PEV  | C38-C39-C40 | 2.66 | 128.16      | 114.45   |
| 61  | A1    | 303  | PGV  | C9-C10-C11  | 2.66 | 126.99      | 112.50   |
| 61  | A0    | 317  | PGV  | C9-C10-C11  | 2.66 | 127.00      | 112.50   |
| 60  | A1    | 307  | PEV  | C39-C40-C41 | 2.67 | 128.19      | 114.45   |
| 61  | AZ    | 207  | PGV  | C9-C10-C11  | 2.67 | 127.02      | 112.50   |
| 60  | BA    | 527  | PEV  | C38-C39-C40 | 2.67 | 128.23      | 114.45   |
| 60  | BA    | 503  | PEV  | C39-C40-C41 | 2.68 | 128.25      | 114.45   |
| 61  | BA    | 501  | PGV  | C9-C10-C11  | 2.68 | 127.09      | 112.50   |
| 61  | BA    | 540  | PGV  | C9-C10-C11  | 2.68 | 127.09      | 112.50   |
| 60  | A0    | 323  | PEV  | C39-C40-C41 | 2.68 | 128.28      | 114.45   |
| 60  | BB    | 211  | PEV  | C39-C40-C41 | 2.68 | 128.28      | 114.45   |
| 61  | A0    | 328  | PGV  | C9-C10-C11  | 2.70 | 127.19      | 112.50   |
| 60  | BB    | 210  | PEV  | C39-C40-C41 | 2.70 | 128.37      | 114.45   |
| 60  | A0    | 323  | PEV  | C38-C39-C40 | 2.70 | 128.37      | 114.45   |
| 61  | BA    | 512  | PGV  | C9-C10-C11  | 2.70 | 127.22      | 112.50   |
| 60  | BA    | 517  | PEV  | C38-C39-C40 | 2.71 | 128.40      | 114.45   |
| 61  | BA    | 505  | PGV  | C9-C10-C11  | 2.71 | 127.24      | 112.50   |
| 61  | BA    | 522  | PGV  | C9-C10-C11  | 2.71 | 127.24      | 112.50   |
| 60  | BA    | 534  | PEV  | C39-C40-C41 | 2.71 | 128.41      | 114.45   |
| 60  | A1    | 307  | PEV  | C38-C39-C40 | 2.71 | 128.44      | 114.45   |
| 61  | BA    | 522  | PGV  | C8-C9-C10   | 2.72 | 124.19      | 113.74   |
| 60  | A1    | 329  | PEV  | C38-C39-C40 | 2.72 | 128.47      | 114.45   |
| 60  | BA    | 503  | PEV  | C38-C39-C40 | 2.72 | 128.49      | 114.45   |
| 61  | BB    | 208  | PGV  | C9-C10-C11  | 2.73 | 127.34      | 112.50   |
| 61  | A0    | 331  | PGV  | C9-C10-C11  | 2.75 | 127.46      | 112.50   |
| 60  | BA    | 532  | PEV  | C38-C39-C40 | 2.75 | 128.64      | 114.45   |
| 61  | BB    | 203  | PGV  | C9-C10-C11  | 2.75 | 127.49      | 112.50   |
| 60  | BB    | 211  | PEV  | C38-C39-C40 | 2.76 | 128.67      | 114.45   |
| 60  | A0    | 308  | PEV  | C38-C39-C40 | 2.76 | 128.67      | 114.45   |
| 61  | BB    | 213  | PGV  | C9-C10-C11  | 2.78 | 127.62      | 112.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 61  | A1    | 311  | PGV  | C9-C10-C11  | 2.78 | 127.65      | 112.50   |
| 61  | A0    | 332  | PGV  | C9-C10-C11  | 2.84 | 127.98      | 112.50   |
| 61  | A0    | 325  | PGV  | C9-C10-C11  | 2.88 | 128.18      | 112.50   |
| 61  | BB    | 207  | PGV  | C9-C10-C11  | 2.89 | 128.21      | 112.50   |
| 61  | BB    | 205  | PGV  | C9-C10-C11  | 2.93 | 128.44      | 112.50   |
| 61  | BA    | 516  | PGV  | C8-C9-C10   | 2.99 | 125.25      | 113.74   |
| 61  | A0    | 305  | PGV  | C8-C9-C10   | 3.02 | 125.37      | 113.74   |
| 60  | A0    | 321  | PEV  | C2-O2-C31   | 3.13 | 125.27      | 117.88   |
| 60  | A0    | 316  | PEV  | C39-C40-C41 | 3.14 | 130.63      | 114.45   |
| 61  | A0    | 327  | PGV  | C8-C9-C10   | 3.14 | 125.81      | 113.74   |
| 61  | BA    | 515  | PGV  | C8-C9-C10   | 3.25 | 126.25      | 113.74   |
| 61  | B8    | 3005 | PGV  | C8-C9-C10   | 3.27 | 126.31      | 113.74   |
| 61  | BB    | 204  | PGV  | C8-C9-C10   | 3.27 | 126.31      | 113.74   |
| 61  | BA    | 536  | PGV  | C8-C9-C10   | 3.28 | 126.34      | 113.74   |
| 61  | A1    | 303  | PGV  | C8-C9-C10   | 3.33 | 126.54      | 113.74   |
| 61  | AZ    | 207  | PGV  | C8-C9-C10   | 3.34 | 126.57      | 113.74   |
| 61  | A0    | 331  | PGV  | C8-C9-C10   | 3.35 | 126.63      | 113.74   |
| 61  | BB    | 207  | PGV  | C8-C9-C10   | 3.36 | 126.65      | 113.74   |
| 61  | BB    | 217  | PGV  | C8-C9-C10   | 3.37 | 126.69      | 113.74   |
| 61  | BA    | 540  | PGV  | C8-C9-C10   | 3.38 | 126.73      | 113.74   |
| 61  | AZ    | 205  | PGV  | C8-C9-C10   | 3.39 | 126.77      | 113.74   |
| 61  | A1    | 318  | PGV  | C8-C9-C10   | 3.42 | 126.88      | 113.74   |
| 61  | A0    | 306  | PGV  | C8-C9-C10   | 3.42 | 126.90      | 113.74   |
| 61  | A0    | 317  | PGV  | C8-C9-C10   | 3.43 | 126.94      | 113.74   |
| 61  | A0    | 318  | PGV  | C8-C9-C10   | 3.46 | 127.03      | 113.74   |
| 61  | A1    | 315  | PGV  | C8-C9-C10   | 3.47 | 127.08      | 113.74   |
| 61  | BB    | 208  | PGV  | C8-C9-C10   | 3.48 | 127.10      | 113.74   |
| 61  | BA    | 501  | PGV  | C8-C9-C10   | 3.49 | 127.16      | 113.74   |
| 61  | A0    | 304  | PGV  | C8-C9-C10   | 3.50 | 127.21      | 113.74   |
| 61  | BB    | 203  | PGV  | C8-C9-C10   | 3.51 | 127.24      | 113.74   |
| 60  | A0    | 316  | PEV  | C38-C39-C40 | 3.51 | 132.56      | 114.45   |
| 61  | BA    | 512  | PGV  | C8-C9-C10   | 3.52 | 127.27      | 113.74   |
| 61  | BA    | 505  | PGV  | C8-C9-C10   | 3.59 | 127.53      | 113.74   |
| 61  | BB    | 213  | PGV  | C8-C9-C10   | 3.64 | 127.73      | 113.74   |
| 61  | A0    | 328  | PGV  | C8-C9-C10   | 3.65 | 127.78      | 113.74   |
| 61  | A1    | 311  | PGV  | C8-C9-C10   | 3.66 | 127.80      | 113.74   |
| 61  | A0    | 332  | PGV  | C8-C9-C10   | 3.67 | 127.84      | 113.74   |
| 61  | BB    | 205  | PGV  | C8-C9-C10   | 3.70 | 127.98      | 113.74   |
| 61  | A0    | 325  | PGV  | C8-C9-C10   | 3.80 | 128.33      | 113.74   |
| 60  | BA    | 533  | PEV  | C38-C39-C40 | 5.45 | 142.55      | 114.45   |
| 60  | BA    | 533  | PEV  | C39-C40-C41 | 5.96 | 145.17      | 114.45   |

All (78) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 60  | A1    | 301 | PEV  | C2   |
| 61  | BA    | 540 | PGV  | C05  |
| 61  | BA    | 540 | PGV  | C02  |
| 61  | A1    | 318 | PGV  | C05  |
| 61  | A1    | 318 | PGV  | C02  |
| 61  | A0    | 327 | PGV  | C05  |
| 61  | A0    | 327 | PGV  | C02  |
| 61  | BB    | 208 | PGV  | C05  |
| 61  | BB    | 208 | PGV  | C02  |
| 61  | A1    | 303 | PGV  | C05  |
| 61  | A1    | 303 | PGV  | C02  |
| 60  | A0    | 323 | PEV  | C2   |
| 61  | BA    | 512 | PGV  | C05  |
| 60  | A1    | 313 | PEV  | C2   |
| 61  | A1    | 311 | PGV  | C05  |
| 61  | A1    | 311 | PGV  | C02  |
| 60  | BA    | 538 | PEV  | C2   |
| 61  | BA    | 515 | PGV  | C05  |
| 61  | BA    | 515 | PGV  | C02  |
| 61  | BB    | 207 | PGV  | C05  |
| 61  | BB    | 207 | PGV  | C02  |
| 61  | BA    | 505 | PGV  | C05  |
| 61  | BA    | 505 | PGV  | C02  |
| 61  | A0    | 304 | PGV  | C05  |
| 61  | A0    | 304 | PGV  | C02  |
| 61  | A0    | 325 | PGV  | C05  |
| 61  | A0    | 325 | PGV  | C02  |
| 61  | A0    | 305 | PGV  | C05  |
| 61  | BA    | 501 | PGV  | C05  |
| 61  | A0    | 317 | PGV  | C05  |
| 61  | A0    | 317 | PGV  | C02  |
| 61  | A0    | 318 | PGV  | C05  |
| 61  | A0    | 318 | PGV  | C02  |
| 61  | A0    | 332 | PGV  | C05  |
| 61  | A0    | 332 | PGV  | C02  |
| 60  | BA    | 502 | PEV  | C2   |
| 61  | BB    | 204 | PGV  | C05  |
| 61  | BB    | 204 | PGV  | C02  |
| 61  | AZ    | 207 | PGV  | C05  |
| 61  | AZ    | 207 | PGV  | C02  |
| 60  | BB    | 202 | PEV  | C2   |
| 60  | A0    | 314 | PEV  | C2   |
| 60  | A0    | 308 | PEV  | C2   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 61  | B8    | 3005 | PGV  | C05  |
| 61  | B8    | 3005 | PGV  | C02  |
| 60  | A1    | 305  | PEV  | C2   |
| 61  | BA    | 536  | PGV  | C05  |
| 61  | BA    | 536  | PGV  | C02  |
| 60  | BA    | 535  | PEV  | C2   |
| 61  | BA    | 522  | PGV  | C05  |
| 61  | BA    | 522  | PGV  | C02  |
| 61  | A1    | 315  | PGV  | C05  |
| 61  | A1    | 315  | PGV  | C02  |
| 60  | BB    | 206  | PEV  | C2   |
| 60  | BA    | 537  | PEV  | C2   |
| 61  | A0    | 331  | PGV  | C05  |
| 61  | A0    | 331  | PGV  | C02  |
| 60  | AZ    | 204  | PEV  | C2   |
| 60  | BA    | 526  | PEV  | C2   |
| 61  | BB    | 203  | PGV  | C05  |
| 61  | BB    | 203  | PGV  | C02  |
| 60  | A1    | 317  | PEV  | C2   |
| 60  | B8    | 3001 | PEV  | C2   |
| 61  | BB    | 217  | PGV  | C05  |
| 61  | BB    | 217  | PGV  | C02  |
| 61  | A0    | 328  | PGV  | C05  |
| 61  | A0    | 328  | PGV  | C02  |
| 60  | BA    | 508  | PEV  | C2   |
| 61  | BB    | 205  | PGV  | C05  |
| 61  | BB    | 205  | PGV  | C02  |
| 61  | BA    | 516  | PGV  | C05  |
| 61  | BA    | 516  | PGV  | C02  |
| 61  | A0    | 306  | PGV  | C05  |
| 61  | A0    | 306  | PGV  | C02  |
| 60  | BA    | 530  | PEV  | C2   |
| 61  | AZ    | 205  | PGV  | C05  |
| 61  | AZ    | 205  | PGV  | C02  |
| 61  | BB    | 213  | PGV  | C05  |

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 60  | A0    | 321 | PEV  | C2-O2-C31-O31 |
| 60  | A0    | 321 | PEV  | C2-O2-C31-C32 |

There are no ring outliers.

17 monomers are involved in 41 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 60  | A0    | 315  | PEV  | 1       | 0            |
| 60  | A1    | 301  | PEV  | 1       | 0            |
| 60  | A1    | 302  | PEV  | 1       | 0            |
| 61  | A1    | 303  | PGV  | 1       | 0            |
| 61  | A1    | 315  | PGV  | 1       | 0            |
| 60  | A1    | 319  | PEV  | 1       | 0            |
| 60  | A1    | 323  | PEV  | 1       | 0            |
| 60  | B8    | 3001 | PEV  | 1       | 0            |
| 60  | B8    | 3002 | PEV  | 2       | 0            |
| 60  | BA    | 503  | PEV  | 1       | 0            |
| 61  | BA    | 512  | PGV  | 1       | 0            |
| 60  | BA    | 513  | PEV  | 1       | 0            |
| 60  | BA    | 514  | PEV  | 1       | 0            |
| 60  | BA    | 520  | PEV  | 1       | 0            |
| 60  | BA    | 526  | PEV  | 1       | 0            |
| 60  | BA    | 531  | PEV  | 1       | 0            |
| 60  | BA    | 533  | PEV  | 29      | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.