



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 09:02 am GMT

PDB ID : 4V6E  
Title : Crystal structure of the E. coli 70S ribosome in an intermediate state of ratcheting  
Authors : Zhang, W.; Dunkle, J.A.; Cate, J.H.D.  
Deposited on : 2009-06-28  
Resolution : 3.71 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28972

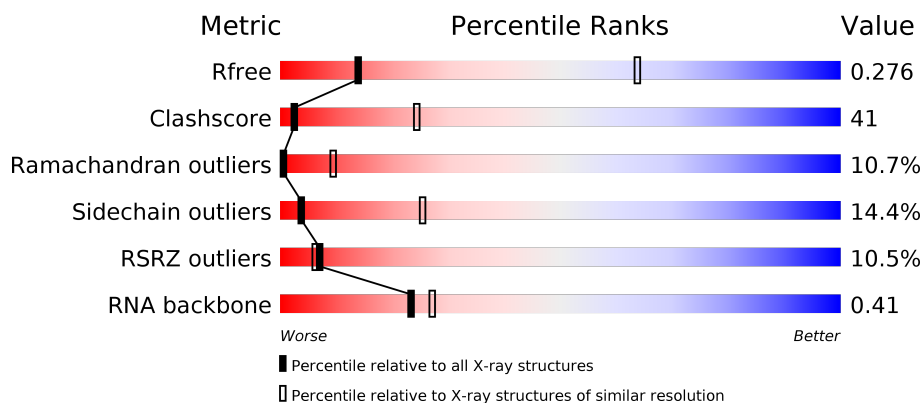
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.71 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1264 (3.94-3.50)                                      |
| Clashscore            | 112137                      | 1408 (3.94-3.50)                                      |
| Ramachandran outliers | 110173                      | 1353 (3.94-3.50)                                      |
| Sidechain outliers    | 110143                      | 1350 (3.94-3.50)                                      |
| RSRZ outliers         | 101464                      | 1293 (3.94-3.50)                                      |
| RNA backbone          | 2435                        | 1012 (4.52-2.90)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | AB    | 241    | <div> <div>34%</div> <div> <div>19%</div> <div>53%</div> <div>17%</div> <div>•</div> <div>10%</div> </div> </div> |
| 1   | CB    | 241    | <div> <div>15%</div> <div> <div>22%</div> <div>55%</div> <div>12%</div> <div>•</div> <div>10%</div> </div> </div> |
| 2   | AC    | 233    | <div> <div>5%</div> <div> <div>33%</div> <div>43%</div> <div>12%</div> <div>12%</div> </div> </div>               |
| 2   | CC    | 233    | <div> <div>7%</div> <div> <div>30%</div> <div>45%</div> <div>12%</div> <div>12%</div> </div> </div>               |

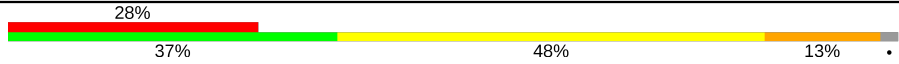
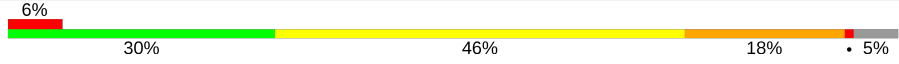
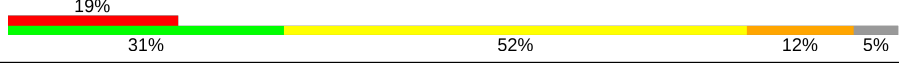
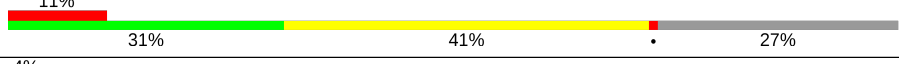
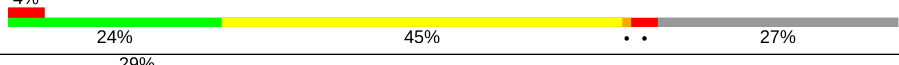
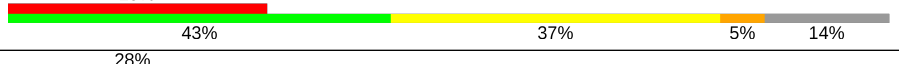
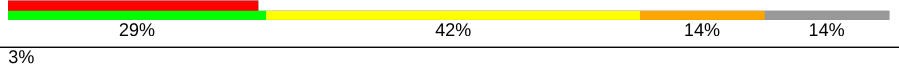

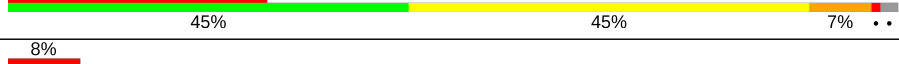
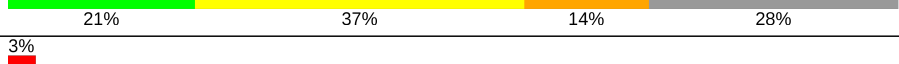

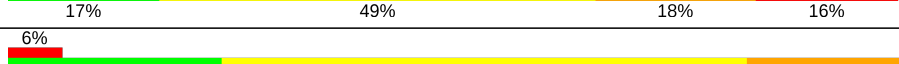
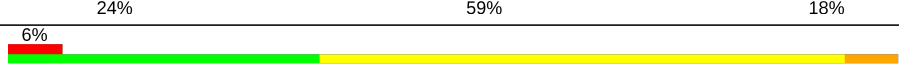
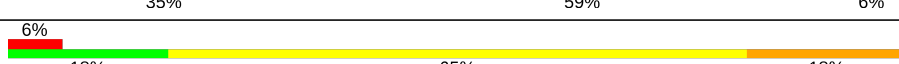
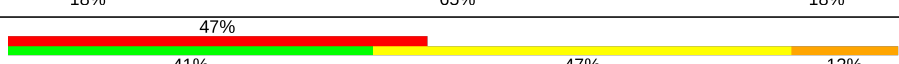

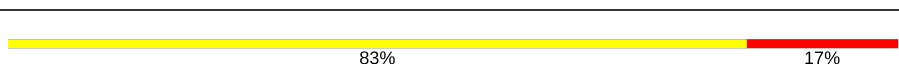
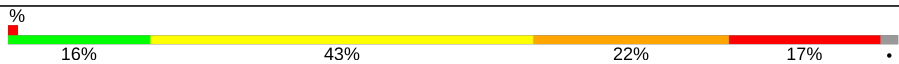
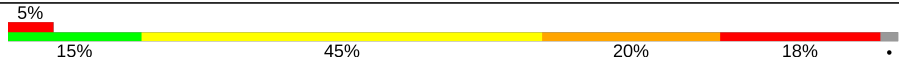
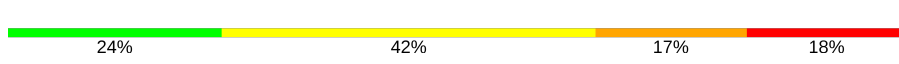

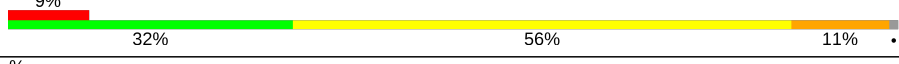



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | AD    | 206    |                  |
| 3   | CD    | 206    |                  |
| 4   | AE    | 167    |                  |
| 4   | CE    | 167    |                  |
| 5   | AF    | 135    |                  |
| 5   | CF    | 135    |                  |
| 6   | AG    | 179    |                  |
| 6   | CG    | 179    |                  |
| 7   | AH    | 130    |                  |
| 7   | CH    | 130    |                  |
| 8   | AI    | 130    |                  |
| 8   | CI    | 130    |                  |
| 9   | AJ    | 103    |                  |
| 9   | CJ    | 103    |                  |
| 10  | AK    | 129    |                  |
| 10  | CK    | 129    |                  |
| 11  | AL    | 124    |                  |
| 11  | CL    | 124    |                  |
| 12  | AM    | 118    |                  |
| 12  | CM    | 118    |                  |
| 13  | AN    | 101    |                  |
| 13  | CN    | 101    |                  |
| 14  | AO    | 89     |                  |
| 14  | CO    | 89     |                  |
| 15  | AP    | 82     |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 15  | CP    | 82     |    |
| 16  | AQ    | 84     |    |
| 16  | CQ    | 84     |    |
| 17  | AR    | 75     |    |
| 17  | CR    | 75     |    |
| 18  | AS    | 92     |    |
| 18  | CS    | 92     |    |
| 19  | AT    | 87     |    |
| 19  | CT    | 87     |    |
| 20  | AU    | 71     |    |
| 20  | CU    | 71     |    |
| 21  | AA    | 1533   |   |
| 22  | AV    | 17     |  |
| 22  | AX    | 17     |  |
| 22  | CV    | 17     |  |
| 22  | CX    | 17     |  |
| 23  | AW    | 6      |  |
| 23  | CW    | 6      |  |
| 24  | BA    | 2903   |  |
| 24  | DA    | 2903   |  |
| 25  | BB    | 118    |  |
| 26  | BC    | 273    |  |
| 26  | DC    | 273    |  |
| 27  | BD    | 209    |  |
| 27  | DD    | 209    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | BE    | 201    |                  |
| 28  | DE    | 201    |                  |
| 29  | BF    | 179    |                  |
| 29  | DF    | 179    |                  |
| 30  | BG    | 177    |                  |
| 30  | DG    | 177    |                  |
| 31  | BH    | 149    |                  |
| 31  | DH    | 149    |                  |
| 32  | BI    | 142    |                  |
| 32  | DI    | 142    |                  |
| 33  | BJ    | 142    |                  |
| 33  | DJ    | 142    |                  |
| 34  | BK    | 123    |                  |
| 34  | DK    | 123    |                  |
| 35  | BL    | 144    |                  |
| 35  | DL    | 144    |                  |
| 36  | BM    | 136    |                  |
| 36  | DM    | 136    |                  |
| 37  | BN    | 127    |                  |
| 37  | DN    | 127    |                  |
| 38  | BO    | 117    |                  |
| 38  | DO    | 117    |                  |
| 39  | BP    | 115    |                  |
| 39  | DP    | 115    |                  |
| 40  | BQ    | 118    |                  |



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40  | DQ    | 118    |                  |
| 41  | BR    | 103    |                  |
| 41  | DR    | 103    |                  |
| 42  | BS    | 110    |                  |
| 42  | DS    | 110    |                  |
| 43  | BT    | 100    |                  |
| 43  | DT    | 100    |                  |
| 44  | BU    | 104    |                  |
| 44  | DU    | 104    |                  |
| 45  | BV    | 94     |                  |
| 45  | DV    | 94     |                  |
| 46  | BW    | 85     |                  |
| 46  | DW    | 85     |                  |
| 47  | BX    | 78     |                  |
| 47  | DX    | 78     |                  |
| 48  | BY    | 63     |                  |
| 48  | DY    | 63     |                  |
| 49  | BZ    | 59     |                  |
| 49  | DZ    | 59     |                  |
| 50  | B0    | 57     |                  |
| 50  | D0    | 57     |                  |
| 51  | B1    | 55     |                  |
| 51  | D1    | 55     |                  |
| 52  | B2    | 46     |                  |
| 52  | D2    | 46     |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 53  | B3    | 65     |  |
| 53  | D3    | 65     |  |
| 54  | B4    | 38     |  |
| 54  | D4    | 38     |  |
| 55  | CA    | 1530   |  |
| 56  | DB    | 117    |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | AA    | 1607 | -         | -        | -       | X                |
| 57  | MG   | AA    | 1625 | -         | -        | -       | X                |
| 57  | MG   | AA    | 1629 | -         | -        | -       | X                |
| 57  | MG   | AA    | 1641 | -         | -        | -       | X                |
| 57  | MG   | AA    | 1642 | -         | -        | -       | X                |
| 57  | MG   | BA    | 3002 | -         | -        | -       | X                |
| 57  | MG   | BA    | 3022 | -         | -        | -       | X                |
| 57  | MG   | BA    | 3028 | -         | -        | -       | X                |
| 57  | MG   | BA    | 3041 | -         | -        | -       | X                |
| 57  | MG   | BA    | 3048 | -         | -        | -       | X                |
| 57  | MG   | BA    | 3056 | -         | -        | -       | X                |
| 57  | MG   | BA    | 3058 | -         | -        | -       | X                |
| 57  | MG   | BA    | 3060 | -         | -        | -       | X                |
| 57  | MG   | BA    | 3072 | -         | -        | -       | X                |
| 57  | MG   | BA    | 3084 | -         | -        | -       | X                |
| 57  | MG   | BA    | 3124 | -         | -        | -       | X                |
| 57  | MG   | BA    | 3136 | -         | -        | -       | X                |
| 57  | MG   | CA    | 1610 | -         | -        | -       | X                |
| 57  | MG   | CA    | 1625 | -         | -        | -       | X                |
| 57  | MG   | CA    | 1628 | -         | -        | -       | X                |
| 57  | MG   | CA    | 1637 | -         | -        | -       | X                |
| 57  | MG   | CA    | 1640 | -         | -        | -       | X                |
| 57  | MG   | DA    | 3002 | -         | -        | -       | X                |
| 57  | MG   | DA    | 3060 | -         | -        | -       | X                |
| 57  | MG   | DA    | 3065 | -         | -        | -       | X                |
| 57  | MG   | DA    | 3068 | -         | -        | -       | X                |
| 57  | MG   | DA    | 3069 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | DA    | 3072 | -         | -        | -       | X                |
| 57  | MG   | DA    | 3075 | -         | -        | -       | X                |
| 57  | MG   | DA    | 3076 | -         | -        | -       | X                |
| 57  | MG   | DA    | 3084 | -         | -        | -       | X                |
| 57  | MG   | DA    | 3104 | -         | -        | -       | X                |
| 57  | MG   | DA    | 3106 | -         | -        | -       | X                |
| 57  | MG   | DA    | 3108 | -         | -        | -       | X                |
| 57  | MG   | DA    | 3124 | -         | -        | -       | X                |
| 57  | MG   | DA    | 3128 | -         | -        | -       | X                |



## 2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 286150 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | AB    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1704  | 1081 | 305 | 311 | 7 |         |         |       |
| 1   | CB    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1704  | 1081 | 305 | 311 | 7 |         |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | AC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |         |       |
| 2   | CC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | AD    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |         |       |
| 3   | CD    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | AE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1105  | 687 | 211 | 201 | 6 |         |         |       |
| 4   | CE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1105  | 687 | 211 | 201 | 6 |         |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | AF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 817   | 515 | 148 | 148 | 6 |         |         |       |
| 5   | CF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 817   | 515 | 148 | 148 | 6 |         |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | AG    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1181  | 735 | 227 | 215 | 4 |         |         |       |
| 6   | CG    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1174  | 730 | 226 | 214 | 4 |         |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AH    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |         |       |
| 7   | CH    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AI    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |         |       |
| 8   | CI    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | AJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |         |       |
| 9   | CJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | AK    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | CK    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | AL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |         |       |
| 11  | CL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AM    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 883   | 546 | 178 | 156 | 3 |         |         |       |
| 12  | CM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 876   | 541 | 177 | 155 | 3 |         |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AN    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 774   | 483 | 160 | 128 | 3 |         |         |       |
| 13  | CN    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 480 | 159 | 127 | 3 |         |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | AO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |         |       |
| 14  | CO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | AP    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |         |       |
| 15  | CP    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 638   | 400 | 126 | 111 | 1 |         |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | AQ    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |         |       |
| 16  | CQ    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 17  | AR    | 55       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 455   | 288 | 86 | 81 |         |         |       |
| 17  | CR    | 55       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 455   | 288 | 86 | 81 |         |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18  | AS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 637   | 408 | 120 | 107 | 2 |         |         |       |
| 18  | CS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 637   | 408 | 120 | 107 | 2 |         |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AT    | 85       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |         |       |
| 19  | CT    | 85       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 20  | AU    | 51       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 425   | 265 | 86 | 73 | 1 |         |         |       |
| 20  | CU    | 51       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 425   | 265 | 86 | 73 | 1 |         |         |       |

- Molecule 21 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 21  | AA    | 1533     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32895 | 14671 | 6036 | 10655 | 1533 |         |         |       |

- Molecule 22 is a RNA chain called P-site tRNA ASL fragment.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 22  | AV    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 365   | 163 | 68 | 117 | 17 |         |         |       |
| 22  | AX    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 365   | 163 | 68 | 117 | 17 |         |         |       |
| 22  | CV    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 365   | 163 | 68 | 117 | 17 |         |         |       |
| 22  | CX    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 365   | 163 | 68 | 117 | 17 |         |         |       |

- Molecule 23 is a RNA chain called messenger RNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 23  | AW    | 6        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 120   | 54 | 12 | 48 | 6 |         |         |       |
| 23  | CW    | 6        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 120   | 54 | 12 | 48 | 6 |         |         |       |

- Molecule 24 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 24  | BA    | 2854     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61274 | 27334 | 11279 | 19807 | 2854 |         |         |       |
| 24  | DA    | 2841     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60995 | 27210 | 11229 | 19715 | 2841 |         |         |       |

- Molecule 25 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 25  | BB    | 118      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2529  | 1126 | 464 | 821 | 118 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 26  | BC    | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 26  | DC    | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27  | BD    | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |         |       |
| 27  | DD    | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | BE    | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |         |       |
| 28  | DE    | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | BF    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |         |       |
| 29  | DF    | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1420  | 905 | 251 | 258 | 6 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | BG    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |         |       |
| 30  | DG    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |         |       |
| 31  | DH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | BI    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |         |       |
| 32  | DI    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | BJ    | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |         |       |
| 33  | DJ    | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | BK    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 938   | 587 | 180 | 165 | 6 |         |         |       |
| 34  | DK    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 938   | 587 | 180 | 165 | 6 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BL    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |         |       |
| 35  | DL    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | BM    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |         |       |
| 36  | DM    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | BN    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 960   | 593 | 196 | 166 | 5 |         |         |       |
| 37  | DN    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 960   | 593 | 196 | 166 | 5 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 38  | BO    | 116      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |  |         |         |       |
| 38  | DO    | 116      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |  |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | BP    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |         |       |
| 39  | DP    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 40  | BQ    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |  |         |         |       |
| 40  | DQ    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |  |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BR    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |         |       |
| 41  | DR    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BS    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | DS    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | BT    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |         |       |
| 43  | DT    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | BU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |   |         |         |       |
| 44  | DU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |   |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | BV    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |         |       |
| 45  | DV    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | BW    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 596   | 367 | 120 | 108 | 1 |         |         |       |
| 46  | DW    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 596   | 367 | 120 | 108 | 1 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | BX    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |         |       |
| 47  | DX    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 48  | BY    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |         |       |
| 48  | DY    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 49  | BZ    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |         |       |
| 49  | DZ    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50  | B0    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |         |       |
| 50  | D0    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 51  | B1    | 50       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 409   | 263 | 75 | 71 |         |         |       |
| 51  | D1    | 50       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 409   | 263 | 75 | 71 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52  | B2    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |         |       |
| 52  | D2    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 53  | B3    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |         |       |
| 53  | D3    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 54  | B4    | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |         |       |
| 54  | D4    | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |         |       |

- Molecule 55 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 55  | CA    | 1530     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32831 | 14642 | 6024 | 10635 | 1530 |         |         |       |

- Molecule 56 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 56  | DB    | 117      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2507  | 1116 | 459 | 815 | 117 |         |         |       |

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57  | BB    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 57  | BA    | 136      | Total | Mg  | 0       | 0       |
|     |       |          | 136   | 136 |         |         |
| 57  | CA    | 42       | Total | Mg  | 0       | 0       |
|     |       |          | 42    | 42  |         |         |
| 57  | DJ    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 57  | BD    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 57  | AA    | 43       | Total | Mg  | 0       | 0       |
|     |       |          | 43    | 43  |         |         |
| 57  | D4    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57  | DA    | 132      | Total<br>132 | Mg<br>132 | 0       | 0       |
| 57  | DC    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | DB    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 58  | B4    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 58  | D4    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

- Molecule 59 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 59  | AE    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 59  | AL    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 59  | AN    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 59  | AT    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 59  | AU    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 59  | AA    | 196      | Total<br>196 | O<br>196 | 0       | 0       |
| 59  | BA    | 615      | Total<br>615 | O<br>615 | 0       | 0       |
| 59  | BB    | 20       | Total<br>20  | O<br>20  | 0       | 0       |
| 59  | BC    | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 59  | BD    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 59  | BE    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 59  | BL    | 3        | Total<br>3   | O<br>3   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 59  | BN    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 59  | BT    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 59  | B2    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 59  | B3    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 59  | B4    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 59  | CE    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 59  | CI    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 59  | CL    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 59  | CN    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 59  | CT    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 59  | CU    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 59  | CA    | 195      | Total<br>195 | O<br>195 | 0       | 0       |
| 59  | DA    | 600      | Total<br>600 | O<br>600 | 0       | 0       |
| 59  | DB    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 59  | DC    | 12       | Total<br>12  | O<br>12  | 0       | 0       |
| 59  | DD    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 59  | DE    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 59  | DJ    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 59  | DL    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 59  | DN    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 59  | DT    | 2        | Total<br>2   | O<br>2   | 0       | 0       |

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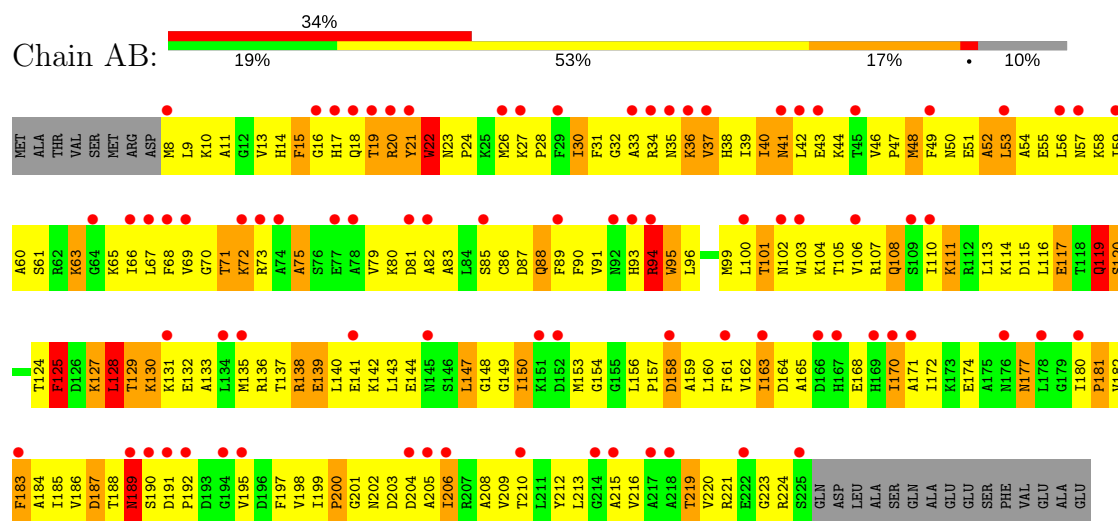
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| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 59  | DU    | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 59  | DV    | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 59  | D2    | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 59  | D3    | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 59  | D4    | 5        | Total<br>5 | O<br>5 | 0       | 0       |

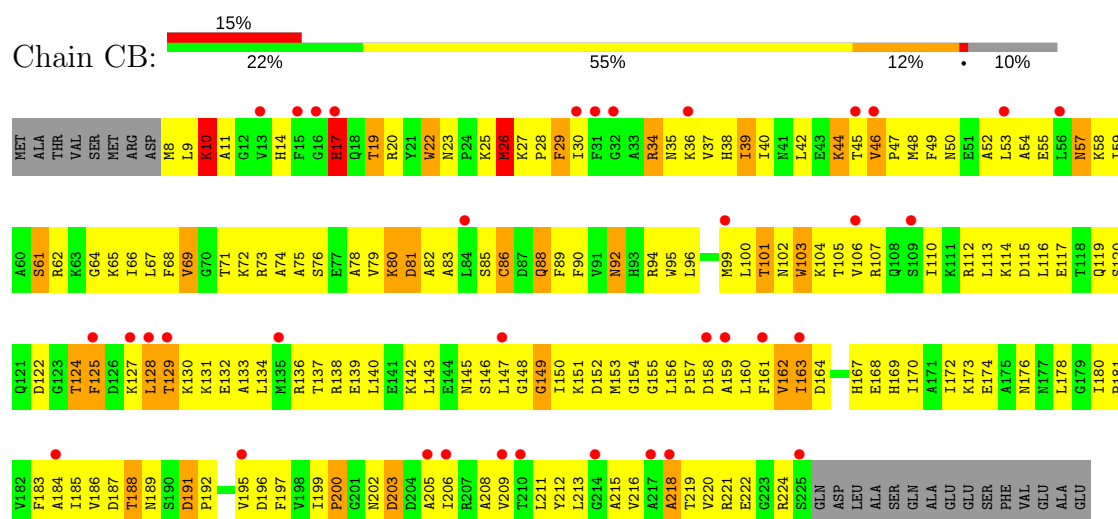
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: 30S ribosomal protein S2

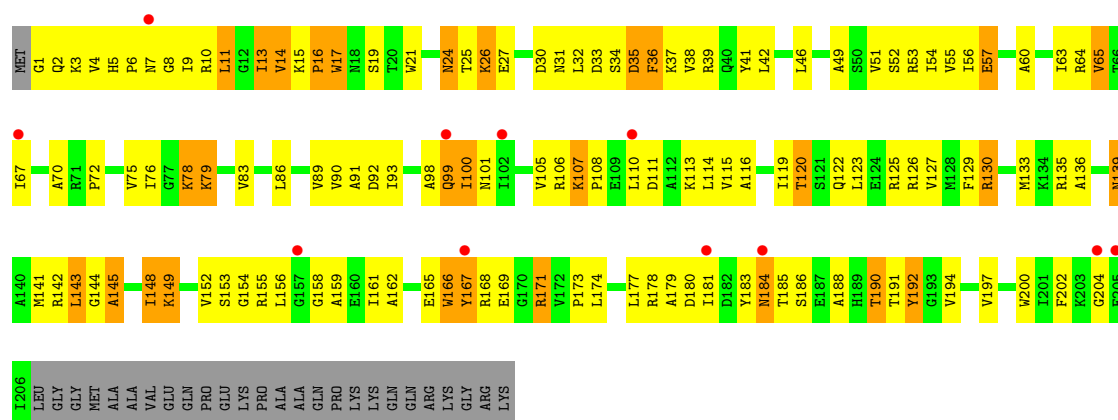


#### • Molecule 1: 30S ribosomal protein S2

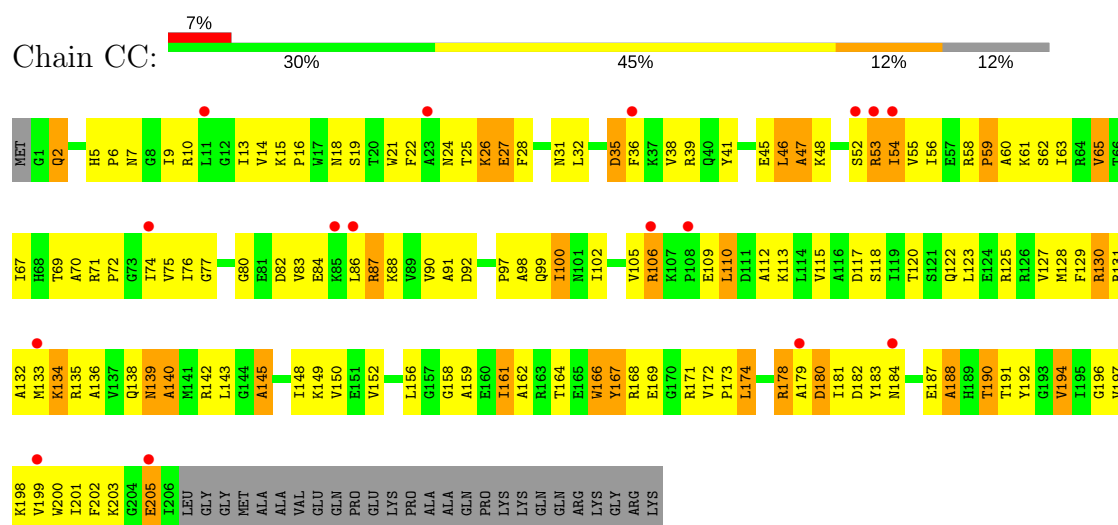


#### • Molecule 2: 30S ribosomal protein S3

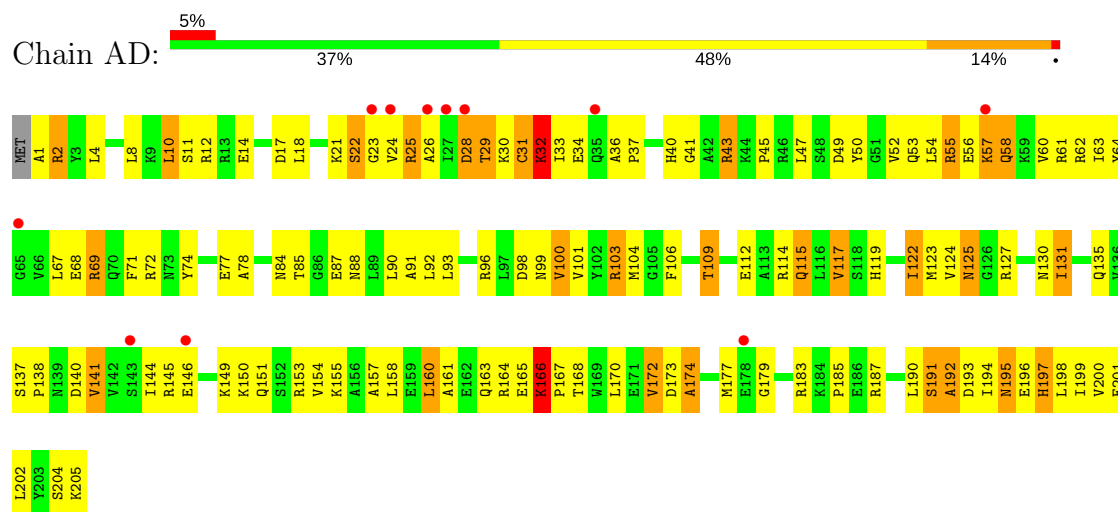




• Molecule 2: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S4



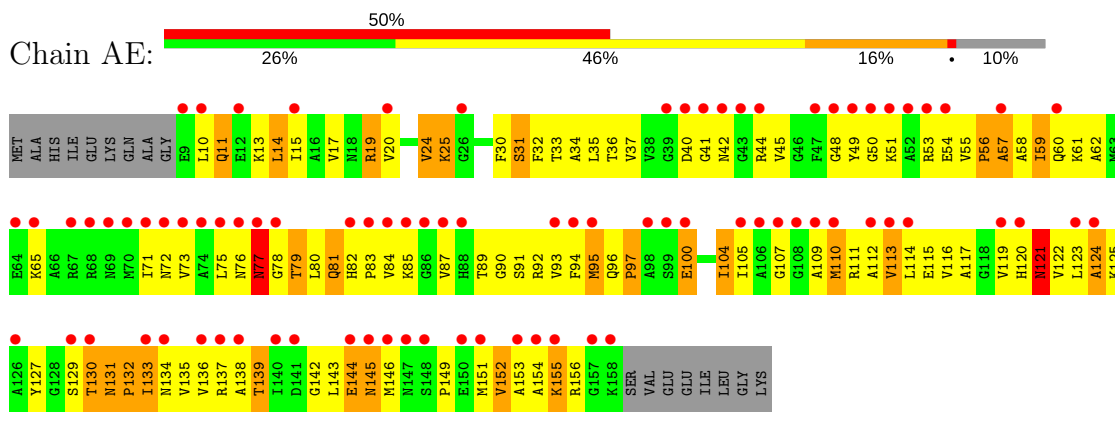
• Molecule 3: 30S ribosomal protein S4



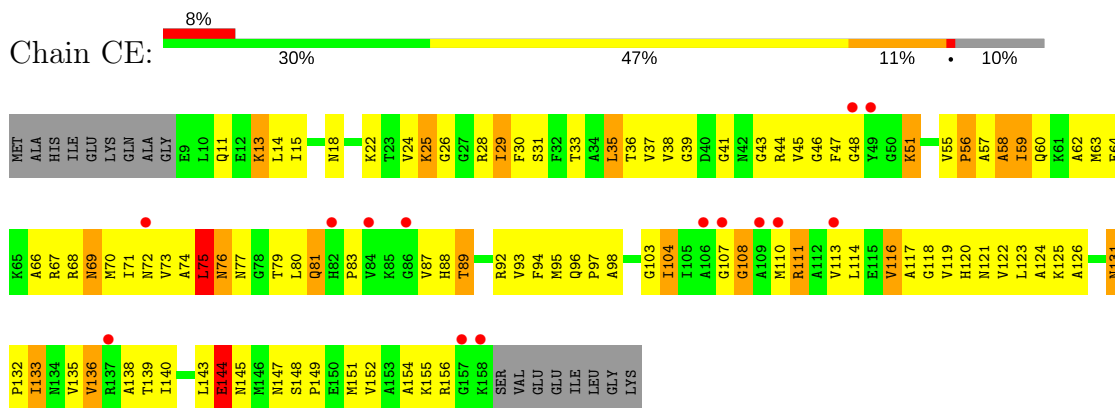




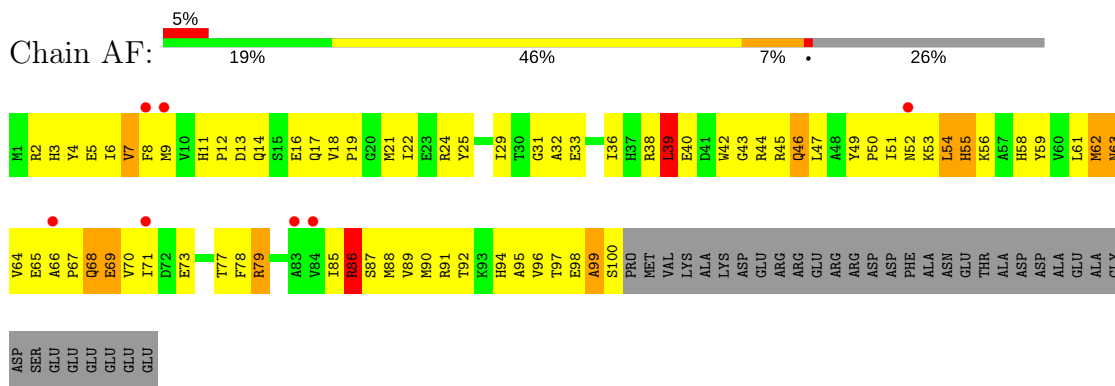
- Molecule 4: 30S ribosomal protein S5



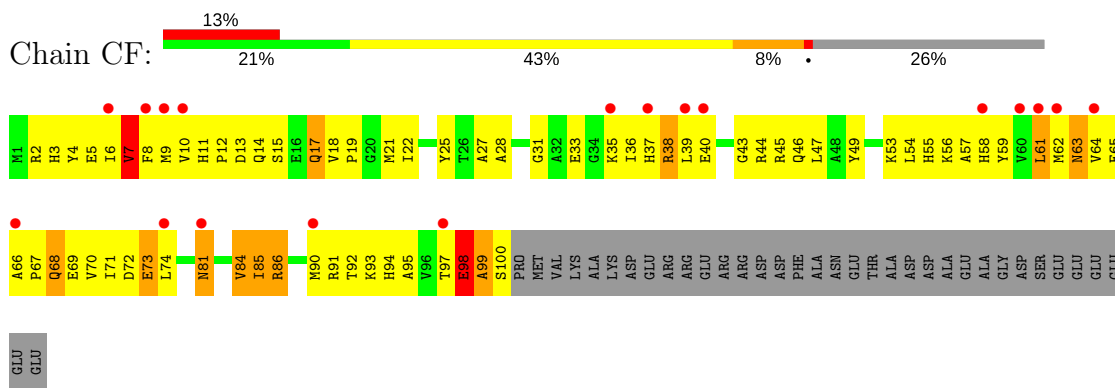
- Molecule 4: 30S ribosomal protein S5



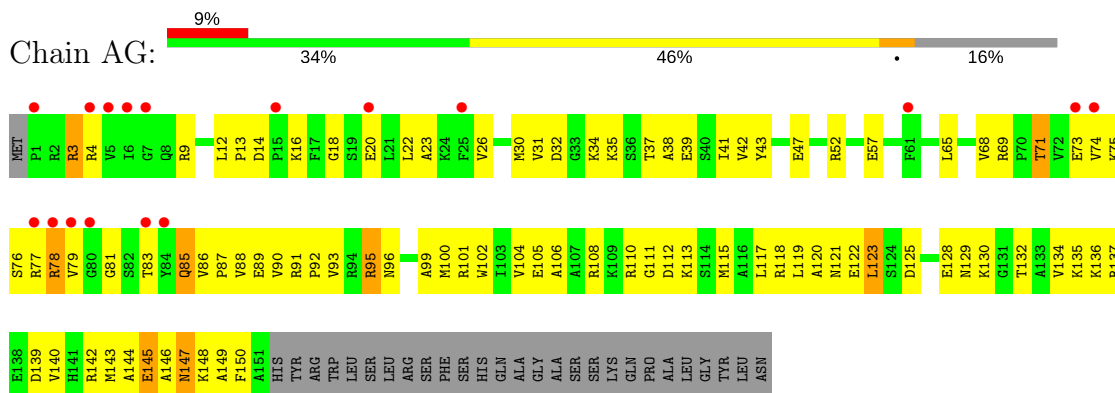
- Molecule 5: 30S ribosomal protein S6



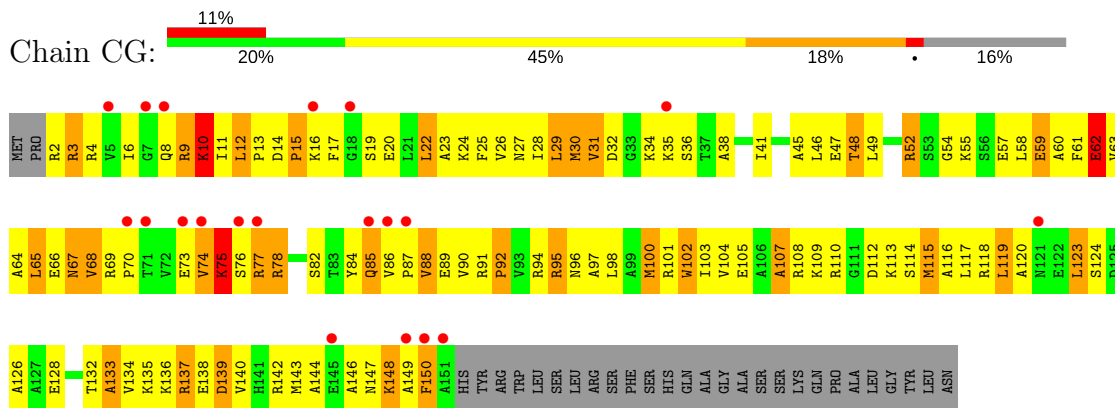
- Molecule 5: 30S ribosomal protein S6



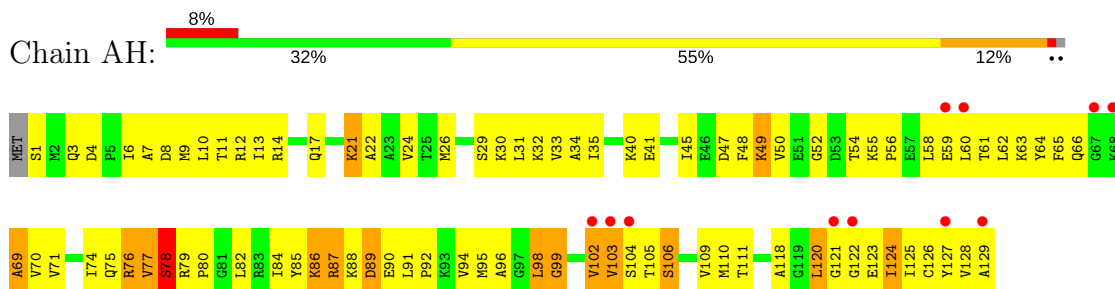
- Molecule 6: 30S ribosomal protein S7



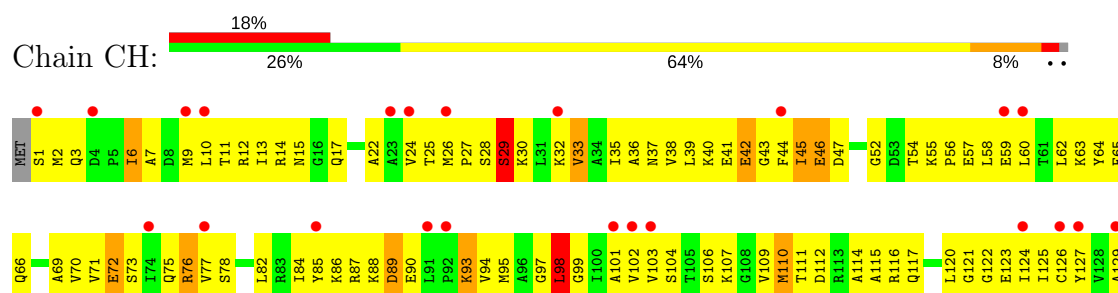
- Molecule 6: 30S ribosomal protein S7



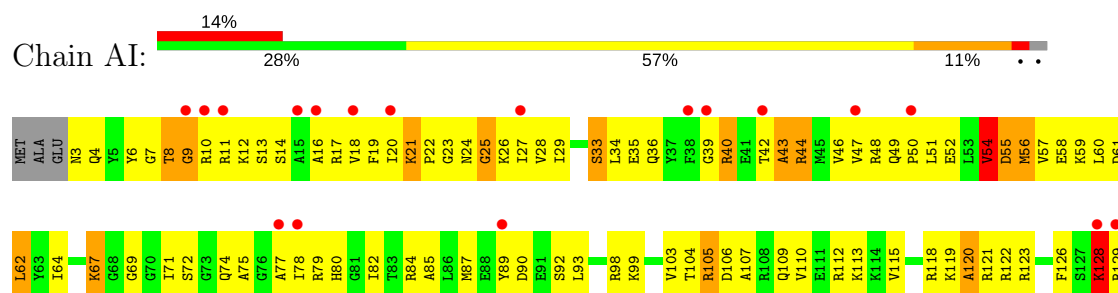
- Molecule 7: 30S ribosomal protein S8



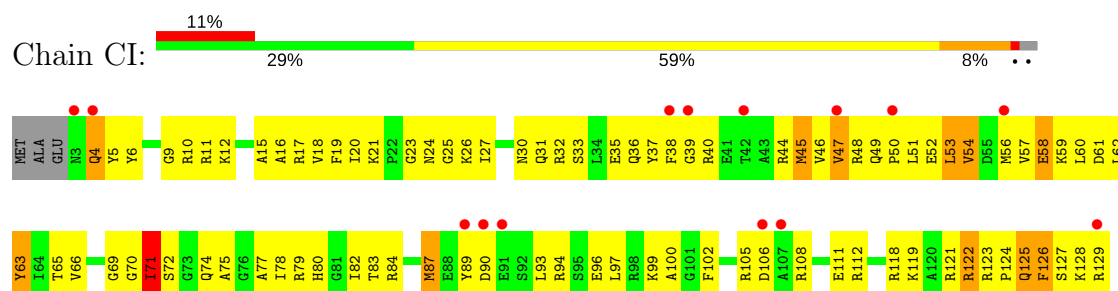
- Molecule 7: 30S ribosomal protein S8



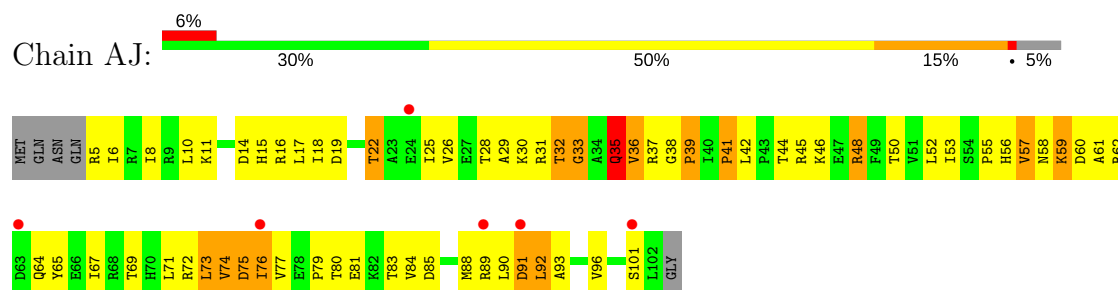
• Molecule 8: 30S ribosomal protein S9



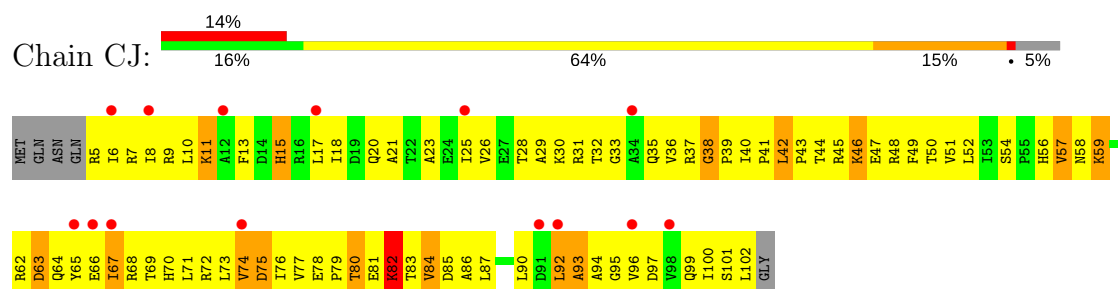
• Molecule 8: 30S ribosomal protein S9



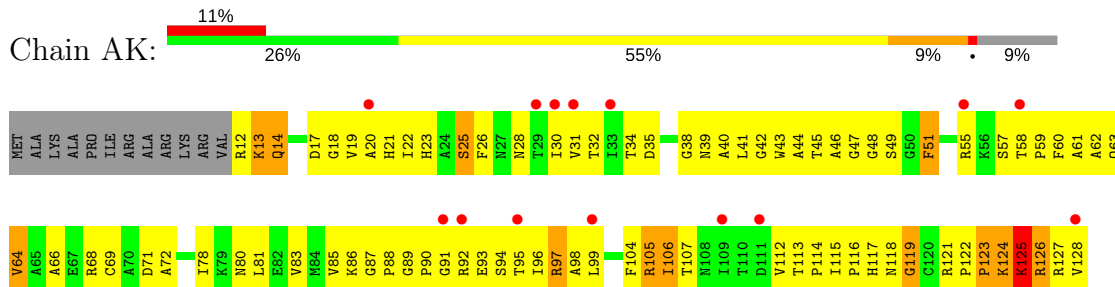
• Molecule 9: 30S ribosomal protein S10



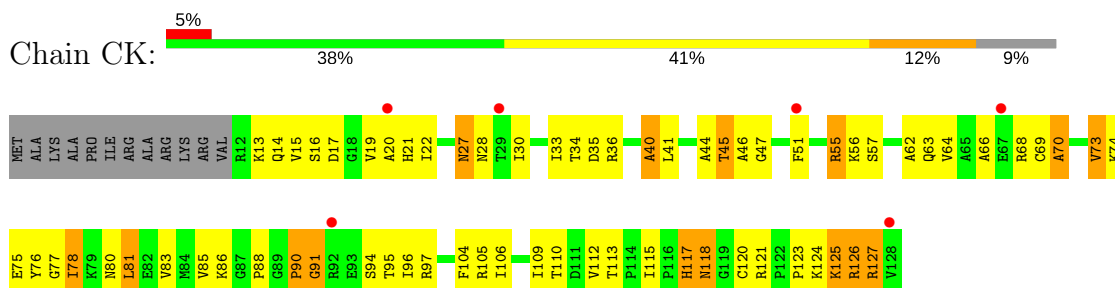
• Molecule 9: 30S ribosomal protein S10



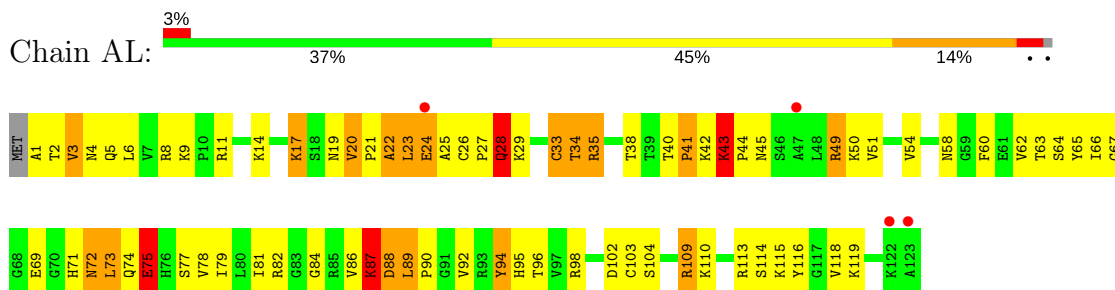
- Molecule 10: 30S ribosomal protein S11



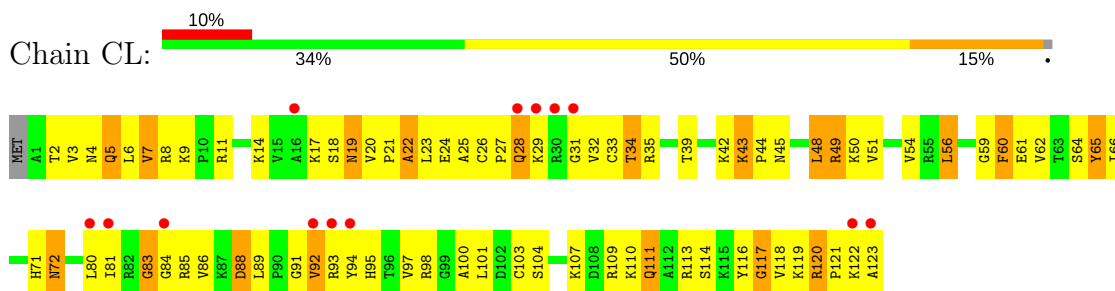
- Molecule 10: 30S ribosomal protein S11



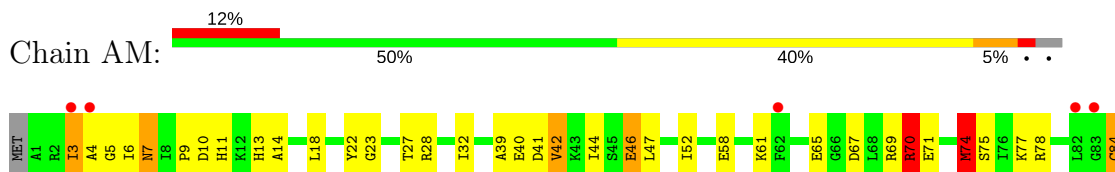
- Molecule 11: 30S ribosomal protein S12

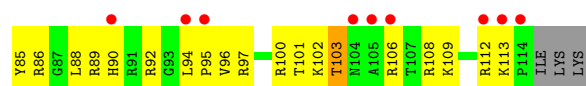


- Molecule 11: 30S ribosomal protein S12

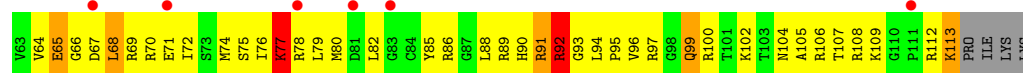


- Molecule 12: 30S ribosomal protein S13

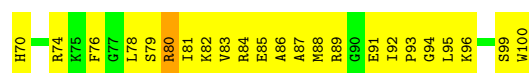
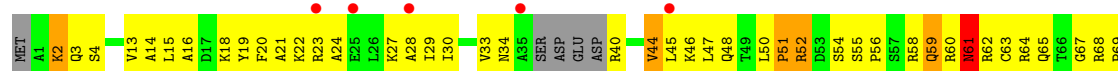




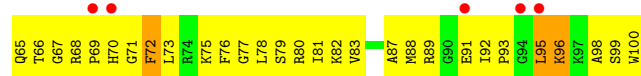
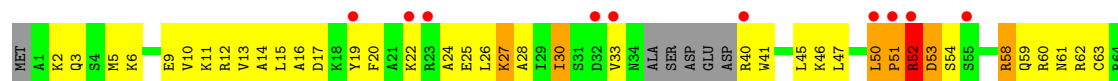
- Molecule 12: 30S ribosomal protein S13



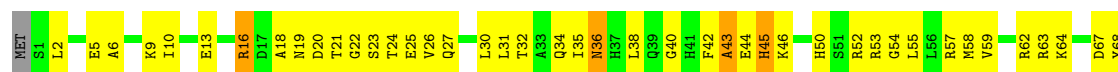
- Molecule 13: 30S ribosomal protein S14



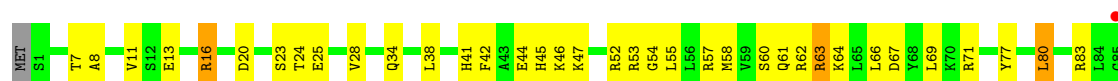
- Molecule 13: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S15

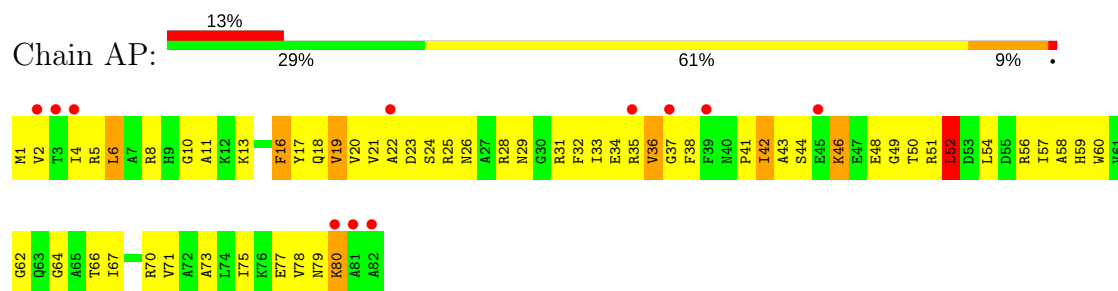


- Molecule 14: 30S ribosomal protein S15

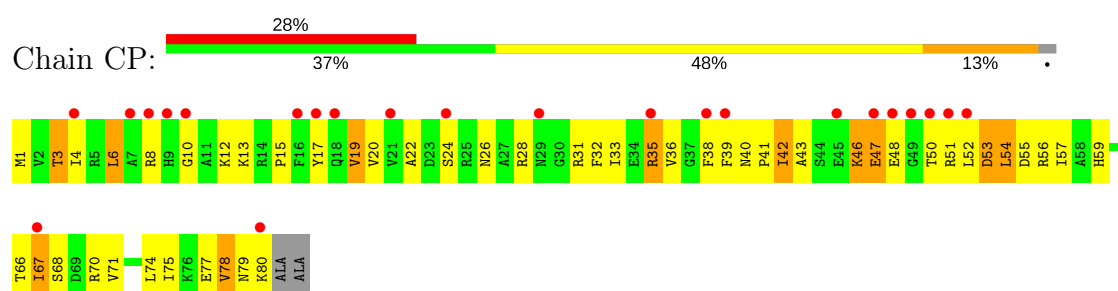




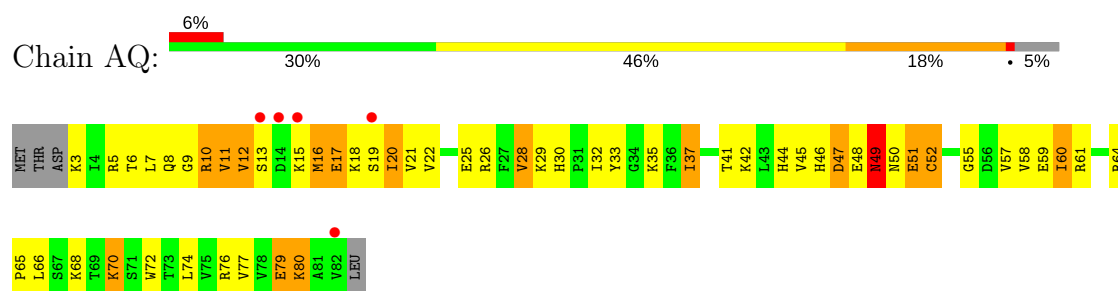
- Molecule 15: 30S ribosomal protein S16



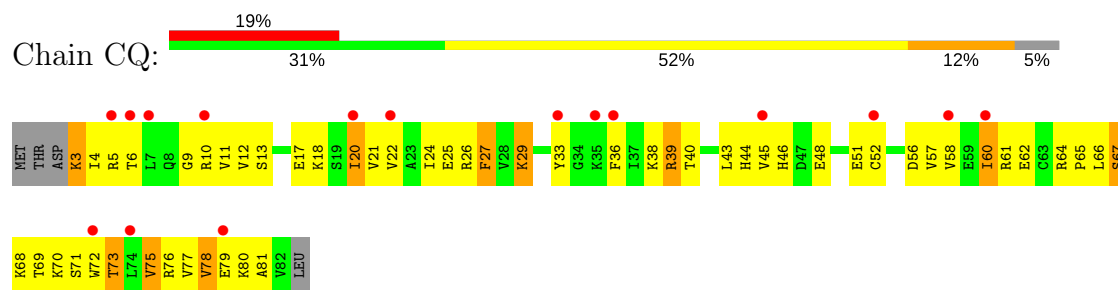
- Molecule 15: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S17

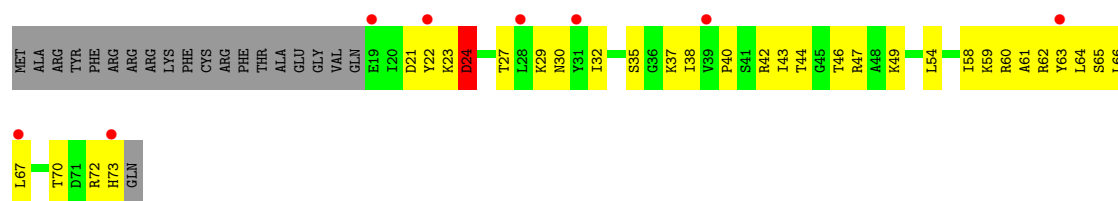


- Molecule 16: 30S ribosomal protein S17

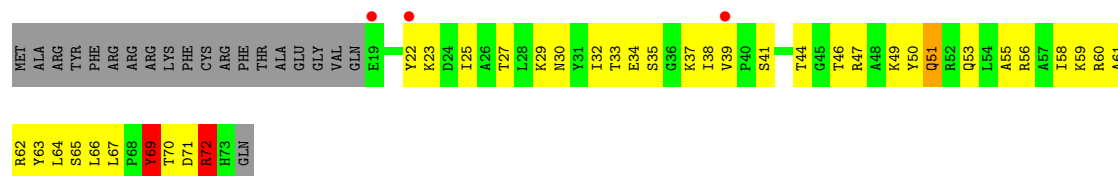


- Molecule 17: 30S ribosomal protein S18

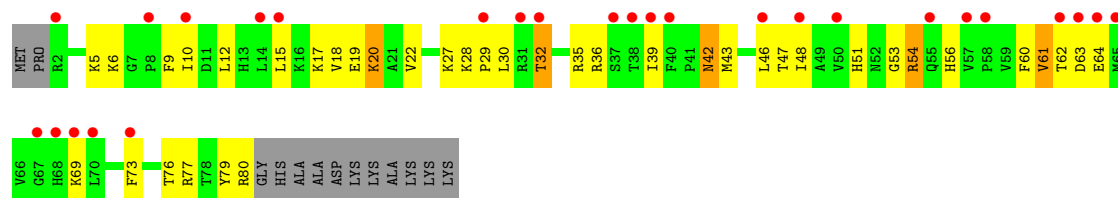
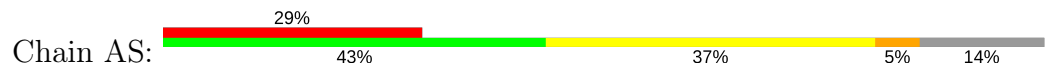




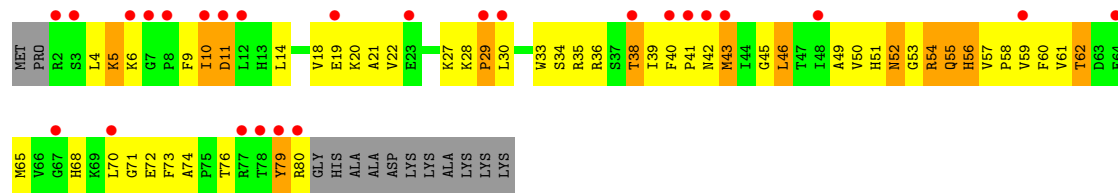
- Molecule 17: 30S ribosomal protein S18



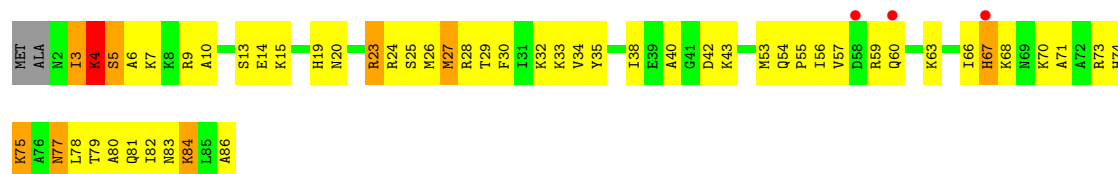
- Molecule 18: 30S ribosomal protein S19



- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



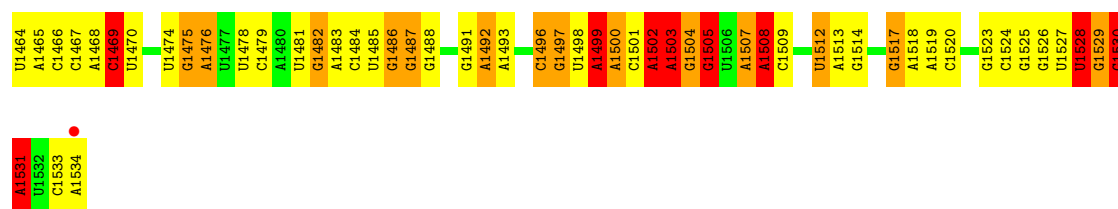
- Molecule 19: 30S ribosomal protein S20



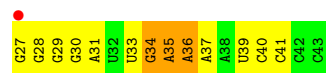




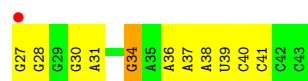
|       |       |       |       |       |       |       |      |      |      |      |      |      |      |
|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|
| C1389 | G1276 | U1211 | C1149 | G1087 | U1025 | U957  | G894 | U827 | A702 | C637 | G570 | A510 | A448 |
| C1400 | C1277 | U1212 | A1150 | G1088 | G1026 | A958  | G895 | U828 | G703 | U638 | U571 | C511 | G449 |
| G1401 | G1278 | C1213 | A1151 | G1089 | C1027 | A959  | C896 | G829 | A704 | G639 | A572 | U512 | G450 |
| C1402 | G1279 | C1214 | A1152 | U1090 | C887  | U960  | C897 | G830 | G705 | A640 | G573 | A451 | A451 |
| C1403 | A1280 | G1215 | G1153 | U1091 | U1029 | U961  | G898 | G831 | A706 | U641 | A574 | C514 | A452 |
| C1404 | C1281 | A1216 | G1154 | U1092 | U1030 | C962  | C899 | G832 | U707 | A642 | G575 | C515 | G453 |
| C1405 | C1282 | C1217 | A1155 | A1093 | C1031 | G963  | A900 | G833 | C708 | C643 | C576 | U516 | G454 |
| U1345 | U1283 | C1218 | G1156 | G1094 | G1032 | A964  | A901 | U834 | U709 | U644 | C577 | G517 | G455 |
| A1408 | C1284 | A1219 | A1157 | U1095 | G1033 | U965  | G902 | U835 | G710 | G645 | C578 | C518 | A456 |
| C1409 | U1285 | G1220 | C1158 | C1096 | G1034 | C966  | G903 | U836 | G711 | G646 | A579 | A520 | U458 |
| A1410 | U1286 | G1221 | A1159 | C1097 | A1035 | C967  | U904 | U837 | A712 | G650 | C580 | G521 | G459 |
| A1349 | A1287 | G1222 | G1160 | C1098 | A1036 | A968  | U908 | G838 | G713 | G651 | G581 | A460 | A460 |
| A1350 | A1288 | C1223 | C1161 | G1099 | C1037 | A969  | A908 | C839 | G714 | U652 | C582 | C522 | A461 |
| U1351 | U1289 | U1224 | C1162 | C1100 | C1038 | A970  | A909 | C841 | A715 | U653 | A583 | A533 | G462 |
| C1352 | G1290 | C1225 | A1163 | A1101 | G1039 | C972  | C910 | U842 | U716 | U654 | C586 | G524 | G463 |
| G1353 | U1291 | C1226 | G1164 | A1102 | U1040 | G973  | C911 | U843 | A717 | C655 | C587 | C525 | U464 |
| G1356 | U1292 | A1227 | U1165 | C1103 | G1043 | A974  | C912 | G844 | C718 | A655 | G587 | C526 | U465 |
| A1357 | G1296 | G1228 | G1166 | G1104 | G1044 | A975  | A913 | A845 | C719 | G656 | G588 | G527 | A466 |
| A1358 | C1297 | A1229 | A1167 | A1105 | A1045 | G976  | A914 | G846 | C720 | U657 | U589 | C528 | A467 |
| U1359 | U1298 | C1230 | U1168 | C1106 | C1046 | A977  | A915 | G847 | G721 | C658 | U590 | G529 | U468 |
| A1360 | G1299 | C1231 | A1169 | C1107 | A1047 | A978  | U916 | C848 | G722 | U662 | U594 | G530 | A468 |
| G1361 | A1300 | U1235 | A1170 | G1108 | G1048 | C979  | G917 | G849 | U723 | U663 | A595 | U531 | C469 |
| G1362 | U1301 | U1236 | A1171 | C1109 | U1049 | C980  | A918 | U889 | G724 | A663 | A596 | A532 | C470 |
| A1363 | C1302 | C1237 | U1172 | A1110 | G1050 | U981  | A919 | A790 | G725 | A664 | A597 | A533 | U471 |
| U1364 | C1303 | A1238 | U1173 | A1111 | C1051 | A983  | U920 | G852 | G726 | A665 | G597 | U534 | U472 |
| C1365 | G1304 | A1239 | G1174 | C1112 | C1052 | C984  | U921 | U854 | G727 | G666 | U598 | A535 | U473 |
| C1366 | U1305 | U1240 | G1175 | C1113 | U1053 | C985  | G922 | U855 | A728 | G667 | C599 | C536 | G474 |
| C1367 | A1306 | G1241 | G1176 | U1117 | C1054 | U986  | C924 | C957 | G731 | G668 | G601 | G537 | C475 |
| A1368 | U1307 | G1242 | G1177 | U1118 | A1055 | C987  | G925 | G858 | G732 | G669 | A602 | A538 | U479 |
| C1369 | U1308 | C1243 | A1178 | C1119 | G1056 | G988  | G926 | G859 | G733 | G671 | G603 | G540 | U480 |
| G1370 | G1309 | G1244 | A1180 | C1120 | G1058 | U991  | G927 | A860 | G734 | U672 | U604 | G541 | G481 |
| A1433 | G1310 | C1245 | G1181 | U1121 | C1059 | U992  | G928 | C866 | C735 | A673 | U605 | G542 | A482 |
| A1434 | A1311 | A1246 | G1182 | U1122 | U1060 | G993  | C929 | G867 | C736 | G674 | G606 | U543 | C483 |
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| U1375 | C1314 | C1249 | G1185 | U1125 | C1063 | C996  | C934 | G869 | C739 | U677 | A609 | A546 | U486 |
| U1376 | U1315 | A1250 | G1186 | U1126 | G1064 | A996  | C935 | U870 | U740 | U678 | U610 | A547 | A487 |
| A1441 | U1316 | A1251 | G1187 | G1127 | U1065 | U997  | A936 | U871 | G741 | C679 | C613 | G548 | C488 |
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| U1443 | A1318 | G1253 | A1191 | C1129 | A1067 | U999  | A937 | A873 | A743 | A681 | C514 | G550 | C490 |
| U1444 | C1319 | G1254 | C1192 | A1130 | G1068 | C1001 | A938 | U874 | C744 | G682 | G615 | U551 | G491 |
| A1446 | A1320 | A1255 | G1193 | G1131 | C1069 | G1002 | G939 | U875 | G745 | G683 | G616 | U552 | C492 |
| C1392 | U1321 | C1256 | U1194 | C1132 | U1070 | G1003 | C940 | C876 | A746 | U684 | U619 | A553 | A493 |
| C1393 | C1322 | G1257 | C1195 | G1133 | C1071 | A1004 | G941 | G877 | A747 | G685 | A554 | A554 | G494 |
| C1394 | G1323 | C1258 | A1196 | G1134 | U1072 | U1005 | G942 | A878 | G748 | U686 | U555 | A495 | A495 |
| G1395 | A1324 | G1260 | A1197 | U1135 | U1073 | G1006 | U943 | C879 | A749 | A687 | A622 | A496 | A496 |
| C1396 | C1325 | A1261 | G1198 | C1136 | G1074 | U1007 | G944 | C880 | C750 | G688 | C523 | G557 | G497 |
| G1397 | U1326 | C1262 | U1199 | G1137 | U1075 | U1008 | G945 | C881 | U751 | C689 | C524 | G558 | A498 |
| C1398 | C1327 | C1263 | C1200 | G1138 | U1076 | U1009 | A946 | U882 | G752 | G690 | U625 | A559 | A499 |
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| U1455 | A1329 | G1265 | U1202 | C1140 | U1078 | G1015 | C948 | G885 | C754 | U692 | G627 | U561 | C501 |
| A1456 | C1203 | C1141 | C1203 | C1141 | G1079 | A1016 | A949 | G886 | G755 | U693 | G628 | U562 | A502 |
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| G1458 | A1332 | G1270 | U1206 | G1144 | A1082 | U952  | A889 | U822 | C531 | A696 | A631 | U565 | G505 |
| C1395 | C1333 | A1271 | G1207 | A1145 | U1083 | A1021 | G890 | G893 | U632 | C532 | U566 | G506 | G506 |
| U1459 | G1334 | G1272 | G1208 | A1146 | U1084 | U1022 | G954 | G894 | G761 | G533 | G533 | G507 | C507 |
| C1460 | U1335 | C1273 | C1209 | C1147 | U1085 | U1023 | A955 | A892 | U762 | G700 | U636 | G508 | U508 |
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- Molecule 22: P-site tRNA ASL fragment



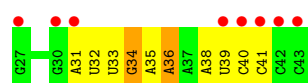
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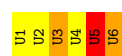
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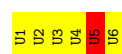
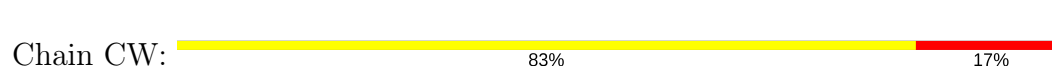
- Molecule 22: P-site tRNA ASL fragment



- Molecule 23: messenger RNA



- Molecule 23: messenger RNA



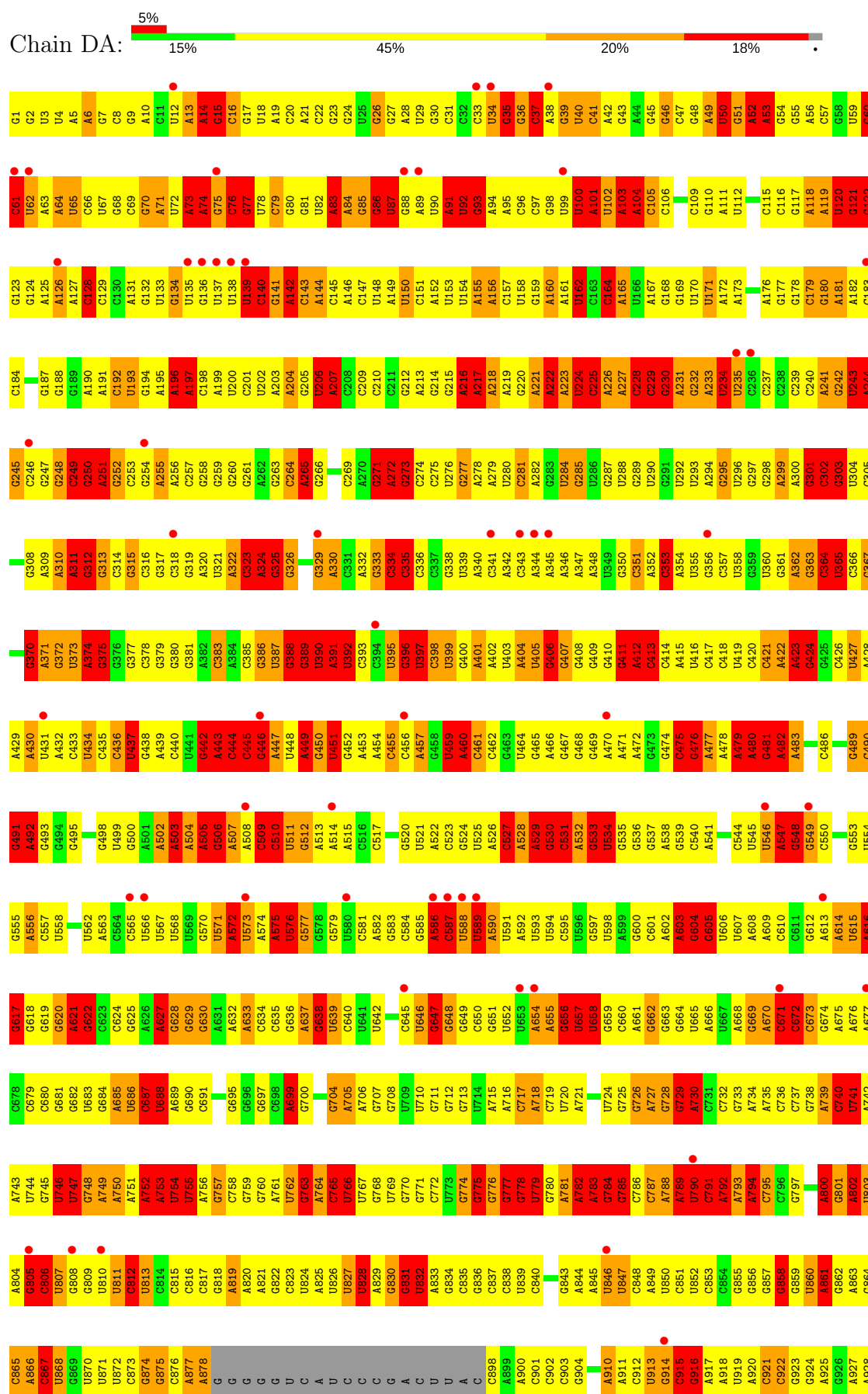
- Molecule 24: 23S rRNA

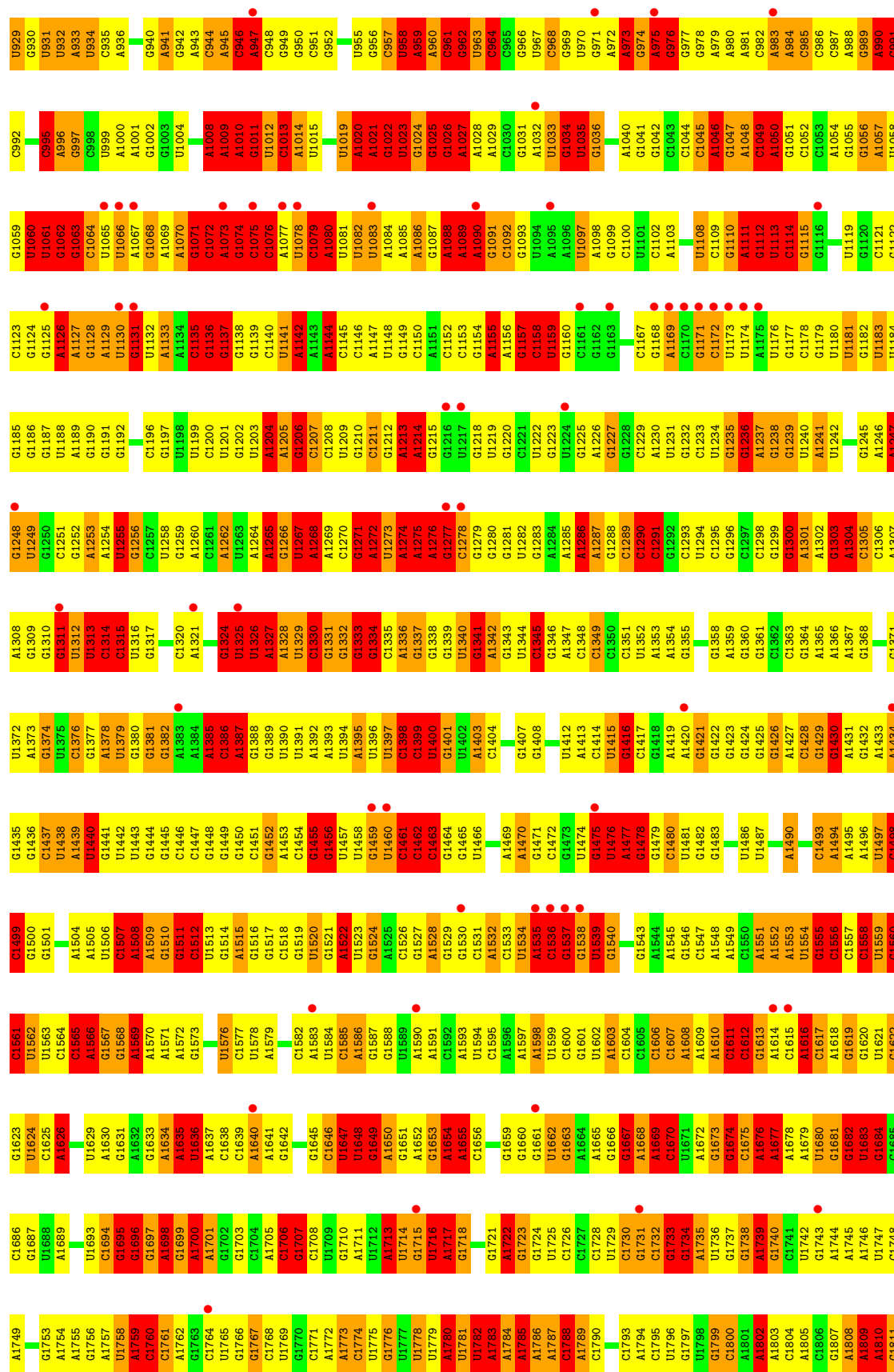


|       |       |       |       |       |       |       |       |       |       |       |       |         |       |       |       |       |       |       |       |       |       |       |       |       |       |
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| A1900 | G1045 | G1046 | G1047 | G1048 | G1049 | G1050 | G1051 | G1052 | G1053 | G1054 | G1055 | G1056   | G1057 | G1058 | G1059 | G1060 | G1061 | G1062 | G1063 | G1064 | G1065 | G1066 | G1067 | G1068 | A1069 |
| A1901 | G1070 | G1071 | G1072 | G1073 | G1074 | G1075 | G1076 | G1077 | G1078 | G1079 | G1080 | G1081   | G1082 | G1083 | G1084 | G1085 | G1086 | G1087 | G1088 | G1089 | G1090 | G1091 | G1092 | G1093 | A1094 |
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| U2849 | U2789 | C2786 | G2720 | A2654 | A2529 | A2469 | A2406 | U2343 | A2281 | U2219 | G2157 | C2096 | A1969 |
| A2850 | G2790 | G2787 | G2721 | G2655 | A2530 | G2470 | A2407 | U2344 | G2282 | U2220 | A     | A2097 | U2033 |
| A2851 | U2791 | C2788 | G2722 | U2656 | A2531 | A2471 | U2408 | G2345 | G2283 | G2221 | G     | U2098 | U1970 |
| G2852 | G2792 | C2789 | G2723 | C2657 | G2532 | G2472 | G2409 | A2346 | G2284 | G2222 | C     | U2099 | G1972 |
| G2853 | U2724 | G2658 | C2723 | U2658 | U2533 | U2473 | G2410 | G2347 | G2285 | G2223 | G     | G2100 | G1973 |
| G2854 | A2725 | G2659 | U2725 | A2534 | U2534 | U2474 | A2411 | U2348 | G2286 | G2224 | A     | A2103 | G1974 |
| C2794 | A2726 | G2660 | G2726 | G2535 | C2475 | A2476 | A2412 | G2349 | A2287 | A2225 | C     | C2104 | G1975 |
| A2855 | A2727 | A2661 | G2727 | U2536 | A2476 | A2477 | G2413 | G2350 | A2288 | G2226 | A     | U2105 | U1976 |
| G2857 | U2728 | A2662 | G2728 | U2537 | U2477 | A2478 | G2414 | G2351 | G2289 | A2227 | C     | U2106 | A1977 |
| G2858 | U2729 | G2663 | G2729 | C2538 | A2478 | A2479 | G2415 | A2352 | G2290 | G2228 | U     | U2107 | A1978 |
| U2796 | G2730 | G2664 | C2730 | C2539 | U2479 | A2480 | G2416 | G2353 | U2291 | U2229 | G     | G2107 | U1979 |
| A2799 | G2731 | A2665 | G2731 | A2540 | G2480 | C2481 | A2417 | G2354 | U2292 | U2230 | A     | A2108 | G1980 |
| A2800 | G2732 | C2666 | U2732 | A2541 | A2482 | C2481 | A2418 | G2355 | G2293 | U2231 | A     | U2109 | A1981 |
| G2801 | A2733 | C2667 | G2733 | U2604 | C2482 | U2419 | A2419 | G2356 | G2294 | G2232 | A     | G2110 | U1982 |
| C2803 | G2734 | G2668 | A2734 | U2605 | C2483 | U2419 | C2420 | G2357 | G2295 | U2233 | A     | U     | G1983 |
| U2804 | G2735 | G2669 | G2735 | G2606 | G2484 | G2484 | U2423 | G2358 | U2296 | G2234 | U     | G     | G1984 |
| G2805 | G2736 | G2670 | G2736 | G2607 | G2485 | G2485 | U2424 | C2359 | A2297 | G2235 | A     | U     | C1985 |
| U2806 | A2738 | G2671 | U2738 | U2545 | U2546 | C2486 | A2425 | G2360 | A2298 | U2236 | C     | A     | G1986 |
| A2807 | U2739 | U2609 | G2739 | A2547 | U2547 | A2487 | A2426 | G2361 | A2299 | G2237 | C     | G     | A1987 |
| G2808 | U2740 | G2675 | A2740 | U2548 | U2548 | G2488 | G2427 | G2362 | G2307 | G2238 | A     | G     | G1988 |
| G2809 | A2741 | G2676 | G2741 | G2549 | G2549 | U2489 | C2428 | G2363 | G2308 | G2239 | A     | A     | G1989 |
| U2810 | G2742 | G2677 | G2742 | G2550 | G2550 | G2490 | G2429 | G2364 | A2309 | U2240 | C     | U     | C1990 |
| U2811 | U2743 | U2680 | U2743 | C2551 | U2491 | U2491 | G2430 | G2365 | U2306 | A2241 | G     | A     | U1991 |
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| A2813 | G2745 | A2682 | G2745 | G2553 | U2493 | G2494 | U2432 | G2367 | G2308 | U2243 | G     | G     | U1993 |
| G2814 | U2746 | U2683 | G2746 | U2554 | G2495 | G2495 | A2434 | G2368 | A2309 | G2246 | U     | U     | U1994 |
| C2815 | A2747 | G2684 | A2747 | U2555 | U2555 | G2496 | A2435 | G2369 | G2310 | A2247 | G     | G     | U1995 |
| U2816 | G2748 | U2685 | G2748 | C2556 | U2556 | A2497 | G2436 | G2370 | A2184 | G2248 | G     | A     | G1996 |
| U2817 | U2749 | U2686 | G2749 | G2557 | G2557 | A2497 | G2437 | G2371 | U2185 | G2249 | G     | G     | C1997 |
| A2818 | G2750 | G2687 | G2750 | C2558 | U2498 | C2498 | U2438 | G2372 | U2186 | U2250 | A     | A     | A2060 |
| U2819 | U2751 | U2688 | G2751 | U2559 | U2499 | U2499 | U2439 | G2373 | U2187 | G2251 | G     | G     | A2062 |
| G2820 | G2752 | G2689 | G2752 | A2560 | U2500 | U2500 | A2439 | A2377 | U2188 | G2252 | G     | G     | A2063 |
| A2821 | U2753 | G2690 | A2753 | G2501 | C2501 | G2501 | C2440 | A2378 | U2189 | G2253 | C     | C     | G2064 |
| G2822 | G2754 | C2691 | G2754 | A2564 | A2502 | A2502 | U2441 | G2379 | U2190 | G2254 | U     | U     | G2065 |
| U2823 | U2755 | G2692 | G2755 | A2565 | A2503 | A2503 | C2442 | G2380 | G2193 | G2255 | U     | U     | G2066 |
| G2824 | U2756 | G2693 | U2756 | A2566 | U2504 | U2504 | G2443 | G2381 | U2194 | G2256 | G     | G     | C2006 |
| A2825 | G2757 | U2694 | G2757 | G2567 | G2505 | G2505 | G2444 | A2382 | U2195 | U2257 | A     | A     | U2007 |
| G2826 | U2758 | G2695 | G2758 | A2568 | C2506 | C2506 | G2445 | G2383 | C2196 | G2258 | G     | G     | G2008 |
| U2827 | G2759 | U2696 | G2759 | G2569 | G2507 | G2507 | G2446 | G2384 | U2197 | U2259 | A     | A     | A2009 |
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| U2829 | A2761 | U2698 | G2761 | U2571 | G2509 | G2509 | A2448 | C2385 | A2199 | U2261 | G     | G     | A2014 |
| A2830 | G2762 | C2699 | G2762 | A2572 | C2510 | C2510 | U2449 | A2386 | G2200 | U2262 | U     | U     | A2015 |
| G2831 | U2763 | U2700 | U2763 | G2573 | U2511 | U2511 | A2450 | U2387 | G2201 | G2263 | G     | G     | U2016 |
| U2832 | G2764 | G2701 | G2764 | C2574 | C2512 | C2512 | A2451 | A2388 | U2199 | G2264 | G     | G     | U2017 |
| G2833 | U2765 | C2702 | U2765 | G2575 | A2513 | A2513 | A2452 | G2389 | U2197 | U2265 | G     | G     | G2018 |
| U2834 | G2766 | G2703 | G2766 | G2576 | U2514 | U2514 | G2453 | U2390 | A2198 | G2266 | A     | A     | U2019 |
| A2835 | A2767 | U2704 | A2767 | A2577 | C2515 | C2515 | A2454 | U2391 | G2202 | A2267 | G     | G     | A2020 |
| G2836 | G2768 | G2705 | G2768 | G2578 | A2516 | A2516 | G2455 | A2392 | G2203 | G2268 | G     | G     | C2021 |
| U2837 | U2769 | U2706 | U2769 | G2579 | C2517 | C2517 | U2456 | G2393 | G2204 | G2269 | G     | G     | U2022 |
| G2838 | G2770 | G2707 | G2770 | U2580 | A2518 | A2518 | U2457 | C2394 | U2210 | U2270 | G     | G     | G2023 |
| U2839 | U2771 | C2708 | U2771 | G2581 | U2519 | U2519 | G2458 | G2395 | A2211 | G2271 | G     | G     | G2024 |
| G2840 | G2772 | G2709 | G2772 | G2582 | C2520 | C2520 | A2459 | U2396 | U2212 | U2272 | G     | G     | G2025 |
| A2841 | A2773 | U2710 | A2773 | G2583 | G2521 | G2521 | U2460 | U2397 | A2213 | A2273 | G     | G     | U2026 |
| G2842 | G2774 | G2711 | G2774 | U2584 | C2522 | C2522 | A2461 | G2398 | A2214 | G2274 | G     | G     | C2091 |
| U2843 | U2775 | U2712 | U2775 | U2585 | U2523 | U2523 | G2462 | U2399 | U2215 | G2275 | G     | G     | U2092 |
| G2844 | G2776 | G2713 | G2776 | G2586 | G2524 | G2524 | U2463 | U2400 | C2215 | G2276 | G     | G     |       |
| U2845 | A2777 | U2714 | A2777 | U2587 | U2525 | U2525 | C2465 | U2402 |       | G2277 |       |       |       |

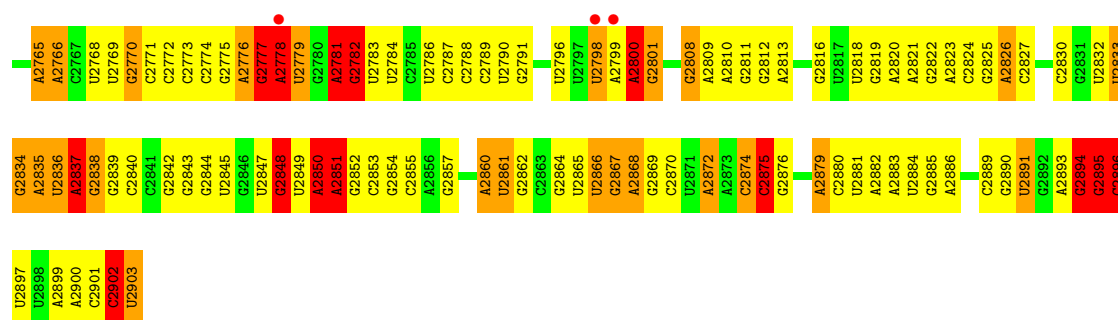
• Molecule 24: 23S rRNA





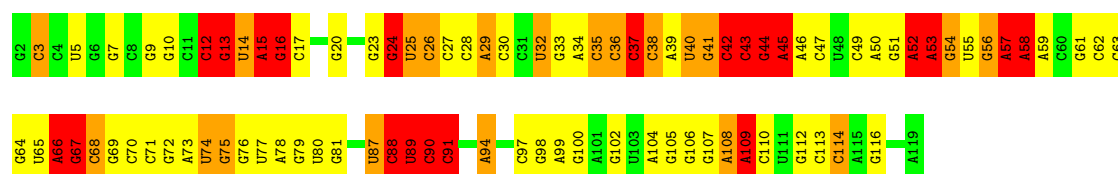
|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| G2697 | G2698 | G2699 | A2700 | G2704 | G2707 | G2708 | G2709 | G2710 | G2711 | G2712 | G2713 | G2714 | G2715 | G2716 | G2717 | G2718 | G2719 | G2720 | G2721 | G2722 | G2723 | G2724 | G2725 | A2726 | A2727 | A2728 | G2729 | G2732 | A2733 | A2734 | G2737 | A2738 | A2739 | A2740 | G2741 | G2742 | G2743 | G2744 | G2745 | G2746 | G2747 | A2748 | A2749 | A2750 | G2751 | G2752 | A2753 | U2754 | G2755 | G2756 | A2757 | A2758 | G2759 | G2760 | A2761 |       |       |       |       |       |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| C2628 | U2629 | G2630 | G2631 | A2632 | A2635 | G2636 | U2637 | G2638 | A2639 | G2640 | G2641 | G2642 | G2643 | G2644 | G2645 | G2646 | G2647 | G2648 | G2649 | U2653 | A2654 | G2655 | U2656 | A2657 | G2658 | G2659 | A2660 | A2661 | A2662 | G2663 | G2664 | G2665 | G2666 | G2667 | U2672 | G2673 | G2674 | A2675 | G2676 | G2677 | G2678 | A2681 | A2682 | G2683 | G2684 | G2685 | G2686 | U2687 | G2688 | G2689 | U2690 | G2691 | G2692 | G2693 | G2694 | U2695 | U2696 |       |       |       |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| G2567 | U2568 | G2569 | G2570 | U2571 | A2572 | G2573 | G2574 | G2575 | G2576 | A2577 | G2578 | G2579 | U2580 | G2581 | G2582 | G2583 | U2584 | U2585 | U2586 | A2587 | U2588 | A2589 | A2590 | G2591 | G2592 | U2593 | G2594 | G2595 | U2596 | G2597 | A2598 | G2599 | A2600 | G2601 | A2602 | A2603 | U2604 | G2605 | A2606 | A2607 | A2608 | A2609 | G2610 | A2611 | G2612 | U2613 | A2614 | U2615 | G2616 | U2617 | G2618 | G2619 | G2620 | G2621 | U2622 | G2623 | G2624 | G2625 | G2626 | G2627 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| U2506 | C2507 | G2508 | G2509 | C2510 | U2511 | G2512 | A2513 | U2514 | C2515 | A2516 | G2517 | A2518 | U2519 | C2520 | G2521 | U2522 | G2523 | G2524 | C2527 | U2528 | G2529 | A2530 | U2531 | G2532 | U2533 | A2534 | G2535 | U2536 | G2537 | U2538 | G2539 | C2540 | A2541 | A2542 | G2543 | G2544 | G2545 | G2546 | A2547 | U2548 | U2549 | G2550 | C2551 | U2552 | U2553 | G2554 | U2555 | G2556 | G2557 | G2558 | C2559 | A2560 | U2561 | U2562 | U2563 | A2564 | U2565 | A2566 |       |       |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| G2445 | G2446 | G2447 | A2448 | U2449 | A2450 | A2451 | G2452 | U2453 | G2454 | G2455 | G2456 | U2457 | G2458 | G2459 | U2460 | A2461 | G2462 | G2463 | C2466 | C2467 | A2468 | A2469 | U2470 | A2471 | G2472 | U2473 | A2474 | G2475 | A2476 | U2477 | A2478 | U2479 | G2480 | U2481 | G2482 | G2483 | G2484 | G2485 | G2486 | G2487 | G2488 | U2489 | G2490 | U2491 | A2492 | U2493 | G2494 | G2495 | G2496 | A2497 | G2498 | G2499 | U2500 | U2501 | G2502 | A2503 | G2504 | G2505 |       |       |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| G2383 | U2384 | G2385 | G2386 | U2387 | A2388 | G2389 | U2390 | G2391 | A2392 | G2393 | U2394 | G2397 | U2398 | G2399 | G2400 | U2401 | U2402 | G2403 | U2404 | G2405 | A2406 | A2407 | U2408 | G2409 | G2410 | A2411 | A2412 | G2413 | G2414 | G2415 | G2416 | U2417 | A2418 | U2419 | G2420 | G2421 | G2422 | U2423 | G2424 | A2425 | A2426 | U2427 | G2428 | G2429 | U2430 | U2431 | A2434 | G2435 | G2436 | G2437 | U2438 | A2439 | G2440 | U2441 | G2442 | G2443 | G2444 |       |       |       |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| U2321 | A2322 | G2323 | U2324 | G2325 | G2326 | A2327 | A2328 | U2329 | G2330 | G2331 | G2332 | A2333 | U2334 | A2335 | A2336 | G2337 | C2338 | G2339 | A2340 | G2341 | G2342 | U2343 | U2344 | G2345 | A2346 | G2347 | U2348 | G2349 | C2350 | G2351 | A2352 | G2355 | U2356 | G2357 | A2358 | G2359 | G2360 | G2361 | G2362 | G2363 | G2364 | G2365 | A2366 | G2367 | G2370 | G2371 | U2372 | G2373 | G2374 | G2375 | A2376 | A2377 | U2378 | G2379 | C2380 | A2381 | G2382 |       |       |       |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| U2259 | C2260 | U2261 | U2262 | G2263 | G2264 | U2265 | A2266 | U2267 | A2268 | G2269 | U2270 | G2271 | U2272 | A2273 | G2274 | C2275 | U2276 | U2277 | U2278 | G2279 | G2280 | A2281 | G2282 | G2283 | A2284 | G2285 | C2286 | A2287 | A2288 | G2289 | G2290 | G2291 | U2292 | G2293 | G2294 | A2297 | A2298 | U2299 | C2300 | C2301 | U2302 | G2303 | G2304 | U2305 | G2306 | G2307 | G2308 | A2309 | C2310 | A2311 | G2312 | C2313 | A2314 | G2315 | G2316 | G2319 | U2320 |       |       |       |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| G2193 | U2194 | U2197 | A2198 | A2199 | G2200 | U2201 | G2202 | U2203 | G2204 | C2208 | G2209 | U2210 | A2211 | U2212 | U2213 | U2214 | U2215 | U2216 | G2217 | G2218 | U2219 | U2220 | A2225 | C2226 | A2227 | U2228 | U2229 | G2230 | U2231 | U2232 | U2233 | U2234 | G2235 | U2236 | G2237 | U2238 | G2239 | U2240 | A2241 | G2242 | U2243 | U2244 | G2245 | U2246 | A2247 | U2248 | U2249 | G2250 | G2251 | G2252 | G2253 | G2254 | G2255 | G2256 | G2258 |       |       |       |       |       |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| G2133 | A2134 | A2135 | U2136 | U2137 | G2138 | U2139 | G2140 | U2141 | A2142 | G2143 | G2144 | G2145 | G2146 | A2147 | U2148 | U2149 | U2151 | G2152 | U2153 | A2154 | U2155 | G2156 | G2157 | A     | G     | C     | C     | G     | U     | U     | G     | A     | A     | A     | A     | A     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C     | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C | C |





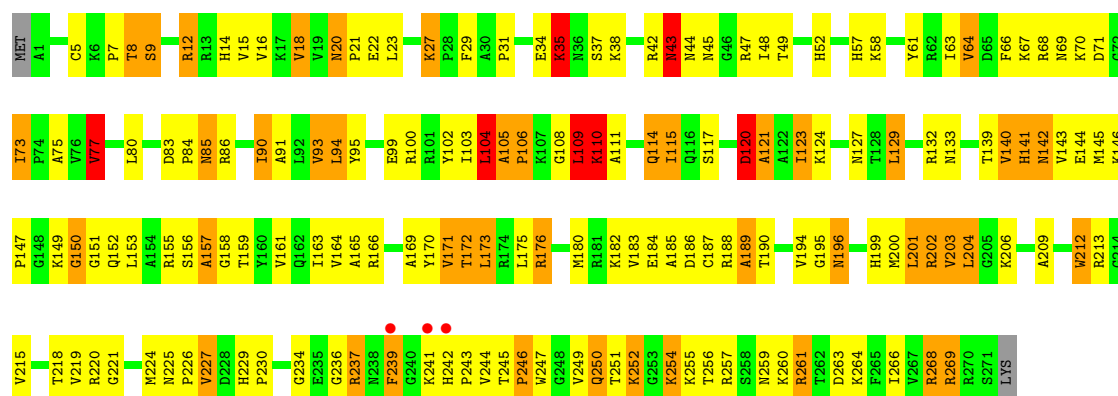
• Molecule 25: 5S rRNA

Chain BB: 24% 42% 17% 18%



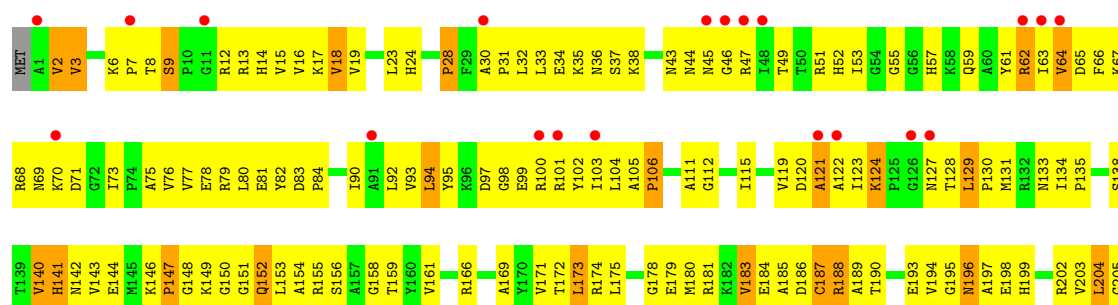
• Molecule 26: 50S ribosomal protein L2

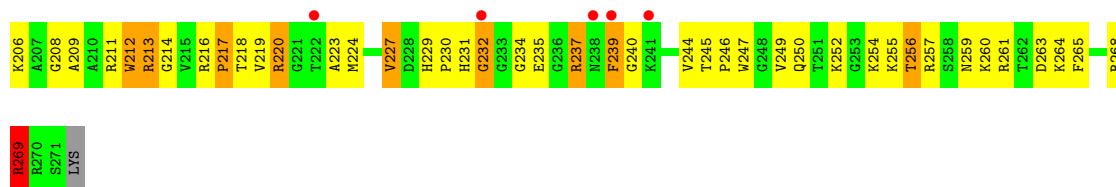
Chain BC: 38% 42% 16%



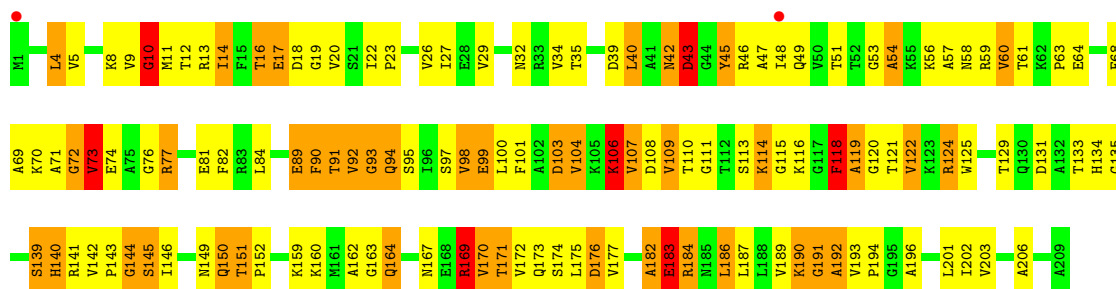
• Molecule 26: 50S ribosomal protein L2

Chain DC: 9% 32% 56% 11%

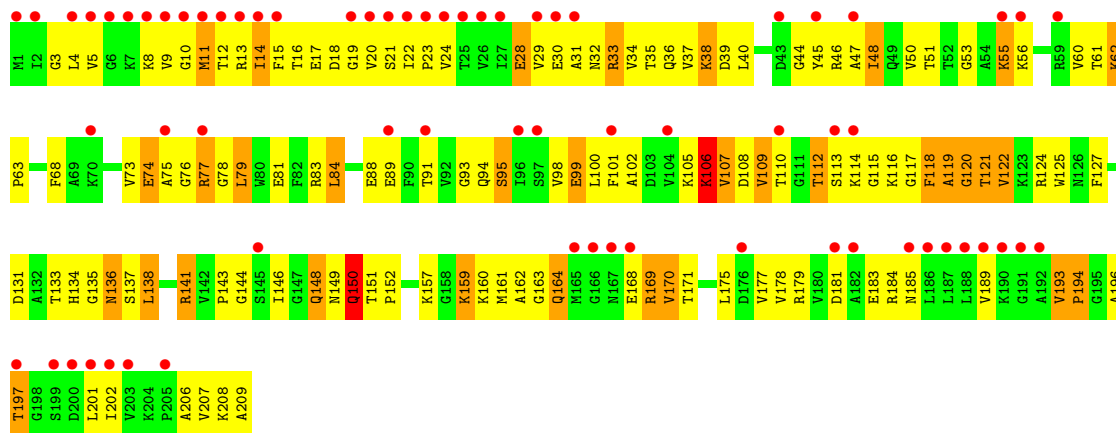




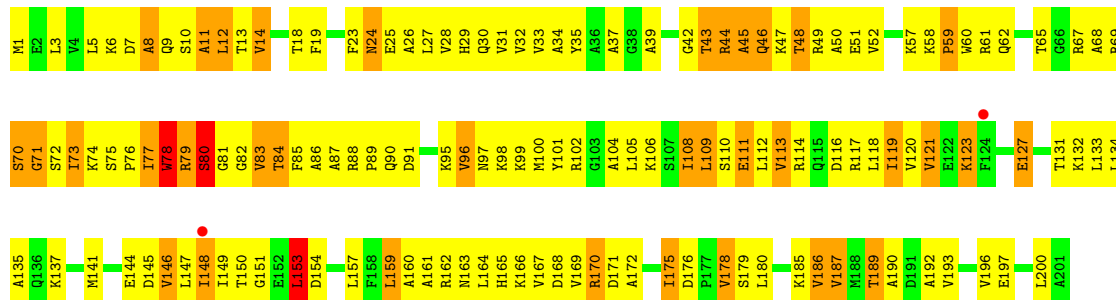
• Molecule 27: 50S ribosomal protein L3



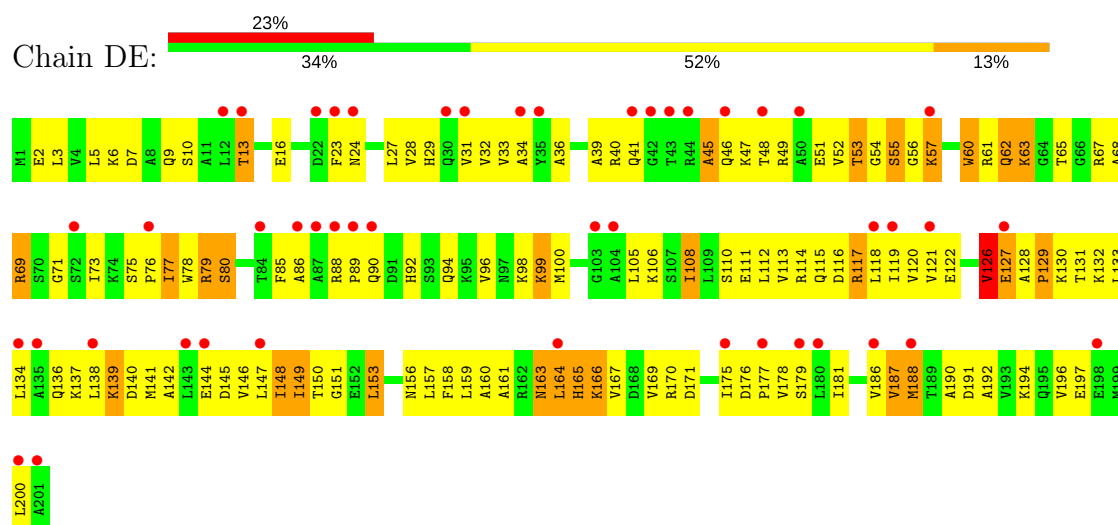
• Molecule 27: 50S ribosomal protein L3



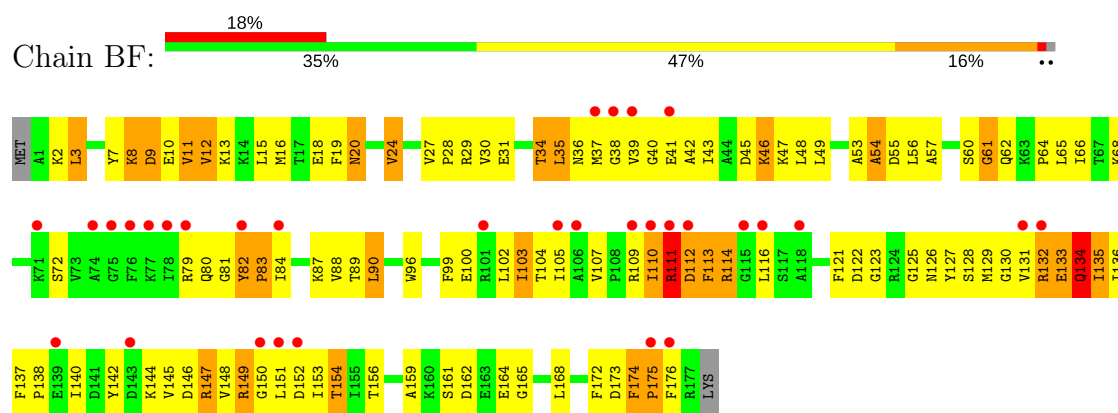
• Molecule 28: 50S ribosomal protein L4



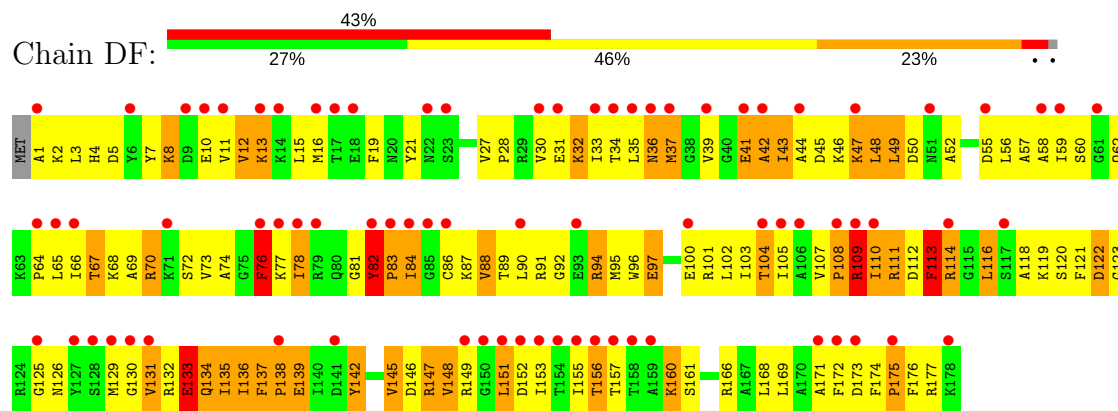
• Molecule 28: 50S ribosomal protein L4



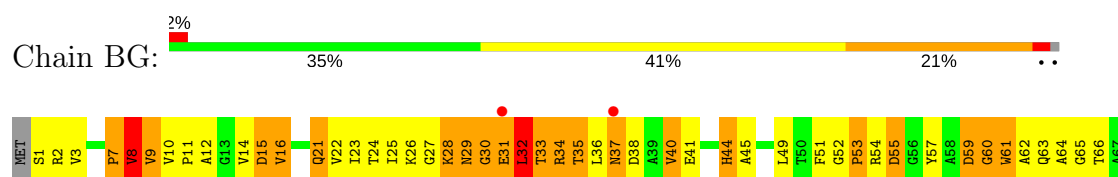
• Molecule 29: 50S ribosomal protein L5

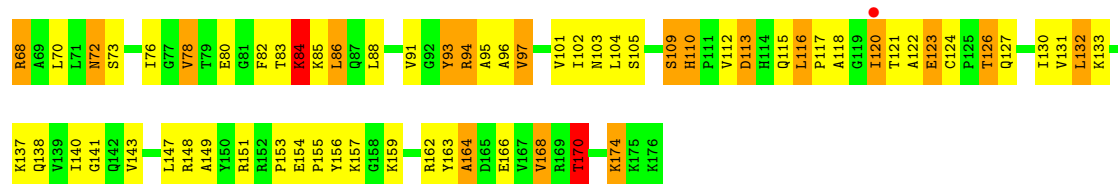


• Molecule 29: 50S ribosomal protein L5

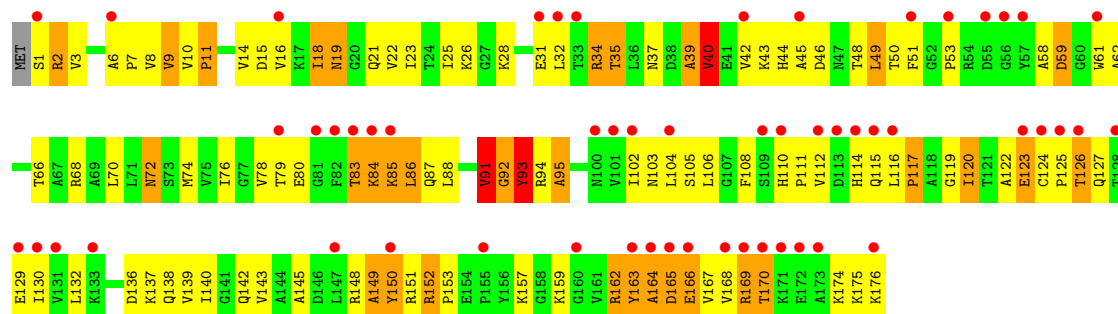


• Molecule 30: 50S ribosomal protein L6

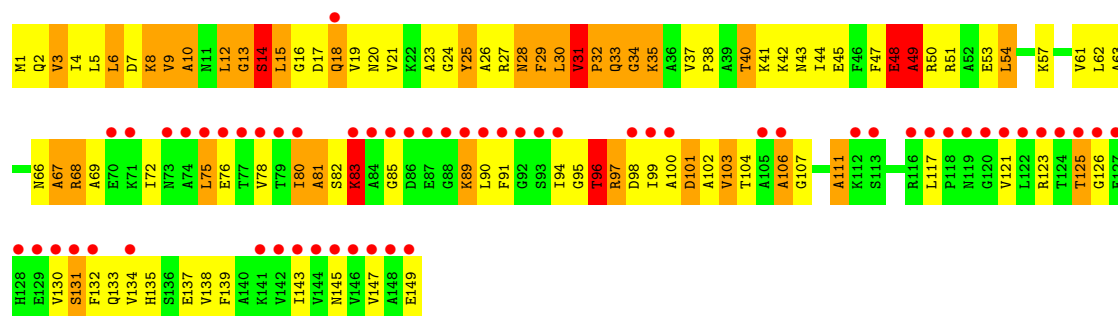




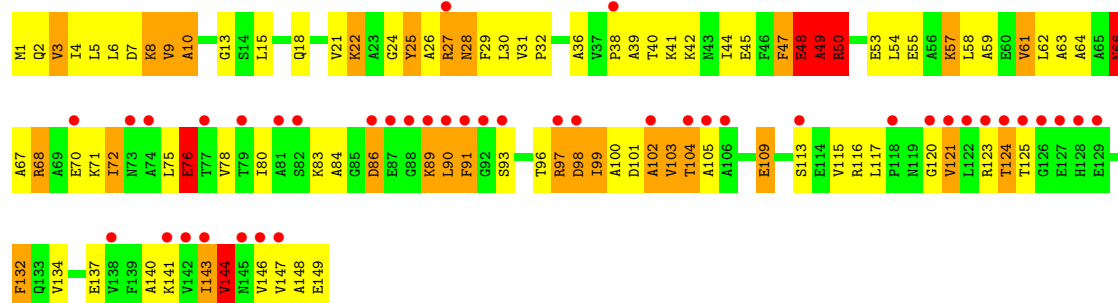
• Molecule 30: 50S ribosomal protein L6



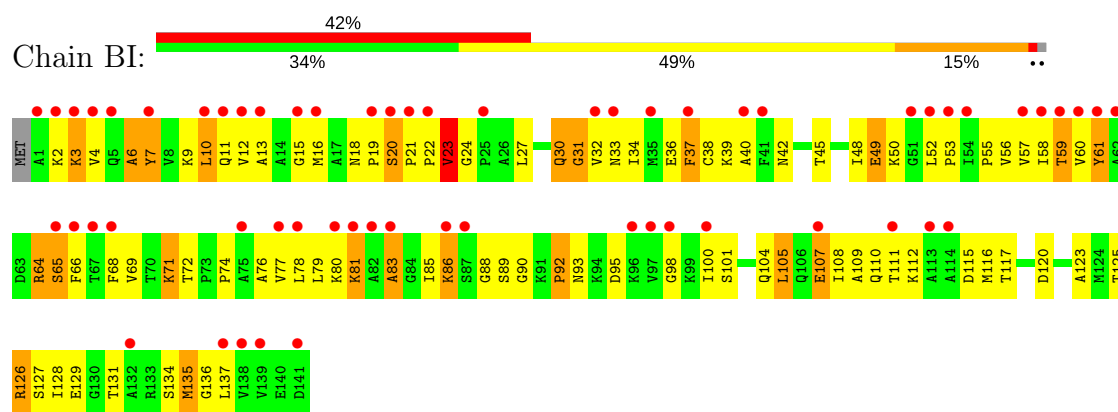
• Molecule 31: 50S ribosomal protein L9



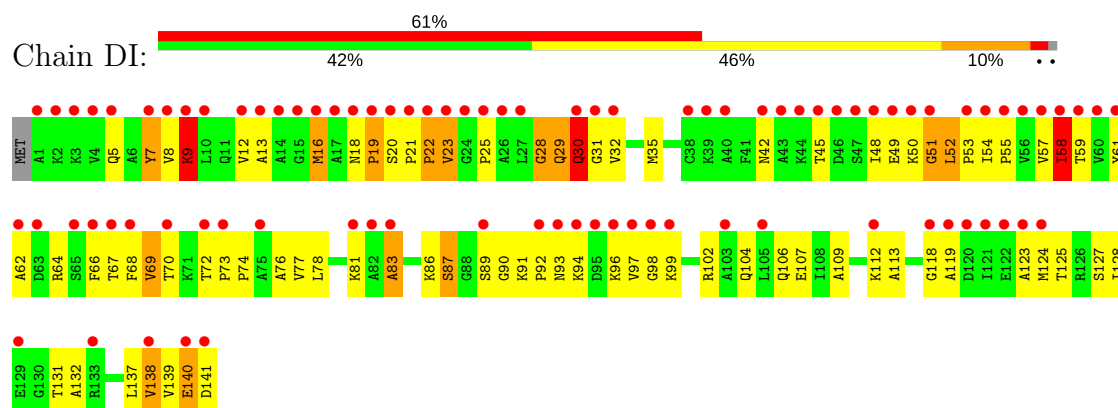
• Molecule 31: 50S ribosomal protein L9



• Molecule 32: 50S ribosomal protein L11



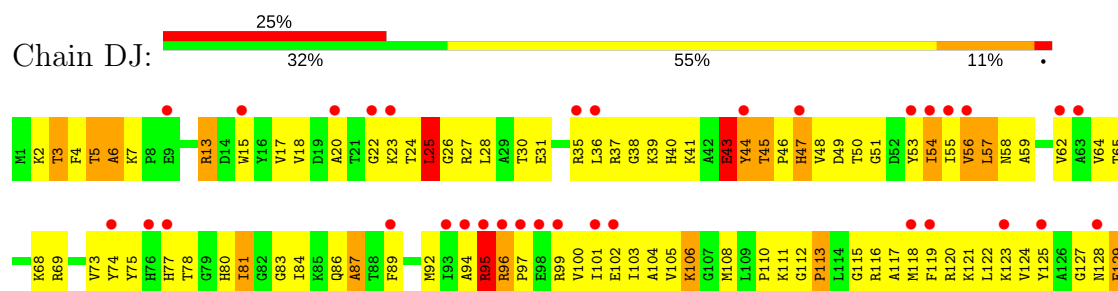
• Molecule 32: 50S ribosomal protein L11



• Molecule 33: 50S ribosomal protein L13

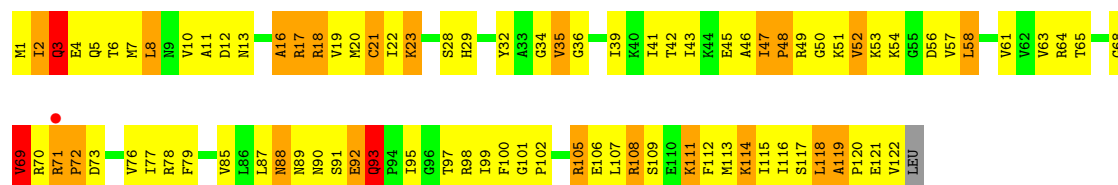


• Molecule 33: 50S ribosomal protein L13

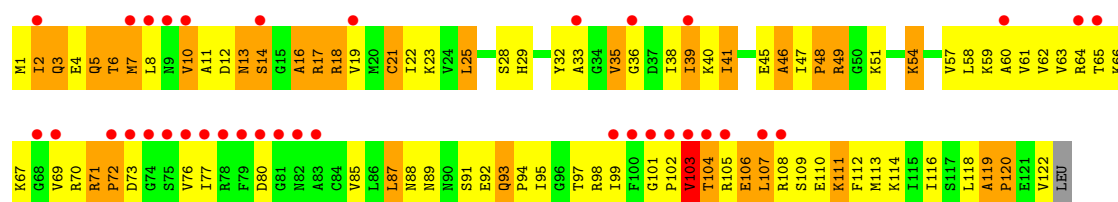




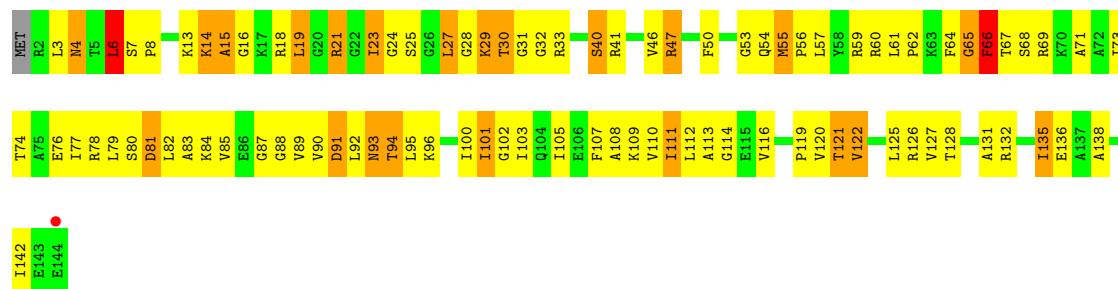
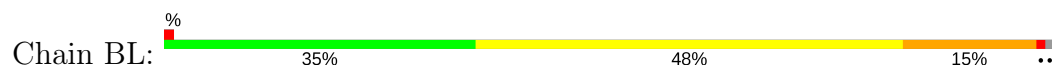
- Molecule 34: 50S ribosomal protein L14



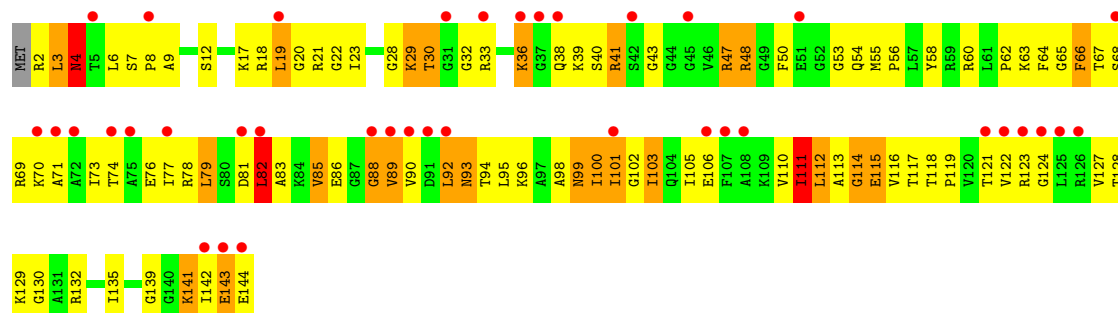
- Molecule 34: 50S ribosomal protein L14



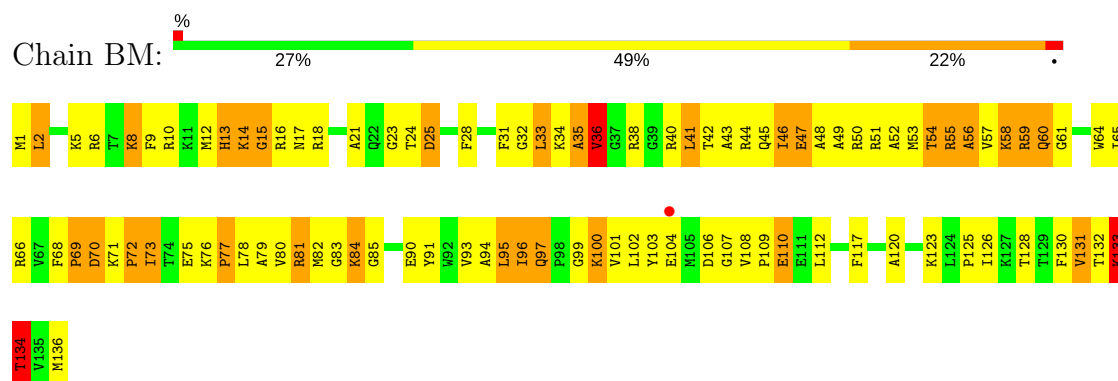
- Molecule 35: 50S ribosomal protein L15



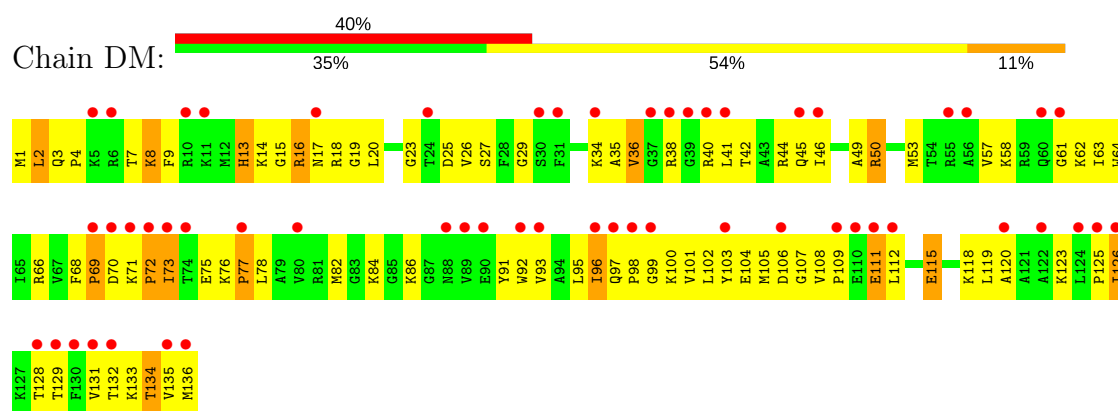
- Molecule 35: 50S ribosomal protein L15



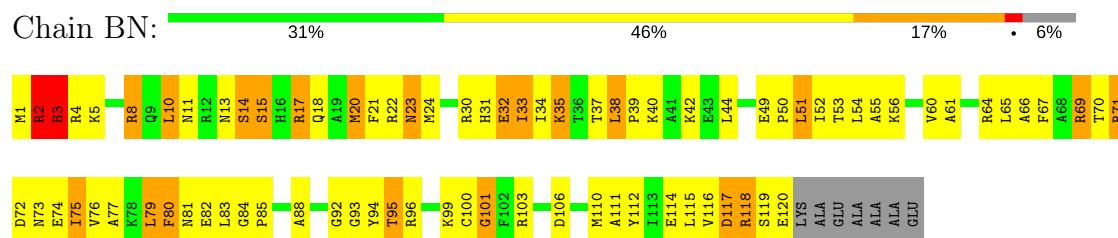
- Molecule 36: 50S ribosomal protein L16



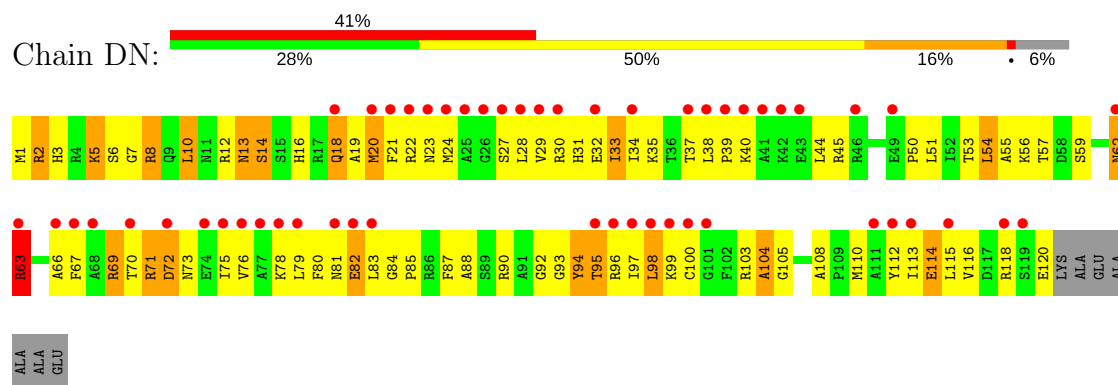
- Molecule 36: 50S ribosomal protein L16



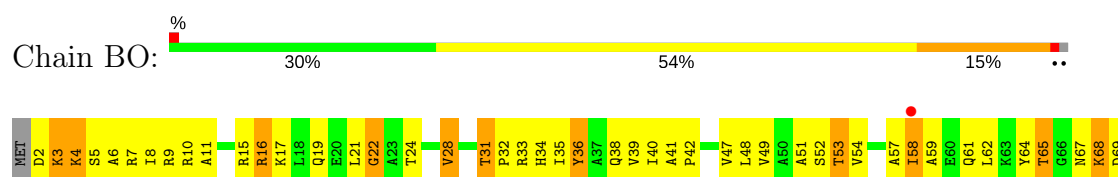
- Molecule 37: 50S ribosomal protein L17



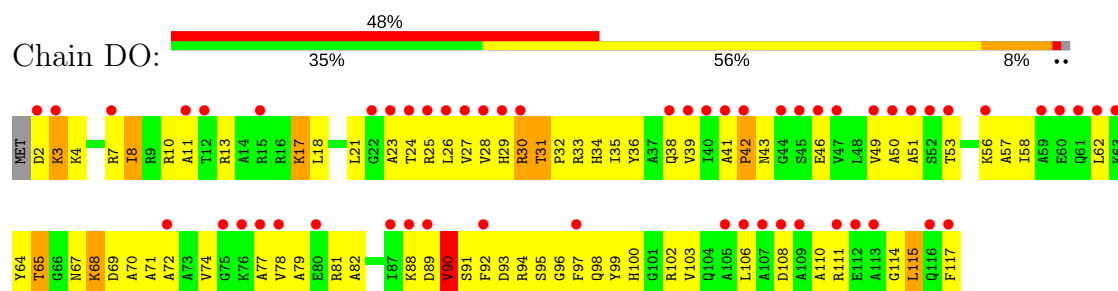
- Molecule 37: 50S ribosomal protein L17



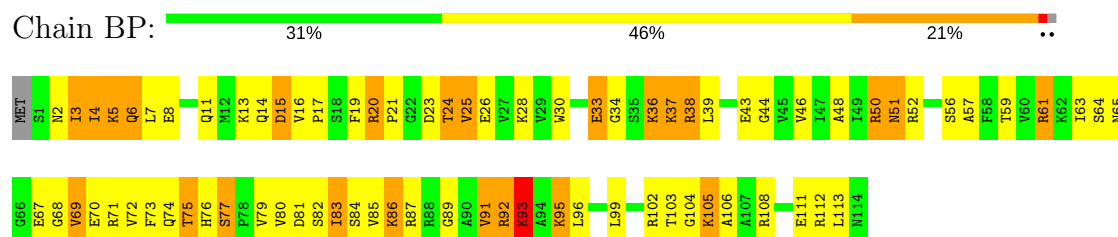
- Molecule 38: 50S ribosomal protein L18



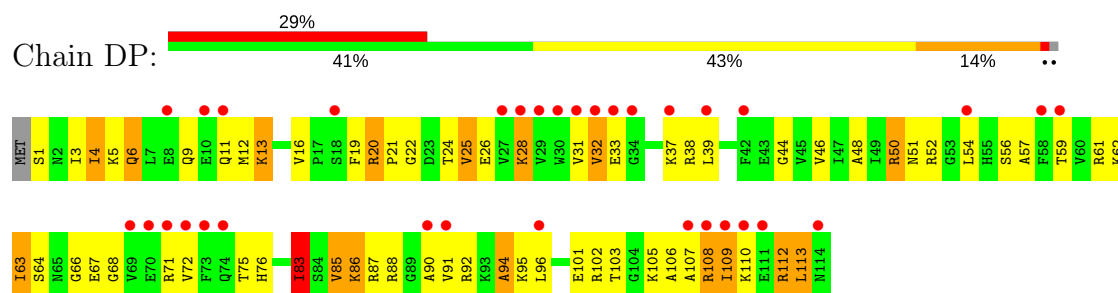
- Molecule 38: 50S ribosomal protein L18



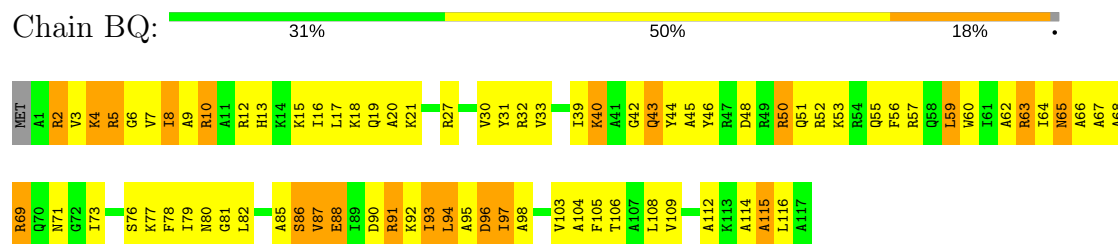
- Molecule 39: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L19

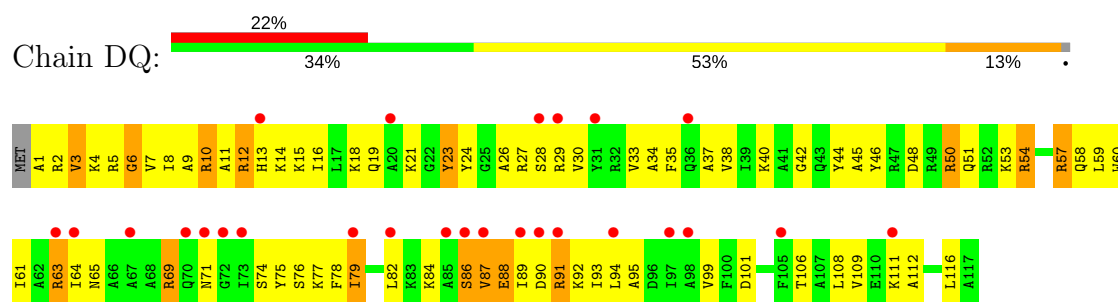


- Molecule 40: 50S ribosomal protein L20

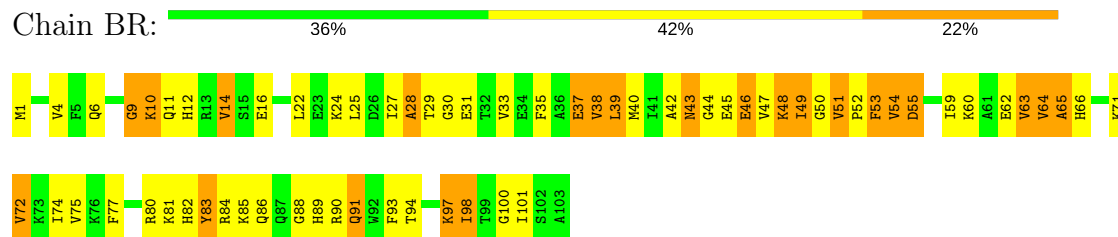


- Molecule 40: 50S ribosomal protein L20

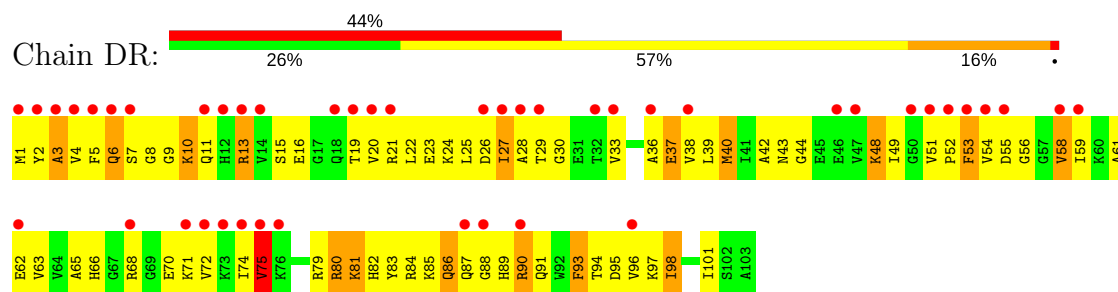




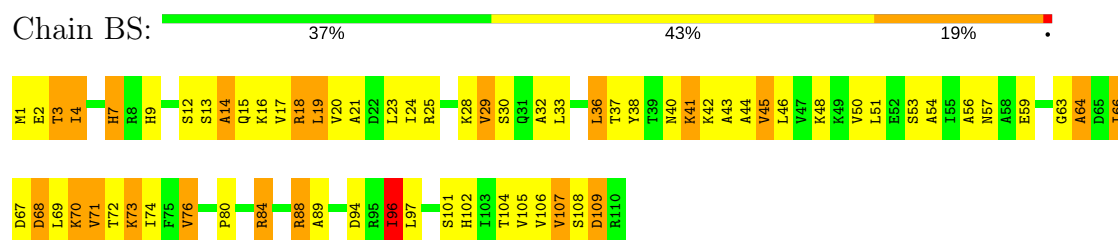
- Molecule 41: 50S ribosomal protein L21



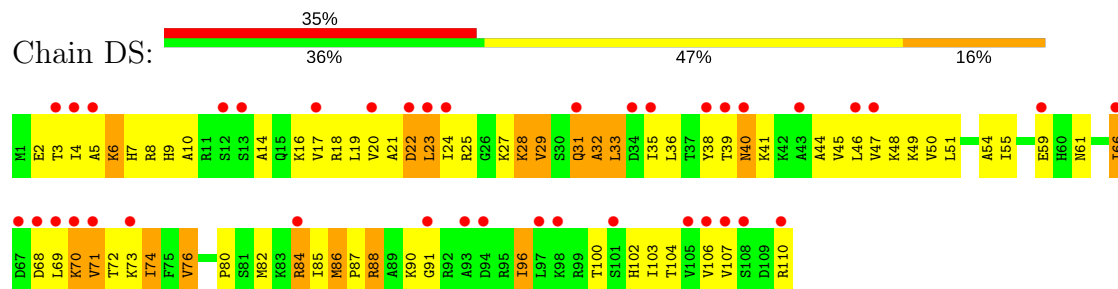
- Molecule 41: 50S ribosomal protein L21



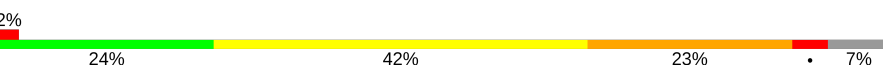
- Molecule 42: 50S ribosomal protein L22

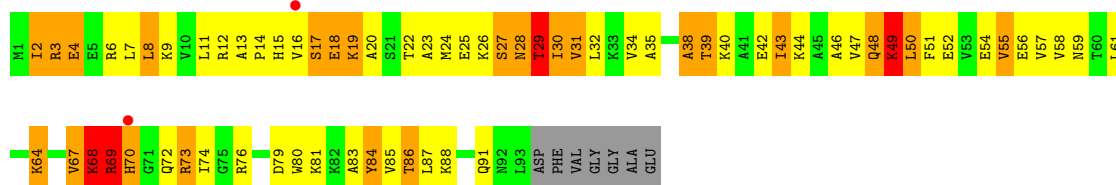


- Molecule 42: 50S ribosomal protein L22



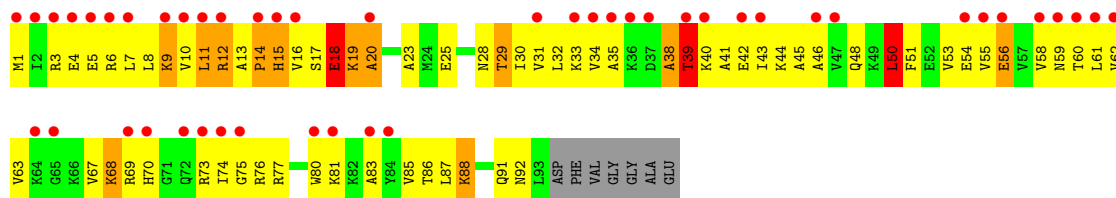
- Molecule 43: 50S ribosomal protein L23

Chain BT: 



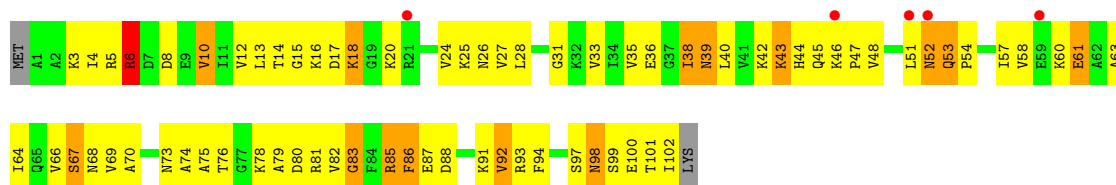
- Molecule 43: 50S ribosomal protein L23

Chain DT: 



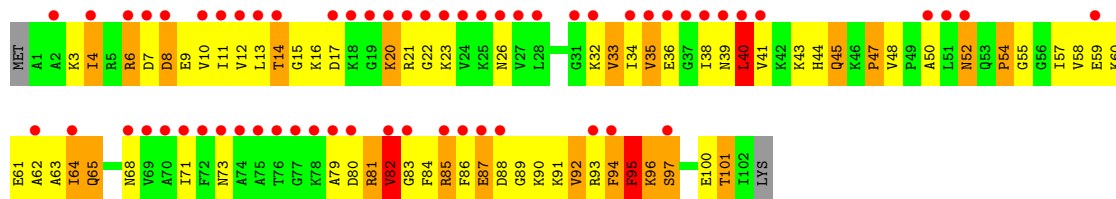
- Molecule 44: 50S ribosomal protein L24

Chain BU: 



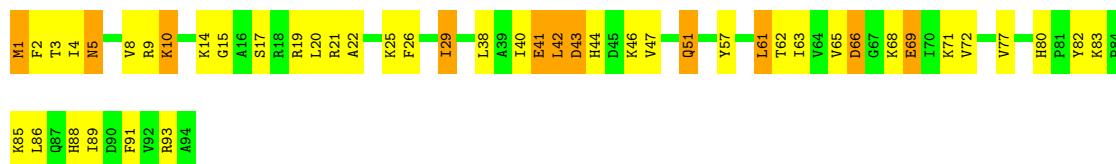
- Molecule 44: 50S ribosomal protein L24

Chain DU: 

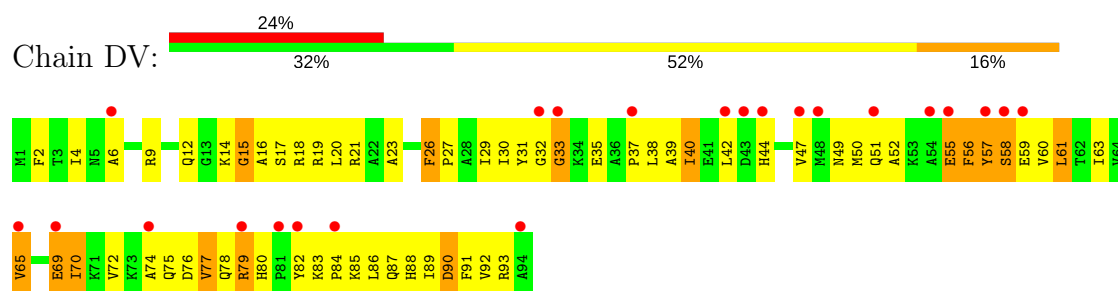


- Molecule 45: 50S ribosomal protein L25

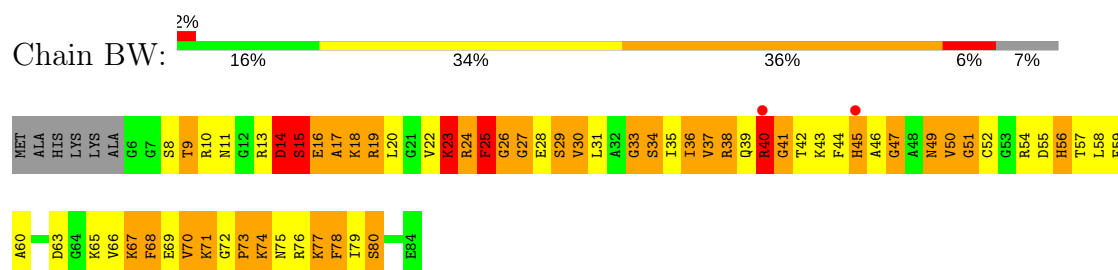
Chain BV: 



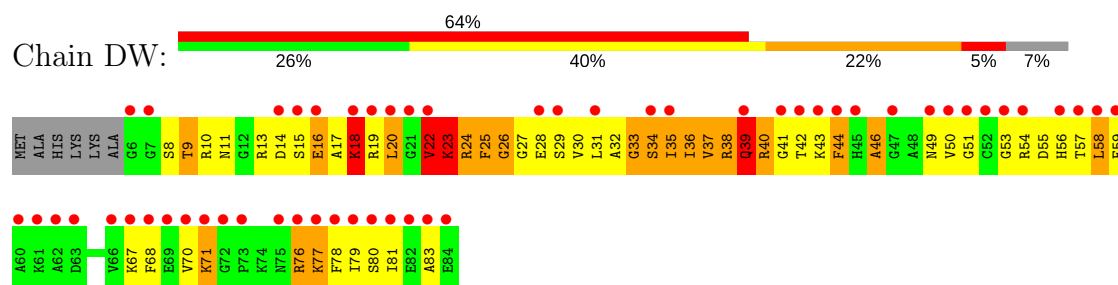
- Molecule 45: 50S ribosomal protein L25



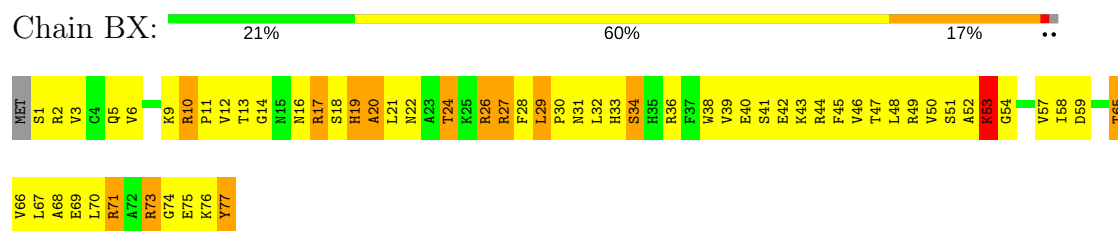
- Molecule 46: 50S ribosomal protein L27



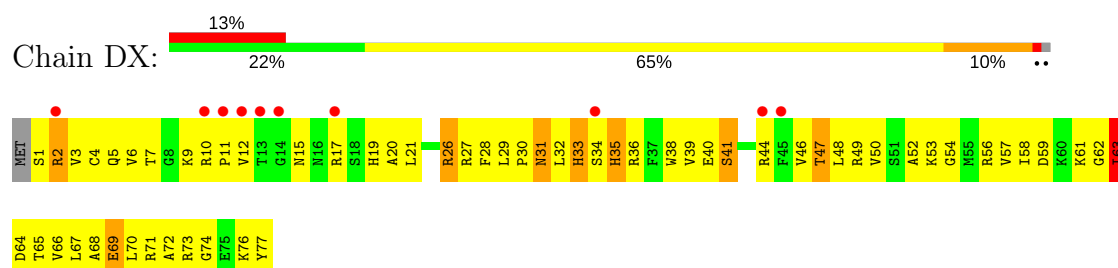
- Molecule 46: 50S ribosomal protein L27



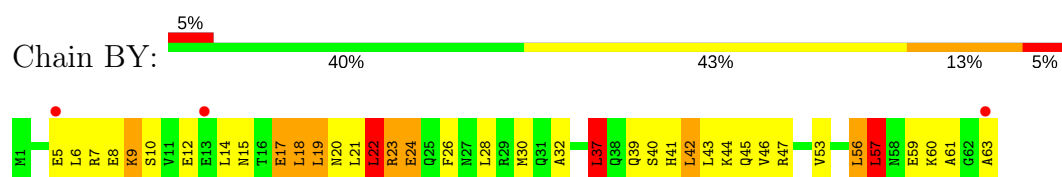
- Molecule 47: 50S ribosomal protein L28



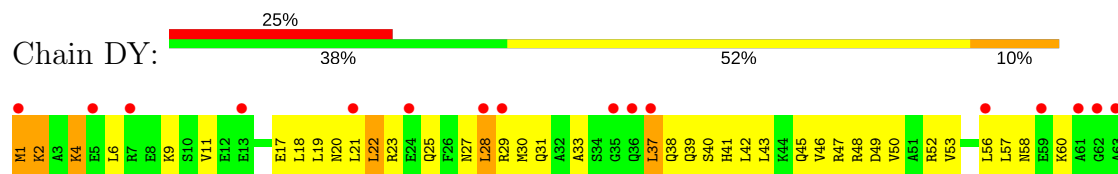
- Molecule 47: 50S ribosomal protein L28



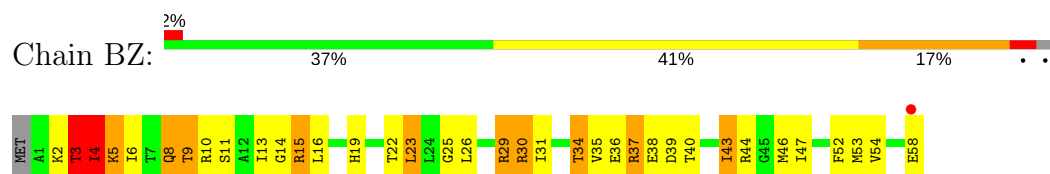
- Molecule 48: 50S ribosomal protein L29



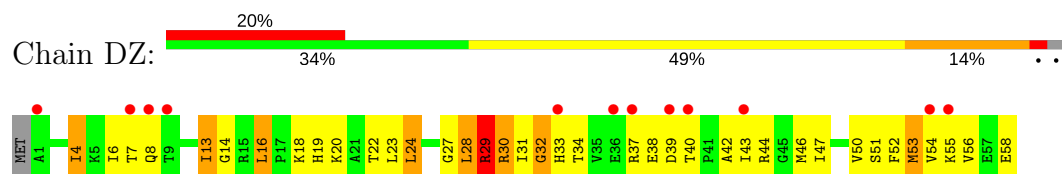
- Molecule 48: 50S ribosomal protein L29



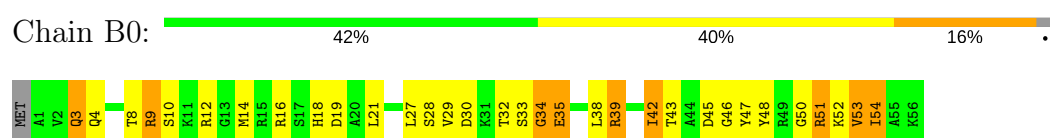
- Molecule 49: 50S ribosomal protein L30



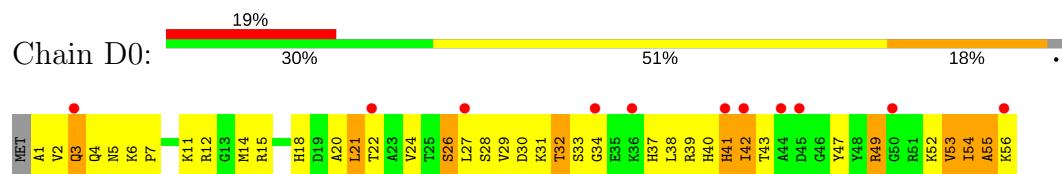
- Molecule 49: 50S ribosomal protein L30



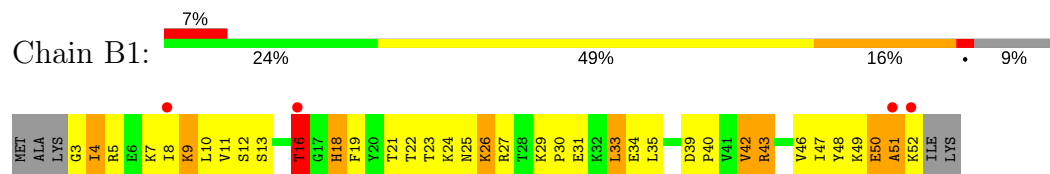
- Molecule 50: 50S ribosomal protein L32



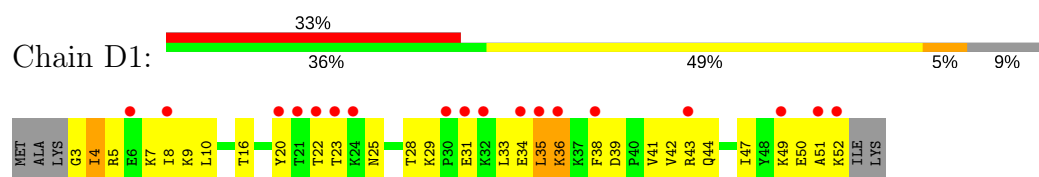
- Molecule 50: 50S ribosomal protein L32



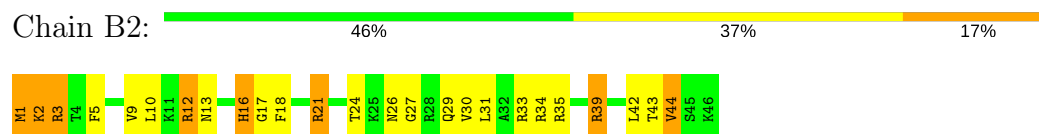
- Molecule 51: 50S ribosomal protein L33



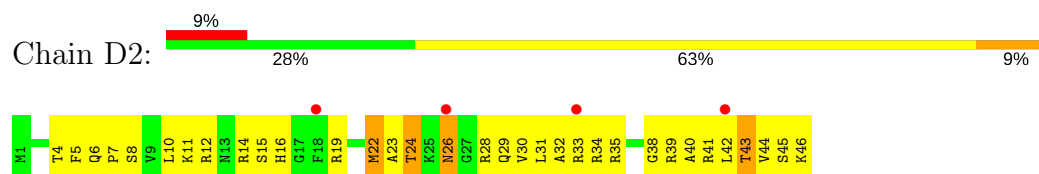
- Molecule 51: 50S ribosomal protein L33



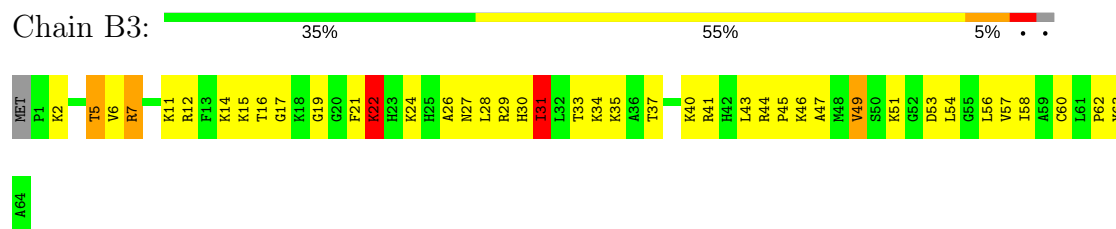
- Molecule 52: 50S ribosomal protein L34



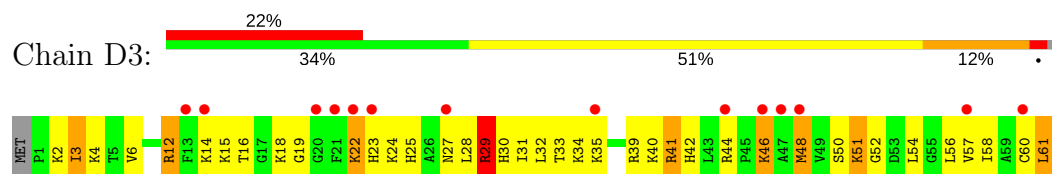
- Molecule 52: 50S ribosomal protein L34



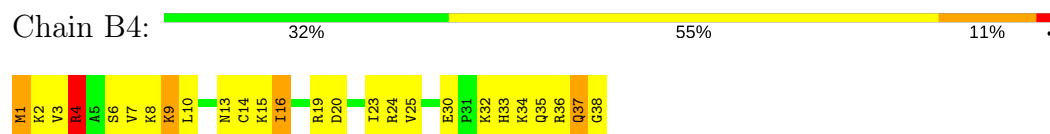
- Molecule 53: 50S ribosomal protein L35



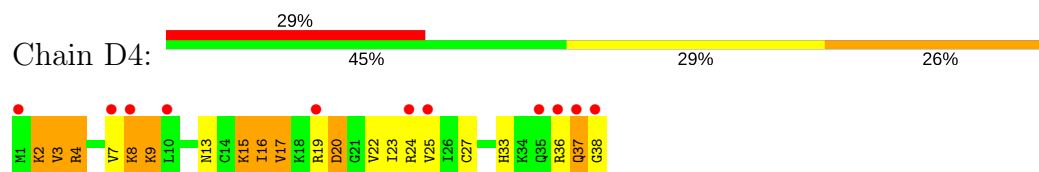
- Molecule 53: 50S ribosomal protein L35



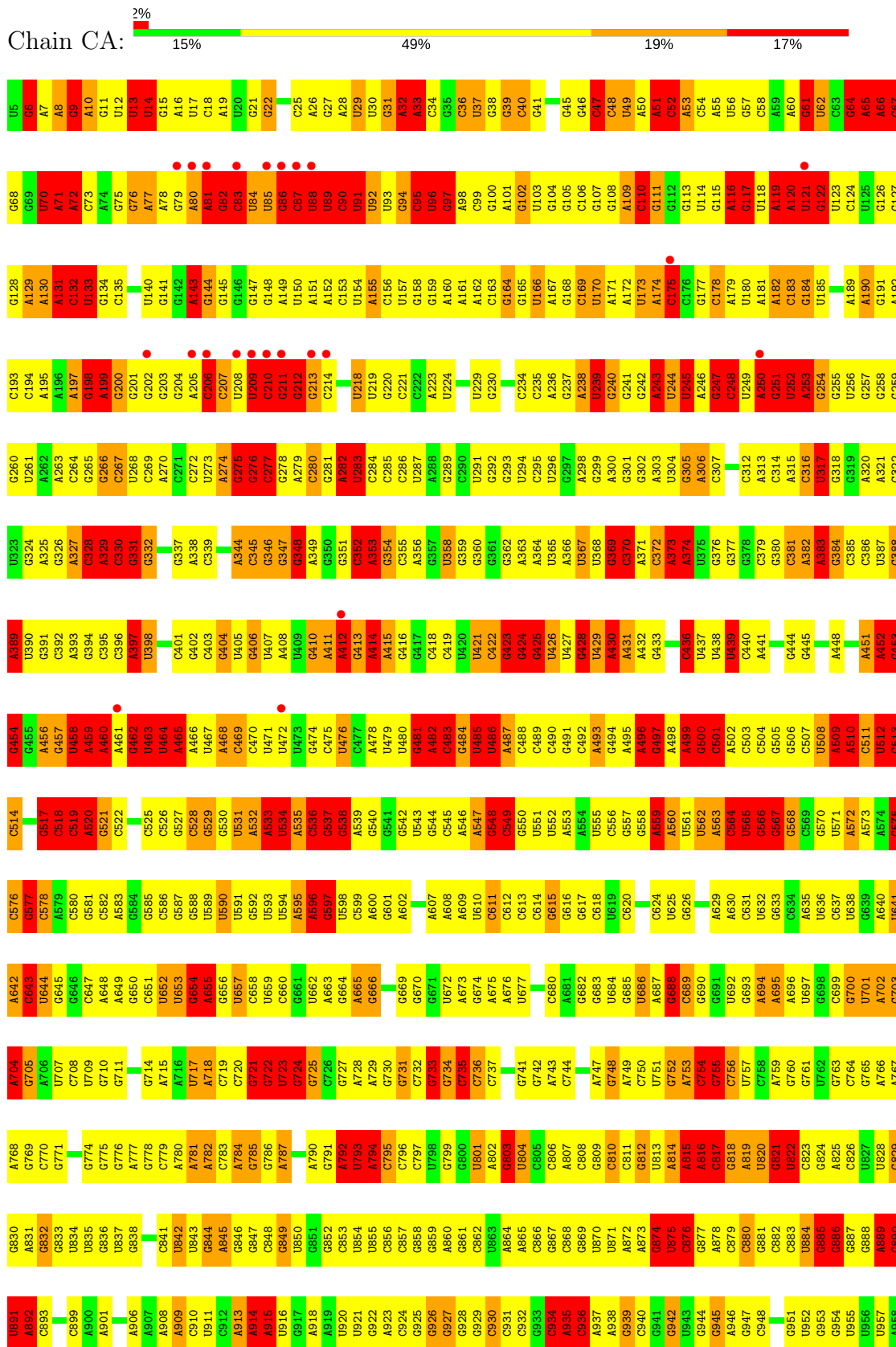
- Molecule 54: 50S ribosomal protein L36

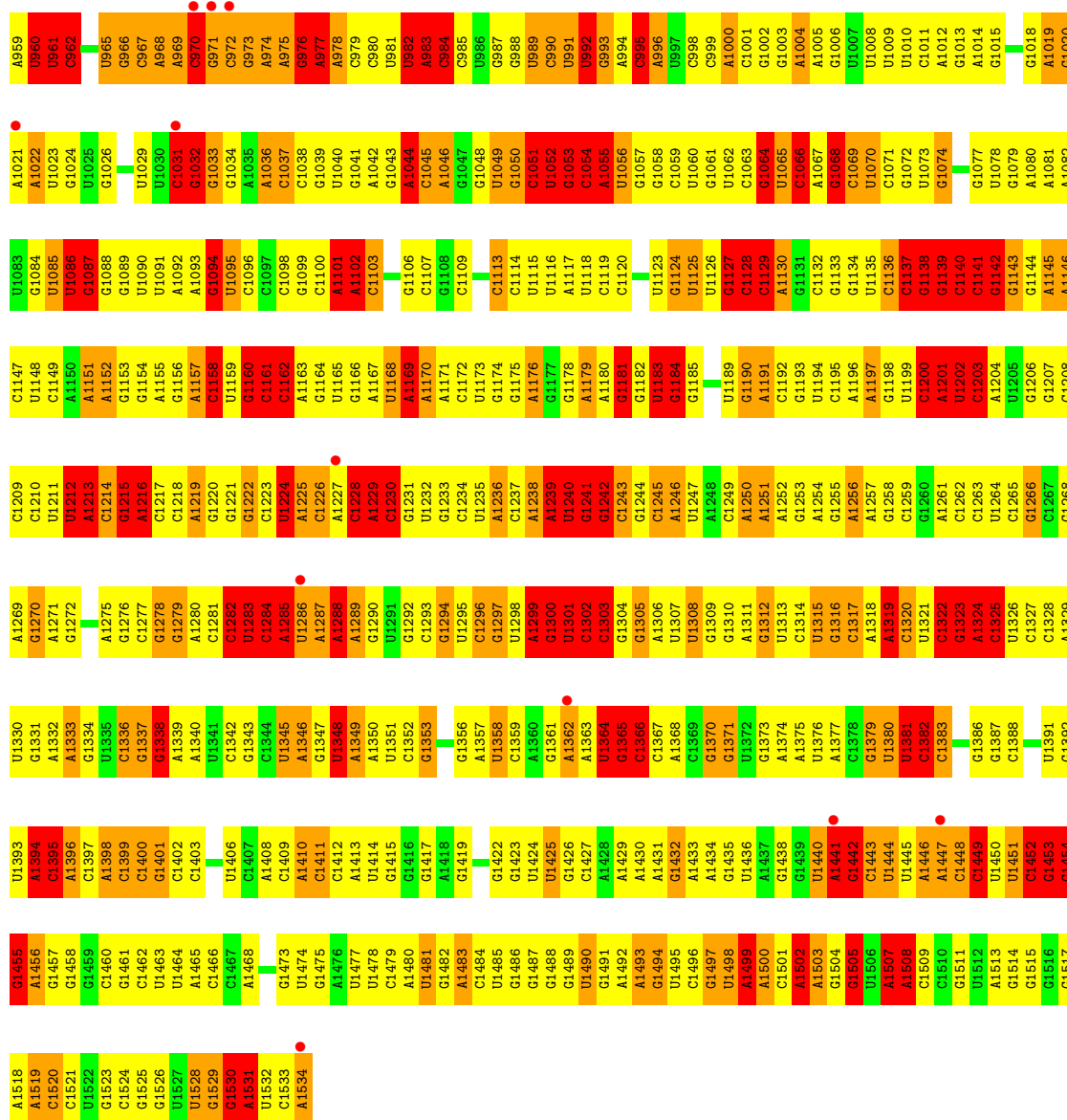


- Molecule 54: 50S ribosomal protein L36

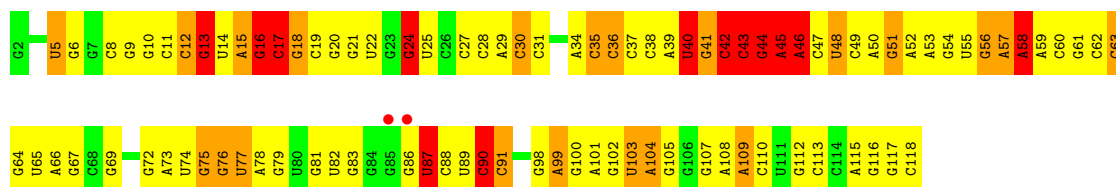


- Molecule 55: 16S rRNA





• Molecule 56: 5S rRNA



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.95Å 433.08Å 624.50Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 73.44 – 3.71<br>73.44 – 3.71                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 75.7 (73.44-3.71)<br>75.7 (73.44-3.71)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.08  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.39 (at 3.67Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine)                                      | Depositor        |
| R, $R_{free}$   | 0.227 , 0.268<br>0.234 , 0.276                              | Depositor<br>DCC |
| $R_{free}$ test set   | 9144 reflections (2.02%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 109.1   | Xtriage          |
| Anisotropy  | 0.249   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.23 , 85.5   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 286150  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 163.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$   |
| 1   | AB    | 0.25         | 0/1735      | 0.47        | 0/2338        |
| 1   | CB    | 0.25         | 0/1735      | 0.46        | 0/2338        |
| 2   | AC    | 0.27         | 0/1651      | 0.48        | 0/2225        |
| 2   | CC    | 0.26         | 0/1651      | 0.47        | 0/2225        |
| 3   | AD    | 0.27         | 0/1665      | 0.48        | 0/2227        |
| 3   | CD    | 0.30         | 0/1665      | 0.50        | 0/2227        |
| 4   | AE    | 0.30         | 0/1118      | 0.54        | 0/1504        |
| 4   | CE    | 0.29         | 0/1118      | 0.53        | 0/1504        |
| 5   | AF    | 0.26         | 0/835       | 0.46        | 0/1128        |
| 5   | CF    | 0.26         | 0/835       | 0.46        | 0/1128        |
| 6   | AG    | 0.25         | 0/1195      | 0.43        | 0/1602        |
| 6   | CG    | 0.27         | 0/1187      | 0.50        | 0/1591        |
| 7   | AH    | 0.27         | 0/989       | 0.50        | 0/1326        |
| 7   | CH    | 0.25         | 0/989       | 0.47        | 0/1326        |
| 8   | AI    | 0.24         | 0/1034      | 0.45        | 0/1375        |
| 8   | CI    | 0.25         | 0/1034      | 0.47        | 0/1375        |
| 9   | AJ    | 0.25         | 0/796       | 0.48        | 0/1077        |
| 9   | CJ    | 0.24         | 0/796       | 0.47        | 0/1077        |
| 10  | AK    | 0.26         | 0/893       | 0.48        | 0/1205        |
| 10  | CK    | 0.26         | 0/893       | 0.50        | 0/1205        |
| 11  | AL    | 0.33         | 0/969       | 0.62        | 0/1300        |
| 11  | CL    | 0.31         | 0/969       | 0.53        | 0/1300        |
| 12  | AM    | 0.36         | 0/892       | 0.64        | 3/1193 (0.3%) |
| 12  | CM    | 0.38         | 0/884       | 0.53        | 0/1181        |
| 13  | AN    | 0.26         | 0/785       | 0.48        | 0/1043        |
| 13  | CN    | 0.25         | 0/780       | 0.43        | 0/1036        |
| 14  | AO    | 0.26         | 0/722       | 0.48        | 0/964         |
| 14  | CO    | 0.24         | 0/722       | 0.46        | 0/964         |
| 15  | AP    | 0.27         | 0/659       | 0.46        | 0/884         |
| 15  | CP    | 0.27         | 0/648       | 0.47        | 0/870         |
| 16  | AQ    | 0.33         | 0/657       | 0.55        | 0/881         |
| 16  | CQ    | 0.26         | 0/657       | 0.46        | 0/881         |

| Mol | Chain | Bond lengths |                 | Bond angles |                    |
|-----|-------|--------------|-----------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5            |
| 17  | AR    | 0.25         | 0/462           | 0.48        | 0/621              |
| 17  | CR    | 0.27         | 0/462           | 0.49        | 0/621              |
| 18  | AS    | 0.24         | 0/652           | 0.43        | 0/877              |
| 18  | CS    | 0.23         | 0/652           | 0.46        | 0/877              |
| 19  | AT    | 0.29         | 0/671           | 0.51        | 0/888              |
| 19  | CT    | 0.24         | 0/671           | 0.44        | 0/888              |
| 20  | AU    | 0.27         | 0/430           | 0.46        | 0/570              |
| 20  | CU    | 0.29         | 0/430           | 0.54        | 0/570              |
| 21  | AA    | 0.55         | 1/36834 (0.0%)  | 1.44        | 678/57462 (1.2%)   |
| 22  | AV    | 0.59         | 0/408           | 1.14        | 1/634 (0.2%)       |
| 22  | AX    | 0.52         | 0/408           | 1.04        | 0/634              |
| 22  | CV    | 0.56         | 0/408           | 1.14        | 0/634              |
| 22  | CX    | 0.41         | 0/408           | 0.82        | 0/634              |
| 23  | AW    | 0.88         | 0/131           | 1.88        | 5/200 (2.5%)       |
| 23  | CW    | 0.73         | 0/131           | 1.93        | 7/200 (3.5%)       |
| 24  | BA    | 0.76         | 12/68626 (0.0%) | 1.69        | 1758/107056 (1.6%) |
| 24  | DA    | 0.53         | 1/68314 (0.0%)  | 1.46        | 1365/106569 (1.3%) |
| 25  | BB    | 0.66         | 0/2828          | 1.67        | 74/4410 (1.7%)     |
| 26  | BC    | 0.45         | 0/2121          | 0.72        | 1/2852 (0.0%)      |
| 26  | DC    | 0.33         | 0/2121          | 0.54        | 0/2852             |
| 27  | BD    | 0.50         | 0/1586          | 0.75        | 1/2134 (0.0%)      |
| 27  | DD    | 0.31         | 0/1586          | 0.55        | 0/2134             |
| 28  | BE    | 0.44         | 0/1571          | 0.67        | 0/2113             |
| 28  | DE    | 0.25         | 0/1571          | 0.47        | 0/2113             |
| 29  | BF    | 0.41         | 0/1434          | 0.68        | 3/1926 (0.2%)      |
| 29  | DF    | 0.35         | 0/1444          | 0.73        | 5/1937 (0.3%)      |
| 30  | BG    | 0.43         | 0/1343          | 0.65        | 0/1816             |
| 30  | DG    | 0.23         | 0/1343          | 0.46        | 0/1816             |
| 31  | BH    | 0.70         | 6/1122 (0.5%)   | 0.83        | 6/1515 (0.4%)      |
| 31  | DH    | 0.53         | 3/1122 (0.3%)   | 0.67        | 3/1515 (0.2%)      |
| 32  | BI    | 0.24         | 0/1046          | 0.50        | 0/1410             |
| 32  | DI    | 0.23         | 0/1046          | 0.44        | 0/1410             |
| 33  | BJ    | 0.55         | 0/1152          | 0.75        | 0/1551             |
| 33  | DJ    | 0.28         | 0/1152          | 0.55        | 0/1551             |
| 34  | BK    | 0.55         | 0/947           | 0.83        | 0/1268             |
| 34  | DK    | 0.31         | 0/947           | 0.54        | 0/1268             |
| 35  | BL    | 0.42         | 0/1054          | 0.77        | 1/1403 (0.1%)      |
| 35  | DL    | 0.27         | 0/1054          | 0.51        | 0/1403             |
| 36  | BM    | 0.51         | 0/1093          | 0.77        | 1/1460 (0.1%)      |
| 36  | DM    | 0.31         | 0/1093          | 0.48        | 0/1460             |
| 37  | BN    | 0.55         | 0/973           | 0.79        | 0/1301             |
| 37  | DN    | 0.27         | 0/973           | 0.49        | 0/1301             |
| 38  | BO    | 0.42         | 0/902           | 0.63        | 0/1209             |

| Mol | Chain | Bond lengths |                  | Bond angles |                    |
|-----|-------|--------------|------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5            |
| 38  | DO    | 0.24         | 0/902            | 0.44        | 0/1209             |
| 39  | BP    | 0.51         | 0/929            | 0.77        | 0/1242             |
| 39  | DP    | 0.28         | 0/929            | 0.49        | 0/1242             |
| 40  | BQ    | 0.60         | 0/960            | 0.71        | 0/1278             |
| 40  | DQ    | 0.28         | 0/960            | 0.46        | 0/1278             |
| 41  | BR    | 0.56         | 0/829            | 0.85        | 1/1107 (0.1%)      |
| 41  | DR    | 0.28         | 0/829            | 0.50        | 0/1107             |
| 42  | BS    | 0.50         | 0/864            | 0.75        | 0/1156             |
| 42  | DS    | 0.29         | 0/864            | 0.54        | 0/1156             |
| 43  | BT    | 0.48         | 0/744            | 0.70        | 0/994              |
| 43  | DT    | 0.25         | 0/744            | 0.49        | 0/994              |
| 44  | BU    | 0.41         | 0/787            | 0.70        | 0/1051             |
| 44  | DU    | 0.25         | 0/787            | 0.47        | 0/1051             |
| 45  | BV    | 0.48         | 0/766            | 0.66        | 0/1025             |
| 45  | DV    | 0.38         | 0/766            | 0.54        | 0/1025             |
| 46  | BW    | 0.51         | 0/603            | 0.76        | 0/797              |
| 46  | DW    | 0.26         | 0/603            | 0.47        | 0/797              |
| 47  | BX    | 0.42         | 0/635            | 0.67        | 0/848              |
| 47  | DX    | 0.30         | 0/635            | 0.55        | 0/848              |
| 48  | BY    | 0.40         | 0/510            | 0.66        | 0/677              |
| 48  | DY    | 0.23         | 0/510            | 0.44        | 0/677              |
| 49  | BZ    | 0.52         | 0/453            | 0.77        | 0/605              |
| 49  | DZ    | 0.28         | 0/453            | 0.51        | 0/605              |
| 50  | B0    | 0.45         | 0/450            | 0.79        | 0/599              |
| 50  | D0    | 0.28         | 0/450            | 0.51        | 0/599              |
| 51  | B1    | 0.40         | 0/416            | 0.63        | 0/554              |
| 51  | D1    | 0.28         | 0/416            | 0.46        | 0/554              |
| 52  | B2    | 0.47         | 0/380            | 0.73        | 0/498              |
| 52  | D2    | 0.28         | 0/380            | 0.55        | 0/498              |
| 53  | B3    | 0.51         | 0/513            | 0.76        | 0/676              |
| 53  | D3    | 0.26         | 0/513            | 0.51        | 0/676              |
| 54  | B4    | 0.47         | 0/303            | 0.76        | 0/397              |
| 54  | D4    | 0.30         | 0/303            | 0.49        | 0/397              |
| 55  | CA    | 0.53         | 0/36762          | 1.45        | 712/57350 (1.2%)   |
| 56  | DB    | 0.52         | 0/2803           | 1.35        | 52/4371 (1.2%)     |
| All | All   | 0.55         | 23/308631 (0.0%) | 1.35        | 4677/461501 (1.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 12  | AM    | 0                   | 1                   |
| 27  | BD    | 0                   | 1                   |
| 31  | BH    | 0                   | 2                   |
| 31  | DH    | 0                   | 3                   |
| 37  | BN    | 0                   | 1                   |
| All | All   | 0                   | 8                   |

All (23) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 24  | BA    | 1142 | A    | N9-C4   | -13.92 | 1.29        | 1.37     |
| 31  | BH    | 48   | GLU  | C-O     | 9.51   | 1.41        | 1.23     |
| 24  | BA    | 2451 | A    | C8-N7   | 9.03   | 1.37        | 1.31     |
| 31  | DH    | 49   | ALA  | CA-CB   | -7.88  | 1.35        | 1.52     |
| 31  | BH    | 48   | GLU  | CA-CB   | 6.93   | 1.69        | 1.53     |
| 24  | DA    | 1060 | U    | C2-N3   | 6.91   | 1.42        | 1.37     |
| 31  | DH    | 48   | GLU  | CB-CG   | 6.81   | 1.65        | 1.52     |
| 31  | BH    | 48   | GLU  | CA-C    | -6.56  | 1.35        | 1.52     |
| 31  | BH    | 49   | ALA  | N-CA    | 6.50   | 1.59        | 1.46     |
| 24  | BA    | 783  | A    | N9-C4   | -6.32  | 1.34        | 1.37     |
| 24  | BA    | 2447 | G    | C6-N1   | 6.31   | 1.44        | 1.39     |
| 24  | BA    | 2860 | A    | C6-N6   | 6.00   | 1.38        | 1.33     |
| 24  | BA    | 1086 | A    | N7-C5   | -5.74  | 1.35        | 1.39     |
| 31  | BH    | 47   | PHE  | CD2-CE2 | 5.54   | 1.50        | 1.39     |
| 24  | BA    | 1876 | A    | N7-C5   | 5.51   | 1.42        | 1.39     |
| 31  | BH    | 48   | GLU  | CD-OE1  | 5.45   | 1.31        | 1.25     |
| 21  | AA    | 1097 | C    | C1'-N1  | 5.33   | 1.56        | 1.48     |
| 24  | BA    | 2275 | C    | C1'-N1  | 5.32   | 1.56        | 1.48     |
| 24  | BA    | 1142 | A    | C8-N7   | 5.29   | 1.35        | 1.31     |
| 24  | BA    | 528  | A    | N7-C5   | -5.26  | 1.36        | 1.39     |
| 31  | DH    | 50   | ARG  | CB-CG   | -5.09  | 1.38        | 1.52     |
| 24  | BA    | 2857 | G    | N3-C4   | 5.05   | 1.39        | 1.35     |
| 24  | BA    | 2884 | U    | C1'-N1  | 5.04   | 1.56        | 1.48     |

All (4677) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 24  | BA    | 2447 | G    | C6-N1-C2   | -22.51 | 111.59      | 125.10   |
| 24  | BA    | 2451 | A    | C5-N7-C8   | -17.23 | 95.28       | 103.90   |
| 24  | BA    | 2347 | C    | N1-C1'-C2' | -16.79 | 92.17       | 114.00   |
| 24  | BA    | 790  | U    | P-O3'-C3'  | -16.12 | 100.36      | 119.70   |
| 25  | BB    | 88   | C    | O4'-C1'-N1 | -15.24 | 96.01       | 108.20   |
| 24  | BA    | 2447 | G    | C5-C6-O6   | -15.23 | 119.46      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 24  | BA    | 2447 | G    | C5-C6-N1   | 15.21  | 119.11      | 111.50   |
| 24  | BA    | 1023 | U    | N1-C1'-C2' | -15.17 | 94.28       | 114.00   |
| 24  | BA    | 2424 | C    | N1-C1'-C2' | -15.08 | 94.40       | 114.00   |
| 24  | BA    | 812  | C    | N1-C1'-C2' | -14.96 | 94.55       | 114.00   |
| 24  | BA    | 740  | C    | N1-C1'-C2' | -14.69 | 94.91       | 114.00   |
| 24  | BA    | 1022 | G    | P-O3'-C3'  | 14.59  | 137.21      | 119.70   |
| 24  | BA    | 206  | U    | N1-C1'-C2' | -14.54 | 95.09       | 114.00   |
| 24  | BA    | 2752 | C    | N1-C1'-C2' | -14.37 | 95.33       | 114.00   |
| 24  | BA    | 1675 | C    | N1-C1'-C2' | -14.18 | 95.56       | 114.00   |
| 29  | DF    | 109  | ARG  | NE-CZ-NH1  | -14.18 | 113.21      | 120.30   |
| 24  | DA    | 2283 | C    | N1-C1'-C2' | -14.13 | 95.63       | 114.00   |
| 24  | BA    | 373  | U    | N1-C1'-C2' | -14.03 | 95.77       | 114.00   |
| 24  | BA    | 805  | G    | P-O3'-C3'  | 14.02  | 136.52      | 119.70   |
| 21  | AA    | 1103 | C    | N1-C1'-C2' | -13.98 | 95.83       | 114.00   |
| 29  | BF    | 112  | ASP  | CB-CG-OD2  | -13.89 | 105.80      | 118.30   |
| 24  | DA    | 861  | A    | P-O3'-C3'  | -13.83 | 103.11      | 119.70   |
| 21  | AA    | 117  | G    | P-O3'-C3'  | -13.79 | 103.16      | 119.70   |
| 24  | DA    | 2586 | U    | N1-C1'-C2' | -13.74 | 96.14       | 114.00   |
| 24  | BA    | 1142 | A    | C5-N7-C8   | -13.73 | 97.04       | 103.90   |
| 55  | CA    | 590  | U    | N1-C1'-C2' | -13.65 | 96.26       | 114.00   |
| 21  | AA    | 1259 | C    | P-O3'-C3'  | -13.62 | 103.36      | 119.70   |
| 21  | AA    | 687  | A    | P-O3'-C3'  | 13.62  | 136.04      | 119.70   |
| 21  | AA    | 795  | C    | N1-C1'-C2' | -13.59 | 96.33       | 114.00   |
| 24  | BA    | 1681 | G    | P-O3'-C3'  | 13.57  | 135.98      | 119.70   |
| 24  | BA    | 1461 | C    | N1-C1'-C2' | -13.54 | 96.41       | 114.00   |
| 24  | BA    | 946  | C    | N1-C1'-C2' | -13.52 | 96.42       | 114.00   |
| 24  | BA    | 435  | C    | N1-C1'-C2' | -13.49 | 96.47       | 114.00   |
| 24  | DA    | 1956 | U    | N1-C1'-C2' | -13.43 | 96.54       | 114.00   |
| 24  | BA    | 2036 | C    | N1-C1'-C2' | -13.41 | 96.57       | 114.00   |
| 24  | DA    | 1499 | C    | N1-C1'-C2' | -13.40 | 96.58       | 114.00   |
| 55  | CA    | 960  | U    | O4'-C1'-N1 | 13.36  | 118.89      | 108.20   |
| 24  | BA    | 2504 | U    | N1-C1'-C2' | -13.29 | 96.72       | 114.00   |
| 29  | DF    | 109  | ARG  | NE-CZ-NH2  | 13.28  | 126.94      | 120.30   |
| 24  | BA    | 249  | C    | P-O3'-C3'  | 13.26  | 135.62      | 119.70   |
| 24  | DA    | 832  | U    | N1-C1'-C2' | -13.26 | 96.76       | 114.00   |
| 21  | AA    | 173  | U    | O4'-C1'-N1 | 13.25  | 118.80      | 108.20   |
| 24  | BA    | 686  | U    | O4'-C1'-N1 | 13.24  | 118.79      | 108.20   |
| 24  | DA    | 1536 | C    | P-O3'-C3'  | 13.22  | 135.57      | 119.70   |
| 24  | BA    | 919  | U    | N1-C2-O2   | 13.20  | 132.04      | 122.80   |
| 24  | DA    | 2441 | U    | N1-C1'-C2' | -13.20 | 96.84       | 114.00   |
| 24  | DA    | 1267 | U    | N1-C1'-C2' | -13.20 | 96.85       | 114.00   |
| 24  | DA    | 741  | U    | N1-C1'-C2' | -13.18 | 96.86       | 114.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 21  | AA    | 891  | U    | N1-C1'-C2' | -13.17 | 96.88       | 114.00   |
| 24  | DA    | 2403 | C    | N1-C1'-C2' | -13.16 | 96.89       | 114.00   |
| 24  | DA    | 964  | C    | N1-C1'-C2' | -13.16 | 96.89       | 114.00   |
| 24  | BA    | 2629 | U    | P-O3'-C3'  | 13.16  | 135.49      | 119.70   |
| 24  | DA    | 1060 | U    | C5-C4-O4   | -13.15 | 118.01      | 125.90   |
| 55  | CA    | 1302 | C    | N1-C1'-C2' | -13.11 | 96.95       | 114.00   |
| 24  | DA    | 1612 | C    | N1-C1'-C2' | -13.10 | 96.97       | 114.00   |
| 25  | BB    | 16   | G    | P-O3'-C3'  | -13.09 | 103.99      | 119.70   |
| 24  | BA    | 1142 | A    | N3-C4-N9   | -13.07 | 116.95      | 127.40   |
| 21  | AA    | 52   | C    | N1-C1'-C2' | -13.00 | 97.09       | 114.00   |
| 55  | CA    | 512  | U    | N1-C1'-C2' | -13.00 | 97.10       | 114.00   |
| 21  | AA    | 169  | C    | O4'-C1'-N1 | 12.99  | 118.59      | 108.20   |
| 24  | BA    | 2068 | U    | N1-C1'-C2' | -12.98 | 97.12       | 114.00   |
| 24  | BA    | 1815 | A    | P-O3'-C3'  | 12.96  | 135.25      | 119.70   |
| 55  | CA    | 1345 | U    | O4'-C1'-N1 | 12.93  | 118.55      | 108.20   |
| 24  | BA    | 1760 | C    | N1-C1'-C2' | -12.90 | 97.22       | 114.00   |
| 24  | DA    | 1556 | C    | N1-C1'-C2' | -12.85 | 97.29       | 114.00   |
| 24  | BA    | 1082 | U    | C2-N3-C4   | -12.85 | 119.29      | 127.00   |
| 24  | DA    | 1023 | U    | N1-C1'-C2' | -12.83 | 97.32       | 114.00   |
| 25  | BB    | 90   | C    | N1-C1'-C2' | -12.82 | 97.33       | 114.00   |
| 24  | BA    | 2575 | C    | C2-N3-C4   | -12.82 | 113.49      | 119.90   |
| 24  | DA    | 2061 | G    | P-O3'-C3'  | 12.80  | 135.06      | 119.70   |
| 24  | BA    | 2238 | G    | P-O3'-C3'  | 12.76  | 135.01      | 119.70   |
| 24  | DA    | 2504 | U    | N1-C1'-C2' | -12.75 | 97.42       | 114.00   |
| 24  | DA    | 1611 | C    | N1-C1'-C2' | -12.74 | 97.43       | 114.00   |
| 24  | BA    | 1019 | U    | C2-N3-C4   | -12.72 | 119.37      | 127.00   |
| 24  | BA    | 646  | U    | N1-C1'-C2' | -12.71 | 97.47       | 114.00   |
| 24  | BA    | 919  | U    | C2-N1-C1'  | 12.71  | 132.95      | 117.70   |
| 24  | DA    | 2063 | C    | N1-C1'-C2' | -12.71 | 97.48       | 114.00   |
| 24  | BA    | 302  | C    | N1-C1'-C2' | -12.68 | 97.52       | 114.00   |
| 24  | BA    | 919  | U    | C5-C6-N1   | 12.66  | 129.03      | 122.70   |
| 55  | CA    | 936  | C    | P-O3'-C3'  | -12.64 | 104.53      | 119.70   |
| 55  | CA    | 891  | U    | N1-C1'-C2' | -12.64 | 97.57       | 114.00   |
| 24  | BA    | 1210 | G    | P-O3'-C3'  | 12.60  | 134.82      | 119.70   |
| 21  | AA    | 327  | A    | P-O3'-C3'  | 12.57  | 134.79      | 119.70   |
| 24  | DA    | 1963 | U    | N1-C1'-C2' | -12.55 | 97.68       | 114.00   |
| 56  | DB    | 90   | C    | N1-C1'-C2' | -12.52 | 97.72       | 114.00   |
| 24  | BA    | 2451 | A    | N7-C8-N9   | 12.51  | 120.05      | 113.80   |
| 55  | CA    | 1325 | C    | N1-C1'-C2' | -12.49 | 97.76       | 114.00   |
| 24  | BA    | 1396 | U    | O4'-C1'-N1 | 12.49  | 118.19      | 108.20   |
| 24  | DA    | 2493 | U    | N1-C1'-C2' | -12.48 | 97.78       | 114.00   |
| 24  | BA    | 2833 | U    | P-O3'-C3'  | 12.47  | 134.66      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 24  | DA    | 2568 | U    | N1-C1'-C2' | -12.46 | 97.80       | 114.00   |
| 24  | DA    | 813  | U    | N1-C1'-C2' | -12.45 | 97.82       | 114.00   |
| 24  | BA    | 2225 | A    | P-O3'-C3'  | 12.42  | 134.61      | 119.70   |
| 24  | BA    | 1247 | A    | P-O3'-C3'  | 12.42  | 134.60      | 119.70   |
| 55  | CA    | 1086 | U    | N1-C1'-C2' | -12.41 | 97.87       | 114.00   |
| 24  | DA    | 784  | G    | P-O3'-C3'  | 12.40  | 134.58      | 119.70   |
| 24  | BA    | 164  | C    | P-O3'-C3'  | -12.39 | 104.83      | 119.70   |
| 24  | BA    | 1965 | C    | P-O3'-C3'  | -12.38 | 104.85      | 119.70   |
| 24  | DA    | 76   | C    | N1-C1'-C2' | -12.37 | 97.92       | 114.00   |
| 24  | DA    | 807  | U    | N1-C1'-C2' | -12.37 | 97.92       | 114.00   |
| 24  | BA    | 1648 | U    | N1-C1'-C2' | -12.36 | 97.93       | 114.00   |
| 24  | BA    | 860  | U    | N1-C1'-C2' | -12.36 | 97.94       | 114.00   |
| 55  | CA    | 133  | U    | N1-C1'-C2' | -12.35 | 97.95       | 114.00   |
| 24  | BA    | 1914 | C    | N1-C1'-C2' | -12.33 | 97.97       | 114.00   |
| 55  | CA    | 483  | C    | N1-C1'-C2' | -12.32 | 97.98       | 114.00   |
| 24  | BA    | 2630 | G    | P-O3'-C3'  | -12.32 | 104.92      | 119.70   |
| 55  | CA    | 1162 | C    | N1-C1'-C2' | -12.28 | 98.04       | 114.00   |
| 24  | DA    | 87   | U    | N1-C1'-C2' | -12.27 | 98.05       | 114.00   |
| 25  | BB    | 37   | C    | N1-C1'-C2' | -12.27 | 98.05       | 114.00   |
| 21  | AA    | 1345 | U    | P-O3'-C3'  | 12.21  | 134.36      | 119.70   |
| 21  | AA    | 915  | A    | P-O3'-C3'  | -12.20 | 105.06      | 119.70   |
| 24  | BA    | 688  | U    | N1-C1'-C2' | -12.17 | 98.17       | 114.00   |
| 24  | DA    | 2520 | C    | N1-C1'-C2' | -12.17 | 98.17       | 114.00   |
| 21  | AA    | 590  | U    | N1-C1'-C2' | -12.16 | 98.19       | 114.00   |
| 24  | DA    | 658  | U    | N1-C1'-C2' | -12.14 | 98.22       | 114.00   |
| 24  | DA    | 375  | G    | P-O3'-C3'  | -12.14 | 105.14      | 119.70   |
| 55  | CA    | 1213 | A    | P-O3'-C3'  | 12.10  | 134.22      | 119.70   |
| 55  | CA    | 67   | C    | O4'-C1'-N1 | 12.07  | 117.86      | 108.20   |
| 21  | AA    | 725  | G    | P-O3'-C3'  | -12.06 | 105.23      | 119.70   |
| 24  | DA    | 460  | A    | P-O3'-C3'  | -12.05 | 105.24      | 119.70   |
| 55  | CA    | 33   | A    | P-O3'-C3'  | -12.04 | 105.25      | 119.70   |
| 55  | CA    | 565  | U    | N1-C1'-C2' | -12.02 | 98.37       | 114.00   |
| 24  | BA    | 1558 | C    | P-O3'-C3'  | 12.02  | 134.12      | 119.70   |
| 21  | AA    | 519  | C    | N1-C1'-C2' | -11.99 | 98.41       | 114.00   |
| 21  | AA    | 1203 | C    | P-O3'-C3'  | -11.98 | 105.32      | 119.70   |
| 24  | BA    | 685  | A    | P-O3'-C3'  | 11.98  | 134.08      | 119.70   |
| 55  | CA    | 348  | G    | P-O3'-C3'  | -11.98 | 105.32      | 119.70   |
| 24  | BA    | 614  | A    | P-O3'-C3'  | 11.97  | 134.07      | 119.70   |
| 24  | BA    | 1142 | A    | N3-C4-C5   | 11.97  | 135.18      | 126.80   |
| 24  | BA    | 1499 | C    | N1-C1'-C2' | -11.97 | 98.44       | 114.00   |
| 55  | CA    | 245  | U    | N1-C1'-C2' | -11.95 | 98.46       | 114.00   |
| 24  | DA    | 534  | U    | N1-C1'-C2' | -11.94 | 98.48       | 114.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 24  | DA    | 2261 | C    | N1-C1'-C2' | -11.94 | 98.48       | 114.00   |
| 24  | BA    | 1145 | C    | P-O5'-C5'  | -11.93 | 101.82      | 120.90   |
| 24  | DA    | 392  | U    | N1-C1'-C2' | -11.91 | 98.51       | 114.00   |
| 24  | DA    | 1539 | U    | N1-C1'-C2' | -11.91 | 98.52       | 114.00   |
| 24  | BA    | 1993 | U    | N1-C1'-C2' | -11.91 | 98.52       | 114.00   |
| 21  | AA    | 110  | C    | N1-C1'-C2' | -11.89 | 98.54       | 114.00   |
| 24  | BA    | 2447 | G    | P-O3'-C3'  | 11.89  | 133.97      | 119.70   |
| 24  | BA    | 2447 | G    | N3-C4-C5   | -11.87 | 122.66      | 128.60   |
| 21  | AA    | 597  | G    | P-O3'-C3'  | -11.87 | 105.46      | 119.70   |
| 24  | BA    | 2023 | C    | N1-C1'-C2' | -11.85 | 98.60       | 114.00   |
| 24  | DA    | 313  | G    | P-O3'-C3'  | -11.85 | 105.48      | 119.70   |
| 21  | AA    | 276  | G    | P-O3'-C3'  | -11.84 | 105.49      | 119.70   |
| 24  | BA    | 2857 | G    | C2-N3-C4   | -11.83 | 105.98      | 111.90   |
| 24  | BA    | 2283 | C    | N1-C1'-C2' | -11.83 | 98.62       | 114.00   |
| 24  | DA    | 1916 | A    | P-O3'-C3'  | -11.83 | 105.51      | 119.70   |
| 21  | AA    | 1182 | G    | P-O3'-C3'  | 11.82  | 133.88      | 119.70   |
| 55  | CA    | 886  | G    | P-O3'-C3'  | -11.80 | 105.53      | 119.70   |
| 24  | DA    | 2429 | G    | P-O3'-C3'  | -11.80 | 105.54      | 119.70   |
| 55  | CA    | 1283 | U    | N1-C1'-C2' | -11.78 | 98.68       | 114.00   |
| 24  | DA    | 576  | U    | N1-C1'-C2' | -11.78 | 98.69       | 114.00   |
| 24  | DA    | 364  | C    | N1-C1'-C2' | -11.77 | 98.70       | 114.00   |
| 24  | DA    | 413  | C    | N1-C1'-C2' | -11.77 | 98.71       | 114.00   |
| 24  | DA    | 1655 | A    | P-O3'-C3'  | -11.75 | 105.60      | 119.70   |
| 21  | AA    | 1348 | U    | N1-C1'-C2' | -11.73 | 98.75       | 114.00   |
| 55  | CA    | 1216 | A    | P-O3'-C3'  | -11.73 | 105.63      | 119.70   |
| 55  | CA    | 132  | C    | N1-C1'-C2' | -11.72 | 98.77       | 114.00   |
| 21  | AA    | 1053 | G    | P-O3'-C3'  | 11.70  | 133.74      | 119.70   |
| 24  | DA    | 1462 | C    | N1-C1'-C2' | -11.68 | 98.81       | 114.00   |
| 24  | DA    | 437  | U    | N1-C1'-C2' | -11.67 | 98.83       | 114.00   |
| 24  | BA    | 1802 | A    | P-O3'-C3'  | -11.66 | 105.70      | 119.70   |
| 55  | CA    | 876  | C    | N1-C1'-C2' | -11.66 | 98.84       | 114.00   |
| 24  | DA    | 1683 | U    | N1-C1'-C2' | -11.65 | 98.85       | 114.00   |
| 24  | BA    | 1965 | C    | N1-C1'-C2' | -11.64 | 98.87       | 114.00   |
| 21  | AA    | 352  | C    | N1-C1'-C2' | -11.61 | 98.91       | 114.00   |
| 21  | AA    | 422  | C    | P-O3'-C3'  | 11.60  | 133.62      | 119.70   |
| 24  | BA    | 2425 | A    | P-O3'-C3'  | 11.60  | 133.62      | 119.70   |
| 24  | DA    | 128  | C    | N1-C1'-C2' | -11.59 | 98.93       | 114.00   |
| 24  | BA    | 1962 | C    | P-O3'-C3'  | 11.59  | 133.60      | 119.70   |
| 24  | BA    | 138  | U    | N1-C1'-C2' | -11.57 | 98.96       | 114.00   |
| 24  | BA    | 2848 | G    | P-O3'-C3'  | 11.54  | 133.55      | 119.70   |
| 55  | CA    | 352  | C    | N1-C1'-C2' | -11.54 | 99.00       | 114.00   |
| 24  | BA    | 2638 | G    | P-O3'-C3'  | 11.53  | 133.54      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 24  | BA    | 1956 | U    | N1-C1'-C2' | -11.53 | 99.01       | 114.00   |
| 24  | DA    | 2402 | U    | N1-C1'-C2' | -11.52 | 99.03       | 114.00   |
| 55  | CA    | 328  | C    | P-O3'-C3'  | 11.50  | 133.50      | 119.70   |
| 24  | DA    | 225  | C    | N1-C1'-C2' | -11.47 | 99.08       | 114.00   |
| 55  | CA    | 1381 | U    | N1-C1'-C2' | -11.45 | 99.11       | 114.00   |
| 24  | DA    | 2348 | U    | N1-C1'-C2' | -11.45 | 99.11       | 114.00   |
| 24  | DA    | 617  | G    | P-O3'-C3'  | -11.44 | 105.97      | 119.70   |
| 24  | DA    | 325  | G    | P-O3'-C3'  | -11.44 | 105.97      | 119.70   |
| 24  | DA    | 672  | C    | N1-C1'-C2' | -11.44 | 99.13       | 114.00   |
| 55  | CA    | 792  | A    | P-O3'-C3'  | 11.43  | 133.42      | 119.70   |
| 24  | BA    | 633  | A    | N1-C6-N6   | 11.42  | 125.45      | 118.60   |
| 24  | BA    | 442  | G    | P-O3'-C3'  | 11.40  | 133.38      | 119.70   |
| 24  | BA    | 934  | U    | N1-C1'-C2' | -11.40 | 99.19       | 114.00   |
| 24  | BA    | 1142 | A    | C4-C5-C6   | -11.39 | 111.30      | 117.00   |
| 21  | AA    | 1398 | A    | P-O3'-C3'  | -11.37 | 106.06      | 119.70   |
| 55  | CA    | 992  | U    | P-O3'-C3'  | 11.36  | 133.34      | 119.70   |
| 24  | DA    | 1799 | G    | P-O3'-C3'  | 11.35  | 133.32      | 119.70   |
| 24  | DA    | 2339 | C    | N1-C1'-C2' | -11.34 | 99.25       | 114.00   |
| 55  | CA    | 439  | U    | N1-C1'-C2' | -11.34 | 99.26       | 114.00   |
| 55  | CA    | 520  | A    | P-O3'-C3'  | -11.34 | 106.10      | 119.70   |
| 24  | BA    | 654  | A    | P-O3'-C3'  | -11.33 | 106.11      | 119.70   |
| 55  | CA    | 1366 | C    | P-O3'-C3'  | -11.33 | 106.11      | 119.70   |
| 24  | BA    | 200  | U    | N1-C1'-C2' | -11.31 | 99.30       | 114.00   |
| 24  | DA    | 2896 | C    | N1-C1'-C2' | -11.31 | 99.30       | 114.00   |
| 55  | CA    | 961  | U    | N1-C1'-C2' | -11.30 | 99.31       | 114.00   |
| 24  | BA    | 2581 | G    | P-O3'-C3'  | 11.29  | 133.24      | 119.70   |
| 24  | DA    | 1788 | C    | N1-C1'-C2' | -11.28 | 99.34       | 114.00   |
| 21  | AA    | 719  | C    | N1-C1'-C2' | -11.26 | 99.36       | 114.00   |
| 55  | CA    | 117  | G    | P-O3'-C3'  | -11.25 | 106.20      | 119.70   |
| 55  | CA    | 65   | A    | P-O3'-C3'  | 11.25  | 133.20      | 119.70   |
| 24  | BA    | 436  | C    | N1-C1'-C2' | -11.24 | 99.39       | 114.00   |
| 24  | BA    | 858  | G    | O4'-C1'-N9 | 11.24  | 117.19      | 108.20   |
| 24  | BA    | 1380 | G    | P-O3'-C3'  | -11.20 | 106.26      | 119.70   |
| 24  | BA    | 1708 | C    | P-O3'-C3'  | -11.18 | 106.28      | 119.70   |
| 21  | AA    | 984  | C    | N1-C1'-C2' | -11.18 | 99.47       | 114.00   |
| 24  | BA    | 489  | G    | P-O3'-C3'  | 11.17  | 133.11      | 119.70   |
| 21  | AA    | 130  | A    | P-O3'-C3'  | 11.16  | 133.10      | 119.70   |
| 21  | AA    | 374  | A    | P-O3'-C3'  | -11.16 | 106.31      | 119.70   |
| 24  | BA    | 303  | G    | P-O3'-C3'  | -11.16 | 106.31      | 119.70   |
| 24  | BA    | 957  | C    | P-O3'-C3'  | 11.15  | 133.09      | 119.70   |
| 24  | BA    | 2440 | C    | N1-C1'-C2' | -11.15 | 99.50       | 114.00   |
| 24  | BA    | 1971 | U    | N1-C1'-C2' | -11.15 | 99.51       | 114.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 24  | BA    | 2691 | C    | N1-C1'-C2' | -11.13 | 99.54       | 114.00   |
| 24  | DA    | 2616 | C    | N1-C1'-C2' | -11.12 | 99.55       | 114.00   |
| 24  | BA    | 1329 | U    | N1-C1'-C2' | 11.09  | 128.41      | 114.00   |
| 24  | DA    | 1997 | C    | N1-C1'-C2' | -11.07 | 99.61       | 114.00   |
| 21  | AA    | 1168 | U    | P-O3'-C3'  | 11.06  | 132.97      | 119.70   |
| 24  | BA    | 2645 | G    | O4'-C1'-N9 | 11.06  | 117.05      | 108.20   |
| 21  | AA    | 185  | U    | N1-C1'-C2' | -11.06 | 99.62       | 114.00   |
| 55  | CA    | 52   | C    | N1-C1'-C2' | -11.06 | 99.63       | 114.00   |
| 24  | DA    | 1556 | C    | P-O3'-C3'  | -11.05 | 106.44      | 119.70   |
| 24  | BA    | 2051 | A    | P-O3'-C3'  | 11.05  | 132.96      | 119.70   |
| 24  | BA    | 783  | A    | P-O3'-C3'  | -11.04 | 106.45      | 119.70   |
| 24  | DA    | 1046 | A    | P-O3'-C3'  | 11.04  | 132.95      | 119.70   |
| 55  | CA    | 962  | C    | P-O3'-C3'  | -11.04 | 106.45      | 119.70   |
| 24  | BA    | 2385 | C    | P-O3'-C3'  | -11.03 | 106.46      | 119.70   |
| 21  | AA    | 109  | A    | P-O3'-C3'  | 11.03  | 132.93      | 119.70   |
| 24  | DA    | 946  | C    | N1-C1'-C2' | -11.03 | 99.67       | 114.00   |
| 55  | CA    | 590  | U    | P-O3'-C3'  | -11.02 | 106.47      | 119.70   |
| 31  | BH    | 49   | ALA  | CB-CA-C    | 11.02  | 126.63      | 110.10   |
| 24  | DA    | 234  | U    | N1-C1'-C2' | -11.02 | 99.68       | 114.00   |
| 55  | CA    | 1228 | C    | N1-C1'-C2' | -11.01 | 99.69       | 114.00   |
| 24  | DA    | 789  | A    | P-O3'-C3'  | 11.01  | 132.91      | 119.70   |
| 24  | DA    | 1478 | G    | P-O3'-C3'  | -11.01 | 106.49      | 119.70   |
| 24  | BA    | 2458 | G    | P-O3'-C3'  | 11.00  | 132.90      | 119.70   |
| 24  | BA    | 1344 | U    | N1-C1'-C2' | -11.00 | 99.70       | 114.00   |
| 24  | BA    | 671  | C    | N1-C1'-C2' | -11.00 | 99.70       | 114.00   |
| 24  | DA    | 991  | C    | N1-C1'-C2' | -11.00 | 99.70       | 114.00   |
| 24  | BA    | 1816 | C    | N1-C1'-C2' | -10.98 | 99.73       | 114.00   |
| 24  | DA    | 1300 | G    | P-O3'-C3'  | 10.98  | 132.88      | 119.70   |
| 24  | DA    | 2499 | C    | N1-C1'-C2' | -10.96 | 99.75       | 114.00   |
| 24  | BA    | 784  | G    | P-O3'-C3'  | 10.96  | 132.85      | 119.70   |
| 24  | BA    | 2866 | U    | O4'-C1'-N1 | 10.96  | 116.96      | 108.20   |
| 24  | BA    | 1250 | G    | P-O3'-C3'  | 10.95  | 132.84      | 119.70   |
| 55  | CA    | 962  | C    | N1-C1'-C2' | -10.95 | 99.77       | 114.00   |
| 55  | CA    | 1449 | C    | N1-C1'-C2' | -10.94 | 99.77       | 114.00   |
| 55  | CA    | 1045 | C    | N1-C1'-C2' | -10.94 | 99.78       | 114.00   |
| 21  | AA    | 967  | C    | N1-C1'-C2' | -10.94 | 99.78       | 114.00   |
| 24  | DA    | 765  | C    | N1-C1'-C2' | -10.93 | 99.79       | 114.00   |
| 24  | DA    | 311  | A    | P-O3'-C3'  | 10.92  | 132.80      | 119.70   |
| 21  | AA    | 14   | U    | N1-C1'-C2' | -10.91 | 99.81       | 114.00   |
| 55  | CA    | 317  | U    | N1-C1'-C2' | -10.91 | 99.82       | 114.00   |
| 24  | BA    | 2498 | C    | P-O5'-C5'  | -10.91 | 103.45      | 120.90   |
| 21  | AA    | 246  | A    | P-O3'-C3'  | 10.90  | 132.78      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 24  | BA    | 858  | G    | N1-C6-O6   | -10.90 | 113.36      | 119.90   |
| 24  | BA    | 1072 | C    | N1-C1'-C2' | -10.90 | 99.83       | 114.00   |
| 24  | BA    | 1145 | C    | P-O3'-C3'  | -10.90 | 106.62      | 119.70   |
| 24  | BA    | 1539 | U    | N1-C1'-C2' | -10.89 | 99.85       | 114.00   |
| 25  | BB    | 88   | C    | P-O3'-C3'  | 10.88  | 132.76      | 119.70   |
| 24  | DA    | 444  | C    | N1-C1'-C2' | -10.88 | 99.85       | 114.00   |
| 24  | BA    | 621  | A    | P-O3'-C3'  | -10.88 | 106.64      | 119.70   |
| 24  | BA    | 1060 | U    | C5-C4-O4   | -10.88 | 119.37      | 125.90   |
| 24  | BA    | 1265 | A    | P-O3'-C3'  | 10.86  | 132.73      | 119.70   |
| 56  | DB    | 46   | A    | P-O3'-C3'  | -10.86 | 106.67      | 119.70   |
| 31  | BH    | 48   | GLU  | CB-CA-C    | -10.85 | 88.70       | 110.40   |
| 24  | DA    | 775  | G    | P-O3'-C3'  | 10.85  | 132.72      | 119.70   |
| 24  | BA    | 1330 | C    | N1-C1'-C2' | -10.84 | 99.90       | 114.00   |
| 24  | BA    | 2609 | U    | O4'-C1'-N1 | 10.84  | 116.87      | 108.20   |
| 24  | DA    | 2612 | C    | N1-C1'-C2' | -10.84 | 99.91       | 114.00   |
| 21  | AA    | 1259 | C    | N1-C1'-C2' | -10.83 | 99.92       | 114.00   |
| 21  | AA    | 373  | A    | P-O3'-C3'  | -10.81 | 106.73      | 119.70   |
| 21  | AA    | 969  | A    | P-O3'-C3'  | -10.81 | 106.73      | 119.70   |
| 24  | BA    | 2451 | A    | C8-N9-C4   | -10.81 | 101.48      | 105.80   |
| 55  | CA    | 1141 | C    | N1-C1'-C2' | -10.81 | 99.95       | 114.00   |
| 24  | BA    | 962  | G    | P-O3'-C3'  | -10.79 | 106.76      | 119.70   |
| 24  | DA    | 1400 | U    | N1-C1'-C2' | -10.79 | 99.98       | 114.00   |
| 24  | DA    | 1552 | A    | O4'-C1'-N9 | 10.78  | 116.82      | 108.20   |
| 24  | DA    | 1439 | A    | C5-C6-N1   | -10.77 | 112.31      | 117.70   |
| 24  | DA    | 1956 | U    | O4'-C1'-N1 | 10.77  | 116.81      | 108.20   |
| 24  | DA    | 2240 | U    | O4'-C1'-N1 | 10.77  | 116.81      | 108.20   |
| 24  | DA    | 1566 | A    | P-O3'-C3'  | 10.76  | 132.62      | 119.70   |
| 24  | BA    | 1865 | U    | C2-N3-C4   | -10.74 | 120.56      | 127.00   |
| 24  | BA    | 1758 | U    | P-O3'-C3'  | 10.73  | 132.58      | 119.70   |
| 24  | DA    | 1684 | G    | P-O3'-C3'  | -10.73 | 106.83      | 119.70   |
| 21  | AA    | 1161 | C    | O4'-C1'-N1 | 10.71  | 116.77      | 108.20   |
| 24  | DA    | 2728 | U    | O4'-C1'-N1 | 10.70  | 116.76      | 108.20   |
| 24  | DA    | 1967 | C    | N1-C1'-C2' | -10.69 | 100.10      | 114.00   |
| 24  | DA    | 1013 | C    | N1-C1'-C2' | -10.69 | 100.11      | 114.00   |
| 55  | CA    | 1202 | U    | N1-C1'-C2' | -10.68 | 100.11      | 114.00   |
| 24  | DA    | 1304 | A    | P-O3'-C3'  | -10.68 | 106.88      | 119.70   |
| 24  | DA    | 2586 | U    | P-O3'-C3'  | -10.68 | 106.89      | 119.70   |
| 24  | DA    | 1816 | C    | N1-C1'-C2' | -10.67 | 100.13      | 114.00   |
| 24  | DA    | 397  | U    | N1-C1'-C2' | -10.66 | 100.14      | 114.00   |
| 24  | BA    | 2681 | C    | P-O3'-C3'  | 10.66  | 132.49      | 119.70   |
| 24  | DA    | 1708 | C    | N1-C1'-C2' | -10.65 | 100.16      | 114.00   |
| 21  | AA    | 1170 | A    | P-O3'-C3'  | -10.65 | 106.92      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 24  | DA    | 2778 | A    | P-O3'-C3'  | 10.64  | 132.47      | 119.70   |
| 24  | DA    | 2314 | A    | P-O3'-C3'  | -10.63 | 106.94      | 119.70   |
| 55  | CA    | 1528 | U    | P-O3'-C3'  | 10.63  | 132.46      | 119.70   |
| 24  | BA    | 1126 | A    | P-O3'-C3'  | 10.62  | 132.44      | 119.70   |
| 24  | DA    | 622  | G    | P-O3'-C3'  | -10.61 | 106.97      | 119.70   |
| 21  | AA    | 1140 | C    | O4'-C1'-N1 | 10.60  | 116.68      | 108.20   |
| 24  | BA    | 1286 | A    | P-O3'-C3'  | 10.60  | 132.41      | 119.70   |
| 24  | BA    | 2428 | G    | P-O3'-C3'  | -10.59 | 106.99      | 119.70   |
| 24  | BA    | 491  | G    | P-O3'-C3'  | -10.58 | 107.01      | 119.70   |
| 24  | BA    | 1329 | U    | P-O3'-C3'  | 10.57  | 132.38      | 119.70   |
| 24  | DA    | 1126 | A    | P-O3'-C3'  | 10.57  | 132.39      | 119.70   |
| 21  | AA    | 1141 | C    | N1-C1'-C2' | -10.54 | 100.30      | 114.00   |
| 21  | AA    | 1203 | C    | N1-C1'-C2' | -10.54 | 100.30      | 114.00   |
| 24  | BA    | 2383 | G    | P-O3'-C3'  | -10.52 | 107.07      | 119.70   |
| 24  | DA    | 1648 | U    | N1-C1'-C2' | -10.52 | 100.33      | 114.00   |
| 24  | BA    | 2573 | C    | N1-C1'-C2' | -10.51 | 100.33      | 114.00   |
| 24  | BA    | 1178 | C    | O4'-C1'-N1 | 10.51  | 116.60      | 108.20   |
| 55  | CA    | 72   | A    | P-O3'-C3'  | -10.50 | 107.10      | 119.70   |
| 24  | BA    | 1717 | A    | P-O3'-C3'  | -10.50 | 107.10      | 119.70   |
| 24  | DA    | 421  | C    | P-O3'-C3'  | 10.49  | 132.29      | 119.70   |
| 24  | BA    | 687  | C    | N1-C1'-C2' | -10.48 | 100.38      | 114.00   |
| 24  | BA    | 1957 | C    | P-O3'-C3'  | -10.47 | 107.13      | 119.70   |
| 24  | BA    | 2214 | C    | N1-C1'-C2' | -10.47 | 100.39      | 114.00   |
| 55  | CA    | 1161 | C    | N1-C1'-C2' | -10.47 | 100.39      | 114.00   |
| 21  | AA    | 1283 | U    | N1-C1'-C2' | -10.46 | 100.40      | 114.00   |
| 55  | CA    | 97   | G    | P-O3'-C3'  | -10.46 | 107.15      | 119.70   |
| 21  | AA    | 1366 | C    | P-O3'-C3'  | -10.46 | 107.15      | 119.70   |
| 21  | AA    | 995  | C    | N1-C1'-C2' | -10.45 | 100.41      | 114.00   |
| 23  | AW    | 5    | U    | N1-C1'-C2' | -10.45 | 100.42      | 114.00   |
| 24  | DA    | 2267 | A    | N1-C6-N6   | 10.43  | 124.86      | 118.60   |
| 24  | BA    | 2333 | A    | P-O3'-C3'  | 10.42  | 132.21      | 119.70   |
| 24  | BA    | 2200 | C    | N1-C1'-C2' | -10.42 | 100.45      | 114.00   |
| 24  | DA    | 964  | C    | O4'-C1'-N1 | 10.41  | 116.53      | 108.20   |
| 55  | CA    | 970  | C    | P-O3'-C3'  | -10.41 | 107.21      | 119.70   |
| 24  | DA    | 1499 | C    | O4'-C1'-N1 | 10.41  | 116.53      | 108.20   |
| 24  | BA    | 100  | U    | P-O3'-C3'  | 10.41  | 132.19      | 119.70   |
| 24  | BA    | 781  | A    | P-O3'-C3'  | 10.41  | 132.19      | 119.70   |
| 24  | DA    | 321  | U    | O4'-C1'-N1 | 10.41  | 116.53      | 108.20   |
| 24  | DA    | 225  | C    | O4'-C1'-N1 | 10.40  | 116.52      | 108.20   |
| 24  | BA    | 726  | G    | P-O3'-C3'  | 10.40  | 132.18      | 119.70   |
| 55  | CA    | 501  | C    | O4'-C1'-N1 | 10.40  | 116.52      | 108.20   |
| 21  | AA    | 590  | U    | P-O3'-C3'  | -10.39 | 107.23      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 21  | AA    | 753  | A    | P-O3'-C3'  | 10.39  | 132.17      | 119.70   |
| 21  | AA    | 1202 | U    | N1-C1'-C2' | -10.39 | 100.49      | 114.00   |
| 24  | BA    | 164  | C    | N1-C1'-C2' | -10.39 | 100.49      | 114.00   |
| 24  | BA    | 730  | A    | P-O3'-C3'  | -10.39 | 107.23      | 119.70   |
| 24  | DA    | 2692 | G    | P-O3'-C3'  | -10.38 | 107.24      | 119.70   |
| 21  | AA    | 87   | C    | N1-C1'-C2' | -10.38 | 100.51      | 114.00   |
| 21  | AA    | 122  | G    | P-O3'-C3'  | -10.38 | 107.25      | 119.70   |
| 24  | DA    | 206  | U    | N1-C1'-C2' | -10.38 | 100.51      | 114.00   |
| 24  | BA    | 1490 | A    | P-O3'-C3'  | 10.36  | 132.14      | 119.70   |
| 24  | BA    | 92   | U    | N1-C1'-C2' | -10.36 | 100.53      | 114.00   |
| 24  | DA    | 2068 | U    | N1-C1'-C2' | -10.36 | 100.53      | 114.00   |
| 55  | CA    | 370  | C    | N1-C1'-C2' | -10.36 | 100.53      | 114.00   |
| 24  | BA    | 2326 | C    | P-O3'-C3'  | 10.36  | 132.13      | 119.70   |
| 55  | CA    | 723  | U    | P-O3'-C3'  | -10.36 | 107.27      | 119.70   |
| 24  | DA    | 436  | C    | O4'-C1'-N1 | 10.36  | 116.48      | 108.20   |
| 24  | DA    | 2261 | C    | P-O3'-C3'  | -10.34 | 107.29      | 119.70   |
| 55  | CA    | 643  | C    | N1-C1'-C2' | -10.34 | 100.56      | 114.00   |
| 24  | DA    | 2226 | C    | N1-C1'-C2' | -10.33 | 100.57      | 114.00   |
| 24  | DA    | 2611 | C    | N1-C1'-C2' | -10.33 | 100.57      | 114.00   |
| 24  | DA    | 2447 | G    | P-O3'-C3'  | 10.32  | 132.09      | 119.70   |
| 55  | CA    | 519  | C    | N1-C1'-C2' | -10.31 | 100.59      | 114.00   |
| 21  | AA    | 1449 | C    | N1-C1'-C2' | -10.31 | 100.60      | 114.00   |
| 55  | CA    | 283  | U    | N1-C1'-C2' | -10.31 | 100.60      | 114.00   |
| 21  | AA    | 547  | A    | P-O3'-C3'  | 10.31  | 132.07      | 119.70   |
| 24  | DA    | 1315 | C    | N1-C1'-C2' | -10.31 | 100.60      | 114.00   |
| 24  | BA    | 1556 | C    | N1-C1'-C2' | -10.30 | 100.61      | 114.00   |
| 24  | DA    | 1561 | C    | N1-C1'-C2' | -10.29 | 100.62      | 114.00   |
| 21  | AA    | 705  | G    | P-O3'-C3'  | -10.28 | 107.36      | 119.70   |
| 55  | CA    | 84   | U    | P-O3'-C3'  | 10.28  | 132.04      | 119.70   |
| 24  | BA    | 2336 | A    | P-O3'-C3'  | 10.27  | 132.03      | 119.70   |
| 24  | DA    | 1667 | G    | P-O3'-C3'  | 10.27  | 132.03      | 119.70   |
| 55  | CA    | 936  | C    | N1-C1'-C2' | -10.26 | 100.66      | 114.00   |
| 24  | DA    | 2064 | C    | N1-C1'-C2' | -10.25 | 100.67      | 114.00   |
| 24  | BA    | 2447 | G    | N1-C2-N3   | 10.25  | 130.05      | 123.90   |
| 24  | BA    | 302  | C    | O4'-C1'-N1 | 10.24  | 116.40      | 108.20   |
| 24  | BA    | 1810 | A    | P-O3'-C3'  | -10.24 | 107.41      | 119.70   |
| 55  | CA    | 501  | C    | N1-C1'-C2' | -10.24 | 100.69      | 114.00   |
| 21  | AA    | 60   | A    | P-O3'-C3'  | 10.23  | 131.98      | 119.70   |
| 21  | AA    | 995  | C    | P-O3'-C3'  | -10.23 | 107.42      | 119.70   |
| 24  | DA    | 2064 | C    | P-O3'-C3'  | -10.23 | 107.42      | 119.70   |
| 24  | DA    | 687  | C    | N1-C1'-C2' | -10.22 | 100.71      | 114.00   |
| 24  | DA    | 2214 | C    | N1-C1'-C2' | -10.22 | 100.71      | 114.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 24  | BA    | 500  | G    | C2-N3-C4   | -10.22 | 106.79      | 111.90   |
| 21  | AA    | 1196 | A    | P-O3'-C3'  | 10.22  | 131.96      | 119.70   |
| 24  | DA    | 234  | U    | O4'-C1'-N1 | 10.21  | 116.37      | 108.20   |
| 55  | CA    | 1170 | A    | P-O3'-C3'  | -10.20 | 107.47      | 119.70   |
| 24  | BA    | 1478 | G    | N3-C4-N9   | -10.19 | 119.88      | 126.00   |
| 24  | BA    | 630  | G    | C2-N3-C4   | -10.18 | 106.81      | 111.90   |
| 55  | CA    | 508  | U    | P-O3'-C3'  | 10.18  | 131.92      | 119.70   |
| 55  | CA    | 1203 | C    | N1-C1'-C2' | -10.18 | 100.77      | 114.00   |
| 24  | BA    | 2880 | C    | P-O3'-C3'  | -10.18 | 107.49      | 119.70   |
| 24  | DA    | 53   | A    | P-O3'-C3'  | -10.18 | 107.49      | 119.70   |
| 24  | DA    | 792  | A    | P-O3'-C3'  | 10.18  | 131.91      | 119.70   |
| 24  | DA    | 1049 | C    | N1-C1'-C2' | -10.16 | 100.79      | 114.00   |
| 24  | BA    | 2451 | A    | C5-C6-N1   | 10.15  | 122.78      | 117.70   |
| 55  | CA    | 735  | C    | P-O3'-C3'  | -10.15 | 107.52      | 119.70   |
| 24  | BA    | 2210 | U    | P-O3'-C3'  | 10.15  | 131.88      | 119.70   |
| 24  | BA    | 2880 | C    | N1-C1'-C2' | -10.15 | 100.81      | 114.00   |
| 55  | CA    | 96   | U    | N1-C1'-C2' | -10.14 | 100.81      | 114.00   |
| 55  | CA    | 248  | C    | N1-C1'-C2' | -10.14 | 100.82      | 114.00   |
| 24  | BA    | 86   | G    | P-O3'-C3'  | -10.12 | 107.55      | 119.70   |
| 24  | BA    | 1511 | G    | P-O3'-C3'  | -10.11 | 107.57      | 119.70   |
| 55  | CA    | 347  | G    | P-O3'-C3'  | -10.11 | 107.57      | 119.70   |
| 24  | DA    | 1957 | C    | P-O3'-C3'  | -10.11 | 107.57      | 119.70   |
| 24  | DA    | 2064 | C    | O4'-C1'-N1 | 10.11  | 116.28      | 108.20   |
| 24  | BA    | 1732 | C    | P-O3'-C3'  | 10.10  | 131.82      | 119.70   |
| 24  | BA    | 142  | A    | P-O3'-C3'  | -10.10 | 107.58      | 119.70   |
| 24  | BA    | 548  | G    | P-O3'-C3'  | -10.09 | 107.59      | 119.70   |
| 24  | DA    | 548  | G    | P-O3'-C3'  | -10.09 | 107.59      | 119.70   |
| 55  | CA    | 1052 | U    | N1-C1'-C2' | -10.09 | 100.89      | 114.00   |
| 24  | DA    | 1114 | C    | N1-C1'-C2' | -10.08 | 100.90      | 114.00   |
| 21  | AA    | 1366 | C    | N1-C1'-C2' | -10.07 | 100.90      | 114.00   |
| 24  | DA    | 2581 | G    | P-O3'-C3'  | 10.06  | 131.77      | 119.70   |
| 24  | BA    | 1475 | G    | P-O3'-C3'  | 10.06  | 131.77      | 119.70   |
| 24  | BA    | 2266 | A    | P-O3'-C3'  | 10.05  | 131.76      | 119.70   |
| 24  | DA    | 459  | U    | N1-C1'-C2' | -10.05 | 100.93      | 114.00   |
| 24  | DA    | 2440 | C    | N1-C1'-C2' | -10.05 | 100.94      | 114.00   |
| 55  | CA    | 874  | G    | P-O3'-C3'  | -10.03 | 107.67      | 119.70   |
| 24  | DA    | 997  | G    | P-O3'-C3'  | -10.03 | 107.67      | 119.70   |
| 24  | BA    | 2645 | G    | P-O3'-C3'  | 10.02  | 131.72      | 119.70   |
| 24  | DA    | 445  | C    | N1-C1'-C2' | -10.01 | 100.99      | 114.00   |
| 55  | CA    | 454  | G    | P-O3'-C3'  | -10.00 | 107.70      | 119.70   |
| 24  | BA    | 279  | A    | P-O3'-C3'  | -10.00 | 107.70      | 119.70   |
| 24  | BA    | 404  | A    | P-O3'-C3'  | 9.99   | 131.69      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | DA    | 2023 | C    | N1-C1'-C2' | -9.99 | 101.01      | 112.00   |
| 21  | AA    | 655  | A    | P-O3'-C3'  | -9.98 | 107.73      | 119.70   |
| 24  | BA    | 482  | A    | P-O3'-C3'  | -9.96 | 107.74      | 119.70   |
| 24  | BA    | 752  | A    | P-O3'-C3'  | 9.96  | 131.65      | 119.70   |
| 24  | DA    | 273  | G    | P-O3'-C3'  | -9.96 | 107.75      | 119.70   |
| 24  | BA    | 1276 | A    | P-O3'-C3'  | -9.95 | 107.76      | 119.70   |
| 55  | CA    | 1508 | A    | P-O3'-C3'  | -9.95 | 107.77      | 119.70   |
| 24  | BA    | 369  | U    | P-O3'-C3'  | 9.94  | 131.63      | 119.70   |
| 24  | BA    | 2732 | G    | P-O3'-C3'  | 9.94  | 131.63      | 119.70   |
| 24  | BA    | 2712 | C    | N1-C1'-C2' | 9.94  | 126.92      | 114.00   |
| 55  | CA    | 132  | C    | O4'-C1'-N1 | 9.94  | 116.15      | 108.20   |
| 24  | DA    | 179  | C    | N1-C1'-C2' | -9.93 | 101.07      | 112.00   |
| 55  | CA    | 892  | A    | P-O3'-C3'  | -9.93 | 107.79      | 119.70   |
| 24  | BA    | 2226 | C    | N1-C1'-C2' | -9.92 | 101.08      | 112.00   |
| 24  | BA    | 301  | G    | P-O3'-C3'  | 9.92  | 131.60      | 119.70   |
| 21  | AA    | 549  | C    | N1-C1'-C2' | -9.92 | 101.09      | 112.00   |
| 24  | DA    | 915  | C    | N1-C1'-C2' | -9.91 | 101.10      | 112.00   |
| 24  | BA    | 479  | A    | P-O3'-C3'  | 9.91  | 131.59      | 119.70   |
| 24  | DA    | 1265 | A    | P-O3'-C3'  | 9.90  | 131.58      | 119.70   |
| 25  | BB    | 52   | A    | P-O3'-C3'  | 9.89  | 131.57      | 119.70   |
| 55  | CA    | 14   | U    | N1-C1'-C2' | -9.89 | 101.12      | 112.00   |
| 24  | DA    | 831  | G    | P-O3'-C3'  | -9.89 | 107.83      | 119.70   |
| 24  | BA    | 1865 | U    | O4'-C1'-N1 | 9.88  | 116.10      | 108.20   |
| 24  | DA    | 229  | C    | N1-C1'-C2' | -9.87 | 101.14      | 112.00   |
| 24  | DA    | 2758 | A    | P-O3'-C3'  | -9.86 | 107.86      | 119.70   |
| 24  | DA    | 2339 | C    | O4'-C1'-N1 | 9.86  | 116.09      | 108.20   |
| 21  | AA    | 1192 | C    | N1-C1'-C2' | -9.84 | 101.17      | 112.00   |
| 55  | CA    | 1455 | G    | P-O3'-C3'  | -9.84 | 107.89      | 119.70   |
| 24  | DA    | 1819 | A    | P-O3'-C3'  | 9.84  | 131.50      | 119.70   |
| 24  | DA    | 860  | U    | N1-C1'-C2' | -9.82 | 101.20      | 112.00   |
| 24  | BA    | 507  | A    | P-O3'-C3'  | -9.82 | 107.92      | 119.70   |
| 24  | DA    | 392  | U    | P-O3'-C3'  | -9.81 | 107.92      | 119.70   |
| 24  | DA    | 2215 | C    | P-O3'-C3'  | -9.81 | 107.92      | 119.70   |
| 25  | BB    | 87   | U    | P-O3'-C3'  | 9.81  | 131.47      | 119.70   |
| 24  | DA    | 916  | G    | P-O3'-C3'  | -9.81 | 107.93      | 119.70   |
| 24  | DA    | 2347 | C    | N1-C1'-C2' | -9.81 | 101.21      | 112.00   |
| 55  | CA    | 67   | C    | N1-C1'-C2' | -9.81 | 101.21      | 112.00   |
| 55  | CA    | 32   | A    | P-O3'-C3'  | -9.80 | 107.93      | 119.70   |
| 55  | CA    | 565  | U    | P-O3'-C3'  | -9.80 | 107.94      | 119.70   |
| 21  | AA    | 306  | A    | P-O3'-C3'  | -9.78 | 107.97      | 119.70   |
| 24  | DA    | 1035 | U    | P-O3'-C3'  | -9.78 | 107.97      | 119.70   |
| 24  | DA    | 2615 | U    | N1-C1'-C2' | -9.78 | 101.25      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 55  | CA    | 510  | A    | P-O3'-C3'  | -9.77 | 107.97      | 119.70   |
| 24  | DA    | 2568 | U    | P-O3'-C3'  | -9.77 | 107.97      | 119.70   |
| 21  | AA    | 577  | G    | P-O3'-C3'  | -9.77 | 107.98      | 119.70   |
| 21  | AA    | 1502 | A    | P-O3'-C3'  | 9.77  | 131.42      | 119.70   |
| 24  | DA    | 1387 | A    | P-O3'-C3'  | -9.76 | 107.99      | 119.70   |
| 24  | DA    | 2408 | U    | N1-C1'-C2' | -9.75 | 101.27      | 112.00   |
| 55  | CA    | 1325 | C    | P-O3'-C3'  | -9.74 | 108.01      | 119.70   |
| 24  | BA    | 2613 | U    | P-O3'-C3'  | 9.74  | 131.39      | 119.70   |
| 24  | BA    | 2902 | C    | O4'-C1'-N1 | 9.74  | 115.99      | 108.20   |
| 24  | DA    | 1476 | U    | O4'-C1'-N1 | 9.74  | 115.99      | 108.20   |
| 21  | AA    | 1241 | G    | P-O3'-C3'  | -9.74 | 108.02      | 119.70   |
| 24  | DA    | 2798 | U    | P-O3'-C3'  | 9.73  | 131.38      | 119.70   |
| 24  | BA    | 227  | A    | P-O3'-C3'  | 9.73  | 131.37      | 119.70   |
| 55  | CA    | 890  | G    | P-O3'-C3'  | 9.73  | 131.37      | 119.70   |
| 24  | BA    | 1156 | A    | P-O3'-C3'  | 9.72  | 131.37      | 119.70   |
| 24  | DA    | 1475 | G    | P-O3'-C3'  | 9.72  | 131.37      | 119.70   |
| 21  | AA    | 467  | U    | N1-C1'-C2' | -9.71 | 101.32      | 112.00   |
| 24  | DA    | 1119 | U    | O4'-C1'-N1 | 9.70  | 115.96      | 108.20   |
| 24  | BA    | 2835 | A    | P-O3'-C3'  | 9.70  | 131.34      | 119.70   |
| 24  | DA    | 790  | U    | O4'-C1'-N1 | 9.69  | 115.95      | 108.20   |
| 24  | DA    | 1137 | G    | P-O3'-C3'  | -9.69 | 108.07      | 119.70   |
| 24  | DA    | 1345 | C    | N1-C1'-C2' | -9.69 | 101.34      | 112.00   |
| 21  | AA    | 422  | C    | O4'-C1'-N1 | 9.68  | 115.95      | 108.20   |
| 55  | CA    | 822  | U    | N1-C1'-C2' | -9.68 | 101.35      | 112.00   |
| 24  | BA    | 2893 | A    | P-O3'-C3'  | 9.68  | 131.31      | 119.70   |
| 24  | BA    | 865  | C    | P-O3'-C3'  | 9.67  | 131.31      | 119.70   |
| 24  | DA    | 2267 | A    | C5-C6-N6   | -9.67 | 115.97      | 123.70   |
| 24  | BA    | 229  | C    | N1-C1'-C2' | -9.66 | 101.37      | 112.00   |
| 24  | DA    | 364  | C    | P-O3'-C3'  | -9.66 | 108.10      | 119.70   |
| 24  | DA    | 179  | C    | O4'-C1'-N1 | 9.66  | 115.92      | 108.20   |
| 24  | DA    | 1399 | C    | N1-C1'-C2' | -9.66 | 101.38      | 112.00   |
| 24  | DA    | 2572 | A    | P-O3'-C3'  | 9.66  | 131.29      | 119.70   |
| 21  | AA    | 812  | G    | P-O3'-C3'  | 9.65  | 131.28      | 119.70   |
| 21  | AA    | 967  | C    | P-O3'-C3'  | -9.65 | 108.12      | 119.70   |
| 24  | BA    | 1236 | G    | P-O3'-C3'  | 9.65  | 131.28      | 119.70   |
| 24  | DA    | 1982 | U    | N1-C1'-C2' | -9.65 | 101.38      | 112.00   |
| 24  | BA    | 1498 | C    | N1-C1'-C2' | -9.65 | 101.39      | 112.00   |
| 24  | DA    | 2868 | A    | P-O3'-C3'  | -9.64 | 108.13      | 119.70   |
| 55  | CA    | 1397 | C    | N1-C1'-C2' | -9.64 | 101.39      | 112.00   |
| 24  | DA    | 1020 | A    | P-O3'-C3'  | 9.64  | 131.27      | 119.70   |
| 24  | BA    | 459  | U    | N1-C1'-C2' | -9.63 | 101.40      | 112.00   |
| 24  | DA    | 2094 | A    | P-O3'-C3'  | -9.63 | 108.14      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | DA    | 766  | U    | N1-C1'-C2' | -9.63 | 101.41      | 112.00   |
| 24  | DA    | 217  | A    | P-O3'-C3'  | -9.62 | 108.16      | 119.70   |
| 24  | BA    | 2384 | U    | P-O3'-C3'  | 9.62  | 131.24      | 119.70   |
| 55  | CA    | 876  | C    | P-O3'-C3'  | -9.60 | 108.18      | 119.70   |
| 56  | DB    | 104  | A    | P-O3'-C3'  | -9.59 | 108.19      | 119.70   |
| 21  | AA    | 875  | U    | O4'-C1'-N1 | 9.59  | 115.87      | 108.20   |
| 24  | BA    | 1045 | C    | P-O3'-C3'  | 9.59  | 131.21      | 119.70   |
| 21  | AA    | 316  | C    | N1-C1'-C2' | -9.58 | 101.47      | 112.00   |
| 24  | BA    | 125  | A    | P-O3'-C3'  | 9.58  | 131.19      | 119.70   |
| 24  | DA    | 688  | U    | N1-C1'-C2' | -9.57 | 101.47      | 112.00   |
| 24  | DA    | 2136 | G    | P-O3'-C3'  | -9.57 | 108.22      | 119.70   |
| 24  | DA    | 589  | U    | N1-C1'-C2' | -9.57 | 101.47      | 112.00   |
| 24  | DA    | 2348 | U    | O4'-C1'-N1 | 9.57  | 115.85      | 108.20   |
| 24  | DA    | 1456 | G    | P-O3'-C3'  | -9.56 | 108.23      | 119.70   |
| 24  | BA    | 1828 | G    | P-O3'-C3'  | 9.56  | 131.17      | 119.70   |
| 24  | BA    | 2199 | A    | P-O3'-C3'  | -9.56 | 108.23      | 119.70   |
| 55  | CA    | 252  | U    | N1-C1'-C2' | -9.56 | 101.49      | 112.00   |
| 21  | AA    | 438  | U    | O4'-C1'-N1 | 9.55  | 115.84      | 108.20   |
| 21  | AA    | 487  | A    | P-O3'-C3'  | -9.55 | 108.23      | 119.70   |
| 24  | DA    | 413  | C    | P-O3'-C3'  | -9.55 | 108.24      | 119.70   |
| 55  | CA    | 344  | A    | P-O3'-C3'  | 9.54  | 131.15      | 119.70   |
| 24  | DA    | 2338 | C    | O4'-C1'-N1 | 9.54  | 115.83      | 108.20   |
| 24  | DA    | 1214 | A    | P-O3'-C3'  | -9.54 | 108.25      | 119.70   |
| 21  | AA    | 132  | C    | N1-C1'-C2' | -9.53 | 101.52      | 112.00   |
| 24  | DA    | 335  | C    | N1-C1'-C2' | -9.53 | 101.52      | 112.00   |
| 55  | CA    | 564  | C    | P-O3'-C3'  | -9.52 | 108.28      | 119.70   |
| 24  | DA    | 688  | U    | P-O3'-C3'  | -9.52 | 108.28      | 119.70   |
| 24  | DA    | 142  | A    | P-O3'-C3'  | -9.51 | 108.29      | 119.70   |
| 55  | CA    | 87   | C    | N1-C1'-C2' | -9.50 | 101.55      | 112.00   |
| 21  | AA    | 530  | G    | P-O3'-C3'  | 9.50  | 131.10      | 119.70   |
| 24  | DA    | 2498 | C    | N1-C1'-C2' | -9.50 | 101.55      | 112.00   |
| 21  | AA    | 961  | U    | N1-C1'-C2' | -9.49 | 101.56      | 112.00   |
| 24  | BA    | 861  | A    | P-O3'-C3'  | -9.49 | 108.31      | 119.70   |
| 24  | DA    | 527  | C    | O4'-C1'-N1 | 9.48  | 115.79      | 108.20   |
| 24  | DA    | 1249 | U    | N1-C1'-C2' | -9.48 | 101.57      | 112.00   |
| 24  | DA    | 1708 | C    | P-O3'-C3'  | -9.48 | 108.33      | 119.70   |
| 24  | DA    | 2875 | C    | N1-C1'-C2' | -9.48 | 101.57      | 112.00   |
| 21  | AA    | 199  | A    | P-O3'-C3'  | -9.47 | 108.33      | 119.70   |
| 24  | DA    | 1498 | C    | N1-C1'-C2' | -9.47 | 101.58      | 112.00   |
| 24  | BA    | 1700 | A    | P-O3'-C3'  | -9.47 | 108.34      | 119.70   |
| 55  | CA    | 1142 | G    | P-O3'-C3'  | -9.46 | 108.34      | 119.70   |
| 24  | DA    | 1810 | A    | P-O3'-C3'  | -9.47 | 108.34      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 55  | CA    | 276  | G    | P-O3'-C3'  | -9.46 | 108.35      | 119.70   |
| 55  | CA    | 721  | G    | P-O3'-C3'  | 9.46  | 131.05      | 119.70   |
| 21  | AA    | 1283 | U    | P-O3'-C3'  | -9.45 | 108.36      | 119.70   |
| 24  | DA    | 2657 | A    | P-O3'-C3'  | -9.45 | 108.36      | 119.70   |
| 24  | BA    | 669  | G    | P-O3'-C3'  | 9.45  | 131.03      | 119.70   |
| 24  | BA    | 1635 | A    | P-O3'-C3'  | -9.45 | 108.36      | 119.70   |
| 21  | AA    | 480  | U    | O4'-C1'-N1 | 9.44  | 115.75      | 108.20   |
| 55  | CA    | 735  | C    | N1-C1'-C2' | -9.44 | 101.62      | 112.00   |
| 24  | BA    | 2860 | A    | N1-C6-N6   | 9.43  | 124.26      | 118.60   |
| 24  | BA    | 620  | G    | P-O3'-C3'  | 9.43  | 131.01      | 119.70   |
| 24  | DA    | 243  | U    | N1-C1'-C2' | -9.42 | 101.64      | 112.00   |
| 24  | DA    | 2497 | A    | P-O3'-C3'  | 9.41  | 130.99      | 119.70   |
| 24  | BA    | 914  | G    | P-O3'-C3'  | -9.41 | 108.41      | 119.70   |
| 24  | DA    | 1980 | G    | P-O3'-C3'  | 9.40  | 130.99      | 119.70   |
| 24  | BA    | 2258 | C    | P-O3'-C3'  | 9.40  | 130.98      | 119.70   |
| 24  | DA    | 1290 | C    | N1-C1'-C2' | -9.40 | 101.66      | 112.00   |
| 24  | DA    | 2493 | U    | P-O3'-C3'  | -9.39 | 108.43      | 119.70   |
| 24  | DA    | 1636 | U    | P-O3'-C3'  | -9.39 | 108.44      | 119.70   |
| 24  | DA    | 741  | U    | O4'-C1'-N1 | 9.38  | 115.71      | 108.20   |
| 24  | DA    | 1072 | C    | N1-C1'-C2' | -9.38 | 101.68      | 112.00   |
| 24  | DA    | 1607 | C    | P-O3'-C3'  | 9.38  | 130.95      | 119.70   |
| 24  | BA    | 2832 | U    | P-O3'-C3'  | 9.37  | 130.95      | 119.70   |
| 24  | BA    | 1082 | U    | O4'-C1'-N1 | 9.37  | 115.69      | 108.20   |
| 24  | BA    | 2725 | A    | P-O3'-C3'  | 9.37  | 130.94      | 119.70   |
| 24  | BA    | 91   | A    | P-O3'-C3'  | 9.36  | 130.93      | 119.70   |
| 21  | AA    | 243  | A    | P-O3'-C3'  | 9.36  | 130.93      | 119.70   |
| 55  | CA    | 1508 | A    | P-O5'-C5'  | -9.36 | 105.93      | 120.90   |
| 24  | DA    | 1131 | G    | P-O3'-C3'  | 9.36  | 130.93      | 119.70   |
| 21  | AA    | 792  | A    | P-O3'-C3'  | 9.36  | 130.93      | 119.70   |
| 24  | DA    | 1400 | U    | P-O3'-C3'  | -9.36 | 108.47      | 119.70   |
| 24  | DA    | 104  | A    | P-O3'-C3'  | -9.35 | 108.48      | 119.70   |
| 24  | DA    | 1867 | G    | P-O3'-C3'  | -9.34 | 108.49      | 119.70   |
| 24  | BA    | 790  | U    | N1-C1'-C2' | -9.34 | 101.72      | 112.00   |
| 24  | DA    | 658  | U    | O4'-C1'-N1 | 9.34  | 115.67      | 108.20   |
| 24  | BA    | 2820 | A    | P-O3'-C3'  | 9.34  | 130.90      | 119.70   |
| 24  | DA    | 1050 | A    | P-O3'-C3'  | -9.33 | 108.50      | 119.70   |
| 55  | CA    | 931  | C    | O4'-C1'-N1 | 9.32  | 115.66      | 108.20   |
| 24  | BA    | 460  | A    | P-O3'-C3'  | -9.32 | 108.51      | 119.70   |
| 24  | BA    | 2682 | A    | P-O3'-C3'  | -9.32 | 108.52      | 119.70   |
| 24  | DA    | 164  | C    | N1-C1'-C2' | -9.31 | 101.76      | 112.00   |
| 21  | AA    | 73   | C    | P-O3'-C3'  | -9.31 | 108.53      | 119.70   |
| 24  | BA    | 49   | A    | P-O3'-C3'  | 9.31  | 130.87      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | BA    | 2296 | U    | N1-C1'-C2' | 9.31  | 126.10      | 114.00   |
| 25  | BB    | 42   | C    | N1-C1'-C2' | -9.31 | 101.76      | 112.00   |
| 24  | BA    | 788  | A    | P-O3'-C3'  | 9.30  | 130.86      | 119.70   |
| 55  | CA    | 169  | C    | O4'-C1'-N1 | 9.30  | 115.64      | 108.20   |
| 24  | BA    | 1378 | A    | P-O3'-C3'  | 9.30  | 130.86      | 119.70   |
| 24  | BA    | 527  | C    | P-O3'-C3'  | 9.29  | 130.85      | 119.70   |
| 55  | CA    | 535  | A    | P-O3'-C3'  | -9.29 | 108.55      | 119.70   |
| 24  | BA    | 1716 | U    | N1-C1'-C2' | -9.28 | 101.79      | 112.00   |
| 55  | CA    | 95   | C    | N1-C1'-C2' | -9.28 | 101.79      | 112.00   |
| 24  | BA    | 1127 | A    | P-O3'-C3'  | -9.28 | 108.57      | 119.70   |
| 21  | AA    | 51   | A    | P-O3'-C3'  | 9.27  | 130.83      | 119.70   |
| 24  | BA    | 2451 | A    | C4-C5-N7   | 9.27  | 115.33      | 110.70   |
| 24  | BA    | 2423 | U    | P-O3'-C3'  | 9.27  | 130.82      | 119.70   |
| 24  | DA    | 730  | A    | P-O3'-C3'  | -9.27 | 108.58      | 119.70   |
| 24  | DA    | 2313 | C    | N1-C1'-C2' | -9.27 | 101.80      | 112.00   |
| 55  | CA    | 1398 | A    | N9-C1'-C2' | -9.27 | 101.81      | 112.00   |
| 24  | BA    | 1158 | C    | P-O3'-C3'  | -9.26 | 108.58      | 119.70   |
| 55  | CA    | 822  | U    | P-O3'-C3'  | -9.26 | 108.58      | 119.70   |
| 24  | BA    | 2857 | G    | N9-C4-C5   | -9.26 | 101.70      | 105.40   |
| 24  | BA    | 2728 | U    | P-O3'-C3'  | -9.25 | 108.59      | 119.70   |
| 55  | CA    | 175  | C    | P-O3'-C3'  | -9.25 | 108.60      | 119.70   |
| 21  | AA    | 1528 | U    | P-O3'-C3'  | 9.25  | 130.80      | 119.70   |
| 24  | DA    | 2334 | U    | P-O3'-C3'  | 9.25  | 130.80      | 119.70   |
| 24  | DA    | 945  | A    | P-O3'-C3'  | 9.24  | 130.79      | 119.70   |
| 24  | DA    | 1080 | A    | P-O3'-C3'  | -9.23 | 108.62      | 119.70   |
| 24  | DA    | 2339 | C    | P-O3'-C3'  | -9.23 | 108.62      | 119.70   |
| 55  | CA    | 184  | G    | P-O3'-C3'  | -9.23 | 108.63      | 119.70   |
| 24  | BA    | 1345 | C    | N1-C1'-C2' | -9.22 | 101.85      | 112.00   |
| 55  | CA    | 1245 | C    | O4'-C1'-N1 | 9.22  | 115.58      | 108.20   |
| 56  | DB    | 17   | C    | O4'-C1'-N1 | 9.22  | 115.58      | 108.20   |
| 24  | BA    | 512  | G    | O4'-C1'-N9 | 9.22  | 115.58      | 108.20   |
| 21  | AA    | 486  | U    | N1-C1'-C2' | -9.21 | 101.87      | 112.00   |
| 24  | BA    | 984  | A    | P-O3'-C3'  | 9.21  | 130.75      | 119.70   |
| 24  | BA    | 2689 | U    | O4'-C1'-N1 | 9.20  | 115.56      | 108.20   |
| 24  | BA    | 1345 | C    | P-O3'-C3'  | -9.19 | 108.67      | 119.70   |
| 24  | DA    | 1019 | U    | O4'-C1'-N1 | 9.19  | 115.56      | 108.20   |
| 24  | DA    | 1815 | A    | P-O3'-C3'  | 9.19  | 130.73      | 119.70   |
| 24  | BA    | 1272 | A    | P-O3'-C3'  | 9.18  | 130.72      | 119.70   |
| 21  | AA    | 704  | A    | P-O3'-C3'  | -9.18 | 108.69      | 119.70   |
| 55  | CA    | 110  | C    | N1-C1'-C2' | -9.18 | 101.91      | 112.00   |
| 25  | BB    | 66   | A    | P-O3'-C3'  | 9.17  | 130.71      | 119.70   |
| 24  | DA    | 2409 | G    | P-O3'-C3'  | -9.17 | 108.70      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25  | BB    | 91   | C    | P-O3'-C3'  | -9.16 | 108.70      | 119.70   |
| 24  | DA    | 1289 | C    | N1-C1'-C2' | -9.16 | 101.92      | 112.00   |
| 55  | CA    | 1398 | A    | P-O3'-C3'  | -9.16 | 108.70      | 119.70   |
| 24  | DA    | 1971 | U    | N1-C1'-C2' | -9.16 | 101.93      | 112.00   |
| 24  | BA    | 1799 | G    | P-O3'-C3'  | 9.15  | 130.68      | 119.70   |
| 55  | CA    | 1161 | C    | O4'-C1'-N1 | 9.15  | 115.52      | 108.20   |
| 25  | BB    | 13   | G    | P-O3'-C3'  | -9.15 | 108.72      | 119.70   |
| 24  | BA    | 829  | A    | P-O3'-C3'  | 9.15  | 130.68      | 119.70   |
| 24  | DA    | 1708 | C    | O4'-C1'-N1 | 9.14  | 115.52      | 108.20   |
| 24  | BA    | 2586 | U    | N1-C1'-C2' | -9.14 | 101.94      | 112.00   |
| 21  | AA    | 73   | C    | N1-C1'-C2' | -9.14 | 101.95      | 112.00   |
| 24  | BA    | 1784 | A    | P-O3'-C3'  | 9.14  | 130.66      | 119.70   |
| 24  | DA    | 424  | G    | P-O3'-C3'  | -9.13 | 108.74      | 119.70   |
| 21  | AA    | 245  | U    | N1-C1'-C2' | -9.13 | 101.95      | 112.00   |
| 24  | BA    | 2520 | C    | N1-C1'-C2' | -9.13 | 101.96      | 112.00   |
| 24  | BA    | 2689 | U    | N1-C1'-C2' | 9.12  | 125.86      | 114.00   |
| 24  | BA    | 1569 | A    | P-O3'-C3'  | -9.12 | 108.76      | 119.70   |
| 55  | CA    | 1240 | U    | P-O3'-C3'  | 9.12  | 130.64      | 119.70   |
| 24  | DA    | 437  | U    | O4'-C1'-N1 | 9.12  | 115.49      | 108.20   |
| 24  | DA    | 2298 | A    | P-O3'-C3'  | -9.11 | 108.76      | 119.70   |
| 24  | DA    | 2198 | A    | P-O3'-C3'  | 9.11  | 130.63      | 119.70   |
| 55  | CA    | 486  | U    | P-O3'-C3'  | -9.10 | 108.78      | 119.70   |
| 55  | CA    | 1380 | U    | P-O3'-C3'  | 9.10  | 130.62      | 119.70   |
| 55  | CA    | 984  | C    | O4'-C1'-N1 | 9.10  | 115.48      | 108.20   |
| 24  | DA    | 483  | A    | P-O3'-C3'  | -9.10 | 108.78      | 119.70   |
| 24  | BA    | 915  | C    | N1-C1'-C2' | -9.09 | 102.00      | 112.00   |
| 24  | BA    | 1993 | U    | P-O5'-C5'  | -9.09 | 106.36      | 120.90   |
| 24  | BA    | 2500 | U    | O4'-C1'-N1 | 9.09  | 115.47      | 108.20   |
| 55  | CA    | 453  | G    | P-O3'-C3'  | -9.08 | 108.80      | 119.70   |
| 24  | BA    | 1385 | A    | P-O3'-C3'  | 9.08  | 130.59      | 119.70   |
| 24  | BA    | 2052 | A    | P-O3'-C3'  | -9.07 | 108.81      | 119.70   |
| 24  | DA    | 1822 | C    | N1-C1'-C2' | -9.07 | 102.02      | 112.00   |
| 24  | BA    | 753  | A    | P-O3'-C3'  | -9.07 | 108.82      | 119.70   |
| 24  | DA    | 77   | G    | P-O3'-C3'  | -9.06 | 108.83      | 119.70   |
| 24  | DA    | 2215 | C    | N1-C1'-C2' | -9.06 | 102.03      | 112.00   |
| 21  | AA    | 1066 | C    | P-O3'-C3'  | -9.06 | 108.83      | 119.70   |
| 24  | BA    | 1427 | A    | P-O3'-C3'  | 9.06  | 130.57      | 119.70   |
| 24  | BA    | 2451 | A    | C4-C5-C6   | -9.06 | 112.47      | 117.00   |
| 55  | CA    | 173  | U    | O4'-C1'-N1 | 9.05  | 115.44      | 108.20   |
| 55  | CA    | 1300 | G    | P-O3'-C3'  | -9.05 | 108.84      | 119.70   |
| 24  | BA    | 1706 | C    | P-O3'-C3'  | 9.05  | 130.56      | 119.70   |
| 21  | AA    | 564  | C    | P-O3'-C3'  | -9.04 | 108.85      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | BA    | 913  | U    | P-O3'-C3'  | 9.04  | 130.54      | 119.70   |
| 55  | CA    | 688  | G    | P-O3'-C3'  | -9.03 | 108.86      | 119.70   |
| 24  | DA    | 1158 | C    | N1-C1'-C2' | -9.03 | 102.07      | 112.00   |
| 21  | AA    | 331  | G    | P-O3'-C3'  | -9.03 | 108.87      | 119.70   |
| 24  | DA    | 73   | A    | P-O3'-C3'  | -9.02 | 108.87      | 119.70   |
| 21  | AA    | 719  | C    | P-O3'-C3'  | -9.02 | 108.88      | 119.70   |
| 24  | DA    | 739  | A    | P-O3'-C3'  | 9.02  | 130.53      | 119.70   |
| 55  | CA    | 1031 | C    | P-O3'-C3'  | 9.02  | 130.52      | 119.70   |
| 55  | CA    | 1395 | C    | N1-C1'-C2' | -9.02 | 102.08      | 112.00   |
| 24  | BA    | 1082 | U    | C5-C4-O4   | -9.02 | 120.49      | 125.90   |
| 24  | BA    | 1566 | A    | P-O3'-C3'  | 9.02  | 130.52      | 119.70   |
| 55  | CA    | 1203 | C    | P-O3'-C3'  | -9.02 | 108.88      | 119.70   |
| 24  | DA    | 867  | C    | N1-C1'-C2' | -9.02 | 102.08      | 112.00   |
| 24  | DA    | 1957 | C    | N1-C1'-C2' | -9.01 | 102.09      | 112.00   |
| 24  | BA    | 747  | U    | N1-C1'-C2' | -9.00 | 102.10      | 112.00   |
| 55  | CA    | 1190 | G    | P-O3'-C3'  | 8.99  | 130.49      | 119.70   |
| 24  | DA    | 1060 | U    | N3-C4-O4   | 8.99  | 125.69      | 119.40   |
| 24  | BA    | 2468 | A    | P-O3'-C3'  | 8.99  | 130.49      | 119.70   |
| 24  | BA    | 1275 | A    | P-O3'-C3'  | 8.99  | 130.48      | 119.70   |
| 24  | DA    | 207  | A    | P-O3'-C3'  | -8.98 | 108.92      | 119.70   |
| 55  | CA    | 133  | U    | P-O3'-C3'  | -8.98 | 108.92      | 119.70   |
| 24  | BA    | 2588 | G    | P-O3'-C3'  | 8.97  | 130.47      | 119.70   |
| 24  | DA    | 976  | G    | P-O3'-C3'  | -8.97 | 108.93      | 119.70   |
| 24  | DA    | 397  | U    | P-O3'-C3'  | -8.97 | 108.94      | 119.70   |
| 24  | BA    | 243  | U    | N1-C1'-C2' | -8.96 | 102.14      | 112.00   |
| 24  | BA    | 2425 | A    | O4'-C1'-N9 | 8.96  | 115.37      | 108.20   |
| 24  | BA    | 2503 | A    | P-O3'-C3'  | 8.96  | 130.45      | 119.70   |
| 24  | BA    | 2609 | U    | P-O3'-C3'  | 8.95  | 130.44      | 119.70   |
| 24  | DA    | 1023 | U    | P-O5'-C5'  | -8.96 | 106.57      | 120.90   |
| 21  | AA    | 190  | A    | N1-C6-N6   | 8.95  | 123.97      | 118.60   |
| 24  | DA    | 2713 | U    | N1-C1'-C2' | 8.95  | 125.64      | 114.00   |
| 24  | DA    | 1079 | C    | N1-C1'-C2' | -8.95 | 102.16      | 112.00   |
| 21  | AA    | 534  | U    | N1-C1'-C2' | -8.95 | 102.16      | 112.00   |
| 24  | BA    | 1142 | A    | C8-N9-C1'  | 8.95  | 143.80      | 127.70   |
| 55  | CA    | 1397 | C    | P-O3'-C3'  | -8.95 | 108.97      | 119.70   |
| 24  | DA    | 128  | C    | P-O3'-C3'  | -8.94 | 108.97      | 119.70   |
| 24  | BA    | 2136 | G    | P-O3'-C3'  | -8.94 | 108.98      | 119.70   |
| 24  | DA    | 2631 | G    | P-O3'-C3'  | -8.93 | 108.98      | 119.70   |
| 24  | BA    | 1522 | A    | P-O3'-C3'  | 8.93  | 130.41      | 119.70   |
| 24  | BA    | 1915 | U    | N1-C1'-C2' | -8.93 | 102.18      | 112.00   |
| 24  | DA    | 1314 | C    | N1-C1'-C2' | -8.93 | 102.18      | 112.00   |
| 24  | DA    | 2713 | U    | P-O3'-C3'  | 8.93  | 130.42      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 479  | U    | O4'-C1'-N1 | 8.92  | 115.34      | 108.20   |
| 24  | BA    | 140  | C    | P-O3'-C3'  | 8.92  | 130.41      | 119.70   |
| 24  | DA    | 1914 | C    | N1-C1'-C2' | -8.92 | 102.18      | 112.00   |
| 24  | DA    | 1315 | C    | P-O3'-C3'  | -8.92 | 108.99      | 119.70   |
| 24  | BA    | 14   | A    | P-O3'-C3'  | -8.92 | 109.00      | 119.70   |
| 55  | CA    | 130  | A    | P-O3'-C3'  | 8.91  | 130.40      | 119.70   |
| 21  | AA    | 169  | C    | C5-C4-N4   | 8.91  | 126.44      | 120.20   |
| 21  | AA    | 1216 | A    | P-O3'-C3'  | -8.91 | 109.01      | 119.70   |
| 21  | AA    | 564  | C    | N1-C1'-C2' | -8.91 | 102.20      | 112.00   |
| 24  | BA    | 958  | U    | N1-C1'-C2' | -8.91 | 102.20      | 112.00   |
| 24  | BA    | 647  | G    | P-O3'-C3'  | -8.90 | 109.02      | 119.70   |
| 24  | BA    | 1606 | C    | P-O3'-C3'  | 8.90  | 130.39      | 119.70   |
| 25  | BB    | 91   | C    | N1-C1'-C2' | -8.90 | 102.20      | 112.00   |
| 24  | BA    | 2068 | U    | P-O3'-C3'  | -8.90 | 109.02      | 119.70   |
| 24  | DA    | 1013 | C    | P-O3'-C3'  | -8.90 | 109.02      | 119.70   |
| 24  | DA    | 754  | U    | N1-C1'-C2' | -8.89 | 102.22      | 112.00   |
| 24  | BA    | 2646 | C    | N1-C1'-C2' | -8.88 | 102.23      | 112.00   |
| 55  | CA    | 534  | U    | N1-C1'-C2' | -8.88 | 102.23      | 112.00   |
| 21  | AA    | 279  | A    | P-O3'-C3'  | 8.88  | 130.35      | 119.70   |
| 55  | CA    | 1528 | U    | O4'-C1'-N1 | 8.88  | 115.30      | 108.20   |
| 24  | DA    | 2021 | C    | N1-C1'-C2' | 8.87  | 125.53      | 114.00   |
| 24  | DA    | 140  | C    | N1-C1'-C2' | 8.85  | 125.51      | 114.00   |
| 55  | CA    | 517  | G    | P-O3'-C3'  | 8.85  | 130.31      | 119.70   |
| 55  | CA    | 590  | U    | O4'-C1'-N1 | 8.83  | 115.27      | 108.20   |
| 24  | DA    | 1271 | G    | P-O3'-C3'  | 8.82  | 130.29      | 119.70   |
| 25  | BB    | 88   | C    | N1-C1'-C2' | 8.82  | 125.47      | 114.00   |
| 55  | CA    | 513  | C    | N1-C1'-C2' | -8.82 | 102.30      | 112.00   |
| 24  | DA    | 2753 | A    | P-O3'-C3'  | -8.82 | 109.11      | 119.70   |
| 55  | CA    | 973  | G    | P-O3'-C3'  | -8.81 | 109.12      | 119.70   |
| 55  | CA    | 90   | C    | N1-C1'-C2' | -8.81 | 102.31      | 112.00   |
| 24  | BA    | 2517 | C    | P-O3'-C3'  | 8.81  | 130.27      | 119.70   |
| 24  | BA    | 1816 | C    | O4'-C1'-N1 | 8.81  | 115.25      | 108.20   |
| 24  | BA    | 324  | A    | P-O3'-C3'  | -8.80 | 109.14      | 119.70   |
| 24  | BA    | 919  | U    | C6-N1-C1'  | -8.80 | 108.88      | 121.20   |
| 24  | DA    | 1076 | C    | P-O3'-C3'  | -8.80 | 109.14      | 119.70   |
| 55  | CA    | 1229 | A    | P-O3'-C3'  | -8.80 | 109.14      | 119.70   |
| 55  | CA    | 370  | C    | P-O3'-C3'  | -8.80 | 109.14      | 119.70   |
| 24  | DA    | 312  | G    | P-O3'-C3'  | -8.79 | 109.14      | 119.70   |
| 55  | CA    | 723  | U    | N1-C1'-C2' | -8.79 | 102.33      | 112.00   |
| 24  | DA    | 1943 | U    | P-O3'-C3'  | 8.78  | 130.24      | 119.70   |
| 55  | CA    | 89   | U    | N1-C1'-C2' | -8.78 | 102.34      | 112.00   |
| 24  | BA    | 1653 | G    | P-O3'-C3'  | 8.78  | 130.24      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | BA    | 2384 | U    | N1-C1'-C2' | 8.77  | 125.41      | 114.00   |
| 21  | AA    | 1483 | A    | N1-C6-N6   | 8.77  | 123.86      | 118.60   |
| 21  | AA    | 1228 | C    | N1-C1'-C2' | -8.77 | 102.36      | 112.00   |
| 21  | AA    | 1161 | C    | N1-C1'-C2' | -8.77 | 102.36      | 112.00   |
| 55  | CA    | 388  | G    | P-O3'-C3'  | 8.77  | 130.22      | 119.70   |
| 24  | BA    | 1913 | A    | P-O3'-C3'  | 8.76  | 130.22      | 119.70   |
| 24  | DA    | 2851 | A    | P-O3'-C3'  | -8.76 | 109.19      | 119.70   |
| 24  | DA    | 510  | C    | N1-C1'-C2' | -8.76 | 102.36      | 112.00   |
| 21  | AA    | 115  | G    | P-O3'-C3'  | 8.76  | 130.21      | 119.70   |
| 21  | AA    | 1215 | G    | P-O3'-C3'  | -8.76 | 109.19      | 119.70   |
| 24  | BA    | 1333 | G    | P-O3'-C3'  | -8.76 | 109.19      | 119.70   |
| 24  | BA    | 1931 | U    | N1-C1'-C2' | -8.75 | 102.38      | 112.00   |
| 24  | DA    | 1239 | G    | P-O3'-C3'  | -8.75 | 109.20      | 119.70   |
| 24  | DA    | 2387 | U    | P-O3'-C3'  | -8.75 | 109.20      | 119.70   |
| 24  | BA    | 120  | U    | O4'-C1'-N1 | -8.74 | 101.20      | 108.20   |
| 21  | AA    | 431  | A    | P-O3'-C3'  | -8.74 | 109.21      | 119.70   |
| 24  | DA    | 755  | U    | P-O3'-C3'  | -8.74 | 109.21      | 119.70   |
| 24  | BA    | 1812 | U    | O4'-C1'-N1 | 8.74  | 115.19      | 108.20   |
| 55  | CA    | 81   | A    | P-O3'-C3'  | 8.74  | 130.18      | 119.70   |
| 24  | DA    | 2322 | A    | P-O3'-C3'  | -8.74 | 109.22      | 119.70   |
| 55  | CA    | 1246 | A    | P-O3'-C3'  | -8.73 | 109.22      | 119.70   |
| 24  | BA    | 1022 | G    | N3-C4-N9   | -8.73 | 120.76      | 126.00   |
| 21  | AA    | 1332 | A    | P-O3'-C3'  | -8.73 | 109.23      | 119.70   |
| 24  | DA    | 2691 | C    | N1-C1'-C2' | -8.72 | 102.41      | 112.00   |
| 23  | CW    | 3    | U    | P-O3'-C3'  | 8.72  | 130.16      | 119.70   |
| 24  | DA    | 2728 | U    | N1-C1'-C2' | -8.71 | 102.42      | 112.00   |
| 24  | BA    | 1303 | G    | P-O3'-C3'  | -8.71 | 109.25      | 119.70   |
| 24  | DA    | 1114 | C    | P-O3'-C3'  | -8.71 | 109.25      | 119.70   |
| 24  | BA    | 919  | U    | N3-C2-O2   | -8.70 | 116.11      | 122.20   |
| 24  | DA    | 2656 | U    | N1-C1'-C2' | -8.70 | 102.43      | 112.00   |
| 24  | BA    | 1788 | C    | O4'-C1'-N1 | -8.70 | 101.24      | 108.20   |
| 21  | AA    | 1066 | C    | N1-C1'-C2' | -8.70 | 102.43      | 112.00   |
| 21  | AA    | 1167 | A    | P-O3'-C3'  | 8.70  | 130.13      | 119.70   |
| 55  | CA    | 1161 | C    | P-O3'-C3'  | -8.70 | 109.27      | 119.70   |
| 55  | CA    | 1499 | A    | P-O3'-C3'  | -8.70 | 109.26      | 119.70   |
| 24  | BA    | 2511 | U    | C2-N3-C4   | -8.69 | 121.79      | 127.00   |
| 24  | DA    | 2837 | A    | P-O3'-C3'  | -8.69 | 109.28      | 119.70   |
| 24  | BA    | 2781 | A    | P-O3'-C3'  | -8.68 | 109.28      | 119.70   |
| 21  | AA    | 875  | U    | N1-C1'-C2' | -8.68 | 102.45      | 112.00   |
| 24  | BA    | 436  | C    | O4'-C1'-N1 | 8.68  | 115.14      | 108.20   |
| 21  | AA    | 1161 | C    | P-O3'-C3'  | -8.67 | 109.29      | 119.70   |
| 21  | AA    | 1303 | C    | N1-C1'-C2' | -8.67 | 102.46      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | BA    | 588  | U    | N1-C1'-C2' | -8.67 | 102.46      | 112.00   |
| 24  | BA    | 2586 | U    | P-O3'-C3'  | -8.67 | 109.30      | 119.70   |
| 24  | DA    | 60   | G    | P-O3'-C3'  | 8.67  | 130.10      | 119.70   |
| 24  | BA    | 1461 | C    | O4'-C1'-N1 | 8.66  | 115.13      | 108.20   |
| 21  | AA    | 344  | A    | O4'-C1'-N9 | 8.66  | 115.13      | 108.20   |
| 24  | BA    | 1398 | C    | N1-C1'-C2' | -8.65 | 102.48      | 112.00   |
| 24  | BA    | 1997 | C    | P-O3'-C3'  | -8.65 | 109.32      | 119.70   |
| 24  | DA    | 1993 | U    | N1-C1'-C2' | -8.64 | 102.49      | 112.00   |
| 24  | DA    | 1606 | C    | O4'-C1'-N1 | 8.64  | 115.11      | 108.20   |
| 24  | BA    | 2836 | U    | N1-C1'-C2' | -8.64 | 102.50      | 112.00   |
| 55  | CA    | 133  | U    | O4'-C1'-N1 | 8.64  | 115.11      | 108.20   |
| 24  | DA    | 1113 | U    | O4'-C1'-N1 | 8.64  | 115.11      | 108.20   |
| 24  | BA    | 509  | C    | P-O3'-C3'  | -8.62 | 109.36      | 119.70   |
| 24  | DA    | 1274 | A    | P-O3'-C3'  | -8.62 | 109.36      | 119.70   |
| 24  | BA    | 1539 | U    | P-O3'-C3'  | -8.61 | 109.36      | 119.70   |
| 24  | DA    | 451  | U    | O4'-C1'-N1 | 8.61  | 115.09      | 108.20   |
| 24  | BA    | 1557 | C    | N1-C1'-C2' | -8.61 | 102.53      | 112.00   |
| 24  | BA    | 1013 | C    | N1-C1'-C2' | -8.60 | 102.54      | 112.00   |
| 24  | BA    | 1675 | C    | P-O3'-C3'  | -8.59 | 109.39      | 119.70   |
| 24  | BA    | 835  | C    | N1-C1'-C2' | -8.59 | 102.55      | 112.00   |
| 24  | DA    | 766  | U    | P-O3'-C3'  | -8.59 | 109.40      | 119.70   |
| 24  | BA    | 1478 | G    | C5-C6-O6   | 8.58  | 133.75      | 128.60   |
| 55  | CA    | 175  | C    | N1-C1'-C2' | -8.58 | 102.57      | 112.00   |
| 24  | BA    | 84   | A    | P-O3'-C3'  | 8.57  | 129.99      | 119.70   |
| 24  | BA    | 2344 | U    | P-O3'-C3'  | 8.57  | 129.99      | 119.70   |
| 24  | DA    | 2612 | C    | P-O3'-C3'  | -8.57 | 109.41      | 119.70   |
| 21  | AA    | 453  | G    | P-O3'-C3'  | -8.57 | 109.42      | 119.70   |
| 24  | BA    | 386  | G    | P-O3'-C3'  | 8.57  | 129.98      | 119.70   |
| 24  | BA    | 443  | A    | P-O3'-C3'  | -8.57 | 109.42      | 119.70   |
| 24  | DA    | 1681 | G    | P-O3'-C3'  | 8.57  | 129.98      | 119.70   |
| 55  | CA    | 251  | G    | P-O3'-C3'  | 8.56  | 129.98      | 119.70   |
| 21  | AA    | 352  | C    | P-O3'-C3'  | -8.56 | 109.42      | 119.70   |
| 24  | DA    | 1386 | C    | N1-C1'-C2' | -8.56 | 102.58      | 112.00   |
| 21  | AA    | 1242 | G    | N9-C1'-C2' | -8.56 | 102.58      | 112.00   |
| 21  | AA    | 984  | C    | O4'-C1'-N1 | 8.55  | 115.04      | 108.20   |
| 24  | DA    | 784  | G    | O4'-C1'-N9 | 8.54  | 115.03      | 108.20   |
| 55  | CA    | 528  | C    | O4'-C1'-N1 | 8.53  | 115.03      | 108.20   |
| 24  | DA    | 791  | C    | P-O3'-C3'  | -8.52 | 109.47      | 119.70   |
| 24  | BA    | 2585 | U    | P-O3'-C3'  | 8.52  | 129.93      | 119.70   |
| 24  | DA    | 749  | A    | P-O3'-C3'  | -8.52 | 109.48      | 119.70   |
| 21  | AA    | 575  | G    | N3-C4-N9   | -8.51 | 120.89      | 126.00   |
| 21  | AA    | 467  | U    | P-O3'-C3'  | -8.51 | 109.48      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | BA    | 2513 | A    | C5-C6-N6   | 8.51  | 130.51      | 123.70   |
| 56  | DB    | 104  | A    | C8-N9-C4   | -8.51 | 102.40      | 105.80   |
| 24  | BA    | 2834 | G    | P-O5'-C5'  | -8.51 | 107.29      | 120.90   |
| 24  | BA    | 645  | C    | N1-C1'-C2' | 8.50  | 125.05      | 114.00   |
| 24  | BA    | 746  | U    | P-O3'-C3'  | 8.50  | 129.90      | 119.70   |
| 24  | DA    | 865  | C    | P-O3'-C3'  | 8.50  | 129.90      | 119.70   |
| 24  | DA    | 2348 | U    | P-O3'-C3'  | -8.50 | 109.50      | 119.70   |
| 55  | CA    | 248  | C    | O4'-C1'-N1 | 8.50  | 115.00      | 108.20   |
| 24  | DA    | 1206 | G    | P-O3'-C3'  | -8.49 | 109.51      | 119.70   |
| 24  | BA    | 1602 | U    | P-O3'-C3'  | 8.49  | 129.88      | 119.70   |
| 24  | BA    | 1856 | U    | O4'-C1'-N1 | 8.49  | 114.99      | 108.20   |
| 21  | AA    | 1530 | G    | N9-C1'-C2' | -8.48 | 102.67      | 112.00   |
| 55  | CA    | 884  | U    | O4'-C1'-N1 | 8.48  | 114.98      | 108.20   |
| 24  | DA    | 100  | U    | P-O3'-C3'  | 8.48  | 129.88      | 119.70   |
| 24  | BA    | 2319 | G    | P-O3'-C3'  | 8.47  | 129.87      | 119.70   |
| 24  | DA    | 1636 | U    | O4'-C1'-N1 | 8.47  | 114.98      | 108.20   |
| 24  | BA    | 531  | C    | N1-C1'-C2' | 8.47  | 125.01      | 114.00   |
| 24  | BA    | 1287 | A    | P-O3'-C3'  | -8.46 | 109.54      | 119.70   |
| 56  | DB    | 24   | G    | P-O3'-C3'  | 8.46  | 129.85      | 119.70   |
| 24  | DA    | 774  | G    | P-O3'-C3'  | 8.46  | 129.85      | 119.70   |
| 24  | BA    | 1635 | A    | N9-C1'-C2' | -8.46 | 102.70      | 112.00   |
| 24  | BA    | 811  | U    | P-O3'-C3'  | 8.46  | 129.85      | 119.70   |
| 24  | DA    | 1141 | U    | P-O3'-C3'  | 8.46  | 129.85      | 119.70   |
| 55  | CA    | 1051 | C    | N1-C1'-C2' | -8.45 | 102.70      | 112.00   |
| 24  | BA    | 506  | G    | P-O3'-C3'  | 8.45  | 129.84      | 119.70   |
| 21  | AA    | 510  | A    | P-O3'-C3'  | -8.45 | 109.57      | 119.70   |
| 24  | DA    | 2031 | A    | P-O3'-C3'  | 8.45  | 129.83      | 119.70   |
| 21  | AA    | 717  | U    | P-O3'-C3'  | 8.44  | 129.83      | 119.70   |
| 55  | CA    | 995  | C    | P-O3'-C3'  | -8.43 | 109.58      | 119.70   |
| 21  | AA    | 1153 | G    | P-O3'-C3'  | -8.43 | 109.58      | 119.70   |
| 24  | BA    | 1174 | U    | N1-C1'-C2' | -8.43 | 102.73      | 112.00   |
| 24  | BA    | 2866 | U    | P-O3'-C3'  | 8.42  | 129.81      | 119.70   |
| 55  | CA    | 1502 | A    | P-O3'-C3'  | 8.42  | 129.80      | 119.70   |
| 24  | BA    | 2520 | C    | O4'-C1'-N1 | 8.42  | 114.93      | 108.20   |
| 55  | CA    | 1449 | C    | O4'-C1'-N1 | 8.42  | 114.93      | 108.20   |
| 24  | DA    | 1636 | U    | N1-C1'-C2' | -8.42 | 102.74      | 112.00   |
| 55  | CA    | 1087 | G    | P-O3'-C3'  | -8.41 | 109.60      | 119.70   |
| 24  | DA    | 778  | G    | P-O3'-C3'  | -8.41 | 109.60      | 119.70   |
| 24  | BA    | 2322 | A    | P-O3'-C3'  | -8.41 | 109.61      | 119.70   |
| 55  | CA    | 1053 | G    | P-O3'-C3'  | 8.41  | 129.79      | 119.70   |
| 21  | AA    | 91   | U    | C5-C4-O4   | -8.40 | 120.86      | 125.90   |
| 24  | BA    | 2392 | A    | P-O3'-C3'  | -8.40 | 109.62      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 315  | A    | P-O3'-C3'  | 8.39  | 129.77      | 119.70   |
| 24  | BA    | 996  | A    | P-O3'-C3'  | -8.38 | 109.64      | 119.70   |
| 55  | CA    | 875  | U    | P-O3'-C3'  | -8.38 | 109.64      | 119.70   |
| 21  | AA    | 1449 | C    | O4'-C1'-N1 | 8.38  | 114.91      | 108.20   |
| 55  | CA    | 913  | A    | P-O3'-C3'  | 8.38  | 129.76      | 119.70   |
| 24  | BA    | 301  | G    | C4-N9-C1'  | -8.38 | 115.61      | 126.50   |
| 24  | BA    | 1020 | A    | P-O3'-C3'  | 8.38  | 129.76      | 119.70   |
| 21  | AA    | 1202 | U    | O4'-C1'-N1 | 8.38  | 114.90      | 108.20   |
| 24  | DA    | 2226 | C    | O4'-C1'-N1 | 8.38  | 114.90      | 108.20   |
| 55  | CA    | 1162 | C    | P-O3'-C3'  | -8.38 | 109.65      | 119.70   |
| 55  | CA    | 1141 | C    | P-O3'-C3'  | -8.37 | 109.65      | 119.70   |
| 21  | AA    | 1140 | C    | N1-C1'-C2' | -8.37 | 102.80      | 112.00   |
| 24  | BA    | 1013 | C    | P-O3'-C3'  | -8.37 | 109.66      | 119.70   |
| 24  | BA    | 1141 | U    | P-O3'-C3'  | 8.36  | 129.74      | 119.70   |
| 24  | DA    | 273  | G    | N9-C1'-C2' | -8.36 | 102.80      | 112.00   |
| 24  | DA    | 2261 | C    | O4'-C1'-N1 | 8.36  | 114.89      | 108.20   |
| 24  | BA    | 2267 | A    | P-O3'-C3'  | -8.36 | 109.67      | 119.70   |
| 21  | AA    | 590  | U    | O4'-C1'-N1 | 8.36  | 114.88      | 108.20   |
| 21  | AA    | 721  | G    | P-O3'-C3'  | 8.35  | 129.72      | 119.70   |
| 55  | CA    | 973  | G    | N9-C1'-C2' | -8.35 | 102.82      | 112.00   |
| 55  | CA    | 459  | A    | P-O3'-C3'  | 8.34  | 129.71      | 119.70   |
| 55  | CA    | 597  | G    | P-O3'-C3'  | -8.34 | 109.69      | 119.70   |
| 24  | DA    | 629  | G    | P-O3'-C3'  | -8.34 | 109.70      | 119.70   |
| 24  | DA    | 1946 | U    | N1-C1'-C2' | -8.34 | 102.83      | 112.00   |
| 24  | DA    | 2458 | G    | P-O3'-C3'  | 8.34  | 129.71      | 119.70   |
| 24  | BA    | 671  | C    | O4'-C1'-N1 | 8.33  | 114.87      | 108.20   |
| 24  | DA    | 1954 | G    | P-O3'-C3'  | 8.33  | 129.70      | 119.70   |
| 24  | BA    | 1033 | U    | P-O3'-C3'  | 8.33  | 129.70      | 119.70   |
| 24  | DA    | 503  | A    | P-O3'-C3'  | 8.33  | 129.69      | 119.70   |
| 55  | CA    | 1224 | U    | P-O3'-C3'  | 8.32  | 129.69      | 119.70   |
| 21  | AA    | 985  | C    | P-O3'-C3'  | -8.32 | 109.72      | 119.70   |
| 24  | BA    | 2490 | G    | P-O3'-C3'  | 8.31  | 129.68      | 119.70   |
| 24  | BA    | 2873 | A    | O4'-C1'-N9 | 8.30  | 114.84      | 108.20   |
| 24  | BA    | 2275 | C    | P-O3'-C3'  | 8.30  | 129.66      | 119.70   |
| 24  | DA    | 957  | C    | P-O3'-C3'  | 8.30  | 129.66      | 119.70   |
| 24  | DA    | 2034 | U    | N1-C1'-C2' | -8.30 | 102.87      | 112.00   |
| 24  | BA    | 278  | A    | P-O3'-C3'  | 8.29  | 129.65      | 119.70   |
| 24  | BA    | 2447 | G    | N3-C4-N9   | 8.29  | 130.97      | 126.00   |
| 55  | CA    | 884  | U    | P-O3'-C3'  | 8.29  | 129.64      | 119.70   |
| 24  | DA    | 2612 | C    | O4'-C1'-N1 | 8.29  | 114.83      | 108.20   |
| 24  | BA    | 613  | A    | P-O3'-C3'  | 8.28  | 129.64      | 119.70   |
| 24  | BA    | 1721 | G    | P-O3'-C3'  | 8.28  | 129.64      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | BA    | 1931 | U    | P-O3'-C3'  | -8.28 | 109.76      | 119.70   |
| 24  | BA    | 749  | A    | P-O3'-C3'  | -8.28 | 109.76      | 119.70   |
| 24  | DA    | 2492 | U    | N1-C1'-C2' | -8.28 | 102.89      | 112.00   |
| 24  | DA    | 445  | C    | O4'-C1'-N1 | 8.28  | 114.82      | 108.20   |
| 21  | AA    | 1101 | A    | P-O3'-C3'  | 8.27  | 129.63      | 119.70   |
| 24  | BA    | 1062 | G    | P-O3'-C3'  | -8.27 | 109.77      | 119.70   |
| 24  | BA    | 162  | U    | P-O3'-C3'  | 8.27  | 129.62      | 119.70   |
| 24  | DA    | 766  | U    | O4'-C1'-N1 | 8.27  | 114.81      | 108.20   |
| 24  | DA    | 2441 | U    | P-O3'-C3'  | -8.27 | 109.78      | 119.70   |
| 55  | CA    | 531  | U    | N1-C1'-C2' | 8.26  | 124.73      | 114.00   |
| 24  | BA    | 2035 | G    | O4'-C1'-N9 | 8.26  | 114.80      | 108.20   |
| 21  | AA    | 344  | A    | P-O3'-C3'  | 8.25  | 129.60      | 119.70   |
| 24  | BA    | 1249 | U    | N1-C1'-C2' | -8.25 | 102.93      | 112.00   |
| 24  | BA    | 1019 | U    | N1-C2-N3   | 8.24  | 119.85      | 114.90   |
| 24  | DA    | 389  | G    | P-O3'-C3'  | -8.24 | 109.81      | 119.70   |
| 24  | BA    | 443  | A    | P-O5'-C5'  | -8.24 | 107.72      | 120.90   |
| 55  | CA    | 486  | U    | N1-C1'-C2' | -8.24 | 102.94      | 112.00   |
| 24  | DA    | 444  | C    | O4'-C1'-N1 | 8.24  | 114.79      | 108.20   |
| 24  | BA    | 645  | C    | P-O3'-C3'  | 8.23  | 129.58      | 119.70   |
| 24  | DA    | 1113 | U    | N1-C1'-C2' | -8.23 | 102.94      | 112.00   |
| 21  | AA    | 116  | A    | N9-C1'-C2' | -8.23 | 102.95      | 112.00   |
| 24  | BA    | 1668 | A    | P-O3'-C3'  | 8.23  | 129.58      | 119.70   |
| 24  | BA    | 688  | U    | P-O3'-C3'  | -8.22 | 109.83      | 119.70   |
| 21  | AA    | 1201 | A    | P-O3'-C3'  | 8.22  | 129.57      | 119.70   |
| 24  | BA    | 858  | G    | P-O3'-C3'  | 8.22  | 129.57      | 119.70   |
| 24  | DA    | 1110 | G    | P-O3'-C3'  | 8.22  | 129.56      | 119.70   |
| 24  | BA    | 2492 | U    | N1-C1'-C2' | -8.22 | 102.96      | 112.00   |
| 55  | CA    | 1449 | C    | P-O3'-C3'  | -8.22 | 109.84      | 119.70   |
| 21  | AA    | 1507 | A    | P-O3'-C3'  | -8.21 | 109.84      | 119.70   |
| 24  | DA    | 2616 | C    | O4'-C1'-N1 | 8.21  | 114.77      | 108.20   |
| 21  | AA    | 1157 | A    | P-O3'-C3'  | 8.21  | 129.55      | 119.70   |
| 24  | DA    | 1760 | C    | N1-C1'-C2' | -8.21 | 102.97      | 112.00   |
| 21  | AA    | 275  | G    | P-O3'-C3'  | -8.21 | 109.85      | 119.70   |
| 24  | BA    | 931  | U    | P-O3'-C3'  | 8.20  | 129.54      | 119.70   |
| 24  | BA    | 1024 | G    | P-O3'-C3'  | -8.20 | 109.86      | 119.70   |
| 21  | AA    | 95   | C    | P-O3'-C3'  | -8.20 | 109.86      | 119.70   |
| 24  | DA    | 1334 | G    | P-O3'-C3'  | -8.20 | 109.86      | 119.70   |
| 21  | AA    | 511  | C    | O4'-C1'-N1 | 8.19  | 114.75      | 108.20   |
| 24  | DA    | 588  | U    | N1-C1'-C2' | -8.19 | 102.99      | 112.00   |
| 24  | DA    | 1063 | G    | P-O3'-C3'  | -8.19 | 109.87      | 119.70   |
| 56  | DB    | 104  | A    | O4'-C1'-N9 | 8.19  | 114.75      | 108.20   |
| 24  | BA    | 1125 | G    | N9-C4-C5   | -8.18 | 102.13      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | BA    | 2215 | C    | N1-C1'-C2' | -8.18 | 103.00      | 112.00   |
| 24  | BA    | 752  | A    | N1-C6-N6   | 8.18  | 123.51      | 118.60   |
| 21  | AA    | 653  | U    | P-O3'-C3'  | 8.18  | 129.51      | 119.70   |
| 24  | BA    | 748  | G    | P-O3'-C3'  | 8.17  | 129.51      | 119.70   |
| 24  | BA    | 2520 | C    | P-O3'-C3'  | -8.17 | 109.89      | 119.70   |
| 24  | DA    | 2387 | U    | N1-C1'-C2' | -8.17 | 103.01      | 112.00   |
| 24  | DA    | 805  | G    | P-O3'-C3'  | 8.17  | 129.50      | 119.70   |
| 21  | AA    | 974  | A    | P-O3'-C3'  | 8.17  | 129.50      | 119.70   |
| 24  | BA    | 811  | U    | O4'-C1'-N1 | 8.17  | 114.73      | 108.20   |
| 24  | BA    | 1647 | U    | P-O3'-C3'  | 8.16  | 129.50      | 119.70   |
| 24  | BA    | 2895 | G    | P-O3'-C3'  | -8.16 | 109.90      | 119.70   |
| 55  | CA    | 70   | U    | P-O3'-C3'  | 8.16  | 129.50      | 119.70   |
| 24  | BA    | 2566 | A    | P-O3'-C3'  | 8.16  | 129.49      | 119.70   |
| 21  | AA    | 931  | C    | O4'-C1'-N1 | 8.16  | 114.73      | 108.20   |
| 55  | CA    | 995  | C    | N1-C1'-C2' | -8.16 | 103.03      | 112.00   |
| 24  | DA    | 1035 | U    | N1-C1'-C2' | -8.15 | 103.03      | 112.00   |
| 21  | AA    | 813  | U    | N1-C1'-C2' | -8.15 | 103.03      | 112.00   |
| 24  | BA    | 2497 | A    | P-O3'-C3'  | 8.15  | 129.48      | 119.70   |
| 24  | DA    | 1616 | A    | P-O3'-C3'  | 8.15  | 129.48      | 119.70   |
| 24  | BA    | 976  | G    | P-O3'-C3'  | -8.14 | 109.93      | 119.70   |
| 24  | BA    | 1996 | C    | O4'-C1'-N1 | 8.14  | 114.71      | 108.20   |
| 24  | BA    | 119  | A    | P-O3'-C3'  | 8.14  | 129.47      | 119.70   |
| 21  | AA    | 874  | G    | P-O3'-C3'  | -8.14 | 109.93      | 119.70   |
| 24  | BA    | 421  | C    | P-O3'-C3'  | 8.14  | 129.47      | 119.70   |
| 24  | BA    | 2424 | C    | O4'-C1'-N1 | 8.14  | 114.71      | 108.20   |
| 55  | CA    | 1284 | C    | P-O3'-C3'  | -8.14 | 109.93      | 119.70   |
| 24  | DA    | 492  | A    | P-O3'-C3'  | -8.14 | 109.93      | 119.70   |
| 24  | BA    | 1698 | A    | P-O3'-C3'  | 8.13  | 129.46      | 119.70   |
| 24  | BA    | 2251 | G    | P-O3'-C3'  | -8.13 | 109.94      | 119.70   |
| 24  | DA    | 2603 | G    | P-O3'-C3'  | -8.13 | 109.94      | 119.70   |
| 24  | BA    | 989  | G    | P-O3'-C3'  | 8.13  | 129.45      | 119.70   |
| 55  | CA    | 1032 | G    | P-O3'-C3'  | 8.13  | 129.45      | 119.70   |
| 24  | DA    | 1782 | U    | N1-C1'-C2' | -8.12 | 103.06      | 112.00   |
| 24  | BA    | 638  | G    | P-O3'-C3'  | -8.12 | 109.95      | 119.70   |
| 24  | DA    | 1073 | A    | P-O3'-C3'  | -8.12 | 109.95      | 119.70   |
| 24  | BA    | 2611 | C    | N1-C1'-C2' | -8.12 | 103.07      | 112.00   |
| 24  | DA    | 1415 | U    | P-O3'-C3'  | 8.11  | 129.44      | 119.70   |
| 24  | DA    | 1839 | G    | P-O3'-C3'  | -8.12 | 109.96      | 119.70   |
| 24  | BA    | 1008 | A    | P-O3'-C3'  | 8.11  | 129.44      | 119.70   |
| 24  | BA    | 2303 | G    | P-O3'-C3'  | -8.11 | 109.97      | 119.70   |
| 24  | DA    | 2902 | C    | O4'-C1'-N1 | 8.11  | 114.69      | 108.20   |
| 24  | DA    | 1499 | C    | P-O3'-C3'  | -8.11 | 109.97      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 1064 | G    | P-O3'-C3'  | 8.11  | 129.43      | 119.70   |
| 24  | BA    | 2283 | C    | O4'-C1'-N1 | 8.11  | 114.69      | 108.20   |
| 24  | DA    | 755  | U    | N1-C1'-C2' | -8.11 | 103.08      | 112.00   |
| 24  | DA    | 1838 | C    | O4'-C1'-N1 | 8.10  | 114.68      | 108.20   |
| 55  | CA    | 1052 | U    | P-O3'-C3'  | -8.10 | 109.98      | 119.70   |
| 24  | BA    | 1682 | G    | P-O3'-C3'  | -8.10 | 109.99      | 119.70   |
| 24  | DA    | 2277 | G    | P-O3'-C3'  | -8.10 | 109.99      | 119.70   |
| 24  | BA    | 945  | A    | O4'-C1'-N9 | 8.09  | 114.67      | 108.20   |
| 21  | AA    | 1278 | G    | P-O3'-C3'  | 8.09  | 129.40      | 119.70   |
| 24  | DA    | 2382 | G    | P-O3'-C3'  | 8.07  | 129.39      | 119.70   |
| 55  | CA    | 934  | C    | P-O3'-C3'  | 8.07  | 129.39      | 119.70   |
| 24  | DA    | 392  | U    | O4'-C1'-N1 | 8.07  | 114.66      | 108.20   |
| 24  | BA    | 2440 | C    | O4'-C1'-N1 | 8.06  | 114.65      | 108.20   |
| 24  | BA    | 2066 | C    | P-O3'-C3'  | -8.06 | 110.03      | 119.70   |
| 24  | BA    | 199  | A    | O4'-C1'-N9 | 8.06  | 114.65      | 108.20   |
| 21  | AA    | 64   | G    | P-O3'-C3'  | 8.06  | 129.37      | 119.70   |
| 24  | BA    | 1981 | A    | P-O3'-C3'  | -8.06 | 110.03      | 119.70   |
| 24  | BA    | 2447 | G    | N3-C2-N2   | -8.06 | 114.26      | 119.90   |
| 55  | CA    | 328  | C    | O4'-C1'-N1 | -8.06 | 101.75      | 108.20   |
| 55  | CA    | 389  | A    | P-O3'-C3'  | -8.06 | 110.03      | 119.70   |
| 55  | CA    | 1530 | G    | P-O3'-C3'  | -8.06 | 110.03      | 119.70   |
| 24  | BA    | 1915 | U    | P-O3'-C3'  | -8.05 | 110.04      | 119.70   |
| 21  | AA    | 1320 | C    | N1-C1'-C2' | -8.05 | 103.14      | 112.00   |
| 24  | BA    | 1876 | A    | C4-C5-C6   | -8.05 | 112.97      | 117.00   |
| 24  | BA    | 2054 | A    | C8-N9-C4   | -8.05 | 102.58      | 105.80   |
| 24  | BA    | 241  | A    | P-O3'-C3'  | 8.05  | 129.36      | 119.70   |
| 24  | DA    | 1076 | C    | O4'-C1'-N1 | 8.05  | 114.64      | 108.20   |
| 24  | DA    | 2782 | G    | P-O3'-C3'  | -8.05 | 110.04      | 119.70   |
| 24  | DA    | 2692 | G    | N9-C1'-C2' | -8.04 | 103.15      | 112.00   |
| 24  | BA    | 2834 | G    | P-O3'-C3'  | -8.04 | 110.06      | 119.70   |
| 55  | CA    | 501  | C    | P-O3'-C3'  | -8.04 | 110.05      | 119.70   |
| 24  | BA    | 959  | A    | P-O3'-C3'  | -8.04 | 110.06      | 119.70   |
| 21  | AA    | 267  | C    | N1-C1'-C2' | -8.03 | 103.16      | 112.00   |
| 21  | AA    | 1362 | A    | O4'-C1'-N9 | 8.03  | 114.63      | 108.20   |
| 24  | BA    | 13   | A    | P-O3'-C3'  | 8.03  | 129.34      | 119.70   |
| 55  | CA    | 81   | A    | O4'-C1'-N9 | 8.03  | 114.62      | 108.20   |
| 55  | CA    | 722  | G    | P-O3'-C3'  | -8.03 | 110.07      | 119.70   |
| 55  | CA    | 1033 | G    | P-O3'-C3'  | -8.02 | 110.08      | 119.70   |
| 24  | BA    | 743  | A    | P-O3'-C3'  | 8.02  | 129.32      | 119.70   |
| 24  | BA    | 2462 | C    | P-O3'-C3'  | -8.02 | 110.08      | 119.70   |
| 31  | BH    | 48   | GLU  | CA-C-O     | -8.02 | 103.26      | 120.10   |
| 55  | CA    | 1228 | C    | O4'-C1'-N1 | 8.02  | 114.61      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 184  | G    | P-O3'-C3'  | -8.02 | 110.08      | 119.70   |
| 24  | BA    | 571  | U    | P-O3'-C3'  | 8.01  | 129.31      | 119.70   |
| 24  | BA    | 1942 | C    | N1-C1'-C2' | -8.01 | 103.19      | 112.00   |
| 24  | BA    | 310  | A    | P-O3'-C3'  | 8.01  | 129.31      | 119.70   |
| 21  | AA    | 1408 | A    | P-O3'-C3'  | -8.01 | 110.09      | 119.70   |
| 21  | AA    | 14   | U    | P-O3'-C3'  | -8.00 | 110.09      | 119.70   |
| 24  | BA    | 1019 | U    | C5-C4-O4   | -8.00 | 121.10      | 125.90   |
| 24  | BA    | 1782 | U    | N1-C1'-C2' | -8.00 | 103.20      | 112.00   |
| 24  | DA    | 122  | G    | P-O3'-C3'  | -8.00 | 110.10      | 119.70   |
| 24  | DA    | 411  | G    | P-O3'-C3'  | 8.00  | 129.30      | 119.70   |
| 24  | BA    | 2406 | A    | P-O3'-C3'  | 8.00  | 129.30      | 119.70   |
| 55  | CA    | 697  | U    | O4'-C1'-N1 | 8.00  | 114.60      | 108.20   |
| 24  | DA    | 658  | U    | P-O3'-C3'  | -8.00 | 110.10      | 119.70   |
| 24  | BA    | 390  | U    | P-O3'-C3'  | 7.99  | 129.29      | 119.70   |
| 56  | DB    | 40   | U    | P-O3'-C3'  | 7.99  | 129.29      | 119.70   |
| 24  | BA    | 2386 | A    | N9-C1'-C2' | -7.99 | 103.21      | 112.00   |
| 24  | DA    | 1290 | C    | O4'-C1'-N1 | 7.99  | 114.59      | 108.20   |
| 24  | DA    | 2499 | C    | P-O3'-C3'  | -7.99 | 110.11      | 119.70   |
| 55  | CA    | 248  | C    | P-O3'-C3'  | -7.99 | 110.11      | 119.70   |
| 24  | BA    | 1602 | U    | O4'-C1'-N1 | 7.98  | 114.59      | 108.20   |
| 24  | BA    | 2093 | G    | N9-C1'-C2' | -7.98 | 103.22      | 112.00   |
| 21  | AA    | 1395 | C    | N1-C1'-C2' | -7.98 | 103.22      | 112.00   |
| 24  | BA    | 406  | G    | P-O3'-C3'  | -7.98 | 110.12      | 119.70   |
| 21  | AA    | 934  | C    | O4'-C1'-N1 | 7.98  | 114.58      | 108.20   |
| 23  | AW    | 3    | U    | P-O3'-C3'  | 7.98  | 129.27      | 119.70   |
| 24  | BA    | 1857 | G    | P-O3'-C3'  | 7.98  | 129.27      | 119.70   |
| 24  | DA    | 50   | U    | P-O3'-C3'  | 7.97  | 129.27      | 119.70   |
| 23  | CW    | 5    | U    | P-O3'-C3'  | -7.97 | 110.13      | 119.70   |
| 24  | DA    | 2712 | C    | P-O3'-C3'  | 7.97  | 129.27      | 119.70   |
| 21  | AA    | 1451 | U    | P-O3'-C3'  | 7.97  | 129.26      | 119.70   |
| 24  | BA    | 1048 | A    | P-O3'-C3'  | -7.97 | 110.14      | 119.70   |
| 24  | DA    | 335  | C    | P-O3'-C3'  | -7.97 | 110.14      | 119.70   |
| 21  | AA    | 451  | A    | P-O3'-C3'  | 7.97  | 129.26      | 119.70   |
| 24  | DA    | 1325 | U    | P-O3'-C3'  | 7.97  | 129.26      | 119.70   |
| 24  | BA    | 301  | G    | N3-C4-N9   | -7.96 | 121.22      | 126.00   |
| 24  | BA    | 2062 | A    | N1-C6-N6   | 7.96  | 123.38      | 118.60   |
| 24  | DA    | 527  | C    | P-O3'-C3'  | 7.96  | 129.26      | 119.70   |
| 24  | DA    | 2249 | U    | P-O3'-C3'  | 7.96  | 129.26      | 119.70   |
| 24  | DA    | 2503 | A    | P-O3'-C3'  | 7.96  | 129.26      | 119.70   |
| 24  | BA    | 1954 | G    | P-O3'-C3'  | 7.96  | 129.25      | 119.70   |
| 24  | BA    | 1619 | G    | P-O3'-C3'  | -7.96 | 110.15      | 119.70   |
| 24  | DA    | 1330 | C    | N1-C1'-C2' | -7.96 | 103.24      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | BA    | 2239 | G    | P-O3'-C3'  | -7.96 | 110.15      | 119.70   |
| 24  | BA    | 2879 | A    | P-O3'-C3'  | 7.95  | 129.25      | 119.70   |
| 24  | BA    | 1967 | C    | N1-C1'-C2' | -7.95 | 103.25      | 112.00   |
| 24  | BA    | 2593 | U    | P-O3'-C3'  | -7.95 | 110.16      | 119.70   |
| 24  | DA    | 605  | G    | N9-C1'-C2' | -7.95 | 103.26      | 112.00   |
| 55  | CA    | 1211 | U    | P-O3'-C3'  | 7.95  | 129.23      | 119.70   |
| 24  | DA    | 2024 | G    | P-O3'-C3'  | -7.94 | 110.18      | 119.70   |
| 55  | CA    | 1365 | G    | P-O3'-C3'  | -7.94 | 110.18      | 119.70   |
| 24  | BA    | 2513 | A    | N1-C6-N6   | -7.93 | 113.84      | 118.60   |
| 24  | DA    | 633  | A    | N1-C6-N6   | 7.93  | 123.36      | 118.60   |
| 21  | AA    | 330  | C    | N1-C1'-C2' | -7.93 | 103.28      | 112.00   |
| 21  | AA    | 500  | G    | P-O3'-C3'  | -7.93 | 110.18      | 119.70   |
| 55  | CA    | 755  | G    | P-O3'-C3'  | -7.93 | 110.18      | 119.70   |
| 24  | DA    | 1440 | U    | O4'-C1'-N1 | 7.93  | 114.55      | 108.20   |
| 24  | BA    | 2734 | A    | P-O3'-C3'  | -7.93 | 110.19      | 119.70   |
| 24  | DA    | 2728 | U    | P-O3'-C3'  | -7.92 | 110.19      | 119.70   |
| 55  | CA    | 875  | U    | O4'-C1'-N1 | 7.92  | 114.54      | 108.20   |
| 24  | BA    | 1330 | C    | O4'-C1'-N1 | 7.92  | 114.53      | 108.20   |
| 24  | BA    | 1647 | U    | O4'-C1'-N1 | 7.92  | 114.53      | 108.20   |
| 24  | DA    | 1539 | U    | P-O3'-C3'  | -7.92 | 110.20      | 119.70   |
| 23  | AW    | 5    | U    | P-O3'-C3'  | -7.92 | 110.20      | 119.70   |
| 55  | CA    | 462  | G    | P-O3'-C3'  | 7.91  | 129.20      | 119.70   |
| 24  | DA    | 534  | U    | P-O3'-C3'  | -7.91 | 110.21      | 119.70   |
| 24  | DA    | 2559 | C    | P-O3'-C3'  | -7.90 | 110.22      | 119.70   |
| 24  | BA    | 1111 | A    | P-O3'-C3'  | 7.90  | 129.18      | 119.70   |
| 24  | DA    | 2505 | G    | P-O3'-C3'  | -7.90 | 110.22      | 119.70   |
| 24  | DA    | 1942 | C    | P-O3'-C3'  | -7.89 | 110.23      | 119.70   |
| 55  | CA    | 915  | A    | P-O3'-C3'  | -7.89 | 110.23      | 119.70   |
| 24  | BA    | 1965 | C    | P-O5'-C5'  | -7.89 | 108.28      | 120.90   |
| 25  | BB    | 26   | C    | O4'-C1'-N1 | 7.89  | 114.51      | 108.20   |
| 24  | DA    | 2267 | A    | C6-C5-N7   | -7.89 | 126.78      | 132.30   |
| 21  | AA    | 252  | U    | N1-C1'-C2' | -7.89 | 103.33      | 112.00   |
| 21  | AA    | 884  | U    | P-O3'-C3'  | 7.88  | 129.16      | 119.70   |
| 24  | DA    | 2023 | C    | O4'-C1'-N1 | 7.88  | 114.51      | 108.20   |
| 24  | DA    | 2238 | G    | P-O3'-C3'  | 7.88  | 129.16      | 119.70   |
| 24  | BA    | 776  | G    | O4'-C1'-N9 | -7.88 | 101.90      | 108.20   |
| 24  | BA    | 1971 | U    | P-O3'-C3'  | -7.88 | 110.25      | 119.70   |
| 24  | DA    | 1430 | G    | P-O3'-C3'  | -7.88 | 110.25      | 119.70   |
| 24  | BA    | 1865 | U    | C5-C4-O4   | -7.88 | 121.17      | 125.90   |
| 24  | DA    | 2629 | U    | P-O3'-C3'  | 7.88  | 129.15      | 119.70   |
| 55  | CA    | 822  | U    | O4'-C1'-N1 | 7.87  | 114.50      | 108.20   |
| 24  | BA    | 866  | A    | N9-C1'-C2' | -7.87 | 103.34      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | BA    | 1012 | U    | O4'-C1'-N1 | 7.87  | 114.50      | 108.20   |
| 24  | BA    | 656  | G    | P-O3'-C3'  | -7.87 | 110.26      | 119.70   |
| 21  | AA    | 369  | G    | P-O3'-C3'  | -7.87 | 110.26      | 119.70   |
| 55  | CA    | 724  | G    | P-O3'-C3'  | -7.87 | 110.26      | 119.70   |
| 24  | DA    | 61   | C    | N1-C1'-C2' | -7.86 | 103.35      | 112.00   |
| 24  | BA    | 1997 | C    | N1-C1'-C2' | -7.86 | 103.35      | 112.00   |
| 55  | CA    | 183  | C    | O4'-C1'-N1 | 7.86  | 114.49      | 108.20   |
| 55  | CA    | 1364 | U    | P-O3'-C3'  | 7.86  | 129.13      | 119.70   |
| 24  | BA    | 2518 | A    | P-O5'-C5'  | -7.86 | 108.33      | 120.90   |
| 24  | BA    | 1029 | A    | N1-C6-N6   | 7.85  | 123.31      | 118.60   |
| 24  | DA    | 811  | U    | P-O3'-C3'  | 7.85  | 129.12      | 119.70   |
| 24  | BA    | 1266 | G    | P-O3'-C3'  | 7.84  | 129.11      | 119.70   |
| 21  | AA    | 1282 | C    | N1-C1'-C2' | -7.84 | 103.37      | 112.00   |
| 55  | CA    | 1128 | C    | N1-C1'-C2' | -7.84 | 103.37      | 112.00   |
| 55  | CA    | 1087 | G    | N9-C1'-C2' | -7.83 | 103.38      | 112.00   |
| 21  | AA    | 194  | C    | C5-C4-N4   | 7.83  | 125.68      | 120.20   |
| 24  | BA    | 2575 | C    | C5-C6-N1   | -7.83 | 117.08      | 121.00   |
| 24  | BA    | 15   | G    | C5-C6-O6   | 7.83  | 133.30      | 128.60   |
| 24  | BA    | 1649 | G    | P-O3'-C3'  | -7.83 | 110.31      | 119.70   |
| 24  | BA    | 264  | C    | O4'-C1'-N1 | 7.83  | 114.46      | 108.20   |
| 24  | DA    | 2585 | U    | P-O3'-C3'  | 7.83  | 129.09      | 119.70   |
| 21  | AA    | 372  | C    | P-O3'-C3'  | 7.82  | 129.09      | 119.70   |
| 24  | DA    | 224  | U    | N1-C1'-C2' | -7.82 | 103.39      | 112.00   |
| 24  | BA    | 1142 | A    | C4-N9-C1'  | -7.81 | 112.23      | 126.30   |
| 24  | BA    | 2060 | A    | P-O3'-C3'  | 7.81  | 129.08      | 119.70   |
| 21  | AA    | 1239 | A    | P-O3'-C3'  | 7.81  | 129.07      | 119.70   |
| 24  | BA    | 1147 | A    | N1-C6-N6   | -7.81 | 113.91      | 118.60   |
| 24  | DA    | 828  | U    | O4'-C1'-N1 | 7.81  | 114.45      | 108.20   |
| 21  | AA    | 1365 | G    | P-O3'-C3'  | -7.80 | 110.33      | 119.70   |
| 55  | CA    | 428  | G    | P-O3'-C3'  | 7.80  | 129.06      | 119.70   |
| 24  | DA    | 423  | A    | P-O3'-C3'  | -7.80 | 110.34      | 119.70   |
| 24  | BA    | 1716 | U    | O4'-C1'-N1 | 7.80  | 114.44      | 108.20   |
| 24  | DA    | 646  | U    | P-O3'-C3'  | 7.80  | 129.06      | 119.70   |
| 24  | BA    | 1963 | U    | N1-C1'-C2' | -7.79 | 103.43      | 112.00   |
| 25  | BB    | 25   | U    | P-O3'-C3'  | -7.79 | 110.35      | 119.70   |
| 24  | DA    | 2860 | A    | N1-C6-N6   | 7.79  | 123.28      | 118.60   |
| 24  | BA    | 1112 | G    | P-O3'-C3'  | -7.79 | 110.35      | 119.70   |
| 55  | CA    | 1162 | C    | O4'-C1'-N1 | 7.79  | 114.43      | 108.20   |
| 24  | DA    | 1462 | C    | O4'-C1'-N1 | 7.79  | 114.43      | 108.20   |
| 24  | DA    | 1913 | A    | P-O3'-C3'  | 7.79  | 129.05      | 119.70   |
| 21  | AA    | 436  | C    | O4'-C1'-N1 | 7.79  | 114.43      | 108.20   |
| 24  | BA    | 531  | C    | P-O3'-C3'  | 7.79  | 129.05      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | BA    | 1810 | A    | N9-C1'-C2' | -7.79 | 103.43      | 112.00   |
| 55  | CA    | 330  | C    | N1-C1'-C2' | -7.78 | 103.44      | 112.00   |
| 56  | DB    | 17   | C    | N1-C1'-C2' | -7.78 | 103.44      | 112.00   |
| 23  | CW    | 5    | U    | N1-C1'-C2' | -7.78 | 103.44      | 112.00   |
| 24  | BA    | 1351 | C    | O4'-C1'-N1 | 7.78  | 114.42      | 108.20   |
| 24  | BA    | 1872 | A    | P-O3'-C3'  | -7.78 | 110.36      | 119.70   |
| 25  | BB    | 12   | C    | O4'-C1'-N1 | 7.78  | 114.42      | 108.20   |
| 21  | AA    | 97   | G    | P-O3'-C3'  | -7.77 | 110.37      | 119.70   |
| 24  | BA    | 2275 | C    | N1-C1'-C2' | 7.77  | 124.10      | 114.00   |
| 55  | CA    | 1138 | G    | P-O3'-C3'  | 7.77  | 129.02      | 119.70   |
| 24  | BA    | 2836 | U    | P-O5'-C5'  | -7.77 | 108.47      | 120.90   |
| 24  | DA    | 2758 | A    | N9-C1'-C2' | -7.77 | 103.46      | 112.00   |
| 24  | DA    | 990  | A    | P-O3'-C3'  | -7.76 | 110.39      | 119.70   |
| 24  | BA    | 449  | A    | P-O3'-C3'  | -7.76 | 110.39      | 119.70   |
| 24  | BA    | 451  | U    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |
| 24  | BA    | 1272 | A    | O4'-C1'-N9 | 7.76  | 114.41      | 108.20   |
| 24  | BA    | 1714 | U    | N1-C1'-C2' | -7.76 | 103.47      | 112.00   |
| 24  | DA    | 1463 | C    | O4'-C1'-N1 | 7.76  | 114.41      | 108.20   |
| 24  | DA    | 1674 | G    | P-O3'-C3'  | 7.76  | 129.01      | 119.70   |
| 24  | DA    | 271  | G    | P-O3'-C3'  | 7.75  | 129.01      | 119.70   |
| 21  | AA    | 1200 | C    | N1-C1'-C2' | 7.75  | 124.08      | 114.00   |
| 24  | DA    | 1088 | A    | C5-C6-N1   | -7.75 | 113.82      | 117.70   |
| 24  | BA    | 519  | U    | N1-C1'-C2' | -7.75 | 103.47      | 112.00   |
| 55  | CA    | 704  | A    | P-O3'-C3'  | -7.75 | 110.40      | 119.70   |
| 24  | DA    | 1816 | C    | P-O3'-C3'  | -7.75 | 110.40      | 119.70   |
| 55  | CA    | 481  | G    | P-O3'-C3'  | 7.75  | 129.00      | 119.70   |
| 24  | DA    | 1946 | U    | P-O3'-C3'  | -7.75 | 110.40      | 119.70   |
| 24  | DA    | 1972 | G    | P-O3'-C3'  | -7.75 | 110.40      | 119.70   |
| 24  | BA    | 2615 | U    | P-O3'-C3'  | -7.75 | 110.40      | 119.70   |
| 24  | DA    | 91   | A    | P-O3'-C3'  | 7.75  | 129.00      | 119.70   |
| 55  | CA    | 389  | A    | N9-C4-C5   | 7.75  | 108.90      | 105.80   |
| 24  | BA    | 479  | A    | O4'-C1'-N9 | 7.74  | 114.39      | 108.20   |
| 24  | BA    | 2259 | U    | N1-C1'-C2' | -7.74 | 103.49      | 112.00   |
| 55  | CA    | 53   | A    | P-O3'-C3'  | -7.74 | 110.42      | 119.70   |
| 24  | BA    | 266  | G    | P-O3'-C3'  | -7.74 | 110.42      | 119.70   |
| 24  | BA    | 2501 | C    | N1-C1'-C2' | 7.73  | 124.05      | 114.00   |
| 24  | BA    | 2791 | G    | P-O3'-C3'  | -7.73 | 110.42      | 119.70   |
| 24  | DA    | 1075 | C    | N1-C1'-C2' | -7.73 | 103.50      | 112.00   |
| 55  | CA    | 643  | C    | O4'-C1'-N1 | 7.72  | 114.38      | 108.20   |
| 24  | BA    | 2035 | G    | P-O3'-C3'  | 7.72  | 128.97      | 119.70   |
| 24  | BA    | 474  | G    | P-O3'-C3'  | 7.72  | 128.96      | 119.70   |
| 24  | BA    | 1693 | U    | P-O3'-C3'  | 7.72  | 128.96      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | DA    | 395  | U    | N1-C1'-C2' | 7.71  | 124.03      | 114.00   |
| 24  | DA    | 1010 | A    | P-O3'-C3'  | -7.71 | 110.44      | 119.70   |
| 24  | BA    | 1458 | U    | P-O3'-C3'  | 7.71  | 128.95      | 119.70   |
| 24  | BA    | 1957 | C    | N1-C1'-C2' | -7.71 | 103.52      | 112.00   |
| 24  | BA    | 791  | C    | O4'-C1'-N1 | 7.70  | 114.36      | 108.20   |
| 24  | DA    | 1089 | A    | P-O3'-C3'  | 7.70  | 128.94      | 119.70   |
| 24  | DA    | 688  | U    | O4'-C1'-N1 | 7.69  | 114.35      | 108.20   |
| 24  | DA    | 2460 | U    | O4'-C1'-N1 | 7.69  | 114.35      | 108.20   |
| 24  | BA    | 2056 | G    | O4'-C1'-N9 | -7.68 | 102.05      | 108.20   |
| 24  | BA    | 2459 | A    | P-O3'-C3'  | -7.68 | 110.48      | 119.70   |
| 55  | CA    | 283  | U    | P-O3'-C3'  | -7.68 | 110.48      | 119.70   |
| 21  | AA    | 575  | G    | P-O3'-C3'  | 7.68  | 128.91      | 119.70   |
| 24  | DA    | 1941 | C    | N1-C1'-C2' | -7.68 | 103.55      | 112.00   |
| 21  | AA    | 1323 | G    | P-O3'-C3'  | -7.68 | 110.49      | 119.70   |
| 25  | BB    | 12   | C    | P-O3'-C3'  | 7.68  | 128.91      | 119.70   |
| 24  | BA    | 481  | G    | P-O3'-C3'  | 7.67  | 128.91      | 119.70   |
| 24  | BA    | 1180 | U    | P-O3'-C3'  | 7.67  | 128.90      | 119.70   |
| 24  | DA    | 1937 | A    | P-O3'-C3'  | 7.67  | 128.90      | 119.70   |
| 24  | DA    | 1971 | U    | P-O3'-C3'  | -7.66 | 110.51      | 119.70   |
| 24  | BA    | 2250 | G    | O4'-C1'-N9 | -7.66 | 102.07      | 108.20   |
| 24  | BA    | 2874 | C    | N1-C1'-C2' | -7.65 | 103.58      | 112.00   |
| 24  | DA    | 1684 | G    | N9-C1'-C2' | -7.65 | 103.58      | 112.00   |
| 24  | DA    | 2143 | C    | P-O3'-C3'  | 7.65  | 128.88      | 119.70   |
| 24  | DA    | 2347 | C    | P-O3'-C3'  | -7.65 | 110.52      | 119.70   |
| 55  | CA    | 91   | U    | N1-C1'-C2' | -7.65 | 103.59      | 112.00   |
| 24  | DA    | 1236 | G    | P-O3'-C3'  | 7.64  | 128.87      | 119.70   |
| 24  | DA    | 2093 | G    | N9-C1'-C2' | -7.64 | 103.59      | 112.00   |
| 21  | AA    | 266  | G    | P-O3'-C3'  | 7.64  | 128.87      | 119.70   |
| 24  | BA    | 1021 | A    | P-O5'-C5'  | -7.64 | 108.68      | 120.90   |
| 24  | DA    | 1963 | U    | O4'-C1'-N1 | 7.64  | 114.31      | 108.20   |
| 24  | DA    | 2726 | A    | P-O3'-C3'  | 7.64  | 128.86      | 119.70   |
| 24  | BA    | 961  | C    | P-O3'-C3'  | 7.63  | 128.86      | 119.70   |
| 55  | CA    | 936  | C    | O4'-C1'-N1 | 7.63  | 114.31      | 108.20   |
| 24  | DA    | 813  | U    | P-O3'-C3'  | -7.63 | 110.54      | 119.70   |
| 24  | DA    | 2896 | C    | O4'-C1'-N1 | 7.63  | 114.31      | 108.20   |
| 55  | CA    | 655  | A    | P-O3'-C3'  | -7.63 | 110.54      | 119.70   |
| 21  | AA    | 131  | A    | P-O3'-C3'  | -7.63 | 110.55      | 119.70   |
| 24  | BA    | 1022 | G    | N3-C2-N2   | -7.63 | 114.56      | 119.90   |
| 24  | DA    | 1272 | A    | P-O3'-C3'  | 7.63  | 128.85      | 119.70   |
| 24  | BA    | 1996 | C    | P-O3'-C3'  | 7.62  | 128.85      | 119.70   |
| 24  | BA    | 475  | C    | N1-C1'-C2' | -7.62 | 103.62      | 112.00   |
| 24  | BA    | 2613 | U    | N1-C1'-C2' | 7.62  | 123.91      | 114.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 55  | CA    | 373  | A    | P-O3'-C3'  | -7.62 | 110.56      | 119.70   |
| 55  | CA    | 1201 | A    | P-O3'-C3'  | 7.62  | 128.84      | 119.70   |
| 24  | DA    | 762  | U    | P-O3'-C3'  | 7.62  | 128.84      | 119.70   |
| 24  | DA    | 777  | G    | N9-C1'-C2' | -7.62 | 103.62      | 112.00   |
| 24  | DA    | 1565 | C    | P-O3'-C3'  | 7.62  | 128.84      | 119.70   |
| 24  | DA    | 741  | U    | P-O3'-C3'  | -7.62 | 110.56      | 119.70   |
| 24  | DA    | 958  | U    | N1-C1'-C2' | -7.61 | 103.63      | 112.00   |
| 24  | BA    | 2439 | A    | P-O3'-C3'  | 7.61  | 128.83      | 119.70   |
| 24  | DA    | 2210 | U    | P-O3'-C3'  | 7.61  | 128.83      | 119.70   |
| 24  | BA    | 1478 | G    | C8-N9-C1'  | 7.61  | 136.89      | 127.00   |
| 55  | CA    | 480  | U    | C2-N3-C4   | -7.60 | 122.44      | 127.00   |
| 24  | BA    | 35   | G    | P-O3'-C3'  | -7.60 | 110.58      | 119.70   |
| 24  | BA    | 2733 | A    | N9-C1'-C2' | -7.60 | 103.64      | 112.00   |
| 24  | BA    | 2259 | U    | P-O3'-C3'  | -7.60 | 110.58      | 119.70   |
| 24  | BA    | 1759 | A    | P-O3'-C3'  | -7.59 | 110.58      | 119.70   |
| 55  | CA    | 1229 | A    | N9-C1'-C2' | -7.59 | 103.65      | 112.00   |
| 24  | BA    | 1006 | C    | P-O3'-C3'  | -7.58 | 110.60      | 119.70   |
| 55  | CA    | 83   | C    | O4'-C1'-N1 | 7.58  | 114.27      | 108.20   |
| 24  | BA    | 2757 | A    | P-O3'-C3'  | -7.58 | 110.61      | 119.70   |
| 24  | BA    | 2567 | G    | P-O3'-C3'  | -7.58 | 110.61      | 119.70   |
| 55  | CA    | 1215 | G    | P-O3'-C3'  | -7.58 | 110.61      | 119.70   |
| 24  | BA    | 1654 | A    | P-O3'-C3'  | -7.57 | 110.61      | 119.70   |
| 24  | DA    | 1439 | A    | C4-C5-C6   | 7.57  | 120.79      | 117.00   |
| 24  | DA    | 2035 | G    | P-O3'-C3'  | -7.57 | 110.61      | 119.70   |
| 24  | BA    | 199  | A    | P-O3'-C3'  | 7.57  | 128.79      | 119.70   |
| 31  | BH    | 49   | ALA  | N-CA-C     | -7.57 | 90.56       | 111.00   |
| 25  | BB    | 43   | C    | O4'-C1'-N1 | 7.57  | 114.25      | 108.20   |
| 21  | AA    | 968  | A    | P-O3'-C3'  | 7.57  | 128.78      | 119.70   |
| 24  | BA    | 2611 | C    | P-O3'-C3'  | -7.57 | 110.62      | 119.70   |
| 24  | BA    | 1839 | G    | P-O3'-C3'  | -7.56 | 110.62      | 119.70   |
| 55  | CA    | 327  | A    | P-O3'-C3'  | 7.56  | 128.77      | 119.70   |
| 24  | BA    | 1615 | C    | P-O3'-C3'  | 7.56  | 128.77      | 119.70   |
| 24  | BA    | 2791 | G    | N9-C1'-C2' | -7.56 | 103.69      | 112.00   |
| 21  | AA    | 1184 | G    | P-O3'-C3'  | -7.55 | 110.64      | 119.70   |
| 24  | BA    | 1964 | G    | P-O3'-C3'  | 7.55  | 128.76      | 119.70   |
| 21  | AA    | 1418 | A    | N1-C6-N6   | 7.55  | 123.13      | 118.60   |
| 24  | BA    | 2555 | U    | O4'-C1'-N1 | 7.54  | 114.24      | 108.20   |
| 24  | DA    | 2850 | A    | P-O3'-C3'  | -7.54 | 110.65      | 119.70   |
| 56  | DB    | 43   | C    | P-O3'-C3'  | -7.54 | 110.65      | 119.70   |
| 24  | DA    | 1320 | C    | P-O3'-C3'  | 7.54  | 128.75      | 119.70   |
| 24  | BA    | 301  | G    | C8-N9-C1'  | 7.54  | 136.80      | 127.00   |
| 24  | BA    | 2542 | A    | O4'-C1'-N9 | 7.54  | 114.23      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | BA    | 739  | A    | P-O3'-C3'  | 7.53  | 128.74      | 119.70   |
| 55  | CA    | 1345 | U    | P-O3'-C3'  | 7.53  | 128.74      | 119.70   |
| 55  | CA    | 1358 | U    | O4'-C1'-N1 | 7.53  | 114.22      | 108.20   |
| 24  | DA    | 2447 | G    | C6-N1-C2   | -7.53 | 120.58      | 125.10   |
| 24  | DA    | 2566 | A    | P-O3'-C3'  | 7.53  | 128.73      | 119.70   |
| 21  | AA    | 1451 | U    | N1-C1'-C2' | 7.53  | 123.78      | 114.00   |
| 24  | BA    | 272  | A    | P-O3'-C3'  | -7.53 | 110.67      | 119.70   |
| 24  | DA    | 480  | A    | P-O3'-C3'  | -7.53 | 110.67      | 119.70   |
| 24  | BA    | 1478 | G    | N3-C4-C5   | 7.52  | 132.36      | 128.60   |
| 24  | DA    | 1276 | A    | P-O3'-C3'  | -7.52 | 110.67      | 119.70   |
| 24  | DA    | 93   | G    | P-O3'-C3'  | -7.52 | 110.67      | 119.70   |
| 25  | BB    | 26   | C    | N1-C1'-C2' | -7.52 | 103.73      | 112.00   |
| 25  | BB    | 26   | C    | P-O3'-C3'  | -7.52 | 110.68      | 119.70   |
| 55  | CA    | 566  | G    | P-O3'-C3'  | 7.52  | 128.72      | 119.70   |
| 55  | CA    | 885  | G    | P-O3'-C3'  | -7.51 | 110.69      | 119.70   |
| 55  | CA    | 421  | U    | P-O3'-C3'  | 7.51  | 128.71      | 119.70   |
| 24  | BA    | 2777 | G    | O4'-C1'-N9 | -7.50 | 102.20      | 108.20   |
| 55  | CA    | 1285 | A    | P-O3'-C3'  | 7.50  | 128.70      | 119.70   |
| 21  | AA    | 821  | G    | P-O3'-C3'  | -7.50 | 110.70      | 119.70   |
| 24  | BA    | 2884 | U    | O4'-C1'-N1 | 7.50  | 114.20      | 108.20   |
| 24  | DA    | 482  | A    | P-O3'-C3'  | -7.50 | 110.70      | 119.70   |
| 55  | CA    | 1055 | A    | P-O3'-C3'  | -7.50 | 110.70      | 119.70   |
| 55  | CA    | 977  | A    | P-O3'-C3'  | -7.49 | 110.72      | 119.70   |
| 24  | DA    | 1326 | U    | N1-C1'-C2' | -7.48 | 103.77      | 112.00   |
| 24  | DA    | 1535 | A    | P-O3'-C3'  | 7.48  | 128.68      | 119.70   |
| 24  | DA    | 1674 | G    | C4-N9-C1'  | 7.48  | 136.22      | 126.50   |
| 24  | DA    | 2310 | C    | N1-C1'-C2' | -7.48 | 103.77      | 112.00   |
| 24  | DA    | 1782 | U    | O4'-C1'-N1 | 7.48  | 114.18      | 108.20   |
| 24  | BA    | 1557 | C    | P-O3'-C3'  | -7.47 | 110.73      | 119.70   |
| 56  | DB    | 56   | G    | P-O3'-C3'  | 7.47  | 128.66      | 119.70   |
| 55  | CA    | 13   | U    | P-O3'-C3'  | 7.46  | 128.66      | 119.70   |
| 55  | CA    | 426  | U    | P-O3'-C3'  | -7.46 | 110.74      | 119.70   |
| 24  | DA    | 1649 | G    | P-O3'-C3'  | -7.46 | 110.75      | 119.70   |
| 55  | CA    | 500  | G    | N9-C1'-C2' | -7.46 | 103.79      | 112.00   |
| 24  | BA    | 1496 | A    | P-O3'-C3'  | -7.46 | 110.75      | 119.70   |
| 55  | CA    | 984  | C    | N1-C1'-C2' | -7.46 | 103.79      | 112.00   |
| 21  | AA    | 1382 | C    | N1-C1'-C2' | -7.46 | 103.80      | 112.00   |
| 24  | DA    | 1387 | A    | N9-C1'-C2' | -7.46 | 103.80      | 112.00   |
| 24  | BA    | 919  | U    | C2-N3-C4   | 7.46  | 131.47      | 127.00   |
| 24  | DA    | 2713 | U    | O4'-C1'-N1 | -7.46 | 102.23      | 108.20   |
| 24  | BA    | 1207 | C    | P-O3'-C3'  | -7.45 | 110.75      | 119.70   |
| 55  | CA    | 1129 | C    | P-O3'-C3'  | 7.45  | 128.64      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | DA    | 92   | U    | N1-C1'-C2' | -7.45 | 103.80      | 112.00   |
| 24  | BA    | 1708 | C    | N1-C1'-C2' | -7.45 | 103.80      | 112.00   |
| 24  | DA    | 963  | U    | O4'-C1'-N1 | 7.45  | 114.16      | 108.20   |
| 24  | DA    | 995  | C    | P-O3'-C3'  | 7.45  | 128.64      | 119.70   |
| 24  | DA    | 2716 | C    | O4'-C1'-N1 | 7.45  | 114.16      | 108.20   |
| 24  | BA    | 588  | U    | P-O3'-C3'  | -7.45 | 110.77      | 119.70   |
| 55  | CA    | 1045 | C    | P-O3'-C3'  | -7.45 | 110.76      | 119.70   |
| 24  | DA    | 1696 | G    | P-O3'-C3'  | -7.45 | 110.77      | 119.70   |
| 24  | BA    | 633  | A    | O4'-C1'-N9 | -7.44 | 102.25      | 108.20   |
| 24  | DA    | 2282 | G    | P-O3'-C3'  | 7.44  | 128.63      | 119.70   |
| 21  | AA    | 985  | C    | N1-C1'-C2' | -7.44 | 103.81      | 112.00   |
| 24  | BA    | 764  | A    | P-O3'-C3'  | 7.44  | 128.63      | 119.70   |
| 24  | DA    | 2307 | G    | P-O3'-C3'  | 7.44  | 128.62      | 119.70   |
| 24  | BA    | 139  | U    | O4'-C1'-N1 | 7.43  | 114.15      | 108.20   |
| 21  | AA    | 1190 | G    | P-O3'-C3'  | 7.43  | 128.62      | 119.70   |
| 24  | BA    | 73   | A    | N9-C1'-C2' | -7.43 | 103.83      | 112.00   |
| 24  | BA    | 1345 | C    | P-O5'-C5'  | -7.43 | 109.02      | 120.90   |
| 21  | AA    | 1476 | A    | P-O3'-C3'  | -7.43 | 110.79      | 119.70   |
| 24  | BA    | 1011 | G    | P-O3'-C3'  | 7.43  | 128.61      | 119.70   |
| 24  | BA    | 2072 | C    | O4'-C1'-N1 | -7.43 | 102.26      | 108.20   |
| 24  | BA    | 2385 | C    | N1-C1'-C2' | -7.43 | 103.83      | 112.00   |
| 24  | BA    | 2572 | A    | P-O3'-C3'  | 7.43  | 128.61      | 119.70   |
| 24  | BA    | 2868 | A    | P-O3'-C3'  | -7.43 | 110.79      | 119.70   |
| 55  | CA    | 1200 | C    | P-O3'-C3'  | 7.43  | 128.61      | 119.70   |
| 25  | BB    | 43   | C    | N1-C1'-C2' | -7.42 | 103.83      | 112.00   |
| 24  | DA    | 1345 | C    | O4'-C1'-N1 | 7.42  | 114.14      | 108.20   |
| 24  | BA    | 855  | G    | C8-N9-C4   | -7.41 | 103.44      | 106.40   |
| 24  | BA    | 1086 | A    | N1-C2-N3   | 7.41  | 133.01      | 129.30   |
| 24  | BA    | 1499 | C    | O4'-C1'-N1 | 7.41  | 114.13      | 108.20   |
| 24  | DA    | 2874 | C    | P-O3'-C3'  | -7.41 | 110.81      | 119.70   |
| 24  | DA    | 404  | A    | P-O3'-C3'  | 7.41  | 128.59      | 119.70   |
| 24  | DA    | 989  | G    | P-O3'-C3'  | 7.41  | 128.59      | 119.70   |
| 24  | BA    | 2215 | C    | P-O3'-C3'  | -7.40 | 110.82      | 119.70   |
| 24  | BA    | 913  | U    | N1-C1'-C2' | 7.39  | 123.61      | 114.00   |
| 24  | DA    | 1477 | A    | P-O3'-C3'  | -7.39 | 110.83      | 119.70   |
| 21  | AA    | 1097 | C    | O4'-C1'-N1 | 7.39  | 114.11      | 108.20   |
| 21  | AA    | 913  | A    | P-O3'-C3'  | 7.39  | 128.57      | 119.70   |
| 24  | DA    | 777  | G    | P-O3'-C3'  | -7.39 | 110.84      | 119.70   |
| 24  | BA    | 279  | A    | N9-C1'-C2' | -7.38 | 103.88      | 112.00   |
| 24  | BA    | 1340 | U    | N1-C1'-C2' | 7.38  | 123.60      | 114.00   |
| 24  | BA    | 2822 | G    | N1-C6-O6   | 7.38  | 124.33      | 119.90   |
| 24  | BA    | 2603 | G    | P-O3'-C3'  | -7.38 | 110.84      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | DA    | 1312 | U    | P-O3'-C3'  | 7.38  | 128.56      | 119.70   |
| 24  | DA    | 534  | U    | O4'-C1'-N1 | 7.38  | 114.10      | 108.20   |
| 24  | DA    | 1076 | C    | N1-C1'-C2' | -7.38 | 103.89      | 112.00   |
| 55  | CA    | 717  | U    | P-O3'-C3'  | 7.38  | 128.55      | 119.70   |
| 21  | AA    | 1054 | C    | P-O3'-C3'  | 7.37  | 128.55      | 119.70   |
| 24  | BA    | 206  | U    | P-O3'-C3'  | -7.37 | 110.86      | 119.70   |
| 24  | DA    | 830  | G    | P-O3'-C3'  | 7.37  | 128.54      | 119.70   |
| 21  | AA    | 210  | C    | P-O3'-C3'  | 7.37  | 128.54      | 119.70   |
| 55  | CA    | 317  | U    | O4'-C1'-N1 | 7.36  | 114.09      | 108.20   |
| 24  | BA    | 459  | U    | P-O5'-C5'  | -7.36 | 109.12      | 120.90   |
| 24  | BA    | 2337 | G    | P-O5'-C5'  | -7.36 | 109.12      | 120.90   |
| 24  | BA    | 995  | C    | P-O3'-C3'  | 7.36  | 128.53      | 119.70   |
| 24  | BA    | 1268 | A    | P-O3'-C3'  | -7.36 | 110.87      | 119.70   |
| 24  | BA    | 1086 | A    | C8-N9-C4   | -7.35 | 102.86      | 105.80   |
| 24  | BA    | 2903 | U    | O4'-C1'-N1 | 7.35  | 114.08      | 108.20   |
| 55  | CA    | 1124 | G    | P-O3'-C3'  | 7.34  | 128.51      | 119.70   |
| 21  | AA    | 934  | C    | P-O3'-C3'  | 7.34  | 128.51      | 119.70   |
| 24  | DA    | 2428 | G    | P-O3'-C3'  | -7.34 | 110.89      | 119.70   |
| 21  | AA    | 1505 | G    | P-O3'-C3'  | -7.34 | 110.89      | 119.70   |
| 24  | BA    | 915  | C    | P-O3'-C3'  | -7.33 | 110.90      | 119.70   |
| 55  | CA    | 1212 | U    | O4'-C1'-N1 | -7.33 | 102.33      | 108.20   |
| 24  | DA    | 1286 | A    | P-O3'-C3'  | 7.33  | 128.50      | 119.70   |
| 24  | BA    | 763  | G    | C6-C5-N7   | -7.33 | 126.00      | 130.40   |
| 24  | BA    | 2211 | A    | P-O3'-C3'  | 7.33  | 128.50      | 119.70   |
| 24  | DA    | 86   | G    | P-O3'-C3'  | -7.33 | 110.90      | 119.70   |
| 21  | AA    | 1053 | G    | O3'-P-O5'  | -7.33 | 90.08       | 104.00   |
| 24  | DA    | 321  | U    | P-O3'-C3'  | 7.33  | 128.50      | 119.70   |
| 24  | DA    | 325  | G    | N9-C1'-C2' | -7.32 | 103.94      | 112.00   |
| 24  | BA    | 454  | A    | P-O3'-C3'  | 7.32  | 128.49      | 119.70   |
| 55  | CA    | 575  | G    | P-O3'-C3'  | 7.32  | 128.48      | 119.70   |
| 21  | AA    | 173  | U    | P-O3'-C3'  | 7.31  | 128.48      | 119.70   |
| 24  | DA    | 958  | U    | P-O3'-C3'  | -7.31 | 110.92      | 119.70   |
| 24  | BA    | 391  | A    | P-O3'-C3'  | -7.31 | 110.93      | 119.70   |
| 24  | BA    | 1799 | G    | O4'-C1'-N9 | 7.31  | 114.05      | 108.20   |
| 24  | BA    | 2275 | C    | O4'-C1'-N1 | 7.30  | 114.04      | 108.20   |
| 24  | DA    | 2037 | A    | P-O3'-C3'  | -7.30 | 110.93      | 119.70   |
| 24  | BA    | 204  | A    | P-O3'-C3'  | 7.30  | 128.46      | 119.70   |
| 24  | BA    | 475  | C    | P-O5'-C5'  | -7.29 | 109.23      | 120.90   |
| 25  | BB    | 108  | A    | P-O3'-C3'  | 7.29  | 128.45      | 119.70   |
| 24  | DA    | 2069 | G    | N9-C1'-C2' | -7.29 | 103.98      | 112.00   |
| 21  | AA    | 1531 | A    | P-O3'-C3'  | -7.29 | 110.95      | 119.70   |
| 24  | DA    | 2460 | U    | N1-C1'-C2' | -7.29 | 103.98      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 465  | A    | P-O3'-C3'  | -7.29 | 110.95      | 119.70   |
| 24  | DA    | 2283 | C    | P-O3'-C3'  | -7.29 | 110.95      | 119.70   |
| 24  | BA    | 2007 | U    | P-O3'-C3'  | -7.29 | 110.96      | 119.70   |
| 24  | BA    | 221  | A    | P-O3'-C3'  | 7.28  | 128.44      | 119.70   |
| 24  | BA    | 1615 | C    | N1-C1'-C2' | 7.28  | 123.46      | 114.00   |
| 24  | DA    | 991  | C    | P-O3'-C3'  | -7.28 | 110.96      | 119.70   |
| 21  | AA    | 566  | G    | P-O3'-C3'  | 7.28  | 128.43      | 119.70   |
| 21  | AA    | 724  | G    | P-O3'-C3'  | -7.28 | 110.97      | 119.70   |
| 55  | CA    | 1202 | U    | P-O3'-C3'  | -7.28 | 110.97      | 119.70   |
| 24  | BA    | 1072 | C    | P-O3'-C3'  | -7.27 | 110.97      | 119.70   |
| 55  | CA    | 1337 | G    | P-O3'-C3'  | 7.27  | 128.43      | 119.70   |
| 24  | DA    | 2521 | C    | N1-C1'-C2' | -7.27 | 104.00      | 112.00   |
| 55  | CA    | 564  | C    | N1-C1'-C2' | -7.27 | 104.00      | 112.00   |
| 21  | AA    | 1085 | U    | N1-C1'-C2' | 7.27  | 123.45      | 114.00   |
| 55  | CA    | 122  | G    | N9-C1'-C2' | -7.26 | 104.01      | 112.00   |
| 55  | CA    | 984  | C    | P-O3'-C3'  | -7.26 | 110.98      | 119.70   |
| 25  | BB    | 109  | A    | P-O3'-C3'  | -7.26 | 110.99      | 119.70   |
| 24  | DA    | 2439 | A    | P-O3'-C3'  | 7.26  | 128.41      | 119.70   |
| 21  | AA    | 1046 | A    | O4'-C1'-N9 | 7.26  | 114.00      | 108.20   |
| 24  | DA    | 973  | A    | P-O3'-C3'  | 7.26  | 128.41      | 119.70   |
| 24  | BA    | 1372 | U    | C2-N3-C4   | -7.25 | 122.65      | 127.00   |
| 24  | DA    | 1936 | A    | P-O3'-C3'  | 7.25  | 128.40      | 119.70   |
| 24  | DA    | 589  | U    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 24  | DA    | 603  | A    | P-O3'-C3'  | 7.25  | 128.40      | 119.70   |
| 24  | BA    | 1706 | C    | N1-C1'-C2' | 7.25  | 123.42      | 114.00   |
| 24  | DA    | 2181 | U    | O4'-C1'-N1 | 7.25  | 114.00      | 108.20   |
| 21  | AA    | 66   | A    | P-O3'-C3'  | -7.25 | 111.01      | 119.70   |
| 24  | BA    | 2307 | G    | P-O3'-C3'  | 7.25  | 128.40      | 119.70   |
| 24  | BA    | 1732 | C    | N1-C2-O2   | -7.24 | 114.56      | 118.90   |
| 24  | DA    | 2391 | G    | P-O3'-C3'  | 7.23  | 128.38      | 119.70   |
| 21  | AA    | 1051 | C    | P-O3'-C3'  | -7.23 | 111.03      | 119.70   |
| 55  | CA    | 430  | A    | N9-C1'-C2' | -7.23 | 104.05      | 112.00   |
| 21  | AA    | 1382 | C    | O4'-C1'-N1 | 7.23  | 113.98      | 108.20   |
| 24  | DA    | 445  | C    | P-O3'-C3'  | -7.23 | 111.03      | 119.70   |
| 55  | CA    | 122  | G    | P-O3'-C3'  | -7.22 | 111.03      | 119.70   |
| 24  | DA    | 945  | A    | O4'-C1'-N9 | 7.22  | 113.98      | 108.20   |
| 24  | DA    | 1758 | U    | P-O3'-C3'  | 7.22  | 128.37      | 119.70   |
| 24  | DA    | 1965 | C    | N1-C1'-C2' | -7.22 | 104.06      | 112.00   |
| 21  | AA    | 1417 | G    | C5-C6-O6   | -7.22 | 124.27      | 128.60   |
| 24  | BA    | 1082 | U    | N1-C2-N3   | 7.21  | 119.23      | 114.90   |
| 24  | BA    | 2862 | G    | P-O3'-C3'  | -7.21 | 111.04      | 119.70   |
| 55  | CA    | 1212 | U    | N1-C1'-C2' | 7.21  | 123.38      | 114.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | BA    | 1555 | G    | P-O5'-C5'  | -7.21 | 109.36      | 120.90   |
| 24  | BA    | 1634 | A    | P-O3'-C3'  | 7.21  | 128.35      | 119.70   |
| 24  | DA    | 1780 | A    | P-O3'-C3'  | 7.21  | 128.35      | 119.70   |
| 55  | CA    | 1228 | C    | P-O3'-C3'  | -7.21 | 111.05      | 119.70   |
| 21  | AA    | 1336 | C    | P-O3'-C3'  | 7.21  | 128.35      | 119.70   |
| 24  | BA    | 233  | A    | P-O3'-C3'  | -7.20 | 111.06      | 119.70   |
| 24  | DA    | 396  | G    | N9-C1'-C2' | -7.20 | 104.08      | 112.00   |
| 24  | BA    | 125  | A    | O4'-C1'-N1 | 7.20  | 113.96      | 108.20   |
| 24  | BA    | 528  | A    | P-O3'-C3'  | -7.20 | 111.06      | 119.70   |
| 24  | BA    | 1451 | C    | N1-C1'-C2' | 7.20  | 123.36      | 114.00   |
| 24  | BA    | 812  | C    | P-O3'-C3'  | -7.20 | 111.06      | 119.70   |
| 55  | CA    | 597  | G    | N9-C1'-C2' | -7.20 | 104.08      | 112.00   |
| 55  | CA    | 64   | G    | P-O3'-C3'  | 7.19  | 128.33      | 119.70   |
| 21  | AA    | 960  | U    | N1-C1'-C2' | 7.19  | 123.35      | 114.00   |
| 24  | DA    | 1158 | C    | O4'-C1'-N1 | 7.19  | 113.95      | 108.20   |
| 24  | DA    | 436  | C    | N1-C1'-C2' | -7.19 | 104.09      | 112.00   |
| 24  | BA    | 616  | A    | P-O3'-C3'  | -7.19 | 111.07      | 119.70   |
| 24  | BA    | 2053 | G    | P-O3'-C3'  | -7.19 | 111.07      | 119.70   |
| 24  | BA    | 1213 | A    | P-O3'-C3'  | -7.19 | 111.07      | 119.70   |
| 24  | DA    | 975  | A    | P-O3'-C3'  | -7.18 | 111.08      | 119.70   |
| 24  | DA    | 627  | A    | P-O3'-C3'  | 7.18  | 128.31      | 119.70   |
| 21  | AA    | 199  | A    | N9-C1'-C2' | -7.18 | 104.11      | 112.00   |
| 24  | BA    | 1714 | U    | P-O3'-C3'  | -7.18 | 111.09      | 119.70   |
| 24  | BA    | 2595 | G    | P-O3'-C3'  | -7.18 | 111.09      | 119.70   |
| 24  | DA    | 790  | U    | P-O3'-C3'  | -7.18 | 111.09      | 119.70   |
| 21  | AA    | 453  | G    | N9-C1'-C2' | -7.17 | 104.11      | 112.00   |
| 55  | CA    | 1200 | C    | O4'-C1'-N1 | -7.17 | 102.46      | 108.20   |
| 55  | CA    | 1137 | C    | N1-C1'-C2' | 7.17  | 123.33      | 114.00   |
| 21  | AA    | 1531 | A    | N9-C1'-C2' | -7.17 | 104.11      | 112.00   |
| 24  | BA    | 2199 | A    | P-O5'-C5'  | -7.17 | 109.43      | 120.90   |
| 24  | BA    | 2427 | C    | P-O3'-C3'  | -7.17 | 111.10      | 119.70   |
| 21  | AA    | 1170 | A    | N9-C1'-C2' | -7.17 | 104.12      | 112.00   |
| 24  | BA    | 1091 | G    | P-O3'-C3'  | -7.17 | 111.10      | 119.70   |
| 24  | BA    | 974  | G    | P-O3'-C3'  | 7.17  | 128.30      | 119.70   |
| 24  | DA    | 1946 | U    | O4'-C1'-N1 | 7.16  | 113.93      | 108.20   |
| 55  | CA    | 595  | A    | P-O3'-C3'  | 7.16  | 128.29      | 119.70   |
| 24  | DA    | 1576 | U    | O4'-C1'-N1 | 7.16  | 113.92      | 108.20   |
| 24  | BA    | 2063 | C    | O4'-C1'-N1 | -7.15 | 102.48      | 108.20   |
| 55  | CA    | 1283 | U    | P-O3'-C3'  | -7.15 | 111.12      | 119.70   |
| 55  | CA    | 14   | U    | P-O3'-C3'  | -7.15 | 111.12      | 119.70   |
| 24  | DA    | 1249 | U    | O4'-C1'-N1 | 7.15  | 113.92      | 108.20   |
| 24  | BA    | 1669 | A    | P-O3'-C3'  | -7.14 | 111.13      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | DA    | 1931 | U    | N1-C1'-C2' | -7.14 | 104.14      | 112.00   |
| 24  | BA    | 1060 | U    | N3-C4-O4   | 7.14  | 124.40      | 119.40   |
| 24  | DA    | 832  | U    | P-O5'-C5'  | -7.14 | 109.47      | 120.90   |
| 21  | AA    | 885  | G    | N9-C1'-C2' | -7.14 | 104.15      | 112.00   |
| 24  | BA    | 1238 | G    | N9-C1'-C2' | -7.14 | 104.15      | 112.00   |
| 24  | BA    | 2772 | C    | C6-N1-C2   | 7.14  | 123.16      | 120.30   |
| 24  | BA    | 163  | C    | P-O3'-C3'  | -7.14 | 111.13      | 119.70   |
| 24  | BA    | 1022 | G    | N3-C4-C5   | 7.14  | 132.17      | 128.60   |
| 55  | CA    | 1336 | C    | P-O3'-C3'  | 7.14  | 128.27      | 119.70   |
| 21  | AA    | 78   | A    | C6-N1-C2   | -7.14 | 114.32      | 118.60   |
| 21  | AA    | 1169 | A    | P-O3'-C3'  | -7.13 | 111.14      | 119.70   |
| 55  | CA    | 998  | C    | O4'-C1'-N1 | 7.13  | 113.91      | 108.20   |
| 55  | CA    | 870  | U    | P-O3'-C3'  | 7.13  | 128.26      | 119.70   |
| 24  | BA    | 704  | G    | P-O3'-C3'  | 7.13  | 128.25      | 119.70   |
| 24  | DA    | 647  | G    | P-O3'-C3'  | -7.13 | 111.15      | 119.70   |
| 24  | DA    | 1569 | A    | P-O3'-C3'  | -7.13 | 111.14      | 119.70   |
| 24  | BA    | 2821 | A    | P-O3'-C3'  | -7.13 | 111.15      | 119.70   |
| 24  | DA    | 2350 | C    | O4'-C1'-N1 | 7.13  | 113.90      | 108.20   |
| 56  | DB    | 58   | A    | P-O3'-C3'  | -7.12 | 111.15      | 119.70   |
| 24  | BA    | 1779 | U    | C5-C6-N1   | -7.12 | 119.14      | 122.70   |
| 24  | BA    | 301  | G    | C6-C5-N7   | 7.12  | 134.67      | 130.40   |
| 21  | AA    | 533  | A    | P-O3'-C3'  | 7.12  | 128.24      | 119.70   |
| 24  | BA    | 2857 | G    | C4-C5-N7   | 7.12  | 113.65      | 110.80   |
| 21  | AA    | 253  | A    | N9-C1'-C2' | -7.11 | 104.17      | 112.00   |
| 55  | CA    | 47   | C    | P-O3'-C3'  | 7.11  | 128.24      | 119.70   |
| 55  | CA    | 212  | G    | P-O3'-C3'  | -7.11 | 111.16      | 119.70   |
| 24  | DA    | 1304 | A    | N9-C1'-C2' | -7.11 | 104.17      | 112.00   |
| 24  | DA    | 1615 | C    | P-O3'-C3'  | 7.11  | 128.24      | 119.70   |
| 21  | AA    | 517  | G    | P-O3'-C3'  | 7.11  | 128.23      | 119.70   |
| 24  | BA    | 1633 | G    | P-O3'-C3'  | 7.11  | 128.23      | 119.70   |
| 24  | BA    | 1664 | A    | P-O3'-C3'  | 7.11  | 128.23      | 119.70   |
| 24  | DA    | 1822 | C    | O4'-C1'-N1 | 7.11  | 113.88      | 108.20   |
| 24  | BA    | 1654 | A    | N9-C1'-C2' | -7.10 | 104.19      | 112.00   |
| 55  | CA    | 1382 | C    | N1-C1'-C2' | -7.10 | 104.19      | 112.00   |
| 24  | BA    | 1129 | A    | P-O3'-C3'  | -7.10 | 111.18      | 119.70   |
| 24  | BA    | 61   | C    | P-O5'-C5'  | -7.10 | 109.54      | 120.90   |
| 55  | CA    | 83   | C    | P-O3'-C3'  | 7.10  | 128.22      | 119.70   |
| 21  | AA    | 1496 | C    | C6-N1-C2   | 7.10  | 123.14      | 120.30   |
| 24  | BA    | 628  | G    | P-O3'-C3'  | -7.10 | 111.18      | 119.70   |
| 55  | CA    | 374  | A    | P-O3'-C3'  | -7.10 | 111.18      | 119.70   |
| 24  | DA    | 2069 | G    | P-O3'-C3'  | -7.09 | 111.19      | 119.70   |
| 24  | DA    | 2267 | A    | N9-C4-C5   | -7.09 | 102.96      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 2275 | C    | O4'-C1'-N1  | 7.09  | 113.88      | 108.20   |
| 24  | BA    | 907  | G    | N3-C4-C5    | 7.09  | 132.15      | 128.60   |
| 55  | CA    | 1169 | A    | P-O3'-C3'   | 7.09  | 128.21      | 119.70   |
| 24  | DA    | 228  | C    | O4'-C1'-N1  | 7.09  | 113.87      | 108.20   |
| 24  | BA    | 1311 | G    | P-O3'-C3'   | 7.09  | 128.20      | 119.70   |
| 24  | DA    | 2408 | U    | O4'-C1'-N1  | 7.09  | 113.87      | 108.20   |
| 21  | AA    | 81   | A    | O4'-C1'-N9  | 7.08  | 113.87      | 108.20   |
| 55  | CA    | 549  | C    | N1-C1'-C2'  | -7.08 | 104.21      | 112.00   |
| 55  | CA    | 1240 | U    | O4'-C1'-N1  | 7.08  | 113.86      | 108.20   |
| 21  | AA    | 329  | A    | O4'-C1'-N9  | -7.07 | 102.54      | 108.20   |
| 24  | BA    | 455  | C    | O4'-C1'-N1  | -7.07 | 102.54      | 108.20   |
| 24  | DA    | 1287 | A    | P-O3'-C3'   | 7.07  | 128.18      | 119.70   |
| 24  | BA    | 685  | A    | O3'-P-O5'   | 7.07  | 117.43      | 104.00   |
| 24  | BA    | 1805 | A    | N9-C4-C5    | 7.07  | 108.63      | 105.80   |
| 24  | BA    | 2724 | U    | P-O3'-C3'   | 7.06  | 128.18      | 119.70   |
| 55  | CA    | 458  | U    | P-O3'-C3'   | 7.06  | 128.18      | 119.70   |
| 24  | BA    | 774  | G    | P-O3'-C3'   | 7.06  | 128.18      | 119.70   |
| 24  | BA    | 2857 | G    | C6-C5-N7    | -7.06 | 126.17      | 130.40   |
| 55  | CA    | 1381 | U    | P-O3'-C3'   | -7.06 | 111.23      | 119.70   |
| 24  | BA    | 1499 | C    | P-O3'-C3'   | -7.06 | 111.23      | 119.70   |
| 24  | BA    | 919  | U    | O4'-C1'-N1  | -7.05 | 102.56      | 108.20   |
| 55  | CA    | 210  | C    | P-O3'-C3'   | 7.05  | 128.17      | 119.70   |
| 55  | CA    | 465  | A    | P-O3'-C3'   | -7.05 | 111.23      | 119.70   |
| 21  | AA    | 549  | C    | P-O3'-C3'   | -7.05 | 111.24      | 119.70   |
| 24  | DA    | 15   | G    | P-O3'-C3'   | -7.05 | 111.24      | 119.70   |
| 21  | AA    | 185  | U    | P-O3'-C3'   | -7.05 | 111.24      | 119.70   |
| 24  | BA    | 2321 | U    | P-O3'-C3'   | -7.05 | 111.24      | 119.70   |
| 24  | DA    | 1674 | G    | C8-N9-C1'   | -7.05 | 117.84      | 127.00   |
| 55  | CA    | 1074 | G    | P-O3'-C3'   | -7.04 | 111.25      | 119.70   |
| 24  | DA    | 933  | A    | P-O3'-C3'   | -7.04 | 111.25      | 119.70   |
| 21  | AA    | 1131 | G    | P-O3'-C3'   | -7.04 | 111.25      | 119.70   |
| 24  | BA    | 1298 | C    | P-O5'-C5'   | -7.04 | 109.63      | 120.90   |
| 55  | CA    | 934  | C    | O4'-C1'-N1  | 7.04  | 113.83      | 108.20   |
| 24  | BA    | 2808 | G    | P-O3'-C3'   | 7.04  | 128.15      | 119.70   |
| 21  | AA    | 567  | G    | C3'-C2'-C1' | 7.04  | 107.13      | 101.50   |
| 24  | DA    | 2447 | G    | C5-C6-N1    | 7.03  | 115.02      | 111.50   |
| 24  | DA    | 2542 | A    | P-O3'-C3'   | 7.03  | 128.14      | 119.70   |
| 24  | BA    | 621  | A    | N9-C1'-C2'  | -7.03 | 104.27      | 112.00   |
| 24  | BA    | 2860 | A    | C5-C6-N1    | -7.03 | 114.19      | 117.70   |
| 24  | DA    | 984  | A    | P-O3'-C3'   | 7.03  | 128.13      | 119.70   |
| 55  | CA    | 1296 | C    | O4'-C1'-N1  | 7.03  | 113.82      | 108.20   |
| 24  | BA    | 1326 | U    | P-O3'-C3'   | -7.02 | 111.27      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | AA    | 78   | A    | C5-C6-N6   | -7.02 | 118.08      | 123.70   |
| 21  | AA    | 1137 | C    | P-O3'-C3'  | 7.02  | 128.13      | 119.70   |
| 24  | BA    | 85   | G    | P-O3'-C3'  | -7.02 | 111.27      | 119.70   |
| 24  | BA    | 216  | A    | N9-C1'-C2' | -7.02 | 104.28      | 112.00   |
| 24  | DA    | 1758 | U    | N1-C1'-C2' | 7.02  | 123.13      | 114.00   |
| 21  | AA    | 81   | A    | P-O3'-C3'  | 7.02  | 128.12      | 119.70   |
| 24  | BA    | 1936 | A    | P-O3'-C3'  | 7.02  | 128.12      | 119.70   |
| 31  | BH    | 48   | GLU  | N-CA-CB    | -7.02 | 97.97       | 110.60   |
| 24  | DA    | 265  | A    | O4'-C1'-N9 | 7.02  | 113.81      | 108.20   |
| 21  | AA    | 559  | A    | P-O3'-C3'  | 7.02  | 128.12      | 119.70   |
| 21  | AA    | 1054 | C    | P-O5'-C5'  | -7.01 | 109.68      | 120.90   |
| 21  | AA    | 1031 | C    | P-O3'-C3'  | 7.01  | 128.11      | 119.70   |
| 24  | DA    | 755  | U    | O4'-C1'-N1 | 7.01  | 113.81      | 108.20   |
| 24  | DA    | 2611 | C    | P-O3'-C3'  | -7.01 | 111.29      | 119.70   |
| 24  | DA    | 437  | U    | P-O3'-C3'  | -7.00 | 111.30      | 119.70   |
| 24  | DA    | 1108 | U    | O4'-C1'-N1 | 7.00  | 113.80      | 108.20   |
| 55  | CA    | 464  | U    | N1-C1'-C2' | -7.00 | 104.30      | 112.00   |
| 24  | DA    | 775  | G    | O4'-C1'-N9 | 6.99  | 113.80      | 108.20   |
| 24  | BA    | 2044 | C    | O4'-C1'-N1 | -6.99 | 102.61      | 108.20   |
| 24  | DA    | 1716 | U    | N1-C1'-C2' | -6.99 | 104.31      | 112.00   |
| 24  | BA    | 299  | A    | C5-N7-C8   | -6.99 | 100.41      | 103.90   |
| 24  | DA    | 2613 | U    | P-O3'-C3'  | 6.99  | 128.09      | 119.70   |
| 24  | DA    | 1539 | U    | O4'-C1'-N1 | 6.99  | 113.79      | 108.20   |
| 24  | BA    | 1324 | G    | P-O3'-C3'  | 6.99  | 128.09      | 119.70   |
| 24  | DA    | 740  | C    | P-O3'-C3'  | 6.99  | 128.08      | 119.70   |
| 24  | DA    | 617  | G    | N9-C1'-C2' | -6.97 | 104.33      | 112.00   |
| 24  | DA    | 1669 | A    | P-O3'-C3'  | -6.97 | 111.33      | 119.70   |
| 24  | DA    | 2616 | C    | P-O3'-C3'  | -6.97 | 111.33      | 119.70   |
| 24  | DA    | 335  | C    | O4'-C1'-N1 | 6.97  | 113.78      | 108.20   |
| 24  | BA    | 752  | A    | O4'-C1'-N9 | 6.97  | 113.78      | 108.20   |
| 24  | BA    | 945  | A    | P-O3'-C3'  | 6.97  | 128.06      | 119.70   |
| 24  | BA    | 396  | G    | N9-C1'-C2' | -6.96 | 104.34      | 112.00   |
| 24  | BA    | 868  | U    | P-O3'-C3'  | 6.96  | 128.06      | 119.70   |
| 24  | BA    | 2610 | C    | P-O3'-C3'  | 6.96  | 128.06      | 119.70   |
| 24  | DA    | 302  | C    | N1-C1'-C2' | -6.96 | 104.34      | 112.00   |
| 24  | BA    | 530  | G    | C4-N9-C1'  | 6.96  | 135.54      | 126.50   |
| 55  | CA    | 348  | G    | N9-C1'-C2' | -6.96 | 104.35      | 112.00   |
| 55  | CA    | 1399 | C    | P-O3'-C3'  | 6.96  | 128.05      | 119.70   |
| 24  | DA    | 2225 | A    | P-O3'-C3'  | 6.96  | 128.05      | 119.70   |
| 24  | DA    | 1256 | G    | P-O3'-C3'  | -6.95 | 111.36      | 119.70   |
| 24  | DA    | 2334 | U    | O4'-C1'-N1 | 6.95  | 113.76      | 108.20   |
| 24  | BA    | 1073 | A    | P-O3'-C3'  | -6.95 | 111.36      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 232  | G    | P-O3'-C3'   | 6.95  | 128.04      | 119.70   |
| 25  | BB    | 3    | C    | P-O3'-C3'   | -6.95 | 111.36      | 119.70   |
| 24  | BA    | 61   | C    | N1-C1'-C2'  | -6.95 | 104.36      | 112.00   |
| 24  | BA    | 1707 | G    | P-O3'-C3'   | -6.95 | 111.36      | 119.70   |
| 24  | BA    | 2691 | C    | P-O3'-C3'   | -6.94 | 111.37      | 119.70   |
| 24  | BA    | 1523 | U    | O4'-C1'-N1  | 6.94  | 113.75      | 108.20   |
| 21  | AA    | 213  | G    | N9-C1'-C2'  | -6.94 | 104.36      | 112.00   |
| 24  | BA    | 1782 | U    | P-O3'-C3'   | -6.94 | 111.37      | 119.70   |
| 55  | CA    | 519  | C    | O4'-C1'-N1  | 6.94  | 113.75      | 108.20   |
| 24  | DA    | 807  | U    | P-O3'-C3'   | -6.94 | 111.37      | 119.70   |
| 24  | BA    | 2069 | G    | P-O3'-C3'   | -6.94 | 111.38      | 119.70   |
| 55  | CA    | 885  | G    | N9-C1'-C2'  | -6.94 | 104.37      | 112.00   |
| 24  | BA    | 2034 | U    | N1-C1'-C2'  | -6.93 | 104.37      | 112.00   |
| 24  | BA    | 468  | G    | P-O5'-C5'   | -6.93 | 109.81      | 120.90   |
| 24  | BA    | 2296 | U    | O4'-C1'-N1  | -6.93 | 102.66      | 108.20   |
| 24  | DA    | 2267 | A    | N3-C4-N9    | 6.93  | 132.94      | 127.40   |
| 21  | AA    | 1051 | C    | N1-C1'-C2'  | -6.92 | 104.39      | 112.00   |
| 24  | BA    | 1273 | U    | N1-C1'-C2'  | -6.92 | 104.39      | 112.00   |
| 24  | BA    | 1455 | G    | P-O3'-C3'   | -6.92 | 111.39      | 119.70   |
| 24  | DA    | 1962 | C    | P-O3'-C3'   | 6.92  | 128.00      | 119.70   |
| 24  | BA    | 2576 | G    | P-O3'-C3'   | 6.92  | 128.00      | 119.70   |
| 24  | DA    | 1722 | A    | P-O3'-C3'   | -6.92 | 111.40      | 119.70   |
| 24  | DA    | 1734 | G    | P-O3'-C3'   | -6.92 | 111.40      | 119.70   |
| 24  | BA    | 747  | U    | P-O3'-C3'   | -6.92 | 111.40      | 119.70   |
| 55  | CA    | 1033 | G    | N9-C1'-C2'  | -6.92 | 104.39      | 112.00   |
| 24  | DA    | 2060 | A    | P-O3'-C3'   | 6.92  | 128.00      | 119.70   |
| 21  | AA    | 1417 | G    | C4-C5-N7    | 6.91  | 113.56      | 110.80   |
| 24  | BA    | 777  | G    | N9-C1'-C2'  | -6.91 | 104.39      | 112.00   |
| 24  | DA    | 605  | G    | P-O3'-C3'   | -6.91 | 111.40      | 119.70   |
| 24  | BA    | 1396 | U    | P-O3'-C3'   | 6.91  | 128.00      | 119.70   |
| 24  | BA    | 1526 | C    | C6-N1-C2    | 6.91  | 123.06      | 120.30   |
| 24  | BA    | 1654 | A    | C3'-C2'-C1' | 6.91  | 107.03      | 101.50   |
| 24  | DA    | 2875 | C    | P-O3'-C3'   | -6.91 | 111.41      | 119.70   |
| 21  | AA    | 1345 | U    | O4'-C1'-N1  | 6.91  | 113.73      | 108.20   |
| 24  | BA    | 1073 | A    | N9-C1'-C2'  | -6.91 | 104.40      | 112.00   |
| 55  | CA    | 1366 | C    | N1-C1'-C2'  | -6.91 | 104.40      | 112.00   |
| 56  | DB    | 76   | G    | N3-C4-N9    | -6.91 | 121.86      | 126.00   |
| 24  | BA    | 1478 | G    | C4-N9-C1'   | -6.91 | 117.52      | 126.50   |
| 24  | BA    | 2063 | C    | P-O3'-C3'   | -6.91 | 111.41      | 119.70   |
| 24  | DA    | 2896 | C    | P-O3'-C3'   | -6.91 | 111.41      | 119.70   |
| 24  | BA    | 504  | A    | P-O5'-C5'   | -6.91 | 109.85      | 120.90   |
| 24  | BA    | 1509 | A    | O4'-C1'-N9  | 6.91  | 113.72      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 55  | CA    | 1382 | C    | P-O3'-C3'  | -6.90 | 111.42      | 119.70   |
| 21  | AA    | 1349 | A    | P-O3'-C3'  | -6.90 | 111.42      | 119.70   |
| 24  | BA    | 2382 | G    | P-O3'-C3'  | 6.90  | 127.98      | 119.70   |
| 24  | DA    | 913  | U    | P-O3'-C3'  | 6.90  | 127.98      | 119.70   |
| 24  | DA    | 1460 | U    | P-O3'-C3'  | 6.90  | 127.98      | 119.70   |
| 24  | BA    | 1334 | G    | P-O3'-C3'  | -6.90 | 111.42      | 119.70   |
| 24  | DA    | 2283 | C    | O4'-C1'-N1 | 6.90  | 113.72      | 108.20   |
| 24  | BA    | 1556 | C    | O4'-C1'-N1 | 6.90  | 113.72      | 108.20   |
| 55  | CA    | 131  | A    | P-O5'-C5'  | -6.90 | 109.86      | 120.90   |
| 24  | DA    | 1942 | C    | N1-C1'-C2' | -6.90 | 104.41      | 112.00   |
| 21  | AA    | 332  | G    | N9-C1'-C2' | -6.90 | 104.42      | 112.00   |
| 21  | AA    | 9    | G    | N9-C1'-C2' | -6.89 | 104.42      | 112.00   |
| 24  | DA    | 424  | G    | N9-C1'-C2' | -6.89 | 104.42      | 112.00   |
| 21  | AA    | 1224 | U    | C2-N3-C4   | -6.89 | 122.86      | 127.00   |
| 24  | DA    | 2333 | A    | P-O3'-C3'  | 6.89  | 127.97      | 119.70   |
| 24  | BA    | 232  | G    | P-O3'-C3'  | 6.89  | 127.97      | 119.70   |
| 24  | BA    | 2062 | A    | P-O3'-C3'  | -6.89 | 111.43      | 119.70   |
| 24  | BA    | 2860 | A    | C4-C5-C6   | 6.89  | 120.44      | 117.00   |
| 21  | AA    | 388  | G    | P-O3'-C3'  | 6.89  | 127.97      | 119.70   |
| 55  | CA    | 1288 | A    | P-O3'-C3'  | -6.89 | 111.43      | 119.70   |
| 24  | DA    | 1511 | G    | P-O3'-C3'  | -6.89 | 111.44      | 119.70   |
| 24  | DA    | 1683 | U    | O4'-C1'-N1 | 6.88  | 113.71      | 108.20   |
| 24  | BA    | 2815 | C    | P-O3'-C3'  | -6.88 | 111.44      | 119.70   |
| 55  | CA    | 596  | A    | P-O3'-C3'  | -6.88 | 111.44      | 119.70   |
| 55  | CA    | 717  | U    | N1-C1'-C2' | 6.88  | 122.94      | 114.00   |
| 55  | CA    | 752  | G    | P-O3'-C3'  | 6.88  | 127.95      | 119.70   |
| 55  | CA    | 1284 | C    | O4'-C1'-N1 | 6.88  | 113.70      | 108.20   |
| 24  | DA    | 1839 | G    | N9-C1'-C2' | -6.88 | 104.43      | 112.00   |
| 24  | BA    | 1142 | A    | C4-C5-N7   | 6.87  | 114.14      | 110.70   |
| 24  | BA    | 1247 | A    | O4'-C1'-N9 | 6.87  | 113.70      | 108.20   |
| 24  | BA    | 2513 | A    | N9-C4-C5   | 6.87  | 108.55      | 105.80   |
| 24  | BA    | 974  | G    | N7-C8-N9   | 6.87  | 116.53      | 113.10   |
| 25  | BB    | 36   | C    | O4'-C1'-N1 | -6.87 | 102.71      | 108.20   |
| 55  | CA    | 91   | U    | O4'-C1'-N1 | 6.87  | 113.69      | 108.20   |
| 21  | AA    | 794  | A    | P-O3'-C3'  | -6.87 | 111.46      | 119.70   |
| 24  | BA    | 2822 | G    | P-O3'-C3'  | -6.86 | 111.47      | 119.70   |
| 24  | BA    | 2229 | U    | O4'-C1'-N1 | 6.86  | 113.69      | 108.20   |
| 55  | CA    | 374  | A    | N9-C1'-C2' | -6.86 | 104.46      | 112.00   |
| 21  | AA    | 47   | C    | N1-C1'-C2' | 6.86  | 122.91      | 114.00   |
| 24  | BA    | 2860 | A    | N9-C4-C5   | -6.86 | 103.06      | 105.80   |
| 24  | BA    | 800  | A    | P-O3'-C3'  | 6.85  | 127.92      | 119.70   |
| 24  | BA    | 1019 | U    | N1-C2-O2   | -6.85 | 118.00      | 122.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 1381 | U    | N1-C1'-C2'  | -6.85 | 104.47      | 112.00   |
| 24  | DA    | 1970 | A    | P-O3'-C3'   | 6.85  | 127.92      | 119.70   |
| 24  | BA    | 70   | G    | P-O3'-C3'   | 6.85  | 127.92      | 119.70   |
| 24  | BA    | 137  | U    | O4'-C1'-N1  | -6.85 | 102.72      | 108.20   |
| 24  | BA    | 434  | U    | P-O3'-C3'   | 6.85  | 127.92      | 119.70   |
| 24  | BA    | 1274 | A    | P-O3'-C3'   | -6.85 | 111.48      | 119.70   |
| 24  | BA    | 1495 | A    | P-O3'-C3'   | -6.85 | 111.48      | 119.70   |
| 24  | BA    | 1452 | G    | N3-C4-C5    | 6.84  | 132.02      | 128.60   |
| 24  | BA    | 802  | A    | C3'-C2'-C1' | 6.84  | 106.97      | 101.50   |
| 24  | BA    | 1805 | A    | N1-C6-N6    | -6.84 | 114.50      | 118.60   |
| 24  | DA    | 1556 | C    | O4'-C1'-N1  | 6.84  | 113.67      | 108.20   |
| 21  | AA    | 687  | A    | P-O5'-C5'   | 6.83  | 131.84      | 120.90   |
| 55  | CA    | 252  | U    | O4'-C1'-N1  | 6.83  | 113.67      | 108.20   |
| 21  | AA    | 1228 | C    | P-O3'-C3'   | -6.83 | 111.50      | 119.70   |
| 24  | DA    | 2280 | G    | P-O3'-C3'   | -6.83 | 111.50      | 119.70   |
| 24  | DA    | 2314 | A    | N9-C1'-C2'  | -6.83 | 104.48      | 112.00   |
| 21  | AA    | 575  | G    | N3-C4-C5    | 6.83  | 132.02      | 128.60   |
| 24  | BA    | 2701 | U    | C2-N3-C4    | -6.83 | 122.90      | 127.00   |
| 24  | BA    | 2883 | A    | N1-C6-N6    | 6.83  | 122.70      | 118.60   |
| 21  | AA    | 1432 | G    | P-O3'-C3'   | 6.83  | 127.89      | 119.70   |
| 24  | DA    | 746  | U    | N1-C1'-C2'  | 6.83  | 122.88      | 114.00   |
| 24  | BA    | 1868 | C    | O4'-C1'-N1  | 6.83  | 113.66      | 108.20   |
| 24  | BA    | 2542 | A    | P-O3'-C3'   | 6.83  | 127.89      | 119.70   |
| 55  | CA    | 373  | A    | N9-C1'-C2'  | -6.82 | 104.49      | 112.00   |
| 24  | DA    | 1929 | G    | P-O3'-C3'   | 6.82  | 127.89      | 119.70   |
| 21  | AA    | 1242 | G    | P-O3'-C3'   | -6.82 | 111.51      | 119.70   |
| 24  | BA    | 1359 | A    | C5-N7-C8    | -6.82 | 100.49      | 103.90   |
| 24  | DA    | 2143 | C    | O4'-C1'-N1  | 6.82  | 113.65      | 108.20   |
| 56  | DB    | 44   | G    | P-O3'-C3'   | 6.82  | 127.88      | 119.70   |
| 24  | BA    | 1941 | C    | N1-C1'-C2'  | -6.82 | 104.50      | 112.00   |
| 24  | DA    | 1136 | G    | N9-C1'-C2'  | -6.82 | 104.50      | 112.00   |
| 24  | BA    | 1334 | G    | P-O5'-C5'   | -6.81 | 110.00      | 120.90   |
| 21  | AA    | 89   | U    | O4'-C1'-N1  | 6.81  | 113.65      | 108.20   |
| 24  | BA    | 250  | G    | P-O3'-C3'   | -6.81 | 111.53      | 119.70   |
| 24  | BA    | 1158 | C    | P-O5'-C5'   | -6.81 | 110.00      | 120.90   |
| 24  | BA    | 1757 | A    | P-O3'-C3'   | 6.81  | 127.87      | 119.70   |
| 24  | BA    | 972  | A    | P-O3'-C3'   | 6.80  | 127.86      | 119.70   |
| 24  | DA    | 2753 | A    | N9-C1'-C2'  | -6.80 | 104.52      | 112.00   |
| 24  | BA    | 1125 | G    | C4-C5-N7    | 6.80  | 113.52      | 110.80   |
| 21  | AA    | 32   | A    | P-O3'-C3'   | -6.80 | 111.54      | 119.70   |
| 21  | AA    | 276  | G    | N9-C1'-C2'  | -6.80 | 104.52      | 112.00   |
| 21  | AA    | 512  | U    | O4'-C1'-N1  | 6.80  | 113.64      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 2496 | C    | O4'-C1'-N1  | 6.80  | 113.64      | 108.20   |
| 24  | DA    | 460  | A    | N9-C1'-C2'  | -6.80 | 104.52      | 112.00   |
| 55  | CA    | 1452 | C    | P-O3'-C3'   | 6.80  | 127.86      | 119.70   |
| 24  | BA    | 215  | G    | P-O3'-C3'   | 6.80  | 127.86      | 119.70   |
| 24  | BA    | 2005 | A    | P-O3'-C3'   | 6.80  | 127.86      | 119.70   |
| 24  | DA    | 2682 | A    | C3'-C2'-C1' | 6.80  | 106.94      | 101.50   |
| 31  | DH    | 49   | ALA  | CB-CA-C     | -6.80 | 99.91       | 110.10   |
| 24  | BA    | 1838 | C    | P-O3'-C3'   | 6.79  | 127.85      | 119.70   |
| 24  | DA    | 531  | C    | N1-C1'-C2'  | 6.79  | 122.83      | 114.00   |
| 21  | AA    | 1087 | G    | P-O3'-C3'   | -6.79 | 111.55      | 119.70   |
| 21  | AA    | 1183 | U    | N1-C1'-C2'  | -6.79 | 104.53      | 112.00   |
| 24  | DA    | 2041 | U    | C2-N3-C4    | -6.79 | 122.92      | 127.00   |
| 35  | BL    | 6    | LEU  | CA-CB-CG    | 6.79  | 130.92      | 115.30   |
| 21  | AA    | 430  | A    | N9-C1'-C2'  | -6.79 | 104.53      | 112.00   |
| 24  | DA    | 807  | U    | O4'-C1'-N1  | 6.79  | 113.63      | 108.20   |
| 24  | DA    | 729  | G    | P-O3'-C3'   | -6.79 | 111.55      | 119.70   |
| 24  | DA    | 2021 | C    | O4'-C1'-N1  | 6.79  | 113.63      | 108.20   |
| 24  | BA    | 411  | G    | P-O3'-C3'   | 6.78  | 127.84      | 119.70   |
| 24  | DA    | 2272 | U    | O4'-C1'-N1  | -6.78 | 102.78      | 108.20   |
| 24  | BA    | 459  | U    | P-O3'-C3'   | -6.78 | 111.56      | 119.70   |
| 24  | BA    | 2639 | A    | N9-C1'-C2'  | -6.78 | 104.54      | 112.00   |
| 24  | BA    | 1866 | A    | P-O3'-C3'   | -6.78 | 111.57      | 119.70   |
| 24  | BA    | 373  | U    | P-O3'-C3'   | -6.77 | 111.57      | 119.70   |
| 55  | CA    | 1200 | C    | N1-C1'-C2'  | 6.77  | 122.80      | 114.00   |
| 24  | DA    | 1515 | A    | O4'-C1'-N9  | 6.77  | 113.62      | 108.20   |
| 24  | BA    | 974  | G    | C5-N7-C8    | -6.77 | 100.92      | 104.30   |
| 24  | BA    | 2067 | G    | P-O3'-C3'   | 6.76  | 127.82      | 119.70   |
| 24  | BA    | 2273 | A    | N1-C6-N6    | 6.76  | 122.66      | 118.60   |
| 55  | CA    | 1366 | C    | O4'-C1'-N1  | 6.76  | 113.61      | 108.20   |
| 24  | BA    | 1452 | G    | N3-C4-N9    | -6.76 | 121.94      | 126.00   |
| 24  | DA    | 2289 | G    | P-O3'-C3'   | -6.76 | 111.59      | 119.70   |
| 24  | BA    | 1342 | A    | N1-C6-N6    | 6.76  | 122.65      | 118.60   |
| 24  | DA    | 531  | C    | C2-N1-C1'   | -6.76 | 111.37      | 118.80   |
| 56  | DB    | 16   | G    | P-O3'-C3'   | -6.76 | 111.59      | 119.70   |
| 21  | AA    | 282  | A    | P-O3'-C3'   | -6.75 | 111.59      | 119.70   |
| 21  | AA    | 966  | G    | N9-C1'-C2'  | -6.75 | 104.57      | 112.00   |
| 24  | BA    | 403  | U    | P-O3'-C3'   | 6.75  | 127.81      | 119.70   |
| 24  | DA    | 1554 | U    | O4'-C1'-N1  | 6.75  | 113.60      | 108.20   |
| 24  | BA    | 509  | C    | N1-C1'-C2'  | -6.75 | 104.57      | 112.00   |
| 24  | BA    | 1118 | C    | P-O5'-C5'   | -6.75 | 110.09      | 120.90   |
| 24  | BA    | 2772 | C    | P-O3'-C3'   | -6.75 | 111.60      | 119.70   |
| 24  | DA    | 832  | U    | O4'-C1'-N1  | 6.75  | 113.60      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 1818 | U    | P-O3'-C3'   | 6.75  | 127.80      | 119.70   |
| 55  | CA    | 33   | A    | N9-C1'-C2'  | -6.75 | 104.58      | 112.00   |
| 24  | DA    | 1451 | C    | P-O3'-C3'   | 6.75  | 127.80      | 119.70   |
| 21  | AA    | 452  | A    | C5-N7-C8    | -6.74 | 100.53      | 103.90   |
| 24  | BA    | 1142 | A    | C2-N3-C4    | -6.74 | 107.23      | 110.60   |
| 55  | CA    | 1216 | A    | N9-C1'-C2'  | -6.74 | 104.58      | 112.00   |
| 21  | AA    | 1303 | C    | P-O3'-C3'   | -6.74 | 111.62      | 119.70   |
| 55  | CA    | 389  | A    | N1-C6-N6    | -6.74 | 114.56      | 118.60   |
| 24  | DA    | 1092 | C    | O4'-C1'-N1  | 6.74  | 113.59      | 108.20   |
| 24  | BA    | 1429 | G    | C3'-C2'-C1' | 6.73  | 106.89      | 101.50   |
| 55  | CA    | 876  | C    | O4'-C1'-N1  | 6.73  | 113.59      | 108.20   |
| 24  | DA    | 1456 | G    | N9-C1'-C2'  | -6.73 | 104.59      | 112.00   |
| 21  | AA    | 1046 | A    | N9-C1'-C2'  | -6.73 | 104.60      | 112.00   |
| 24  | DA    | 913  | U    | N1-C1'-C2'  | 6.73  | 122.75      | 114.00   |
| 24  | BA    | 1497 | U    | N1-C1'-C2'  | 6.73  | 122.75      | 114.00   |
| 24  | BA    | 27   | G    | P-O3'-C3'   | 6.73  | 127.77      | 119.70   |
| 24  | DA    | 1738 | G    | P-O3'-C3'   | 6.73  | 127.77      | 119.70   |
| 24  | DA    | 2403 | C    | P-O3'-C3'   | -6.72 | 111.63      | 119.70   |
| 21  | AA    | 960  | U    | O4'-C1'-N1  | 6.72  | 113.58      | 108.20   |
| 24  | BA    | 2893 | A    | C8-N9-C4    | 6.72  | 108.49      | 105.80   |
| 24  | DA    | 196  | A    | P-O3'-C3'   | 6.72  | 127.77      | 119.70   |
| 21  | AA    | 1332 | A    | N9-C1'-C2'  | -6.72 | 104.61      | 112.00   |
| 24  | BA    | 2063 | C    | N1-C1'-C2'  | -6.72 | 104.61      | 112.00   |
| 24  | BA    | 121  | G    | P-O3'-C3'   | -6.72 | 111.64      | 119.70   |
| 24  | BA    | 824  | U    | P-O3'-C3'   | -6.72 | 111.64      | 119.70   |
| 24  | DA    | 2053 | G    | N3-C4-N9    | -6.71 | 121.97      | 126.00   |
| 24  | BA    | 684  | G    | N9-C4-C5    | -6.71 | 102.72      | 105.40   |
| 21  | AA    | 1417 | G    | C6-C5-N7    | -6.71 | 126.37      | 130.40   |
| 21  | AA    | 1417 | G    | N1-C6-O6    | 6.71  | 123.93      | 119.90   |
| 24  | BA    | 1901 | A    | C6-N1-C2    | 6.71  | 122.63      | 118.60   |
| 24  | DA    | 1778 | U    | P-O3'-C3'   | 6.71  | 127.75      | 119.70   |
| 24  | DA    | 116  | C    | O4'-C1'-N1  | 6.71  | 113.57      | 108.20   |
| 24  | DA    | 2021 | C    | P-O3'-C3'   | 6.71  | 127.75      | 119.70   |
| 24  | BA    | 1325 | U    | O4'-C1'-N1  | 6.70  | 113.56      | 108.20   |
| 55  | CA    | 247  | G    | P-O3'-C3'   | -6.70 | 111.66      | 119.70   |
| 55  | CA    | 1212 | U    | P-O3'-C3'   | 6.70  | 127.74      | 119.70   |
| 21  | AA    | 1141 | C    | P-O3'-C3'   | -6.70 | 111.67      | 119.70   |
| 24  | BA    | 671  | C    | C3'-C2'-C1' | 6.69  | 106.86      | 101.50   |
| 24  | BA    | 800  | A    | N1-C6-N6    | -6.69 | 114.59      | 118.60   |
| 21  | AA    | 82   | G    | C3'-C2'-C1' | 6.69  | 106.85      | 101.50   |
| 24  | BA    | 1019 | U    | N3-C4-C5    | 6.69  | 118.61      | 114.60   |
| 24  | BA    | 1155 | A    | N1-C2-N3    | -6.69 | 125.96      | 129.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 37   | U    | O4'-C1'-N1  | 6.68  | 113.55      | 108.20   |
| 55  | CA    | 512  | U    | O4'-C1'-N1  | 6.68  | 113.55      | 108.20   |
| 24  | DA    | 704  | G    | P-O3'-C3'   | 6.68  | 127.72      | 119.70   |
| 21  | AA    | 351  | G    | O4'-C1'-N9  | 6.68  | 113.55      | 108.20   |
| 24  | DA    | 2498 | C    | O4'-C1'-N1  | 6.68  | 113.55      | 108.20   |
| 24  | DA    | 783  | A    | C3'-C2'-C1' | 6.68  | 106.84      | 101.50   |
| 56  | DB    | 91   | C    | O4'-C1'-N1  | 6.68  | 113.54      | 108.20   |
| 24  | BA    | 2451 | A    | N1-C6-N6    | -6.68 | 114.59      | 118.60   |
| 24  | DA    | 2386 | A    | P-O3'-C3'   | -6.68 | 111.69      | 119.70   |
| 24  | DA    | 1268 | A    | P-O3'-C3'   | -6.68 | 111.69      | 119.70   |
| 24  | BA    | 396  | G    | P-O3'-C3'   | -6.67 | 111.69      | 119.70   |
| 55  | CA    | 1094 | G    | P-O3'-C3'   | 6.67  | 127.71      | 119.70   |
| 24  | DA    | 1647 | U    | P-O3'-C3'   | 6.67  | 127.71      | 119.70   |
| 24  | DA    | 60   | G    | O4'-C1'-N9  | 6.67  | 113.54      | 108.20   |
| 24  | DA    | 547  | A    | P-O3'-C3'   | 6.67  | 127.70      | 119.70   |
| 24  | BA    | 73   | A    | C3'-C2'-C1' | 6.67  | 106.84      | 101.50   |
| 25  | BB    | 77   | U    | P-O3'-C3'   | -6.67 | 111.70      | 119.70   |
| 55  | CA    | 210  | C    | N1-C1'-C2'  | 6.67  | 122.67      | 114.00   |
| 24  | DA    | 1536 | C    | O4'-C1'-N1  | -6.67 | 102.87      | 108.20   |
| 24  | BA    | 2093 | G    | P-O3'-C3'   | -6.66 | 111.70      | 119.70   |
| 24  | DA    | 2312 | U    | N3-C2-O2    | -6.66 | 117.53      | 122.20   |
| 24  | BA    | 1731 | G    | N3-C4-N9    | -6.66 | 122.00      | 126.00   |
| 24  | DA    | 1327 | A    | P-O3'-C3'   | -6.66 | 111.71      | 119.70   |
| 55  | CA    | 1068 | G    | P-O3'-C3'   | -6.66 | 111.71      | 119.70   |
| 24  | DA    | 1957 | C    | O4'-C1'-N1  | 6.66  | 113.53      | 108.20   |
| 24  | BA    | 634  | C    | O4'-C1'-N1  | -6.66 | 102.87      | 108.20   |
| 55  | CA    | 1066 | C    | N1-C1'-C2'  | -6.66 | 104.68      | 112.00   |
| 24  | BA    | 1255 | U    | O4'-C1'-N1  | 6.66  | 113.52      | 108.20   |
| 24  | DA    | 509  | C    | C2-N1-C1'   | 6.66  | 126.12      | 118.80   |
| 56  | DB    | 104  | A    | C4-C5-C6    | 6.66  | 120.33      | 117.00   |
| 55  | CA    | 1364 | U    | N1-C1'-C2'  | 6.65  | 122.65      | 114.00   |
| 21  | AA    | 536  | C    | N1-C1'-C2'  | -6.65 | 104.68      | 112.00   |
| 24  | BA    | 2200 | C    | P-O3'-C3'   | -6.65 | 111.72      | 119.70   |
| 25  | BB    | 89   | U    | C3'-C2'-C1' | 6.65  | 106.82      | 101.50   |
| 21  | AA    | 5    | U    | P-O3'-C3'   | 6.65  | 127.68      | 119.70   |
| 24  | DA    | 931  | U    | O4'-C1'-N1  | 6.65  | 113.52      | 108.20   |
| 21  | AA    | 48   | C    | O4'-C1'-N1  | 6.65  | 113.52      | 108.20   |
| 24  | BA    | 989  | G    | O4'-C1'-N9  | 6.65  | 113.52      | 108.20   |
| 24  | BA    | 142  | A    | N9-C1'-C2'  | -6.64 | 104.69      | 112.00   |
| 24  | BA    | 1174 | U    | P-O3'-C3'   | -6.64 | 111.73      | 119.70   |
| 24  | BA    | 1708 | C    | P-O5'-C5'   | -6.64 | 110.27      | 120.90   |
| 24  | BA    | 2293 | G    | P-O3'-C3'   | -6.64 | 111.73      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | CA    | 733  | G    | P-O3'-C3'   | 6.64  | 127.67      | 119.70   |
| 21  | AA    | 70   | U    | P-O3'-C3'   | 6.64  | 127.67      | 119.70   |
| 55  | CA    | 1308 | U    | O4'-C1'-N1  | 6.64  | 113.51      | 108.20   |
| 24  | BA    | 633  | A    | C4-C5-C6    | 6.64  | 120.32      | 117.00   |
| 55  | CA    | 52   | C    | P-O3'-C3'   | -6.64 | 111.74      | 119.70   |
| 56  | DB    | 51   | G    | O4'-C1'-N9  | 6.64  | 113.51      | 108.20   |
| 24  | DA    | 1653 | G    | P-O3'-C3'   | 6.63  | 127.66      | 119.70   |
| 24  | BA    | 2639 | A    | N1-C6-N6    | 6.63  | 122.58      | 118.60   |
| 55  | CA    | 1490 | U    | O4'-C1'-N1  | 6.63  | 113.51      | 108.20   |
| 21  | AA    | 211  | G    | P-O3'-C3'   | 6.63  | 127.66      | 119.70   |
| 21  | AA    | 575  | G    | C4-N9-C1'   | -6.63 | 117.88      | 126.50   |
| 24  | BA    | 1945 | G    | C3'-C2'-C1' | 6.63  | 106.81      | 101.50   |
| 24  | DA    | 301  | G    | N3-C4-N9    | -6.63 | 122.02      | 126.00   |
| 24  | BA    | 1438 | U    | C5-C4-O4    | -6.63 | 121.92      | 125.90   |
| 24  | DA    | 1619 | G    | N9-C1'-C2'  | -6.63 | 104.71      | 112.00   |
| 21  | AA    | 97   | G    | N9-C1'-C2'  | -6.62 | 104.71      | 112.00   |
| 55  | CA    | 119  | A    | P-O3'-C3'   | 6.62  | 127.65      | 119.70   |
| 24  | DA    | 621  | A    | P-O3'-C3'   | -6.62 | 111.75      | 119.70   |
| 55  | CA    | 914  | A    | C3'-C2'-C1' | 6.62  | 106.80      | 101.50   |
| 24  | BA    | 747  | U    | O5'-P-OP2   | -6.62 | 99.75       | 105.70   |
| 24  | BA    | 1661 | G    | N3-C4-C5    | 6.62  | 131.91      | 128.60   |
| 55  | CA    | 1246 | A    | N9-C1'-C2'  | -6.62 | 104.72      | 112.00   |
| 55  | CA    | 1441 | A    | P-O3'-C3'   | 6.62  | 127.64      | 119.70   |
| 24  | DA    | 2857 | G    | C2-N3-C4    | -6.62 | 108.59      | 111.90   |
| 55  | CA    | 1052 | U    | P-O5'-C5'   | -6.62 | 110.31      | 120.90   |
| 24  | BA    | 567  | U    | P-O3'-C3'   | -6.61 | 111.77      | 119.70   |
| 24  | BA    | 2575 | C    | C5-C4-N4    | -6.61 | 115.57      | 120.20   |
| 21  | AA    | 374  | A    | N9-C1'-C2'  | -6.61 | 104.73      | 112.00   |
| 24  | DA    | 251  | A    | C3'-C2'-C1' | 6.61  | 106.79      | 101.50   |
| 21  | AA    | 1394 | A    | P-O3'-C3'   | 6.61  | 127.63      | 119.70   |
| 21  | AA    | 250  | A    | P-O3'-C3'   | 6.61  | 127.63      | 119.70   |
| 21  | AA    | 722  | G    | P-O3'-C3'   | -6.61 | 111.77      | 119.70   |
| 55  | CA    | 381  | C    | N1-C1'-C2'  | 6.60  | 122.58      | 114.00   |
| 24  | BA    | 1145 | C    | N1-C1'-C2'  | -6.60 | 104.74      | 112.00   |
| 24  | DA    | 915  | C    | P-O3'-C3'   | -6.60 | 111.78      | 119.70   |
| 55  | CA    | 641  | U    | P-O3'-C3'   | 6.60  | 127.62      | 119.70   |
| 24  | BA    | 249  | C    | N1-C1'-C2'  | 6.60  | 122.58      | 114.00   |
| 21  | AA    | 110  | C    | P-O3'-C3'   | -6.60 | 111.78      | 119.70   |
| 24  | DA    | 334  | C    | O4'-C1'-N1  | 6.60  | 113.48      | 108.20   |
| 24  | BA    | 1932 | A    | P-O3'-C3'   | -6.59 | 111.79      | 119.70   |
| 24  | DA    | 1561 | C    | P-O3'-C3'   | -6.59 | 111.78      | 119.70   |
| 24  | BA    | 2297 | A    | N9-C1'-C2'  | -6.59 | 104.75      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 74   | A    | P-O3'-C3'   | 6.59  | 127.61      | 119.70   |
| 24  | DA    | 37   | C    | O4'-C1'-N1  | 6.59  | 113.47      | 108.20   |
| 24  | BA    | 628  | G    | N9-C1'-C2'  | -6.59 | 104.75      | 112.00   |
| 24  | DA    | 427  | U    | O4'-C1'-N1  | 6.59  | 113.47      | 108.20   |
| 24  | DA    | 575  | A    | P-O3'-C3'   | -6.59 | 111.79      | 119.70   |
| 24  | BA    | 1786 | A    | O4'-C1'-N9  | 6.59  | 113.47      | 108.20   |
| 21  | AA    | 995  | C    | O4'-C1'-N1  | 6.59  | 113.47      | 108.20   |
| 24  | BA    | 633  | A    | C6-C5-N7    | -6.59 | 127.69      | 132.30   |
| 24  | DA    | 1943 | U    | N1-C1'-C2'  | -6.59 | 104.75      | 112.00   |
| 24  | DA    | 2258 | C    | P-O3'-C3'   | 6.59  | 127.60      | 119.70   |
| 24  | BA    | 268  | C    | O4'-C1'-N1  | -6.58 | 102.94      | 108.20   |
| 25  | BB    | 15   | A    | P-O5'-C5'   | -6.58 | 110.38      | 120.90   |
| 24  | BA    | 349  | U    | O4'-C1'-N1  | -6.58 | 102.94      | 108.20   |
| 24  | BA    | 1478 | G    | C6-C5-N7    | 6.58  | 134.34      | 130.40   |
| 24  | DA    | 2423 | U    | N1-C1'-C2'  | 6.58  | 122.55      | 114.00   |
| 24  | BA    | 1942 | C    | P-O3'-C3'   | -6.57 | 111.81      | 119.70   |
| 24  | BA    | 831  | G    | P-O3'-C3'   | -6.57 | 111.82      | 119.70   |
| 56  | DB    | 43   | C    | O4'-C1'-N1  | 6.57  | 113.45      | 108.20   |
| 24  | BA    | 2391 | G    | O4'-C1'-N9  | 6.57  | 113.45      | 108.20   |
| 24  | DA    | 2266 | A    | P-O3'-C3'   | 6.57  | 127.58      | 119.70   |
| 24  | BA    | 2578 | G    | N1-C6-O6    | -6.56 | 115.96      | 119.90   |
| 25  | BB    | 16   | G    | N9-C1'-C2'  | -6.56 | 104.78      | 112.00   |
| 55  | CA    | 890  | G    | O4'-C1'-N9  | 6.56  | 113.45      | 108.20   |
| 24  | DA    | 461  | C    | C2-N1-C1'   | 6.56  | 126.02      | 118.80   |
| 24  | DA    | 1809 | A    | P-O3'-C3'   | -6.56 | 111.82      | 119.70   |
| 24  | BA    | 2511 | U    | C5-C4-O4    | -6.56 | 121.97      | 125.90   |
| 24  | DA    | 1214 | A    | N9-C1'-C2'  | -6.56 | 104.78      | 112.00   |
| 24  | DA    | 976  | G    | N9-C1'-C2'  | -6.56 | 104.79      | 112.00   |
| 21  | AA    | 991  | U    | O4'-C1'-N1  | 6.56  | 113.44      | 108.20   |
| 24  | BA    | 1867 | G    | P-O3'-C3'   | -6.56 | 111.83      | 119.70   |
| 25  | BB    | 58   | A    | P-O3'-C3'   | -6.56 | 111.83      | 119.70   |
| 55  | CA    | 383  | A    | C3'-C2'-C1' | 6.56  | 106.75      | 101.50   |
| 55  | CA    | 537  | G    | C3'-C2'-C1' | 6.56  | 106.75      | 101.50   |
| 24  | DA    | 1522 | A    | N1-C6-N6    | 6.56  | 122.53      | 118.60   |
| 24  | BA    | 2504 | U    | O4'-C1'-N1  | 6.55  | 113.44      | 108.20   |
| 24  | BA    | 2881 | U    | P-O3'-C3'   | -6.55 | 111.84      | 119.70   |
| 21  | AA    | 1141 | C    | O4'-C1'-N1  | 6.55  | 113.44      | 108.20   |
| 24  | BA    | 1554 | U    | P-O3'-C3'   | 6.55  | 127.56      | 119.70   |
| 24  | BA    | 2556 | C    | O4'-C1'-N1  | 6.55  | 113.44      | 108.20   |
| 25  | BB    | 90   | C    | P-O5'-C5'   | -6.55 | 110.42      | 120.90   |
| 25  | BB    | 57   | A    | P-O5'-C5'   | -6.55 | 110.42      | 120.90   |
| 55  | CA    | 430  | A    | P-O3'-C3'   | -6.55 | 111.84      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | AV    | 35   | A    | N1-C6-N6    | -6.55 | 114.67      | 118.60   |
| 24  | DA    | 250  | G    | P-O3'-C3'   | -6.55 | 111.84      | 119.70   |
| 24  | BA    | 178  | G    | N9-C1'-C2'  | -6.54 | 104.80      | 112.00   |
| 24  | DA    | 1865 | U    | C2-N3-C4    | -6.54 | 123.07      | 127.00   |
| 24  | DA    | 301  | G    | C8-N9-C1'   | 6.54  | 135.50      | 127.00   |
| 55  | CA    | 73   | C    | O4'-C1'-N1  | 6.54  | 113.43      | 108.20   |
| 24  | BA    | 975  | A    | N9-C1'-C2'  | -6.54 | 104.81      | 112.00   |
| 24  | DA    | 53   | A    | N9-C1'-C2'  | -6.54 | 104.81      | 112.00   |
| 24  | DA    | 370  | G    | N3-C4-N9    | -6.54 | 122.08      | 126.00   |
| 24  | DA    | 861  | A    | N9-C1'-C2'  | -6.54 | 104.81      | 112.00   |
| 29  | BF    | 110  | ILE  | CB-CA-C     | -6.54 | 98.53       | 111.60   |
| 55  | CA    | 13   | U    | N1-C1'-C2'  | 6.54  | 122.50      | 114.00   |
| 55  | CA    | 81   | A    | N1-C6-N6    | -6.54 | 114.68      | 118.60   |
| 55  | CA    | 451  | A    | P-O3'-C3'   | 6.54  | 127.54      | 119.70   |
| 24  | DA    | 334  | C    | P-O3'-C3'   | -6.53 | 111.86      | 119.70   |
| 55  | CA    | 109  | A    | P-O3'-C3'   | 6.53  | 127.54      | 119.70   |
| 24  | DA    | 1707 | G    | P-O3'-C3'   | 6.53  | 127.54      | 119.70   |
| 24  | BA    | 957  | C    | O4'-C1'-N1  | 6.53  | 113.42      | 108.20   |
| 21  | AA    | 548  | G    | N9-C1'-C2'  | -6.53 | 104.82      | 112.00   |
| 24  | BA    | 233  | A    | N9-C1'-C2'  | -6.53 | 104.82      | 112.00   |
| 24  | BA    | 1240 | U    | N1-C1'-C2'  | 6.53  | 122.49      | 114.00   |
| 21  | AA    | 1200 | C    | P-O3'-C3'   | 6.53  | 127.53      | 119.70   |
| 24  | DA    | 685  | A    | P-O3'-C3'   | 6.53  | 127.53      | 119.70   |
| 56  | DB    | 46   | A    | N9-C1'-C2'  | -6.53 | 104.82      | 112.00   |
| 24  | BA    | 2779 | U    | O4'-C1'-N1  | 6.52  | 113.42      | 108.20   |
| 55  | CA    | 1230 | C    | O4'-C1'-N1  | -6.52 | 102.98      | 108.20   |
| 24  | DA    | 1275 | A    | P-O3'-C3'   | 6.52  | 127.53      | 119.70   |
| 21  | AA    | 1087 | G    | C3'-C2'-C1' | 6.52  | 106.72      | 101.50   |
| 24  | BA    | 507  | A    | P-O5'-C5'   | -6.52 | 110.47      | 120.90   |
| 24  | BA    | 907  | G    | N3-C4-N9    | -6.52 | 122.09      | 126.00   |
| 24  | BA    | 1695 | G    | P-O3'-C3'   | -6.52 | 111.88      | 119.70   |
| 55  | CA    | 510  | A    | P-O5'-C5'   | -6.52 | 110.47      | 120.90   |
| 24  | DA    | 2092 | U    | P-O3'-C3'   | 6.52  | 127.52      | 119.70   |
| 24  | BA    | 62   | U    | P-O3'-C3'   | 6.52  | 127.52      | 119.70   |
| 24  | BA    | 1430 | G    | C5-C6-O6    | 6.52  | 132.51      | 128.60   |
| 24  | DA    | 2493 | U    | O4'-C1'-N1  | 6.52  | 113.41      | 108.20   |
| 24  | BA    | 2148 | G    | P-O3'-C3'   | -6.52 | 111.88      | 119.70   |
| 24  | BA    | 2894 | G    | N9-C1'-C2'  | -6.52 | 104.83      | 112.00   |
| 24  | DA    | 2681 | C    | P-O3'-C3'   | 6.52  | 127.52      | 119.70   |
| 24  | DA    | 74   | A    | P-O3'-C3'   | 6.51  | 127.52      | 119.70   |
| 24  | BA    | 510  | C    | P-O3'-C3'   | -6.51 | 111.89      | 119.70   |
| 24  | BA    | 2363 | G    | N9-C4-C5    | 6.51  | 108.00      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 531  | C    | C6-N1-C2    | 6.51  | 122.90      | 120.30   |
| 24  | BA    | 683  | U    | N1-C2-N3    | 6.50  | 118.80      | 114.90   |
| 24  | BA    | 528  | A    | N9-C1'-C2'  | -6.50 | 104.85      | 112.00   |
| 24  | BA    | 800  | A    | C5-C6-N6    | 6.50  | 128.90      | 123.70   |
| 24  | BA    | 2728 | U    | O4'-C1'-N1  | 6.50  | 113.40      | 108.20   |
| 24  | BA    | 687  | C    | C3'-C2'-C1' | 6.50  | 106.70      | 101.50   |
| 24  | BA    | 1213 | A    | N9-C1'-C2'  | -6.50 | 104.85      | 112.00   |
| 24  | BA    | 2335 | A    | C3'-C2'-C1' | 6.50  | 106.70      | 101.50   |
| 24  | DA    | 1025 | G    | P-O3'-C3'   | 6.50  | 127.50      | 119.70   |
| 24  | BA    | 1876 | A    | C5-N7-C8    | -6.50 | 100.65      | 103.90   |
| 31  | BH    | 47   | PHE  | C-N-CA      | -6.50 | 105.46      | 121.70   |
| 55  | CA    | 615  | G    | O4'-C1'-N9  | 6.50  | 113.40      | 108.20   |
| 21  | AA    | 121  | U    | O4'-C1'-N1  | -6.50 | 103.00      | 108.20   |
| 21  | AA    | 413  | G    | P-O3'-C3'   | -6.50 | 111.91      | 119.70   |
| 55  | CA    | 131  | A    | P-O3'-C3'   | 6.50  | 127.49      | 119.70   |
| 24  | DA    | 2581 | G    | O4'-C1'-N9  | 6.50  | 113.40      | 108.20   |
| 55  | CA    | 1348 | U    | N1-C1'-C2'  | -6.49 | 104.86      | 112.00   |
| 24  | DA    | 1615 | C    | N1-C1'-C2'  | 6.49  | 122.44      | 114.00   |
| 24  | BA    | 2398 | U    | P-O3'-C3'   | -6.49 | 111.91      | 119.70   |
| 55  | CA    | 283  | U    | O4'-C1'-N1  | 6.49  | 113.39      | 108.20   |
| 21  | AA    | 304  | U    | O4'-C1'-N1  | 6.49  | 113.39      | 108.20   |
| 24  | DA    | 13   | A    | P-O3'-C3'   | 6.49  | 127.49      | 119.70   |
| 24  | DA    | 389  | G    | N9-C1'-C2'  | -6.49 | 104.86      | 112.00   |
| 24  | DA    | 2790 | U    | O4'-C1'-N1  | 6.49  | 113.39      | 108.20   |
| 24  | BA    | 1247 | A    | N1-C6-N6    | 6.49  | 122.49      | 118.60   |
| 24  | BA    | 23   | G    | N1-C6-O6    | -6.49 | 116.01      | 119.90   |
| 24  | BA    | 974  | G    | C8-N9-C4    | -6.49 | 103.81      | 106.40   |
| 24  | DA    | 1478 | G    | N9-C1'-C2'  | -6.49 | 104.87      | 112.00   |
| 24  | BA    | 1611 | C    | C3'-C2'-C1' | 6.48  | 106.69      | 101.50   |
| 24  | BA    | 2347 | C    | C3'-C2'-C1' | 6.48  | 106.69      | 101.50   |
| 24  | BA    | 299  | A    | N7-C8-N9    | 6.48  | 117.04      | 113.80   |
| 24  | BA    | 1760 | C    | O4'-C1'-N1  | 6.48  | 113.39      | 108.20   |
| 24  | DA    | 1674 | G    | C6-C5-N7    | -6.48 | 126.51      | 130.40   |
| 24  | BA    | 1551 | A    | P-O3'-C3'   | -6.48 | 111.93      | 119.70   |
| 24  | DA    | 225  | C    | P-O3'-C3'   | -6.48 | 111.93      | 119.70   |
| 24  | DA    | 931  | U    | P-O3'-C3'   | 6.48  | 127.47      | 119.70   |
| 24  | BA    | 2030 | A    | P-O3'-C3'   | 6.48  | 127.47      | 119.70   |
| 24  | BA    | 2052 | A    | N9-C1'-C2'  | -6.48 | 104.88      | 112.00   |
| 55  | CA    | 1191 | A    | P-O3'-C3'   | 6.48  | 127.47      | 119.70   |
| 24  | DA    | 1277 | G    | C3'-C2'-C1' | 6.47  | 106.68      | 101.50   |
| 24  | BA    | 1435 | G    | P-O3'-C3'   | -6.47 | 111.94      | 119.70   |
| 24  | DA    | 1788 | C    | P-O3'-C3'   | -6.47 | 111.94      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 31  | DH    | 48   | GLU  | CA-C-N      | -6.47 | 102.97      | 117.20   |
| 24  | BA    | 919  | U    | P-O3'-C3'   | -6.46 | 111.94      | 119.70   |
| 55  | CA    | 577  | G    | N9-C1'-C2'  | -6.46 | 104.89      | 112.00   |
| 24  | DA    | 1717 | A    | P-O3'-C3'   | -6.46 | 111.94      | 119.70   |
| 21  | AA    | 1197 | A    | P-O3'-C3'   | -6.46 | 111.95      | 119.70   |
| 24  | BA    | 556  | A    | P-O3'-C3'   | 6.46  | 127.45      | 119.70   |
| 24  | BA    | 1238 | G    | P-O3'-C3'   | -6.46 | 111.95      | 119.70   |
| 24  | DA    | 1437 | C    | O4'-C1'-N1  | 6.46  | 113.36      | 108.20   |
| 24  | BA    | 503  | A    | P-O3'-C3'   | 6.45  | 127.44      | 119.70   |
| 24  | BA    | 2656 | U    | N1-C1'-C2'  | -6.45 | 104.90      | 112.00   |
| 55  | CA    | 243  | A    | N1-C6-N6    | -6.45 | 114.73      | 118.60   |
| 24  | DA    | 2043 | C    | O4'-C1'-N1  | -6.45 | 103.04      | 108.20   |
| 24  | BA    | 1818 | U    | P-O3'-C3'   | -6.45 | 111.96      | 119.70   |
| 21  | AA    | 914  | A    | C3'-C2'-C1' | 6.45  | 106.66      | 101.50   |
| 24  | BA    | 196  | A    | P-O3'-C3'   | 6.45  | 127.44      | 119.70   |
| 24  | BA    | 35   | G    | C3'-C2'-C1' | 6.45  | 106.66      | 101.50   |
| 24  | BA    | 2307 | G    | O4'-C1'-N9  | 6.45  | 113.36      | 108.20   |
| 24  | DA    | 961  | C    | P-O3'-C3'   | 6.45  | 127.44      | 119.70   |
| 24  | BA    | 587  | C    | C6-N1-C2    | 6.44  | 122.88      | 120.30   |
| 24  | BA    | 2332 | C    | O4'-C1'-N1  | 6.44  | 113.35      | 108.20   |
| 24  | DA    | 239  | C    | O4'-C1'-N1  | 6.44  | 113.35      | 108.20   |
| 24  | DA    | 1962 | C    | N1-C1'-C2'  | 6.44  | 122.38      | 114.00   |
| 24  | BA    | 2249 | U    | O4'-C1'-N1  | 6.44  | 113.35      | 108.20   |
| 24  | BA    | 2447 | G    | C2-N3-C4    | 6.44  | 115.12      | 111.90   |
| 25  | BB    | 68   | C    | O4'-C1'-N1  | 6.44  | 113.35      | 108.20   |
| 55  | CA    | 460  | A    | P-O3'-C3'   | -6.44 | 111.97      | 119.70   |
| 24  | DA    | 230  | G    | P-O3'-C3'   | -6.44 | 111.97      | 119.70   |
| 24  | DA    | 1049 | C    | O4'-C1'-N1  | 6.44  | 113.35      | 108.20   |
| 24  | BA    | 1688 | U    | O4'-C1'-N1  | 6.44  | 113.35      | 108.20   |
| 24  | DA    | 1082 | U    | O4'-C1'-N1  | 6.44  | 113.35      | 108.20   |
| 24  | BA    | 505  | A    | C3'-C2'-C1' | 6.43  | 106.65      | 101.50   |
| 24  | BA    | 265  | A    | P-O3'-C3'   | 6.43  | 127.42      | 119.70   |
| 55  | CA    | 577  | G    | C3'-C2'-C1' | 6.43  | 106.64      | 101.50   |
| 55  | CA    | 821  | G    | N9-C1'-C2'  | -6.43 | 104.93      | 112.00   |
| 24  | BA    | 2385 | C    | O4'-C1'-N1  | -6.42 | 103.06      | 108.20   |
| 24  | BA    | 2546 | U    | O4'-C1'-N1  | -6.42 | 103.06      | 108.20   |
| 24  | DA    | 302  | C    | O4'-C1'-N1  | 6.42  | 113.34      | 108.20   |
| 56  | DB    | 104  | A    | N1-C6-N6    | 6.42  | 122.45      | 118.60   |
| 24  | BA    | 63   | A    | P-O3'-C3'   | -6.42 | 112.00      | 119.70   |
| 24  | BA    | 1731 | G    | N9-C4-C5    | 6.42  | 107.97      | 105.40   |
| 24  | DA    | 2199 | A    | P-O3'-C3'   | -6.42 | 112.00      | 119.70   |
| 24  | BA    | 271  | G    | P-O3'-C3'   | 6.42  | 127.40      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25  | BB    | 24   | G    | P-O3'-C3'  | 6.42  | 127.40      | 119.70   |
| 55  | CA    | 67   | C    | P-O3'-C3'  | -6.42 | 112.00      | 119.70   |
| 24  | BA    | 60   | G    | P-O3'-C3'  | 6.42  | 127.40      | 119.70   |
| 24  | BA    | 633  | A    | C5-C6-N1   | -6.42 | 114.49      | 117.70   |
| 24  | DA    | 140  | C    | P-O3'-C3'  | 6.42  | 127.40      | 119.70   |
| 21  | AA    | 805  | C    | O4'-C1'-N1 | -6.41 | 103.07      | 108.20   |
| 55  | CA    | 81   | A    | C5-C6-N6   | 6.41  | 128.83      | 123.70   |
| 21  | AA    | 1395 | C    | P-O3'-C3'  | -6.41 | 112.01      | 119.70   |
| 21  | AA    | 90   | C    | N1-C1'-C2' | -6.41 | 104.95      | 112.00   |
| 24  | DA    | 2573 | C    | C6-N1-C2   | -6.41 | 117.73      | 120.30   |
| 24  | BA    | 752  | A    | C4-C5-N7   | 6.41  | 113.90      | 110.70   |
| 24  | BA    | 1060 | U    | C2-N3-C4   | -6.41 | 123.16      | 127.00   |
| 24  | DA    | 1925 | C    | O4'-C1'-N1 | 6.41  | 113.33      | 108.20   |
| 24  | DA    | 2311 | A    | P-O5'-C5'  | 6.41  | 131.15      | 120.90   |
| 21  | AA    | 232  | G    | P-O3'-C3'  | -6.41 | 112.01      | 119.70   |
| 24  | DA    | 301  | G    | C4-N9-C1'  | -6.41 | 118.17      | 126.50   |
| 24  | BA    | 995  | C    | O4'-C1'-N1 | -6.40 | 103.08      | 108.20   |
| 24  | BA    | 2239 | G    | P-O5'-C5'  | -6.40 | 110.66      | 120.90   |
| 55  | CA    | 452  | A    | C5-N7-C8   | -6.40 | 100.70      | 103.90   |
| 55  | CA    | 875  | U    | N1-C1'-C2' | -6.40 | 104.96      | 112.00   |
| 24  | DA    | 2030 | A    | P-O3'-C3'  | 6.40  | 127.38      | 119.70   |
| 55  | CA    | 1301 | U    | P-O3'-C3'  | 6.40  | 127.38      | 119.70   |
| 55  | CA    | 14   | U    | O4'-C1'-N1 | 6.40  | 113.32      | 108.20   |
| 55  | CA    | 52   | C    | O4'-C1'-N1 | 6.39  | 113.32      | 108.20   |
| 55  | CA    | 1324 | A    | P-O5'-C5'  | -6.39 | 110.67      | 120.90   |
| 55  | CA    | 1323 | G    | P-O3'-C3'  | 6.39  | 127.37      | 119.70   |
| 24  | DA    | 2352 | A    | N1-C6-N6   | 6.39  | 122.44      | 118.60   |
| 21  | AA    | 808  | C    | N1-C2-O2   | -6.39 | 115.07      | 118.90   |
| 24  | BA    | 1551 | A    | C6-N1-C2   | 6.39  | 122.43      | 118.60   |
| 24  | BA    | 2528 | U    | P-O3'-C3'  | 6.39  | 127.37      | 119.70   |
| 24  | BA    | 2822 | G    | C5-C6-O6   | -6.39 | 124.77      | 128.60   |
| 55  | CA    | 90   | C    | P-O3'-C3'  | -6.39 | 112.04      | 119.70   |
| 24  | DA    | 2094 | A    | N9-C1'-C2' | -6.39 | 104.97      | 112.00   |
| 21  | AA    | 132  | C    | P-O3'-C3'  | -6.38 | 112.04      | 119.70   |
| 24  | BA    | 2543 | G    | N9-C1'-C2' | -6.38 | 104.98      | 112.00   |
| 21  | AA    | 368  | U    | N1-C1'-C2' | -6.38 | 104.98      | 112.00   |
| 55  | CA    | 436  | C    | O4'-C1'-N1 | -6.38 | 103.09      | 108.20   |
| 55  | CA    | 1301 | U    | O4'-C1'-N1 | 6.38  | 113.31      | 108.20   |
| 24  | DA    | 964  | C    | P-O3'-C3'  | -6.38 | 112.04      | 119.70   |
| 24  | DA    | 1867 | G    | N9-C1'-C2' | -6.38 | 104.98      | 112.00   |
| 21  | AA    | 1449 | C    | P-O3'-C3'  | -6.38 | 112.05      | 119.70   |
| 21  | AA    | 1417 | G    | N9-C4-C5   | -6.38 | 102.85      | 105.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 2427 | C    | C3'-C2'-C1' | 6.38  | 106.60      | 101.50   |
| 55  | CA    | 1053 | G    | O3'-P-O5'   | -6.38 | 91.88       | 104.00   |
| 55  | CA    | 803  | G    | P-O3'-C3'   | -6.37 | 112.05      | 119.70   |
| 24  | DA    | 61   | C    | C3'-C2'-C1' | 6.37  | 106.60      | 101.50   |
| 21  | AA    | 966  | G    | C3'-C2'-C1' | 6.37  | 106.60      | 101.50   |
| 24  | BA    | 460  | A    | P-O5'-C5'   | -6.37 | 110.71      | 120.90   |
| 24  | BA    | 1142 | A    | N7-C8-N9    | 6.37  | 116.98      | 113.80   |
| 24  | DA    | 2387 | U    | O4'-C1'-N1  | 6.37  | 113.30      | 108.20   |
| 24  | BA    | 1324 | G    | O4'-C1'-N9  | 6.37  | 113.29      | 108.20   |
| 24  | DA    | 2092 | U    | O4'-C1'-N1  | 6.37  | 113.29      | 108.20   |
| 24  | BA    | 783  | A    | C5-N7-C8    | -6.36 | 100.72      | 103.90   |
| 24  | DA    | 396  | G    | C3'-C2'-C1' | 6.36  | 106.59      | 101.50   |
| 24  | DA    | 947  | A    | P-O3'-C3'   | -6.36 | 112.06      | 119.70   |
| 24  | DA    | 1786 | A    | O4'-C1'-N9  | 6.36  | 113.29      | 108.20   |
| 24  | BA    | 1277 | G    | P-O3'-C3'   | -6.36 | 112.07      | 119.70   |
| 24  | BA    | 2790 | U    | N1-C1'-C2'  | 6.36  | 122.27      | 114.00   |
| 24  | DA    | 1385 | A    | C6-N1-C2    | 6.36  | 122.42      | 118.60   |
| 24  | BA    | 1491 | G    | C3'-C2'-C1' | 6.36  | 106.59      | 101.50   |
| 21  | AA    | 169  | C    | N3-C4-N4    | -6.36 | 113.55      | 118.00   |
| 24  | DA    | 2403 | C    | O4'-C1'-N1  | 6.36  | 113.29      | 108.20   |
| 21  | AA    | 545  | C    | C6-N1-C2    | 6.36  | 122.84      | 120.30   |
| 24  | DA    | 249  | C    | P-O3'-C3'   | 6.36  | 127.33      | 119.70   |
| 24  | DA    | 1079 | C    | P-O3'-C3'   | -6.36 | 112.07      | 119.70   |
| 55  | CA    | 567  | G    | C3'-C2'-C1' | 6.35  | 106.58      | 101.50   |
| 24  | BA    | 2857 | G    | N1-C2-N2    | -6.35 | 110.48      | 116.20   |
| 24  | BA    | 1089 | A    | P-O3'-C3'   | 6.35  | 127.32      | 119.70   |
| 21  | AA    | 688  | G    | N9-C1'-C2'  | -6.35 | 105.02      | 112.00   |
| 24  | BA    | 496  | G    | P-O3'-C3'   | -6.35 | 112.08      | 119.70   |
| 21  | AA    | 109  | A    | O4'-C1'-N9  | 6.34  | 113.28      | 108.20   |
| 21  | AA    | 960  | U    | P-O3'-C3'   | 6.34  | 127.31      | 119.70   |
| 21  | AA    | 1256 | A    | P-O3'-C3'   | 6.34  | 127.31      | 119.70   |
| 24  | DA    | 2275 | C    | P-O3'-C3'   | 6.34  | 127.31      | 119.70   |
| 24  | BA    | 958  | U    | P-O3'-C3'   | -6.34 | 112.09      | 119.70   |
| 24  | BA    | 968  | C    | N1-C2-O2    | 6.34  | 122.70      | 118.90   |
| 55  | CA    | 212  | G    | N9-C1'-C2'  | -6.34 | 105.02      | 112.00   |
| 24  | DA    | 271  | G    | C4-N9-C1'   | -6.34 | 118.26      | 126.50   |
| 24  | BA    | 395  | U    | P-O3'-C3'   | 6.34  | 127.31      | 119.70   |
| 24  | DA    | 2800 | A    | C3'-C2'-C1' | 6.34  | 106.57      | 101.50   |
| 24  | BA    | 2575 | C    | P-O3'-C3'   | 6.33  | 127.30      | 119.70   |
| 55  | CA    | 424  | G    | P-O3'-C3'   | -6.33 | 112.10      | 119.70   |
| 24  | DA    | 531  | C    | P-O3'-C3'   | 6.33  | 127.30      | 119.70   |
| 24  | BA    | 243  | U    | C3'-C2'-C1' | 6.33  | 106.57      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 860  | U    | P-O3'-C3'   | -6.33 | 112.10      | 119.70   |
| 24  | DA    | 1607 | C    | N1-C1'-C2'  | 6.33  | 122.23      | 114.00   |
| 21  | AA    | 1129 | C    | P-O3'-C3'   | 6.33  | 127.30      | 119.70   |
| 24  | BA    | 934  | U    | P-O3'-C3'   | -6.33 | 112.10      | 119.70   |
| 24  | BA    | 1496 | A    | N9-C1'-C2'  | -6.33 | 105.04      | 112.00   |
| 24  | BA    | 1805 | A    | C5-C6-N6    | 6.33  | 128.77      | 123.70   |
| 24  | DA    | 1996 | C    | P-O3'-C3'   | 6.33  | 127.30      | 119.70   |
| 24  | DA    | 2401 | U    | P-O3'-C3'   | 6.33  | 127.30      | 119.70   |
| 24  | BA    | 1115 | G    | O4'-C1'-N9  | 6.33  | 113.26      | 108.20   |
| 24  | DA    | 121  | G    | P-O3'-C3'   | -6.33 | 112.11      | 119.70   |
| 24  | BA    | 2492 | U    | C3'-C2'-C1' | 6.33  | 106.56      | 101.50   |
| 21  | AA    | 1130 | A    | P-O3'-C3'   | 6.33  | 127.29      | 119.70   |
| 24  | BA    | 229  | C    | C3'-C2'-C1' | 6.33  | 106.56      | 101.50   |
| 24  | DA    | 216  | A    | P-O3'-C3'   | -6.33 | 112.11      | 119.70   |
| 21  | AA    | 70   | U    | N1-C1'-C2'  | 6.32  | 122.22      | 114.00   |
| 24  | DA    | 1291 | C    | O4'-C1'-N1  | 6.32  | 113.26      | 108.20   |
| 24  | BA    | 729  | G    | C3'-C2'-C1' | 6.32  | 106.56      | 101.50   |
| 24  | DA    | 2267 | A    | C6-N1-C2    | -6.32 | 114.81      | 118.60   |
| 24  | BA    | 2210 | U    | O4'-C1'-N1  | 6.32  | 113.26      | 108.20   |
| 21  | AA    | 560  | A    | P-O3'-C3'   | -6.32 | 112.12      | 119.70   |
| 24  | BA    | 1619 | G    | N9-C1'-C2'  | -6.32 | 105.05      | 112.00   |
| 21  | AA    | 119  | A    | P-O3'-C3'   | 6.32  | 127.28      | 119.70   |
| 21  | AA    | 1225 | A    | P-O3'-C3'   | -6.32 | 112.12      | 119.70   |
| 24  | BA    | 1858 | A    | C3'-C2'-C1' | 6.31  | 106.55      | 101.50   |
| 24  | BA    | 2272 | U    | P-O3'-C3'   | 6.31  | 127.27      | 119.70   |
| 24  | BA    | 2520 | C    | C3'-C2'-C1' | 6.31  | 106.55      | 101.50   |
| 24  | BA    | 2850 | A    | P-O3'-C3'   | -6.31 | 112.12      | 119.70   |
| 24  | DA    | 1802 | A    | C3'-C2'-C1' | 6.31  | 106.55      | 101.50   |
| 24  | DA    | 1996 | C    | O4'-C1'-N1  | 6.31  | 113.25      | 108.20   |
| 21  | AA    | 890  | G    | P-O3'-C3'   | 6.31  | 127.27      | 119.70   |
| 21  | AA    | 1401 | G    | P-O3'-C3'   | -6.31 | 112.13      | 119.70   |
| 24  | BA    | 1125 | G    | C2-N3-C4    | -6.31 | 108.75      | 111.90   |
| 24  | DA    | 749  | A    | N9-C1'-C2'  | -6.31 | 105.06      | 112.00   |
| 24  | BA    | 2034 | U    | N3-C2-O2    | -6.31 | 117.78      | 122.20   |
| 55  | CA    | 891  | U    | C3'-C2'-C1' | 6.31  | 106.55      | 101.50   |
| 24  | DA    | 234  | U    | P-O3'-C3'   | -6.31 | 112.13      | 119.70   |
| 24  | DA    | 370  | G    | C4-N9-C1'   | -6.31 | 118.30      | 126.50   |
| 24  | BA    | 302  | C    | C3'-C2'-C1' | 6.30  | 106.54      | 101.50   |
| 55  | CA    | 512  | U    | C3'-C2'-C1' | 6.30  | 106.54      | 101.50   |
| 24  | DA    | 1722 | A    | N9-C1'-C2'  | -6.30 | 105.06      | 112.00   |
| 21  | AA    | 1125 | U    | P-O3'-C3'   | 6.30  | 127.26      | 119.70   |
| 24  | BA    | 1009 | A    | C3'-C2'-C1' | 6.30  | 106.54      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 1246 | A    | C6-N1-C2    | -6.30 | 114.82      | 118.60   |
| 24  | BA    | 212  | G    | P-O3'-C3'   | -6.30 | 112.14      | 119.70   |
| 24  | BA    | 1552 | A    | P-O3'-C3'   | -6.30 | 112.14      | 119.70   |
| 24  | DA    | 2630 | G    | C3'-C2'-C1' | 6.30  | 106.54      | 101.50   |
| 55  | CA    | 1139 | G    | P-O3'-C3'   | 6.30  | 127.26      | 119.70   |
| 24  | BA    | 1829 | A    | C3'-C2'-C1' | 6.30  | 106.54      | 101.50   |
| 24  | DA    | 222  | A    | P-O3'-C3'   | 6.30  | 127.26      | 119.70   |
| 21  | AA    | 1337 | G    | P-O3'-C3'   | 6.29  | 127.25      | 119.70   |
| 21  | AA    | 183  | C    | O4'-C1'-N1  | 6.29  | 113.23      | 108.20   |
| 23  | CW    | 3    | U    | N1-C1'-C2'  | 6.29  | 122.18      | 114.00   |
| 21  | AA    | 47   | C    | O4'-C1'-N1  | 6.29  | 113.23      | 108.20   |
| 55  | CA    | 14   | U    | C3'-C2'-C1' | 6.29  | 106.53      | 101.50   |
| 55  | CA    | 82   | G    | C3'-C2'-C1' | 6.29  | 106.53      | 101.50   |
| 24  | DA    | 206  | U    | P-O3'-C3'   | -6.29 | 112.15      | 119.70   |
| 24  | DA    | 1828 | G    | P-O3'-C3'   | 6.29  | 127.25      | 119.70   |
| 24  | DA    | 1324 | G    | P-O3'-C3'   | 6.29  | 127.25      | 119.70   |
| 24  | BA    | 1816 | C    | C3'-C2'-C1' | 6.29  | 106.53      | 101.50   |
| 24  | DA    | 1993 | U    | C3'-C2'-C1' | 6.29  | 106.53      | 101.50   |
| 24  | BA    | 759  | G    | P-O5'-C5'   | -6.28 | 110.85      | 120.90   |
| 21  | AA    | 368  | U    | O4'-C1'-N1  | 6.28  | 113.23      | 108.20   |
| 21  | AA    | 480  | U    | C2-N3-C4    | -6.28 | 123.23      | 127.00   |
| 21  | AA    | 116  | A    | C3'-C2'-C1' | 6.28  | 106.53      | 101.50   |
| 21  | AA    | 575  | G    | C8-N9-C1'   | 6.28  | 135.17      | 127.00   |
| 21  | AA    | 1288 | A    | C3'-C2'-C1' | 6.28  | 106.53      | 101.50   |
| 21  | AA    | 1366 | C    | O4'-C1'-N1  | 6.28  | 113.22      | 108.20   |
| 21  | AA    | 1399 | C    | N1-C1'-C2'  | 6.28  | 122.16      | 114.00   |
| 24  | BA    | 2545 | G    | C8-N9-C4    | -6.28 | 103.89      | 106.40   |
| 24  | BA    | 858  | G    | C5-C6-N1    | 6.28  | 114.64      | 111.50   |
| 55  | CA    | 1241 | G    | C3'-C2'-C1' | 6.28  | 106.52      | 101.50   |
| 24  | DA    | 1945 | G    | C3'-C2'-C1' | 6.28  | 106.52      | 101.50   |
| 24  | DA    | 1021 | A    | N9-C1'-C2'  | -6.28 | 105.10      | 112.00   |
| 24  | DA    | 1915 | U    | N1-C1'-C2'  | -6.28 | 105.10      | 112.00   |
| 24  | DA    | 2260 | C    | O4'-C1'-N1  | 6.28  | 113.22      | 108.20   |
| 24  | DA    | 2457 | U    | O4'-C1'-N1  | 6.28  | 113.22      | 108.20   |
| 21  | AA    | 559  | A    | O4'-C1'-N9  | 6.27  | 113.22      | 108.20   |
| 24  | DA    | 1832 | C    | O4'-C1'-N1  | 6.27  | 113.22      | 108.20   |
| 24  | BA    | 2517 | C    | O4'-C1'-N1  | 6.27  | 113.22      | 108.20   |
| 55  | CA    | 1127 | G    | P-O3'-C3'   | -6.27 | 112.17      | 119.70   |
| 24  | DA    | 1461 | C    | P-O3'-C3'   | -6.27 | 112.17      | 119.70   |
| 21  | AA    | 253  | A    | P-O3'-C3'   | -6.27 | 112.17      | 119.70   |
| 24  | BA    | 740  | C    | O4'-C1'-N1  | 6.27  | 113.22      | 108.20   |
| 55  | CA    | 1531 | A    | N9-C1'-C2'  | -6.27 | 105.10      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 959  | A    | P-O3'-C3'   | -6.27 | 112.18      | 119.70   |
| 24  | DA    | 1398 | C    | P-O3'-C3'   | -6.27 | 112.18      | 119.70   |
| 24  | BA    | 802  | A    | P-O3'-C3'   | -6.27 | 112.18      | 119.70   |
| 24  | BA    | 946  | C    | C3'-C2'-C1' | 6.27  | 106.51      | 101.50   |
| 24  | BA    | 763  | G    | C4-N9-C1'   | 6.27  | 134.65      | 126.50   |
| 56  | DB    | 41   | G    | P-O3'-C3'   | -6.27 | 112.18      | 119.70   |
| 24  | BA    | 1568 | G    | O4'-C1'-N9  | -6.26 | 103.19      | 108.20   |
| 21  | AA    | 452  | A    | C3'-C2'-C1' | 6.26  | 106.51      | 101.50   |
| 55  | CA    | 86   | G    | P-O3'-C3'   | 6.26  | 127.22      | 119.70   |
| 24  | BA    | 2036 | C    | C3'-C2'-C1' | 6.26  | 106.51      | 101.50   |
| 24  | BA    | 2427 | C    | C6-N1-C2    | -6.26 | 117.80      | 120.30   |
| 24  | DA    | 1816 | C    | O4'-C1'-N1  | 6.26  | 113.21      | 108.20   |
| 24  | DA    | 2214 | C    | P-O3'-C3'   | -6.26 | 112.19      | 119.70   |
| 21  | AA    | 652  | U    | P-O3'-C3'   | 6.26  | 127.21      | 119.70   |
| 21  | AA    | 935  | A    | P-O3'-C3'   | -6.26 | 112.19      | 119.70   |
| 24  | DA    | 303  | G    | C3'-C2'-C1' | 6.26  | 106.50      | 101.50   |
| 24  | DA    | 2277 | G    | N9-C1'-C2'  | -6.26 | 105.12      | 112.00   |
| 24  | BA    | 1962 | C    | O4'-C1'-N1  | 6.25  | 113.20      | 108.20   |
| 21  | AA    | 655  | A    | N9-C1'-C2'  | -6.25 | 105.12      | 112.00   |
| 24  | DA    | 2144 | G    | P-O3'-C3'   | 6.25  | 127.20      | 119.70   |
| 24  | DA    | 2460 | U    | C3'-C2'-C1' | 6.25  | 106.50      | 101.50   |
| 21  | AA    | 1216 | A    | N9-C1'-C2'  | -6.25 | 105.12      | 112.00   |
| 21  | AA    | 520  | A    | P-O3'-C3'   | -6.25 | 112.20      | 119.70   |
| 24  | BA    | 1568 | G    | P-O3'-C3'   | -6.25 | 112.20      | 119.70   |
| 24  | DA    | 1993 | U    | O4'-C1'-N1  | 6.25  | 113.20      | 108.20   |
| 24  | BA    | 119  | A    | O3'-P-O5'   | 6.25  | 115.87      | 104.00   |
| 24  | DA    | 2053 | G    | N9-C4-C5    | 6.25  | 107.90      | 105.40   |
| 24  | BA    | 2511 | U    | C2-N1-C1'   | 6.25  | 125.19      | 117.70   |
| 24  | DA    | 1090 | A    | C3'-C2'-C1' | 6.25  | 106.50      | 101.50   |
| 21  | AA    | 339  | C    | O4'-C1'-N1  | 6.24  | 113.19      | 108.20   |
| 24  | BA    | 763  | G    | C3'-C2'-C1' | 6.24  | 106.50      | 101.50   |
| 24  | BA    | 2001 | C    | P-O3'-C3'   | -6.24 | 112.21      | 119.70   |
| 24  | DA    | 647  | G    | C3'-C2'-C1' | 6.24  | 106.49      | 101.50   |
| 55  | CA    | 282  | A    | P-O3'-C3'   | -6.24 | 112.21      | 119.70   |
| 55  | CA    | 209  | U    | P-O3'-C3'   | 6.24  | 127.19      | 119.70   |
| 55  | CA    | 1124 | G    | O4'-C1'-N9  | 6.24  | 113.19      | 108.20   |
| 24  | DA    | 1341 | G    | C3'-C2'-C1' | 6.24  | 106.49      | 101.50   |
| 24  | BA    | 684  | G    | N3-C2-N2    | 6.24  | 124.27      | 119.90   |
| 24  | DA    | 1733 | G    | P-O3'-C3'   | -6.24 | 112.22      | 119.70   |
| 55  | CA    | 801  | U    | P-O3'-C3'   | -6.24 | 112.22      | 119.70   |
| 24  | BA    | 2359 | C    | C6-N1-C2    | 6.23  | 122.79      | 120.30   |
| 55  | CA    | 1326 | U    | O4'-C1'-N1  | 6.23  | 113.19      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 1733 | G    | P-O3'-C3'   | -6.23 | 112.22      | 119.70   |
| 55  | CA    | 1184 | G    | C3'-C2'-C1' | 6.23  | 106.48      | 101.50   |
| 29  | DF    | 109  | ARG  | CG-CD-NE    | -6.23 | 98.72       | 111.80   |
| 24  | BA    | 1137 | G    | P-O3'-C3'   | -6.23 | 112.23      | 119.70   |
| 24  | BA    | 389  | G    | P-O3'-C3'   | -6.22 | 112.23      | 119.70   |
| 24  | DA    | 2895 | G    | C3'-C2'-C1' | 6.22  | 106.48      | 101.50   |
| 24  | DA    | 301  | G    | P-O3'-C3'   | 6.22  | 127.17      | 119.70   |
| 21  | AA    | 247  | G    | N9-C1'-C2'  | -6.22 | 105.16      | 112.00   |
| 24  | BA    | 1142 | A    | C6-N1-C2    | 6.22  | 122.33      | 118.60   |
| 24  | BA    | 2800 | A    | C3'-C2'-C1' | 6.22  | 106.48      | 101.50   |
| 55  | CA    | 1181 | G    | P-O3'-C3'   | 6.22  | 127.16      | 119.70   |
| 55  | CA    | 410  | G    | C5-C6-O6    | -6.22 | 124.87      | 128.60   |
| 24  | DA    | 375  | G    | N9-C1'-C2'  | -6.22 | 105.16      | 112.00   |
| 24  | DA    | 1839 | G    | C3'-C2'-C1' | 6.22  | 106.47      | 101.50   |
| 24  | BA    | 162  | U    | O4'-C1'-N1  | 6.21  | 113.17      | 108.20   |
| 24  | DA    | 1416 | G    | O4'-C1'-N9  | 6.21  | 113.17      | 108.20   |
| 21  | AA    | 705  | G    | N9-C1'-C2'  | -6.21 | 105.17      | 112.00   |
| 24  | BA    | 967  | U    | P-O5'-C5'   | -6.21 | 110.96      | 120.90   |
| 55  | CA    | 1481 | U    | O4'-C1'-N1  | 6.21  | 113.17      | 108.20   |
| 24  | DA    | 1341 | G    | P-O3'-C3'   | 6.21  | 127.15      | 119.70   |
| 24  | DA    | 2447 | G    | O4'-C1'-N9  | 6.21  | 113.17      | 108.20   |
| 24  | DA    | 2656 | U    | P-O3'-C3'   | -6.21 | 112.25      | 119.70   |
| 24  | DA    | 2610 | C    | N1-C1'-C2'  | 6.21  | 122.07      | 114.00   |
| 24  | BA    | 2780 | G    | P-O5'-C5'   | -6.21 | 110.97      | 120.90   |
| 55  | CA    | 754  | C    | N1-C1'-C2'  | -6.21 | 105.17      | 112.00   |
| 21  | AA    | 281  | G    | P-O3'-C3'   | -6.21 | 112.25      | 119.70   |
| 24  | BA    | 75   | G    | P-O3'-C3'   | -6.21 | 112.25      | 119.70   |
| 24  | BA    | 2812 | G    | C4-N9-C1'   | 6.21  | 134.57      | 126.50   |
| 24  | BA    | 1809 | A    | C3'-C2'-C1' | 6.20  | 106.46      | 101.50   |
| 24  | BA    | 2801 | G    | N9-C1'-C2'  | -6.20 | 105.18      | 112.00   |
| 24  | DA    | 1315 | C    | P-O5'-C5'   | -6.20 | 110.97      | 120.90   |
| 24  | DA    | 2459 | A    | C3'-C2'-C1' | 6.20  | 106.46      | 101.50   |
| 24  | BA    | 2750 | A    | P-O3'-C3'   | 6.20  | 127.14      | 119.70   |
| 21  | AA    | 267  | C    | C3'-C2'-C1' | 6.20  | 106.46      | 101.50   |
| 24  | BA    | 1110 | G    | P-O3'-C3'   | 6.20  | 127.14      | 119.70   |
| 21  | AA    | 110  | C    | C3'-C2'-C1' | 6.20  | 106.46      | 101.50   |
| 21  | AA    | 1297 | G    | P-O3'-C3'   | 6.20  | 127.14      | 119.70   |
| 55  | CA    | 198  | G    | C3'-C2'-C1' | 6.20  | 106.46      | 101.50   |
| 55  | CA    | 688  | G    | N9-C1'-C2'  | -6.20 | 105.19      | 112.00   |
| 21  | AA    | 1212 | U    | O4'-C1'-N1  | -6.19 | 103.24      | 108.20   |
| 24  | BA    | 1914 | C    | C3'-C2'-C1' | 6.19  | 106.45      | 101.50   |
| 12  | AM    | 70   | ARG  | CG-CD-NE    | -6.19 | 98.80       | 111.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 94   | G    | P-O3'-C3'   | 6.19  | 127.13      | 119.70   |
| 24  | BA    | 858  | G    | N3-C4-C5    | -6.19 | 125.50      | 128.60   |
| 24  | BA    | 2066 | C    | C2-N3-C4    | 6.19  | 123.00      | 119.90   |
| 55  | CA    | 97   | G    | N9-C1'-C2'  | -6.19 | 105.19      | 112.00   |
| 24  | DA    | 763  | G    | P-O3'-C3'   | -6.19 | 112.27      | 119.70   |
| 24  | DA    | 794  | A    | C3'-C2'-C1' | 6.19  | 106.45      | 101.50   |
| 21  | AA    | 90   | C    | P-O3'-C3'   | -6.19 | 112.28      | 119.70   |
| 21  | AA    | 13   | U    | P-O3'-C3'   | 6.18  | 127.12      | 119.70   |
| 24  | BA    | 333  | G    | C3'-C2'-C1' | 6.18  | 106.45      | 101.50   |
| 24  | BA    | 449  | A    | C3'-C2'-C1' | 6.18  | 106.45      | 101.50   |
| 24  | BA    | 1915 | U    | O4'-C1'-N1  | 6.18  | 113.15      | 108.20   |
| 21  | AA    | 13   | U    | O4'-C1'-N1  | 6.18  | 113.15      | 108.20   |
| 24  | BA    | 530  | G    | C3'-C2'-C1' | 6.18  | 106.45      | 101.50   |
| 55  | CA    | 91   | U    | P-O3'-C3'   | -6.18 | 112.28      | 119.70   |
| 21  | AA    | 884  | U    | O4'-C1'-N1  | 6.18  | 113.14      | 108.20   |
| 24  | BA    | 1733 | G    | C3'-C2'-C1' | 6.18  | 106.44      | 101.50   |
| 24  | BA    | 1812 | U    | C5-C4-O4    | 6.18  | 129.61      | 125.90   |
| 24  | DA    | 35   | G    | P-O3'-C3'   | -6.18 | 112.29      | 119.70   |
| 24  | BA    | 858  | G    | C2-N3-C4    | 6.17  | 114.99      | 111.90   |
| 55  | CA    | 275  | G    | P-O3'-C3'   | -6.17 | 112.29      | 119.70   |
| 21  | AA    | 351  | G    | C4-N9-C1'   | 6.17  | 134.52      | 126.50   |
| 24  | BA    | 1644 | C    | O4'-C1'-N1  | -6.17 | 103.26      | 108.20   |
| 24  | BA    | 1663 | G    | P-O3'-C3'   | 6.17  | 127.10      | 119.70   |
| 24  | BA    | 2582 | G    | P-O3'-C3'   | -6.17 | 112.30      | 119.70   |
| 24  | BA    | 2654 | A    | P-O3'-C3'   | 6.17  | 127.10      | 119.70   |
| 24  | DA    | 2492 | U    | C3'-C2'-C1' | 6.17  | 106.43      | 101.50   |
| 24  | BA    | 2730 | C    | O4'-C1'-N1  | 6.17  | 113.13      | 108.20   |
| 24  | BA    | 301  | G    | N3-C4-C5    | 6.16  | 131.68      | 128.60   |
| 24  | BA    | 1318 | U    | O4'-C1'-N1  | 6.16  | 113.13      | 108.20   |
| 24  | BA    | 1333 | G    | P-O5'-C5'   | -6.16 | 111.04      | 120.90   |
| 24  | BA    | 2498 | C    | N1-C1'-C2'  | -6.16 | 105.22      | 112.00   |
| 21  | AA    | 74   | A    | C6-N1-C2    | 6.16  | 122.30      | 118.60   |
| 55  | CA    | 548  | G    | C3'-C2'-C1' | 6.16  | 106.43      | 101.50   |
| 24  | DA    | 1255 | U    | O4'-C1'-N1  | 6.16  | 113.13      | 108.20   |
| 24  | DA    | 2544 | G    | C3'-C2'-C1' | 6.16  | 106.43      | 101.50   |
| 24  | BA    | 2607 | G    | P-O3'-C3'   | -6.16 | 112.31      | 119.70   |
| 24  | DA    | 87   | U    | O4'-C1'-N1  | 6.16  | 113.13      | 108.20   |
| 24  | DA    | 1206 | G    | N9-C1'-C2'  | -6.16 | 105.22      | 112.00   |
| 21  | AA    | 1098 | C    | O4'-C1'-N1  | 6.16  | 113.12      | 108.20   |
| 24  | BA    | 38   | A    | P-O3'-C3'   | -6.16 | 112.31      | 119.70   |
| 24  | BA    | 2023 | C    | P-O3'-C3'   | -6.16 | 112.31      | 119.70   |
| 21  | AA    | 47   | C    | P-O3'-C3'   | 6.16  | 127.09      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 1144 | A    | C3'-C2'-C1' | 6.16  | 106.42      | 101.50   |
| 24  | BA    | 2655 | G    | P-O3'-C3'   | 6.16  | 127.09      | 119.70   |
| 31  | DH    | 48   | GLU  | CB-CA-C     | -6.16 | 98.09       | 110.40   |
| 24  | DA    | 671  | C    | N1-C1'-C2'  | -6.15 | 105.23      | 112.00   |
| 24  | BA    | 1273 | U    | O4'-C1'-N1  | 6.15  | 113.12      | 108.20   |
| 25  | BB    | 5    | U    | O4'-C1'-N1  | 6.15  | 113.12      | 108.20   |
| 21  | AA    | 509  | A    | C3'-C2'-C1' | 6.15  | 106.42      | 101.50   |
| 21  | AA    | 1091 | U    | O4'-C1'-N1  | 6.15  | 113.12      | 108.20   |
| 21  | AA    | 1380 | U    | P-O3'-C3'   | 6.15  | 127.08      | 119.70   |
| 24  | BA    | 1778 | U    | C2-N3-C4    | -6.15 | 123.31      | 127.00   |
| 55  | CA    | 448  | A    | O4'-C1'-N9  | 6.15  | 113.12      | 108.20   |
| 21  | AA    | 886  | G    | P-O3'-C3'   | -6.15 | 112.32      | 119.70   |
| 24  | BA    | 378  | C    | C6-N1-C2    | 6.15  | 122.76      | 120.30   |
| 24  | BA    | 1498 | C    | C3'-C2'-C1' | 6.15  | 106.42      | 101.50   |
| 24  | BA    | 323  | C    | O4'-C1'-N1  | 6.14  | 113.12      | 108.20   |
| 24  | BA    | 747  | U    | C3'-C2'-C1' | 6.14  | 106.42      | 101.50   |
| 24  | DA    | 1135 | C    | N1-C1'-C2'  | -6.14 | 105.24      | 112.00   |
| 21  | AA    | 1182 | G    | C4-N9-C1'   | -6.14 | 118.52      | 126.50   |
| 24  | BA    | 1340 | U    | P-O3'-C3'   | 6.14  | 127.07      | 119.70   |
| 55  | CA    | 891  | U    | O4'-C1'-N1  | 6.14  | 113.11      | 108.20   |
| 55  | CA    | 1303 | C    | C2-N1-C1'   | 6.14  | 125.56      | 118.80   |
| 24  | DA    | 1137 | G    | N9-C1'-C2'  | -6.14 | 105.24      | 112.00   |
| 24  | DA    | 1739 | A    | P-O3'-C3'   | -6.14 | 112.33      | 119.70   |
| 21  | AA    | 985  | C    | O4'-C1'-N1  | 6.14  | 113.11      | 108.20   |
| 21  | AA    | 1046 | A    | P-O5'-C5'   | -6.14 | 111.07      | 120.90   |
| 24  | DA    | 244  | A    | P-O3'-C3'   | -6.14 | 112.33      | 119.70   |
| 24  | BA    | 411  | G    | O4'-C1'-N9  | 6.14  | 113.11      | 108.20   |
| 24  | BA    | 2641 | G    | N3-C4-N9    | -6.14 | 122.32      | 126.00   |
| 24  | DA    | 1932 | A    | N1-C6-N6    | 6.14  | 122.28      | 118.60   |
| 24  | BA    | 1728 | C    | O4'-C1'-N1  | 6.13  | 113.11      | 108.20   |
| 24  | DA    | 52   | A    | P-O3'-C3'   | -6.13 | 112.34      | 119.70   |
| 24  | BA    | 1760 | C    | C3'-C2'-C1' | 6.13  | 106.41      | 101.50   |
| 24  | BA    | 1885 | A    | C3'-C2'-C1' | 6.13  | 106.41      | 101.50   |
| 24  | BA    | 1943 | U    | N1-C1'-C2'  | 6.13  | 121.97      | 114.00   |
| 24  | BA    | 181  | A    | P-O5'-C5'   | -6.13 | 111.09      | 120.90   |
| 21  | AA    | 1032 | G    | P-O3'-C3'   | -6.13 | 112.35      | 119.70   |
| 24  | BA    | 1305 | C    | P-O3'-C3'   | -6.13 | 112.35      | 119.70   |
| 24  | BA    | 2046 | G    | P-O3'-C3'   | 6.13  | 127.05      | 119.70   |
| 55  | CA    | 1284 | C    | N1-C1'-C2'  | -6.13 | 105.26      | 112.00   |
| 24  | DA    | 2689 | U    | P-O3'-C3'   | 6.13  | 127.05      | 119.70   |
| 24  | BA    | 1478 | G    | C6-N1-C2    | 6.12  | 128.78      | 125.10   |
| 24  | BA    | 2566 | A    | O4'-C1'-N9  | 6.12  | 113.10      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 126  | A    | P-O3'-C3'   | -6.12 | 112.35      | 119.70   |
| 55  | CA    | 1242 | G    | N9-C1'-C2'  | -6.12 | 105.26      | 112.00   |
| 24  | DA    | 1624 | U    | O4'-C1'-N1  | 6.12  | 113.10      | 108.20   |
| 21  | AA    | 1182 | G    | O4'-C1'-N9  | -6.12 | 103.30      | 108.20   |
| 24  | BA    | 1380 | G    | P-O5'-C5'   | -6.12 | 111.11      | 120.90   |
| 55  | CA    | 82   | G    | P-O3'-C3'   | -6.12 | 112.35      | 119.70   |
| 24  | DA    | 1961 | C    | O4'-C1'-N1  | 6.12  | 113.10      | 108.20   |
| 24  | DA    | 2691 | C    | C3'-C2'-C1' | 6.12  | 106.40      | 101.50   |
| 56  | DB    | 42   | C    | P-O3'-C3'   | -6.12 | 112.36      | 119.70   |
| 21  | AA    | 495  | A    | P-O3'-C3'   | 6.12  | 127.04      | 119.70   |
| 24  | BA    | 1944 | U    | N1-C1'-C2'  | 6.12  | 121.95      | 114.00   |
| 24  | BA    | 2450 | A    | C3'-C2'-C1' | 6.12  | 106.39      | 101.50   |
| 55  | CA    | 37   | U    | O4'-C1'-N1  | 6.12  | 113.09      | 108.20   |
| 24  | BA    | 2514 | U    | C2-N3-C4    | -6.12 | 123.33      | 127.00   |
| 24  | BA    | 2812 | G    | N3-C4-C5    | -6.12 | 125.54      | 128.60   |
| 55  | CA    | 1380 | U    | O4'-C1'-N1  | 6.12  | 113.09      | 108.20   |
| 21  | AA    | 885  | G    | P-O3'-C3'   | -6.12 | 112.36      | 119.70   |
| 24  | BA    | 812  | C    | C3'-C2'-C1' | 6.12  | 106.39      | 101.50   |
| 55  | CA    | 404  | G    | P-O3'-C3'   | 6.12  | 127.04      | 119.70   |
| 24  | DA    | 1072 | C    | P-O3'-C3'   | -6.12 | 112.36      | 119.70   |
| 24  | DA    | 2289 | G    | C3'-C2'-C1' | 6.12  | 106.39      | 101.50   |
| 55  | CA    | 654  | G    | C3'-C2'-C1' | 6.11  | 106.39      | 101.50   |
| 55  | CA    | 67   | C    | C6-N1-C2    | -6.11 | 117.86      | 120.30   |
| 24  | BA    | 1643 | G    | P-O3'-C3'   | -6.11 | 112.37      | 119.70   |
| 55  | CA    | 317  | U    | P-O3'-C3'   | -6.11 | 112.37      | 119.70   |
| 24  | DA    | 1802 | A    | P-O3'-C3'   | -6.11 | 112.37      | 119.70   |
| 24  | DA    | 2289 | G    | N9-C1'-C2'  | -6.11 | 105.28      | 112.00   |
| 24  | BA    | 688  | U    | P-O5'-C5'   | -6.11 | 111.13      | 120.90   |
| 24  | BA    | 1060 | U    | N1-C2-O2    | -6.11 | 118.53      | 122.80   |
| 55  | CA    | 71   | A    | C3'-C2'-C1' | 6.11  | 106.39      | 101.50   |
| 24  | DA    | 1960 | A    | N1-C6-N6    | -6.11 | 114.94      | 118.60   |
| 24  | DA    | 1142 | A    | C5-N7-C8    | -6.11 | 100.85      | 103.90   |
| 24  | DA    | 1739 | A    | C3'-C2'-C1' | 6.10  | 106.38      | 101.50   |
| 21  | AA    | 1046 | A    | P-O3'-C3'   | -6.10 | 112.38      | 119.70   |
| 24  | BA    | 2504 | U    | C3'-C2'-C1' | 6.10  | 106.38      | 101.50   |
| 24  | DA    | 446  | G    | P-O3'-C3'   | 6.10  | 127.02      | 119.70   |
| 24  | BA    | 1560 | G    | C3'-C2'-C1' | 6.10  | 106.38      | 101.50   |
| 24  | BA    | 1792 | G    | N9-C1'-C2'  | -6.10 | 105.29      | 112.00   |
| 24  | BA    | 2362 | C    | P-O3'-C3'   | -6.10 | 112.38      | 119.70   |
| 24  | DA    | 1619 | G    | P-O3'-C3'   | -6.10 | 112.38      | 119.70   |
| 21  | AA    | 719  | C    | O4'-C1'-N1  | 6.10  | 113.08      | 108.20   |
| 24  | BA    | 435  | C    | P-O3'-C3'   | -6.10 | 112.38      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 2022 | U    | P-O5'-C5'   | -6.10 | 111.14      | 120.90   |
| 24  | BA    | 2327 | A    | P-O3'-C3'   | -6.10 | 112.38      | 119.70   |
| 24  | DA    | 1303 | G    | P-O3'-C3'   | -6.10 | 112.38      | 119.70   |
| 21  | AA    | 1481 | U    | N1-C2-O2    | -6.10 | 118.53      | 122.80   |
| 24  | BA    | 1015 | U    | P-O3'-C3'   | -6.10 | 112.38      | 119.70   |
| 24  | BA    | 1359 | A    | N7-C8-N9    | 6.10  | 116.85      | 113.80   |
| 24  | BA    | 1956 | U    | C3'-C2'-C1' | 6.10  | 106.38      | 101.50   |
| 24  | BA    | 2347 | C    | O4'-C1'-N1  | 6.10  | 113.08      | 108.20   |
| 24  | BA    | 2797 | U    | P-O3'-C3'   | 6.10  | 127.02      | 119.70   |
| 24  | DA    | 2631 | G    | N9-C1'-C2'  | -6.10 | 105.29      | 112.00   |
| 24  | BA    | 587  | C    | O4'-C1'-N1  | 6.09  | 113.08      | 108.20   |
| 24  | DA    | 2851 | A    | N9-C1'-C2'  | -6.09 | 105.30      | 112.00   |
| 21  | AA    | 1131 | G    | C3'-C2'-C1' | 6.09  | 106.37      | 101.50   |
| 21  | AA    | 1282 | C    | C3'-C2'-C1' | 6.09  | 106.37      | 101.50   |
| 24  | DA    | 1769 | U    | O4'-C1'-N1  | 6.09  | 113.08      | 108.20   |
| 24  | BA    | 1082 | U    | N3-C4-C5    | 6.09  | 118.25      | 114.60   |
| 55  | CA    | 1444 | U    | O4'-C1'-N1  | 6.09  | 113.07      | 108.20   |
| 24  | BA    | 627  | A    | P-O3'-C3'   | 6.09  | 127.01      | 119.70   |
| 24  | BA    | 2061 | G    | C6-N1-C2    | -6.09 | 121.45      | 125.10   |
| 24  | DA    | 65   | U    | O4'-C1'-N1  | 6.09  | 113.07      | 108.20   |
| 24  | DA    | 2250 | G    | O4'-C1'-N9  | -6.09 | 103.33      | 108.20   |
| 24  | BA    | 118  | A    | P-O3'-C3'   | 6.09  | 127.00      | 119.70   |
| 24  | BA    | 2297 | A    | P-O3'-C3'   | -6.09 | 112.40      | 119.70   |
| 55  | CA    | 549  | C    | O4'-C1'-N1  | 6.09  | 113.07      | 108.20   |
| 24  | DA    | 687  | C    | C3'-C2'-C1' | 6.09  | 106.37      | 101.50   |
| 24  | BA    | 1461 | C    | C3'-C2'-C1' | 6.08  | 106.37      | 101.50   |
| 21  | AA    | 1320 | C    | P-O3'-C3'   | -6.08 | 112.40      | 119.70   |
| 55  | CA    | 536  | C    | N1-C1'-C2'  | -6.08 | 105.31      | 112.00   |
| 24  | DA    | 1395 | A    | P-O3'-C3'   | 6.08  | 127.00      | 119.70   |
| 24  | BA    | 2617 | U    | C5-C4-O4    | 6.08  | 129.55      | 125.90   |
| 24  | BA    | 2810 | A    | N9-C1'-C2'  | -6.08 | 105.31      | 112.00   |
| 21  | AA    | 486  | U    | P-O5'-C5'   | -6.08 | 111.17      | 120.90   |
| 24  | BA    | 2573 | C    | C3'-C2'-C1' | 6.08  | 106.36      | 101.50   |
| 24  | BA    | 2823 | A    | P-O3'-C3'   | 6.08  | 126.99      | 119.70   |
| 24  | DA    | 1649 | G    | N9-C1'-C2'  | -6.08 | 105.31      | 112.00   |
| 24  | BA    | 1865 | U    | N1-C2-N3    | 6.08  | 118.55      | 114.90   |
| 24  | BA    | 2092 | U    | N1-C1'-C2'  | 6.08  | 121.90      | 114.00   |
| 55  | CA    | 686  | U    | O4'-C1'-N1  | 6.08  | 113.06      | 108.20   |
| 12  | AM    | 70   | ARG  | NE-CZ-NH2   | -6.08 | 117.26      | 120.30   |
| 21  | AA    | 1285 | A    | P-O3'-C3'   | 6.08  | 126.99      | 119.70   |
| 24  | BA    | 1024 | G    | P-O5'-C5'   | -6.08 | 111.18      | 120.90   |
| 55  | CA    | 89   | U    | C5-C4-O4    | -6.08 | 122.25      | 125.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 1060 | U    | C2-N3-C4    | -6.08 | 123.35      | 127.00   |
| 24  | DA    | 1683 | U    | P-O3'-C3'   | -6.08 | 112.41      | 119.70   |
| 24  | BA    | 1760 | C    | P-O3'-C3'   | -6.07 | 112.41      | 119.70   |
| 24  | BA    | 1980 | G    | P-O3'-C3'   | 6.07  | 126.99      | 119.70   |
| 24  | DA    | 1241 | A    | P-O5'-C5'   | -6.07 | 111.18      | 120.90   |
| 21  | AA    | 982  | U    | P-O3'-C3'   | 6.07  | 126.98      | 119.70   |
| 21  | AA    | 1482 | G    | C2-N3-C4    | -6.07 | 108.86      | 111.90   |
| 24  | BA    | 630  | G    | N9-C4-C5    | -6.07 | 102.97      | 105.40   |
| 24  | BA    | 1182 | G    | C3'-C2'-C1' | 6.07  | 106.36      | 101.50   |
| 24  | DA    | 2582 | G    | C3'-C2'-C1' | 6.07  | 106.36      | 101.50   |
| 21  | AA    | 366  | A    | P-O3'-C3'   | 6.07  | 126.98      | 119.70   |
| 24  | BA    | 1259 | G    | N3-C4-N9    | -6.07 | 122.36      | 126.00   |
| 24  | DA    | 629  | G    | N9-C1'-C2'  | -6.07 | 105.33      | 112.00   |
| 24  | DA    | 1786 | A    | P-O3'-C3'   | 6.07  | 126.98      | 119.70   |
| 24  | BA    | 962  | G    | N3-C4-N9    | -6.06 | 122.36      | 126.00   |
| 24  | BA    | 2578 | G    | N9-C4-C5    | 6.06  | 107.83      | 105.40   |
| 21  | AA    | 1321 | U    | N1-C1'-C2'  | -6.06 | 105.33      | 112.00   |
| 24  | BA    | 1348 | C    | C6-N1-C2    | 6.06  | 122.72      | 120.30   |
| 21  | AA    | 497  | G    | P-O3'-C3'   | -6.06 | 112.43      | 119.70   |
| 24  | BA    | 2514 | U    | N1-C2-O2    | -6.06 | 118.56      | 122.80   |
| 24  | BA    | 529  | A    | C4-C5-C6    | -6.06 | 113.97      | 117.00   |
| 24  | BA    | 1952 | A    | C8-N9-C4    | -6.06 | 103.38      | 105.80   |
| 24  | DA    | 1385 | A    | C5-C6-N6    | 6.06  | 128.55      | 123.70   |
| 24  | DA    | 1314 | C    | C3'-C2'-C1' | 6.06  | 106.34      | 101.50   |
| 24  | BA    | 1611 | C    | N1-C1'-C2'  | -6.05 | 105.34      | 112.00   |
| 24  | BA    | 1731 | G    | C8-N9-C1'   | 6.05  | 134.87      | 127.00   |
| 55  | CA    | 282  | A    | C3'-C2'-C1' | 6.05  | 106.34      | 101.50   |
| 24  | BA    | 1667 | G    | P-O3'-C3'   | 6.05  | 126.96      | 119.70   |
| 24  | DA    | 1760 | C    | C3'-C2'-C1' | 6.05  | 106.34      | 101.50   |
| 24  | DA    | 2440 | C    | C3'-C2'-C1' | 6.05  | 106.34      | 101.50   |
| 21  | AA    | 935  | A    | C3'-C2'-C1' | 6.05  | 106.34      | 101.50   |
| 24  | BA    | 2407 | A    | P-O3'-C3'   | -6.05 | 112.44      | 119.70   |
| 24  | DA    | 1386 | C    | C3'-C2'-C1' | 6.05  | 106.34      | 101.50   |
| 21  | AA    | 1054 | C    | N1-C1'-C2'  | 6.05  | 121.86      | 114.00   |
| 21  | AA    | 1363 | A    | P-O3'-C3'   | 6.05  | 126.96      | 119.70   |
| 24  | BA    | 58   | G    | C8-N9-C4    | -6.05 | 103.98      | 106.40   |
| 24  | BA    | 1767 | G    | C8-N9-C4    | -6.05 | 103.98      | 106.40   |
| 24  | BA    | 2867 | G    | N3-C4-N9    | -6.05 | 122.37      | 126.00   |
| 24  | DA    | 1477 | A    | C3'-C2'-C1' | 6.05  | 106.34      | 101.50   |
| 21  | AA    | 654  | G    | C3'-C2'-C1' | 6.05  | 106.34      | 101.50   |
| 24  | BA    | 513  | A    | P-O3'-C3'   | -6.05 | 112.44      | 119.70   |
| 24  | DA    | 2312 | U    | O5'-P-OP1   | -6.05 | 100.26      | 105.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 423  | G    | C3'-C2'-C1' | 6.04  | 106.34      | 101.50   |
| 24  | BA    | 1188 | U    | C2-N3-C4    | 6.04  | 130.63      | 127.00   |
| 24  | DA    | 197  | A    | C3'-C2'-C1' | 6.04  | 106.33      | 101.50   |
| 24  | BA    | 661  | A    | P-O3'-C3'   | -6.04 | 112.45      | 119.70   |
| 55  | CA    | 329  | A    | N1-C6-N6    | 6.04  | 122.22      | 118.60   |
| 24  | DA    | 443  | A    | P-O3'-C3'   | -6.04 | 112.45      | 119.70   |
| 24  | DA    | 397  | U    | O4'-C1'-N1  | 6.04  | 113.03      | 108.20   |
| 21  | AA    | 174  | A    | P-O3'-C3'   | -6.03 | 112.46      | 119.70   |
| 21  | AA    | 1202 | U    | P-O3'-C3'   | -6.03 | 112.46      | 119.70   |
| 21  | AA    | 131  | A    | C5-C6-N6    | 6.03  | 128.52      | 123.70   |
| 26  | BC    | 109  | LEU  | CA-CB-CG    | 6.03  | 129.17      | 115.30   |
| 55  | CA    | 464  | U    | P-O3'-C3'   | -6.03 | 112.46      | 119.70   |
| 24  | BA    | 548  | G    | N9-C1'-C2'  | -6.03 | 105.37      | 112.00   |
| 24  | BA    | 1770 | G    | C4-C5-N7    | 6.03  | 113.21      | 110.80   |
| 24  | BA    | 177  | G    | P-O3'-C3'   | 6.03  | 126.93      | 119.70   |
| 24  | BA    | 1732 | C    | O4'-C1'-N1  | 6.03  | 113.02      | 108.20   |
| 55  | CA    | 1128 | C    | O4'-C1'-N1  | 6.02  | 113.02      | 108.20   |
| 24  | BA    | 2828 | G    | P-O3'-C3'   | 6.02  | 126.93      | 119.70   |
| 55  | CA    | 116  | A    | C3'-C2'-C1' | 6.02  | 106.32      | 101.50   |
| 55  | CA    | 547  | A    | P-O3'-C3'   | 6.02  | 126.93      | 119.70   |
| 24  | DA    | 622  | G    | N9-C1'-C2'  | -6.02 | 105.38      | 112.00   |
| 55  | CA    | 915  | A    | N9-C1'-C2'  | -6.02 | 105.38      | 112.00   |
| 24  | DA    | 2148 | G    | P-O3'-C3'   | -6.02 | 112.48      | 119.70   |
| 24  | BA    | 216  | A    | C3'-C2'-C1' | 6.02  | 106.31      | 101.50   |
| 24  | BA    | 1716 | U    | C3'-C2'-C1' | 6.02  | 106.31      | 101.50   |
| 24  | BA    | 2148 | G    | C3'-C2'-C1' | 6.02  | 106.31      | 101.50   |
| 24  | BA    | 1    | G    | P-O3'-C3'   | -6.02 | 112.48      | 119.70   |
| 24  | BA    | 1787 | A    | C6-N1-C2    | 6.02  | 122.21      | 118.60   |
| 24  | BA    | 1267 | U    | P-O3'-C3'   | -6.01 | 112.48      | 119.70   |
| 24  | BA    | 1387 | A    | P-O3'-C3'   | -6.01 | 112.48      | 119.70   |
| 24  | DA    | 482  | A    | N9-C1'-C2'  | -6.01 | 105.38      | 112.00   |
| 24  | BA    | 389  | G    | N9-C1'-C2'  | -6.01 | 105.39      | 112.00   |
| 24  | BA    | 1606 | C    | P-O5'-C5'   | -6.01 | 111.28      | 120.90   |
| 55  | CA    | 1324 | A    | P-O3'-C3'   | 6.01  | 126.92      | 119.70   |
| 56  | DB    | 45   | A    | P-O3'-C3'   | -6.01 | 112.48      | 119.70   |
| 24  | BA    | 460  | A    | C3'-C2'-C1' | 6.01  | 106.31      | 101.50   |
| 55  | CA    | 483  | C    | O4'-C1'-N1  | 6.01  | 113.01      | 108.20   |
| 24  | DA    | 2615 | U    | C3'-C2'-C1' | 6.01  | 106.31      | 101.50   |
| 24  | BA    | 121  | G    | C3'-C2'-C1' | 6.01  | 106.31      | 101.50   |
| 24  | BA    | 1040 | A    | O4'-C1'-N9  | 6.01  | 113.01      | 108.20   |
| 25  | BB    | 58   | A    | N9-C1'-C2'  | -6.00 | 105.40      | 112.00   |
| 24  | DA    | 2889 | C    | O4'-C1'-N1  | 6.00  | 113.00      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 934  | U    | C3'-C2'-C1' | 6.00  | 106.30      | 101.50   |
| 24  | BA    | 1817 | G    | N9-C1'-C2'  | -6.00 | 105.40      | 112.00   |
| 24  | DA    | 1158 | C    | C3'-C2'-C1' | 6.00  | 106.30      | 101.50   |
| 55  | CA    | 218  | U    | O4'-C1'-N1  | 6.00  | 113.00      | 108.20   |
| 24  | BA    | 2441 | U    | O4'-C1'-N1  | 6.00  | 113.00      | 108.20   |
| 55  | CA    | 976  | G    | P-O3'-C3'   | -6.00 | 112.50      | 119.70   |
| 56  | DB    | 42   | C    | N1-C1'-C2'  | -6.00 | 105.40      | 112.00   |
| 55  | CA    | 173  | U    | N1-C1'-C2'  | 6.00  | 121.80      | 114.00   |
| 21  | AA    | 245  | U    | P-O3'-C3'   | -6.00 | 112.51      | 119.70   |
| 23  | AW    | 5    | U    | O4'-C1'-N1  | 5.99  | 113.00      | 108.20   |
| 24  | BA    | 2426 | A    | P-O3'-C3'   | 5.99  | 126.89      | 119.70   |
| 24  | DA    | 2251 | G    | C3'-C2'-C1' | 5.99  | 106.30      | 101.50   |
| 24  | DA    | 2611 | C    | C3'-C2'-C1' | 5.99  | 106.29      | 101.50   |
| 25  | BB    | 37   | C    | P-O3'-C3'   | -5.99 | 112.51      | 119.70   |
| 24  | DA    | 2226 | C    | C3'-C2'-C1' | 5.99  | 106.29      | 101.50   |
| 24  | DA    | 303  | G    | P-O3'-C3'   | -5.99 | 112.51      | 119.70   |
| 24  | BA    | 994  | C    | P-O3'-C3'   | -5.99 | 112.51      | 119.70   |
| 24  | BA    | 1157 | G    | P-O3'-C3'   | -5.99 | 112.51      | 119.70   |
| 24  | BA    | 1960 | A    | C6-N1-C2    | 5.99  | 122.19      | 118.60   |
| 24  | DA    | 406  | G    | P-O3'-C3'   | -5.99 | 112.52      | 119.70   |
| 24  | DA    | 1787 | A    | C3'-C2'-C1' | 5.99  | 106.29      | 101.50   |
| 24  | BA    | 1828 | G    | P-O5'-C5'   | 5.98  | 130.47      | 120.90   |
| 55  | CA    | 190  | A    | N1-C6-N6    | 5.98  | 122.19      | 118.60   |
| 55  | CA    | 483  | C    | P-O3'-C3'   | -5.98 | 112.52      | 119.70   |
| 21  | AA    | 1399 | C    | N1-C2-O2    | -5.98 | 115.31      | 118.90   |
| 24  | DA    | 1654 | A    | C3'-C2'-C1' | 5.98  | 106.28      | 101.50   |
| 24  | DA    | 1992 | G    | P-O3'-C3'   | 5.98  | 126.88      | 119.70   |
| 21  | AA    | 686  | U    | O4'-C1'-N1  | 5.98  | 112.98      | 108.20   |
| 24  | BA    | 1135 | C    | C3'-C2'-C1' | 5.98  | 106.28      | 101.50   |
| 24  | DA    | 459  | U    | C3'-C2'-C1' | 5.98  | 106.28      | 101.50   |
| 24  | DA    | 1019 | U    | C2-N3-C4    | -5.98 | 123.41      | 127.00   |
| 24  | BA    | 2543 | G    | C3'-C2'-C1' | 5.98  | 106.28      | 101.50   |
| 55  | CA    | 803  | G    | N9-C1'-C2'  | -5.98 | 105.42      | 112.00   |
| 24  | DA    | 2267 | A    | N9-C1'-C2'  | -5.98 | 105.42      | 112.00   |
| 55  | CA    | 389  | A    | C6-C5-N7    | 5.98  | 136.48      | 132.30   |
| 24  | DA    | 530  | G    | P-O3'-C3'   | -5.98 | 112.53      | 119.70   |
| 24  | DA    | 2257 | U    | P-O3'-C3'   | 5.98  | 126.87      | 119.70   |
| 21  | AA    | 1454 | G    | P-O3'-C3'   | -5.98 | 112.53      | 119.70   |
| 21  | AA    | 1399 | C    | P-O3'-C3'   | 5.97  | 126.87      | 119.70   |
| 24  | BA    | 1508 | A    | P-O3'-C3'   | 5.97  | 126.87      | 119.70   |
| 55  | CA    | 1442 | G    | C3'-C2'-C1' | 5.97  | 106.28      | 101.50   |
| 24  | DA    | 461  | C    | O4'-C1'-N1  | -5.97 | 103.42      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 1788 | C    | O4'-C1'-N1  | 5.97  | 112.98      | 108.20   |
| 24  | BA    | 1963 | U    | P-O3'-C3'   | -5.97 | 112.53      | 119.70   |
| 25  | BB    | 44   | G    | P-O3'-C3'   | 5.97  | 126.87      | 119.70   |
| 24  | DA    | 962  | G    | P-O3'-C3'   | 5.97  | 126.87      | 119.70   |
| 55  | CA    | 935  | A    | P-O3'-C3'   | -5.97 | 112.53      | 119.70   |
| 24  | DA    | 35   | G    | C3'-C2'-C1' | 5.97  | 106.28      | 101.50   |
| 24  | DA    | 449  | A    | P-O3'-C3'   | -5.97 | 112.53      | 119.70   |
| 24  | BA    | 61   | C    | P-O3'-C3'   | -5.97 | 112.54      | 119.70   |
| 21  | AA    | 1258 | G    | C3'-C2'-C1' | 5.97  | 106.28      | 101.50   |
| 24  | DA    | 14   | A    | P-O3'-C3'   | -5.97 | 112.54      | 119.70   |
| 24  | DA    | 421  | C    | N1-C1'-C2'  | 5.97  | 121.76      | 114.00   |
| 24  | DA    | 1694 | C    | N1-C2-O2    | 5.97  | 122.48      | 118.90   |
| 21  | AA    | 1102 | A    | C3'-C2'-C1' | 5.97  | 106.27      | 101.50   |
| 24  | BA    | 1241 | A    | P-O3'-C3'   | 5.97  | 126.86      | 119.70   |
| 24  | BA    | 1399 | C    | P-O3'-C3'   | 5.97  | 126.86      | 119.70   |
| 21  | AA    | 414  | A    | N9-C1'-C2'  | -5.96 | 105.44      | 112.00   |
| 24  | BA    | 2049 | G    | C5-C6-O6    | 5.96  | 132.18      | 128.60   |
| 55  | CA    | 175  | C    | O4'-C1'-N1  | 5.96  | 112.97      | 108.20   |
| 24  | BA    | 744  | U    | N1-C2-N3    | 5.96  | 118.48      | 114.90   |
| 24  | BA    | 2392 | A    | P-O5'-C5'   | -5.96 | 111.36      | 120.90   |
| 24  | BA    | 2727 | A    | P-O3'-C3'   | -5.96 | 112.55      | 119.70   |
| 25  | BB    | 40   | U    | P-O3'-C3'   | 5.96  | 126.85      | 119.70   |
| 55  | CA    | 643  | C    | C3'-C2'-C1' | 5.96  | 106.27      | 101.50   |
| 55  | CA    | 931  | C    | N1-C2-O2    | -5.96 | 115.32      | 118.90   |
| 24  | DA    | 244  | A    | C3'-C2'-C1' | 5.96  | 106.27      | 101.50   |
| 24  | DA    | 1997 | C    | C3'-C2'-C1' | 5.96  | 106.27      | 101.50   |
| 21  | AA    | 1319 | A    | P-O3'-C3'   | 5.96  | 126.85      | 119.70   |
| 24  | BA    | 1204 | A    | O4'-C1'-N9  | 5.96  | 112.97      | 108.20   |
| 24  | DA    | 576  | U    | C3'-C2'-C1' | 5.96  | 106.26      | 101.50   |
| 24  | DA    | 269  | C    | O4'-C1'-N1  | 5.96  | 112.96      | 108.20   |
| 24  | BA    | 1386 | C    | N1-C1'-C2'  | -5.95 | 105.45      | 112.00   |
| 24  | BA    | 1429 | G    | N9-C1'-C2'  | -5.95 | 105.45      | 112.00   |
| 24  | BA    | 1386 | C    | C3'-C2'-C1' | 5.95  | 106.26      | 101.50   |
| 24  | DA    | 947  | A    | C3'-C2'-C1' | 5.95  | 106.26      | 101.50   |
| 21  | AA    | 1283 | U    | O4'-C1'-N1  | 5.95  | 112.96      | 108.20   |
| 24  | BA    | 1585 | C    | O4'-C1'-N1  | -5.95 | 103.44      | 108.20   |
| 55  | CA    | 358  | U    | O4'-C1'-N1  | 5.95  | 112.96      | 108.20   |
| 55  | CA    | 983  | A    | C3'-C2'-C1' | 5.95  | 106.26      | 101.50   |
| 24  | DA    | 2214 | C    | C3'-C2'-C1' | 5.95  | 106.26      | 101.50   |
| 21  | AA    | 1196 | A    | O4'-C1'-N9  | 5.95  | 112.96      | 108.20   |
| 24  | BA    | 1919 | A    | P-O3'-C3'   | -5.95 | 112.56      | 119.70   |
| 24  | BA    | 2022 | U    | P-O3'-C3'   | -5.95 | 112.56      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 2575 | C    | C6-N1-C2    | 5.95  | 122.68      | 120.30   |
| 55  | CA    | 66   | A    | P-O3'-C3'   | -5.95 | 112.56      | 119.70   |
| 24  | DA    | 390  | U    | P-O3'-C3'   | 5.95  | 126.84      | 119.70   |
| 21  | AA    | 808  | C    | O4'-C1'-N1  | 5.95  | 112.96      | 108.20   |
| 24  | BA    | 61   | C    | C3'-C2'-C1' | 5.95  | 106.26      | 101.50   |
| 24  | BA    | 2197 | U    | N1-C1'-C2'  | 5.95  | 121.73      | 114.00   |
| 24  | BA    | 1733 | G    | N9-C1'-C2'  | -5.95 | 105.46      | 112.00   |
| 55  | CA    | 30   | U    | O4'-C1'-N1  | 5.95  | 112.96      | 108.20   |
| 55  | CA    | 686  | U    | N1-C1'-C2'  | 5.95  | 121.73      | 114.00   |
| 55  | CA    | 1160 | G    | N9-C1'-C2'  | -5.95 | 105.46      | 112.00   |
| 55  | CA    | 1296 | C    | P-O3'-C3'   | 5.95  | 126.83      | 119.70   |
| 24  | DA    | 2781 | A    | C3'-C2'-C1' | 5.95  | 106.26      | 101.50   |
| 24  | BA    | 2752 | C    | C3'-C2'-C1' | 5.94  | 106.25      | 101.50   |
| 55  | CA    | 531  | U    | P-O3'-C3'   | 5.94  | 126.83      | 119.70   |
| 24  | DA    | 1676 | A    | C3'-C2'-C1' | 5.94  | 106.25      | 101.50   |
| 24  | BA    | 1026 | G    | C3'-C2'-C1' | 5.94  | 106.25      | 101.50   |
| 24  | BA    | 1568 | G    | P-O5'-C5'   | -5.94 | 111.39      | 120.90   |
| 24  | DA    | 1695 | G    | P-O3'-C3'   | -5.94 | 112.57      | 119.70   |
| 24  | DA    | 1759 | A    | C3'-C2'-C1' | 5.94  | 106.25      | 101.50   |
| 24  | DA    | 2022 | U    | O4'-C1'-N1  | -5.94 | 103.45      | 108.20   |
| 24  | DA    | 2245 | U    | O4'-C1'-N1  | 5.94  | 112.95      | 108.20   |
| 56  | DB    | 58   | A    | C3'-C2'-C1' | 5.94  | 106.25      | 101.50   |
| 24  | BA    | 1838 | C    | O4'-C1'-N1  | 5.94  | 112.95      | 108.20   |
| 24  | DA    | 1330 | C    | P-O3'-C3'   | -5.94 | 112.57      | 119.70   |
| 24  | DA    | 2093 | G    | C3'-C2'-C1' | 5.94  | 106.25      | 101.50   |
| 56  | DB    | 87   | U    | O4'-C1'-N1  | 5.94  | 112.95      | 108.20   |
| 24  | BA    | 365  | U    | C5-C4-O4    | -5.93 | 122.34      | 125.90   |
| 24  | BA    | 633  | A    | N9-C4-C5    | -5.93 | 103.43      | 105.80   |
| 24  | BA    | 1161 | C    | N1-C2-O2    | -5.93 | 115.34      | 118.90   |
| 24  | BA    | 1326 | U    | C3'-C2'-C1' | 5.93  | 106.25      | 101.50   |
| 55  | CA    | 968  | A    | O4'-C1'-N9  | 5.93  | 112.94      | 108.20   |
| 55  | CA    | 1288 | A    | N9-C1'-C2'  | -5.93 | 105.47      | 112.00   |
| 55  | CA    | 1102 | A    | C3'-C2'-C1' | 5.93  | 106.25      | 101.50   |
| 55  | CA    | 1507 | A    | C3'-C2'-C1' | 5.93  | 106.25      | 101.50   |
| 24  | BA    | 1135 | C    | N1-C1'-C2'  | -5.93 | 105.48      | 112.00   |
| 24  | BA    | 1142 | A    | N1-C2-N3    | -5.93 | 126.34      | 129.30   |
| 24  | DA    | 1654 | A    | O4'-C1'-N9  | 5.93  | 112.94      | 108.20   |
| 21  | AA    | 595  | A    | P-O3'-C3'   | 5.93  | 126.81      | 119.70   |
| 24  | DA    | 310  | A    | P-O3'-C3'   | 5.93  | 126.81      | 119.70   |
| 24  | BA    | 197  | A    | N9-C1'-C2'  | -5.93 | 105.48      | 112.00   |
| 24  | BA    | 2199 | A    | O4'-C1'-N9  | -5.93 | 103.46      | 108.20   |
| 55  | CA    | 143  | A    | N1-C6-N6    | -5.93 | 115.04      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | CA    | 794  | A    | C3'-C2'-C1' | 5.93  | 106.24      | 101.50   |
| 24  | DA    | 1821 | A    | P-O3'-C3'   | -5.92 | 112.59      | 119.70   |
| 21  | AA    | 52   | C    | C3'-C2'-C1' | 5.92  | 106.24      | 101.50   |
| 21  | AA    | 1168 | U    | O3'-P-O5'   | -5.92 | 92.75       | 104.00   |
| 24  | DA    | 230  | G    | C3'-C2'-C1' | 5.92  | 106.24      | 101.50   |
| 21  | AA    | 1348 | U    | C3'-C2'-C1' | 5.92  | 106.24      | 101.50   |
| 24  | BA    | 2049 | G    | C5-C6-N1    | -5.92 | 108.54      | 111.50   |
| 21  | AA    | 1229 | A    | P-O3'-C3'   | -5.92 | 112.60      | 119.70   |
| 24  | BA    | 2055 | C    | O4'-C1'-N1  | -5.92 | 103.46      | 108.20   |
| 24  | DA    | 449  | A    | C3'-C2'-C1' | 5.92  | 106.24      | 101.50   |
| 55  | CA    | 704  | A    | C3'-C2'-C1' | 5.92  | 106.23      | 101.50   |
| 24  | DA    | 604  | G    | N9-C1'-C2'  | -5.92 | 105.49      | 112.00   |
| 24  | DA    | 1788 | C    | C3'-C2'-C1' | 5.92  | 106.23      | 101.50   |
| 24  | DA    | 2630 | G    | N9-C1'-C2'  | -5.92 | 105.49      | 112.00   |
| 24  | BA    | 265  | A    | O4'-C1'-N9  | 5.92  | 112.93      | 108.20   |
| 21  | AA    | 194  | C    | O4'-C1'-N1  | 5.91  | 112.93      | 108.20   |
| 55  | CA    | 370  | C    | O4'-C1'-N1  | 5.91  | 112.93      | 108.20   |
| 24  | DA    | 60   | G    | C8-N9-C1'   | 5.91  | 134.69      | 127.00   |
| 24  | BA    | 520  | G    | P-O3'-C3'   | -5.91 | 112.61      | 119.70   |
| 24  | DA    | 1010 | A    | C3'-C2'-C1' | 5.91  | 106.23      | 101.50   |
| 55  | CA    | 110  | C    | C3'-C2'-C1' | 5.91  | 106.23      | 101.50   |
| 21  | AA    | 1064 | G    | O4'-C1'-N9  | 5.91  | 112.93      | 108.20   |
| 24  | BA    | 140  | C    | N1-C1'-C2'  | 5.91  | 121.68      | 114.00   |
| 55  | CA    | 497  | G    | C3'-C2'-C1' | 5.91  | 106.23      | 101.50   |
| 24  | DA    | 1129 | A    | C3'-C2'-C1' | 5.91  | 106.23      | 101.50   |
| 24  | DA    | 2543 | G    | C3'-C2'-C1' | 5.91  | 106.23      | 101.50   |
| 21  | AA    | 430  | A    | P-O3'-C3'   | -5.91 | 112.61      | 119.70   |
| 24  | DA    | 1050 | A    | N9-C1'-C2'  | -5.91 | 105.50      | 112.00   |
| 21  | AA    | 87   | C    | C3'-C2'-C1' | 5.91  | 106.22      | 101.50   |
| 21  | AA    | 1160 | G    | C3'-C2'-C1' | 5.91  | 106.22      | 101.50   |
| 21  | AA    | 1055 | A    | N9-C1'-C2'  | -5.90 | 105.51      | 112.00   |
| 24  | BA    | 2075 | U    | C5-C4-O4    | 5.90  | 129.44      | 125.90   |
| 24  | BA    | 2857 | G    | C8-N9-C4    | 5.90  | 108.76      | 106.40   |
| 24  | BA    | 2860 | A    | O4'-C1'-N9  | -5.90 | 103.48      | 108.20   |
| 24  | DA    | 1706 | C    | O4'-C1'-N1  | 5.90  | 112.92      | 108.20   |
| 21  | AA    | 1461 | G    | N9-C4-C5    | -5.90 | 103.04      | 105.40   |
| 24  | DA    | 2267 | A    | C4-C5-N7    | 5.90  | 113.65      | 110.70   |
| 21  | AA    | 1382 | C    | C3'-C2'-C1' | 5.90  | 106.22      | 101.50   |
| 24  | BA    | 1130 | U    | C2-N1-C1'   | 5.90  | 124.78      | 117.70   |
| 24  | DA    | 271  | G    | C8-N9-C1'   | 5.90  | 134.67      | 127.00   |
| 24  | DA    | 1555 | G    | C3'-C2'-C1' | 5.90  | 106.22      | 101.50   |
| 55  | CA    | 1454 | G    | C3'-C2'-C1' | 5.90  | 106.22      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 390  | U    | N1-C1'-C2'  | 5.90  | 121.67      | 114.00   |
| 24  | DA    | 2521 | C    | O4'-C1'-N1  | 5.90  | 112.92      | 108.20   |
| 21  | AA    | 1323 | G    | C3'-C2'-C1' | 5.89  | 106.22      | 101.50   |
| 24  | BA    | 1303 | G    | C3'-C2'-C1' | 5.89  | 106.22      | 101.50   |
| 24  | BA    | 1800 | C    | O4'-C1'-N1  | -5.89 | 103.48      | 108.20   |
| 24  | BA    | 2574 | G    | C3'-C2'-C1' | 5.89  | 106.22      | 101.50   |
| 55  | CA    | 425  | G    | P-O3'-C3'   | -5.89 | 112.63      | 119.70   |
| 24  | DA    | 779  | U    | O4'-C1'-N1  | 5.89  | 112.92      | 108.20   |
| 24  | DA    | 1290 | C    | C3'-C2'-C1' | 5.89  | 106.22      | 101.50   |
| 24  | DA    | 1626 | A    | P-O3'-C3'   | 5.89  | 126.77      | 119.70   |
| 24  | DA    | 1965 | C    | P-O3'-C3'   | -5.89 | 112.63      | 119.70   |
| 55  | CA    | 250  | A    | P-O3'-C3'   | 5.89  | 126.77      | 119.70   |
| 24  | BA    | 653  | U    | P-O3'-C3'   | -5.89 | 112.63      | 119.70   |
| 24  | BA    | 1147 | A    | N9-C4-C5    | 5.89  | 108.16      | 105.80   |
| 24  | DA    | 1303 | G    | C3'-C2'-C1' | 5.89  | 106.21      | 101.50   |
| 24  | BA    | 2423 | U    | N1-C1'-C2'  | 5.89  | 121.66      | 114.00   |
| 24  | BA    | 2440 | C    | C3'-C2'-C1' | 5.89  | 106.21      | 101.50   |
| 24  | BA    | 1478 | G    | N9-C4-C5    | 5.89  | 107.75      | 105.40   |
| 24  | DA    | 1507 | C    | O4'-C1'-N1  | -5.89 | 103.49      | 108.20   |
| 21  | AA    | 723  | U    | P-O3'-C3'   | -5.89 | 112.64      | 119.70   |
| 24  | BA    | 469  | G    | P-O3'-C3'   | -5.89 | 112.64      | 119.70   |
| 25  | BB    | 89   | U    | N1-C1'-C2'  | -5.88 | 105.53      | 112.00   |
| 24  | DA    | 1670 | C    | P-O3'-C3'   | 5.88  | 126.76      | 119.70   |
| 24  | DA    | 1206 | G    | C3'-C2'-C1' | 5.88  | 106.21      | 101.50   |
| 24  | DA    | 1785 | A    | C3'-C2'-C1' | 5.88  | 106.21      | 101.50   |
| 21  | AA    | 1530 | G    | C3'-C2'-C1' | 5.88  | 106.20      | 101.50   |
| 24  | DA    | 1034 | G    | C3'-C2'-C1' | 5.88  | 106.21      | 101.50   |
| 24  | BA    | 1956 | U    | O4'-C1'-N1  | 5.88  | 112.90      | 108.20   |
| 24  | DA    | 2402 | U    | P-O3'-C3'   | -5.88 | 112.65      | 119.70   |
| 24  | DA    | 2447 | G    | C5-C6-O6    | -5.88 | 125.08      | 128.60   |
| 24  | BA    | 1696 | G    | P-O3'-C3'   | -5.87 | 112.65      | 119.70   |
| 24  | DA    | 374  | A    | C3'-C2'-C1' | 5.87  | 106.20      | 101.50   |
| 24  | DA    | 2312 | U    | P-O3'-C3'   | -5.87 | 112.65      | 119.70   |
| 24  | DA    | 2312 | U    | C6-N1-C2    | -5.87 | 117.47      | 121.00   |
| 24  | BA    | 572  | A    | C3'-C2'-C1' | 5.87  | 106.20      | 101.50   |
| 24  | BA    | 1238 | G    | C3'-C2'-C1' | 5.87  | 106.20      | 101.50   |
| 24  | BA    | 1666 | G    | O4'-C1'-N9  | 5.87  | 112.90      | 108.20   |
| 55  | CA    | 982  | U    | P-O3'-C3'   | 5.87  | 126.75      | 119.70   |
| 24  | DA    | 1114 | C    | O4'-C1'-N1  | 5.87  | 112.90      | 108.20   |
| 24  | BA    | 1379 | U    | C3'-C2'-C1' | 5.87  | 106.20      | 101.50   |
| 55  | CA    | 381  | C    | P-O3'-C3'   | 5.87  | 126.74      | 119.70   |
| 24  | DA    | 2337 | G    | P-O3'-C3'   | -5.87 | 112.66      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 885  | G    | C3'-C2'-C1' | 5.87  | 106.19      | 101.50   |
| 24  | DA    | 2903 | U    | O4'-C1'-N1  | 5.87  | 112.89      | 108.20   |
| 21  | AA    | 1349 | A    | C3'-C2'-C1' | 5.87  | 106.19      | 101.50   |
| 21  | AA    | 1365 | G    | C3'-C2'-C1' | 5.87  | 106.19      | 101.50   |
| 24  | DA    | 2504 | U    | C3'-C2'-C1' | 5.87  | 106.19      | 101.50   |
| 24  | DA    | 2620 | C    | C6-N1-C2    | 5.87  | 122.65      | 120.30   |
| 55  | CA    | 970  | C    | P-O5'-C5'   | -5.86 | 111.52      | 120.90   |
| 55  | CA    | 1242 | G    | C3'-C2'-C1' | 5.86  | 106.19      | 101.50   |
| 24  | DA    | 413  | C    | O4'-C1'-N1  | 5.86  | 112.89      | 108.20   |
| 24  | BA    | 111  | A    | P-O3'-C3'   | -5.86 | 112.67      | 119.70   |
| 21  | AA    | 397  | A    | C6-N1-C2    | -5.86 | 115.08      | 118.60   |
| 24  | BA    | 639  | U    | O4'-C1'-N1  | 5.86  | 112.89      | 108.20   |
| 24  | BA    | 919  | U    | C4-C5-C6    | -5.86 | 116.18      | 119.70   |
| 24  | DA    | 1363 | C    | O4'-C1'-N1  | -5.86 | 103.51      | 108.20   |
| 24  | DA    | 1941 | C    | P-O3'-C3'   | -5.86 | 112.67      | 119.70   |
| 24  | BA    | 460  | A    | N9-C1'-C2'  | -5.86 | 105.56      | 112.00   |
| 24  | BA    | 1707 | G    | C3'-C2'-C1' | 5.86  | 106.19      | 101.50   |
| 24  | BA    | 2276 | G    | P-O3'-C3'   | -5.86 | 112.67      | 119.70   |
| 24  | BA    | 2326 | C    | N1-C1'-C2'  | 5.86  | 121.62      | 114.00   |
| 24  | BA    | 2792 | A    | P-O3'-C3'   | -5.86 | 112.67      | 119.70   |
| 55  | CA    | 565  | U    | O4'-C1'-N1  | 5.86  | 112.89      | 108.20   |
| 55  | CA    | 1151 | A    | P-O3'-C3'   | 5.86  | 126.73      | 119.70   |
| 24  | DA    | 802  | A    | C3'-C2'-C1' | 5.86  | 106.19      | 101.50   |
| 24  | DA    | 2727 | A    | P-O3'-C3'   | -5.86 | 112.67      | 119.70   |
| 24  | BA    | 2868 | A    | C3'-C2'-C1' | 5.85  | 106.18      | 101.50   |
| 24  | BA    | 645  | C    | C2-N1-C1'   | 5.85  | 125.24      | 118.80   |
| 24  | DA    | 1612 | C    | O4'-C1'-N1  | 5.85  | 112.88      | 108.20   |
| 24  | DA    | 370  | G    | C8-N9-C1'   | 5.85  | 134.61      | 127.00   |
| 24  | DA    | 587  | C    | P-O3'-C3'   | 5.85  | 126.72      | 119.70   |
| 24  | DA    | 1812 | U    | O4'-C1'-N1  | 5.85  | 112.88      | 108.20   |
| 25  | BB    | 15   | A    | N1-C6-N6    | 5.85  | 122.11      | 118.60   |
| 24  | DA    | 197  | A    | P-O3'-C3'   | -5.85 | 112.68      | 119.70   |
| 21  | AA    | 197  | A    | P-O3'-C3'   | 5.84  | 126.71      | 119.70   |
| 24  | BA    | 1188 | U    | O4'-C1'-N1  | -5.84 | 103.52      | 108.20   |
| 24  | BA    | 1993 | U    | C3'-C2'-C1' | 5.84  | 106.18      | 101.50   |
| 21  | AA    | 89   | U    | N1-C1'-C2'  | -5.84 | 105.57      | 112.00   |
| 24  | DA    | 1607 | C    | O4'-C1'-N1  | -5.84 | 103.53      | 108.20   |
| 24  | BA    | 86   | G    | N9-C1'-C2'  | -5.84 | 105.57      | 112.00   |
| 24  | BA    | 2712 | C    | P-O3'-C3'   | 5.84  | 126.71      | 119.70   |
| 55  | CA    | 143  | A    | C5-C6-N6    | 5.84  | 128.37      | 123.70   |
| 24  | DA    | 1157 | G    | C3'-C2'-C1' | 5.84  | 106.17      | 101.50   |
| 24  | BA    | 860  | U    | P-O5'-C5'   | -5.84 | 111.56      | 120.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 1510 | G    | C3'-C2'-C1' | 5.84  | 106.17      | 101.50   |
| 24  | BA    | 1326 | U    | N1-C1'-C2'  | -5.84 | 105.58      | 112.00   |
| 24  | BA    | 200  | U    | O4'-C1'-N1  | 5.84  | 112.87      | 108.20   |
| 24  | BA    | 2580 | U    | P-O3'-C3'   | 5.84  | 126.70      | 119.70   |
| 55  | CA    | 1505 | G    | O4'-C1'-N9  | -5.84 | 103.53      | 108.20   |
| 56  | DB    | 17   | C    | P-O3'-C3'   | -5.84 | 112.70      | 119.70   |
| 24  | BA    | 1023 | U    | P-O3'-C3'   | -5.83 | 112.70      | 119.70   |
| 24  | DA    | 2059 | A    | P-O3'-C3'   | 5.83  | 126.70      | 119.70   |
| 24  | BA    | 2281 | A    | C6-N1-C2    | -5.83 | 115.10      | 118.60   |
| 25  | BB    | 32   | U    | C6-N1-C2    | 5.83  | 124.50      | 121.00   |
| 24  | DA    | 858  | G    | P-O3'-C3'   | 5.83  | 126.70      | 119.70   |
| 24  | BA    | 2424 | C    | C3'-C2'-C1' | 5.83  | 106.16      | 101.50   |
| 24  | DA    | 990  | A    | C3'-C2'-C1' | 5.83  | 106.16      | 101.50   |
| 24  | DA    | 1822 | C    | C3'-C2'-C1' | 5.83  | 106.16      | 101.50   |
| 24  | DA    | 2037 | A    | C3'-C2'-C1' | 5.83  | 106.16      | 101.50   |
| 24  | DA    | 2267 | A    | P-O3'-C3'   | -5.83 | 112.70      | 119.70   |
| 24  | BA    | 138  | U    | P-O3'-C3'   | -5.83 | 112.70      | 119.70   |
| 24  | BA    | 813  | U    | O4'-C1'-N1  | -5.83 | 103.54      | 108.20   |
| 24  | BA    | 1942 | C    | C3'-C2'-C1' | 5.83  | 106.16      | 101.50   |
| 24  | DA    | 1716 | U    | P-O3'-C3'   | -5.83 | 112.71      | 119.70   |
| 24  | DA    | 2434 | A    | P-O3'-C3'   | 5.83  | 126.69      | 119.70   |
| 24  | DA    | 2573 | C    | N1-C1'-C2'  | -5.83 | 105.59      | 112.00   |
| 56  | DB    | 45   | A    | C3'-C2'-C1' | 5.83  | 106.16      | 101.50   |
| 21  | AA    | 1102 | A    | P-O3'-C3'   | -5.83 | 112.71      | 119.70   |
| 24  | BA    | 975  | A    | C3'-C2'-C1' | 5.83  | 106.16      | 101.50   |
| 55  | CA    | 1183 | U    | N1-C1'-C2'  | -5.83 | 105.59      | 112.00   |
| 24  | BA    | 1345 | C    | O4'-C1'-N1  | 5.82  | 112.86      | 108.20   |
| 21  | AA    | 548  | G    | C3'-C2'-C1' | 5.82  | 106.16      | 101.50   |
| 21  | AA    | 653  | U    | N1-C1'-C2'  | 5.82  | 121.57      | 114.00   |
| 21  | AA    | 1087 | G    | N9-C1'-C2'  | -5.82 | 105.60      | 112.00   |
| 23  | AW    | 3    | U    | N1-C1'-C2'  | 5.82  | 121.57      | 114.00   |
| 24  | BA    | 1254 | A    | C3'-C2'-C1' | 5.82  | 106.16      | 101.50   |
| 24  | BA    | 1437 | C    | O4'-C1'-N1  | 5.82  | 112.86      | 108.20   |
| 24  | BA    | 2309 | A    | C3'-C2'-C1' | 5.82  | 106.16      | 101.50   |
| 55  | CA    | 1507 | A    | P-O3'-C3'   | -5.82 | 112.72      | 119.70   |
| 21  | AA    | 274  | A    | O4'-C1'-N9  | 5.82  | 112.86      | 108.20   |
| 24  | DA    | 52   | A    | C3'-C2'-C1' | 5.82  | 106.15      | 101.50   |
| 24  | BA    | 395  | U    | N1-C1'-C2'  | 5.82  | 121.56      | 114.00   |
| 24  | BA    | 1229 | C    | C5-C6-N1    | -5.81 | 118.09      | 121.00   |
| 24  | BA    | 589  | U    | P-O3'-C3'   | -5.81 | 112.72      | 119.70   |
| 55  | CA    | 816  | A    | N9-C1'-C2'  | -5.81 | 105.61      | 112.00   |
| 24  | DA    | 2756 | U    | P-O3'-C3'   | 5.81  | 126.68      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 2282 | G    | N3-C4-N9    | -5.81 | 122.51      | 126.00   |
| 24  | BA    | 2860 | A    | C6-C5-N7    | -5.81 | 128.23      | 132.30   |
| 24  | DA    | 221  | A    | P-O3'-C3'   | 5.81  | 126.67      | 119.70   |
| 24  | DA    | 1273 | U    | N1-C1'-C2'  | -5.81 | 105.61      | 112.00   |
| 24  | DA    | 1399 | C    | C3'-C2'-C1' | 5.81  | 106.15      | 101.50   |
| 21  | AA    | 316  | C    | C3'-C2'-C1' | 5.81  | 106.14      | 101.50   |
| 24  | BA    | 2639 | A    | C3'-C2'-C1' | 5.81  | 106.14      | 101.50   |
| 24  | DA    | 1060 | U    | C2-N1-C1'   | 5.81  | 124.67      | 117.70   |
| 24  | BA    | 2896 | C    | C5-C4-N4    | 5.81  | 124.26      | 120.20   |
| 24  | BA    | 1981 | A    | C3'-C2'-C1' | 5.80  | 106.14      | 101.50   |
| 55  | CA    | 247  | G    | C3'-C2'-C1' | 5.80  | 106.14      | 101.50   |
| 55  | CA    | 513  | C    | P-O3'-C3'   | -5.80 | 112.74      | 119.70   |
| 24  | BA    | 12   | U    | N3-C2-O2    | -5.80 | 118.14      | 122.20   |
| 24  | DA    | 2848 | G    | P-O3'-C3'   | 5.80  | 126.66      | 119.70   |
| 21  | AA    | 84   | U    | N1-C1'-C2'  | 5.80  | 121.54      | 114.00   |
| 24  | BA    | 522  | A    | P-O3'-C3'   | -5.80 | 112.74      | 119.70   |
| 24  | BA    | 2092 | U    | P-O3'-C3'   | 5.80  | 126.66      | 119.70   |
| 24  | DA    | 785  | G    | N9-C1'-C2'  | -5.80 | 105.62      | 112.00   |
| 24  | DA    | 1333 | G    | C3'-C2'-C1' | 5.80  | 106.14      | 101.50   |
| 24  | DA    | 476  | G    | P-O3'-C3'   | -5.80 | 112.74      | 119.70   |
| 24  | BA    | 436  | C    | C3'-C2'-C1' | 5.80  | 106.14      | 101.50   |
| 24  | BA    | 2728 | U    | P-O5'-C5'   | -5.80 | 111.63      | 120.90   |
| 24  | DA    | 832  | U    | P-O3'-C3'   | -5.80 | 112.74      | 119.70   |
| 24  | DA    | 2136 | G    | N9-C1'-C2'  | -5.80 | 105.62      | 112.00   |
| 24  | DA    | 2313 | C    | P-O3'-C3'   | -5.80 | 112.74      | 119.70   |
| 55  | CA    | 253  | A    | C3'-C2'-C1' | 5.79  | 106.14      | 101.50   |
| 24  | BA    | 818  | G    | P-O3'-C3'   | -5.79 | 112.75      | 119.70   |
| 24  | BA    | 1060 | U    | N1-C1'-C2'  | 5.79  | 121.53      | 114.00   |
| 24  | DA    | 479  | A    | O4'-C1'-N9  | 5.79  | 112.83      | 108.20   |
| 24  | BA    | 482  | A    | C3'-C2'-C1' | 5.79  | 106.13      | 101.50   |
| 24  | BA    | 514  | A    | P-O3'-C3'   | -5.79 | 112.75      | 119.70   |
| 24  | BA    | 1330 | C    | C3'-C2'-C1' | 5.79  | 106.13      | 101.50   |
| 24  | BA    | 2052 | A    | C5-C6-N6    | 5.79  | 128.33      | 123.70   |
| 24  | BA    | 2797 | U    | O4'-C1'-N1  | 5.79  | 112.83      | 108.20   |
| 55  | CA    | 96   | U    | P-O3'-C3'   | -5.79 | 112.75      | 119.70   |
| 55  | CA    | 87   | C    | C3'-C2'-C1' | 5.79  | 106.13      | 101.50   |
| 24  | DA    | 2039 | U    | O4'-C1'-N1  | 5.79  | 112.83      | 108.20   |
| 24  | BA    | 303  | G    | N9-C1'-C2'  | -5.79 | 105.63      | 112.00   |
| 24  | BA    | 750  | A    | C8-N9-C4    | -5.79 | 103.48      | 105.80   |
| 24  | BA    | 2554 | U    | P-O3'-C3'   | 5.79  | 126.65      | 119.70   |
| 55  | CA    | 945  | G    | C6-N1-C2    | -5.79 | 121.63      | 125.10   |
| 24  | DA    | 1553 | A    | O4'-C1'-N9  | 5.79  | 112.83      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 2638 | G    | P-O3'-C3'   | 5.79  | 126.64      | 119.70   |
| 21  | AA    | 78   | A    | C5-C6-N1    | 5.79  | 120.59      | 117.70   |
| 24  | BA    | 370  | G    | P-O3'-C3'   | 5.79  | 126.64      | 119.70   |
| 25  | BB    | 36   | C    | C2-N1-C1'   | 5.79  | 125.17      | 118.80   |
| 24  | BA    | 860  | U    | C3'-C2'-C1' | 5.78  | 106.13      | 101.50   |
| 55  | CA    | 331  | G    | C3'-C2'-C1' | 5.78  | 106.13      | 101.50   |
| 55  | CA    | 1302 | C    | P-O3'-C3'   | -5.78 | 112.76      | 119.70   |
| 24  | BA    | 200  | U    | P-O3'-C3'   | -5.78 | 112.77      | 119.70   |
| 24  | BA    | 1156 | A    | N1-C6-N6    | 5.78  | 122.07      | 118.60   |
| 24  | BA    | 2650 | U    | P-O5'-C5'   | -5.78 | 111.65      | 120.90   |
| 21  | AA    | 1502 | A    | O4'-C1'-N9  | 5.78  | 112.82      | 108.20   |
| 24  | BA    | 860  | U    | C5'-C4'-O4' | -5.78 | 102.17      | 109.10   |
| 24  | DA    | 672  | C    | C3'-C2'-C1' | 5.78  | 106.12      | 101.50   |
| 24  | DA    | 2267 | A    | C8-N9-C1'   | -5.78 | 117.30      | 127.70   |
| 21  | AA    | 1046 | A    | C3'-C2'-C1' | 5.78  | 106.12      | 101.50   |
| 24  | BA    | 2054 | A    | N1-C2-N3    | 5.78  | 132.19      | 129.30   |
| 55  | CA    | 6    | G    | C3'-C2'-C1' | 5.78  | 106.12      | 101.50   |
| 24  | DA    | 509  | C    | N1-C1'-C2'  | -5.78 | 105.64      | 112.00   |
| 24  | BA    | 1350 | C    | P-O3'-C3'   | -5.78 | 112.77      | 119.70   |
| 55  | CA    | 755  | G    | C3'-C2'-C1' | 5.78  | 106.12      | 101.50   |
| 56  | DB    | 5    | U    | O4'-C1'-N1  | 5.77  | 112.82      | 108.20   |
| 21  | AA    | 185  | U    | P-O5'-C5'   | -5.77 | 111.67      | 120.90   |
| 24  | BA    | 1238 | G    | O4'-C1'-N9  | 5.77  | 112.82      | 108.20   |
| 24  | DA    | 250  | G    | C3'-C2'-C1' | 5.77  | 106.12      | 101.50   |
| 21  | AA    | 794  | A    | C3'-C2'-C1' | 5.77  | 106.12      | 101.50   |
| 21  | AA    | 411  | A    | P-O3'-C3'   | 5.77  | 126.62      | 119.70   |
| 24  | BA    | 1649 | G    | C3'-C2'-C1' | 5.77  | 106.11      | 101.50   |
| 55  | CA    | 1395 | C    | C3'-C2'-C1' | 5.77  | 106.12      | 101.50   |
| 24  | DA    | 656  | G    | C3'-C2'-C1' | 5.77  | 106.12      | 101.50   |
| 24  | DA    | 1021 | A    | C3'-C2'-C1' | 5.77  | 106.12      | 101.50   |
| 21  | AA    | 1363 | A    | O4'-C1'-N9  | 5.77  | 112.81      | 108.20   |
| 24  | BA    | 1331 | G    | P-O3'-C3'   | 5.77  | 126.62      | 119.70   |
| 25  | BB    | 43   | C    | P-O3'-C3'   | -5.77 | 112.78      | 119.70   |
| 55  | CA    | 967  | C    | C6-N1-C2    | 5.77  | 122.61      | 120.30   |
| 24  | DA    | 1008 | A    | P-O3'-C3'   | 5.77  | 126.62      | 119.70   |
| 24  | DA    | 1060 | U    | C6-N1-C1'   | -5.77 | 113.12      | 121.20   |
| 21  | AA    | 961  | U    | C3'-C2'-C1' | 5.77  | 106.11      | 101.50   |
| 24  | BA    | 554  | U    | O4'-C1'-N1  | 5.77  | 112.81      | 108.20   |
| 21  | AA    | 282  | A    | C3'-C2'-C1' | 5.76  | 106.11      | 101.50   |
| 21  | AA    | 536  | C    | C3'-C2'-C1' | 5.76  | 106.11      | 101.50   |
| 55  | CA    | 870  | U    | N1-C1'-C2'  | 5.76  | 121.49      | 114.00   |
| 55  | CA    | 1160 | G    | P-O3'-C3'   | -5.76 | 112.78      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | CA    | 1299 | A    | P-O3'-C3'   | -5.76 | 112.78      | 119.70   |
| 24  | BA    | 2099 | U    | O4'-C1'-N1  | 5.76  | 112.81      | 108.20   |
| 24  | BA    | 2346 | A    | P-O3'-C3'   | 5.76  | 126.62      | 119.70   |
| 24  | DA    | 434  | U    | N1-C1'-C2'  | 5.76  | 121.49      | 114.00   |
| 24  | BA    | 2682 | A    | C3'-C2'-C1' | 5.76  | 106.11      | 101.50   |
| 25  | BB    | 26   | C    | P-O5'-C5'   | -5.76 | 111.68      | 120.90   |
| 55  | CA    | 199  | A    | C3'-C2'-C1' | 5.76  | 106.11      | 101.50   |
| 55  | CA    | 549  | C    | C3'-C2'-C1' | 5.76  | 106.11      | 101.50   |
| 24  | DA    | 1455 | G    | C3'-C2'-C1' | 5.76  | 106.11      | 101.50   |
| 55  | CA    | 382  | A    | C3'-C2'-C1' | 5.76  | 106.11      | 101.50   |
| 55  | CA    | 499  | A    | P-O3'-C3'   | 5.76  | 126.61      | 119.70   |
| 24  | DA    | 726  | G    | O4'-C1'-N9  | 5.76  | 112.81      | 108.20   |
| 24  | DA    | 1717 | A    | C3'-C2'-C1' | 5.76  | 106.11      | 101.50   |
| 24  | DA    | 2033 | A    | C6-N1-C2    | 5.76  | 122.06      | 118.60   |
| 56  | DB    | 45   | A    | N9-C1'-C2'  | -5.76 | 105.67      | 112.00   |
| 24  | BA    | 831  | G    | N9-C1'-C2'  | -5.76 | 105.67      | 112.00   |
| 24  | BA    | 2777 | G    | P-O5'-C5'   | -5.76 | 111.69      | 120.90   |
| 25  | BB    | 56   | G    | O3'-P-O5'   | 5.76  | 114.94      | 104.00   |
| 25  | BB    | 90   | C    | C3'-C2'-C1' | 5.76  | 106.11      | 101.50   |
| 55  | CA    | 439  | U    | P-O3'-C3'   | -5.76 | 112.79      | 119.70   |
| 55  | CA    | 1239 | A    | P-O3'-C3'   | 5.76  | 126.61      | 119.70   |
| 24  | DA    | 2777 | G    | C3'-C2'-C1' | 5.76  | 106.10      | 101.50   |
| 56  | DB    | 87   | U    | P-O3'-C3'   | 5.76  | 126.61      | 119.70   |
| 21  | AA    | 1449 | C    | C3'-C2'-C1' | 5.75  | 106.10      | 101.50   |
| 55  | CA    | 419  | C    | O4'-C1'-N1  | 5.75  | 112.80      | 108.20   |
| 24  | BA    | 92   | U    | P-O3'-C3'   | -5.75 | 112.80      | 119.70   |
| 24  | BA    | 528  | A    | C4-C5-C6    | 5.75  | 119.88      | 117.00   |
| 24  | BA    | 585  | G    | O5'-P-OP2   | -5.75 | 100.52      | 105.70   |
| 24  | DA    | 142  | A    | N9-C1'-C2'  | -5.75 | 105.67      | 112.00   |
| 24  | DA    | 2308 | G    | P-O3'-C3'   | 5.75  | 126.60      | 119.70   |
| 24  | DA    | 2657 | A    | N9-C1'-C2'  | -5.75 | 105.67      | 112.00   |
| 24  | BA    | 1885 | A    | N9-C4-C5    | 5.75  | 108.10      | 105.80   |
| 24  | BA    | 2226 | C    | P-O3'-C3'   | -5.75 | 112.80      | 119.70   |
| 24  | DA    | 271  | G    | N3-C4-N9    | -5.75 | 122.55      | 126.00   |
| 24  | DA    | 1022 | G    | O4'-C1'-N9  | 5.75  | 112.80      | 108.20   |
| 21  | AA    | 1450 | U    | O4'-C1'-N1  | 5.75  | 112.80      | 108.20   |
| 24  | BA    | 369  | U    | N1-C1'-C2'  | 5.75  | 121.47      | 114.00   |
| 24  | DA    | 1647 | U    | O4'-C1'-N1  | 5.75  | 112.80      | 108.20   |
| 24  | BA    | 985  | C    | O4'-C1'-N1  | -5.75 | 103.60      | 108.20   |
| 24  | BA    | 2447 | G    | O4'-C1'-N9  | 5.75  | 112.80      | 108.20   |
| 21  | AA    | 131  | A    | C3'-C2'-C1' | 5.74  | 106.09      | 101.50   |
| 24  | BA    | 1289 | C    | C3'-C2'-C1' | 5.74  | 106.09      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 277  | C    | O4'-C1'-N1  | 5.74  | 112.79      | 108.20   |
| 24  | BA    | 1204 | A    | P-O3'-C3'   | 5.74  | 126.59      | 119.70   |
| 24  | BA    | 2501 | C    | P-O3'-C3'   | 5.74  | 126.59      | 119.70   |
| 24  | BA    | 455  | C    | P-O3'-C3'   | 5.74  | 126.59      | 119.70   |
| 24  | BA    | 763  | G    | N3-C4-N9    | 5.74  | 129.44      | 126.00   |
| 24  | BA    | 1538 | G    | C3'-C2'-C1' | 5.74  | 106.09      | 101.50   |
| 55  | CA    | 1530 | G    | C3'-C2'-C1' | 5.74  | 106.09      | 101.50   |
| 24  | DA    | 572  | A    | C3'-C2'-C1' | 5.74  | 106.09      | 101.50   |
| 24  | DA    | 2549 | G    | P-O3'-C3'   | 5.74  | 126.59      | 119.70   |
| 24  | BA    | 2582 | G    | N9-C1'-C2'  | -5.74 | 105.69      | 112.00   |
| 24  | BA    | 1372 | U    | C5-C4-O4    | -5.74 | 122.46      | 125.90   |
| 24  | BA    | 2441 | U    | C2-N3-C4    | -5.74 | 123.56      | 127.00   |
| 24  | BA    | 2575 | C    | N3-C4-C5    | 5.74  | 124.19      | 121.90   |
| 24  | DA    | 505  | A    | C3'-C2'-C1' | 5.74  | 106.09      | 101.50   |
| 24  | DA    | 1213 | A    | C3'-C2'-C1' | 5.74  | 106.09      | 101.50   |
| 21  | AA    | 1335 | U    | P-O3'-C3'   | 5.73  | 126.58      | 119.70   |
| 24  | BA    | 943  | A    | C8-N9-C4    | -5.73 | 103.51      | 105.80   |
| 24  | BA    | 2727 | A    | C3'-C2'-C1' | 5.73  | 106.09      | 101.50   |
| 25  | BB    | 90   | C    | P-O3'-C3'   | -5.73 | 112.82      | 119.70   |
| 24  | DA    | 491  | G    | P-O3'-C3'   | -5.73 | 112.82      | 119.70   |
| 24  | DA    | 2499 | C    | C3'-C2'-C1' | 5.73  | 106.09      | 101.50   |
| 21  | AA    | 306  | A    | C3'-C2'-C1' | 5.73  | 106.08      | 101.50   |
| 25  | BB    | 42   | C    | P-O3'-C3'   | -5.73 | 112.82      | 119.70   |
| 24  | DA    | 1080 | A    | N9-C1'-C2'  | -5.73 | 105.70      | 112.00   |
| 24  | DA    | 1325 | U    | N1-C1'-C2'  | 5.73  | 121.45      | 114.00   |
| 21  | AA    | 316  | C    | P-O3'-C3'   | -5.73 | 112.83      | 119.70   |
| 24  | BA    | 1866 | A    | C3'-C2'-C1' | 5.73  | 106.08      | 101.50   |
| 55  | CA    | 1348 | U    | C3'-C2'-C1' | 5.73  | 106.08      | 101.50   |
| 24  | BA    | 2618 | G    | N9-C4-C5    | 5.73  | 107.69      | 105.40   |
| 55  | CA    | 559  | A    | P-O3'-C3'   | 5.73  | 126.57      | 119.70   |
| 21  | AA    | 368  | U    | C2-N1-C1'   | 5.72  | 124.57      | 117.70   |
| 24  | BA    | 1379 | U    | N1-C1'-C2'  | -5.72 | 105.70      | 112.00   |
| 24  | BA    | 2034 | U    | C3'-C2'-C1' | 5.72  | 106.08      | 101.50   |
| 21  | AA    | 664  | G    | P-O3'-C3'   | -5.72 | 112.83      | 119.70   |
| 24  | BA    | 1493 | C    | O4'-C1'-N1  | 5.72  | 112.78      | 108.20   |
| 24  | BA    | 1556 | C    | P-O3'-C3'   | -5.72 | 112.83      | 119.70   |
| 21  | AA    | 347  | G    | P-O3'-C3'   | 5.72  | 126.57      | 119.70   |
| 55  | CA    | 1127 | G    | C3'-C2'-C1' | 5.72  | 106.08      | 101.50   |
| 24  | DA    | 1011 | G    | C4-N9-C1'   | -5.72 | 119.06      | 126.50   |
| 21  | AA    | 1503 | A    | P-O3'-C3'   | 5.72  | 126.56      | 119.70   |
| 24  | BA    | 621  | A    | C3'-C2'-C1' | 5.72  | 106.08      | 101.50   |
| 24  | BA    | 2511 | U    | N3-C4-C5    | 5.72  | 118.03      | 114.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 1683 | U    | C3'-C2'-C1' | 5.72  | 106.08      | 101.50   |
| 24  | BA    | 1821 | A    | C5-C6-N1    | -5.72 | 114.84      | 117.70   |
| 24  | BA    | 1829 | A    | N9-C1'-C2'  | -5.72 | 105.71      | 112.00   |
| 55  | CA    | 480  | U    | C5-C4-O4    | -5.72 | 122.47      | 125.90   |
| 24  | BA    | 1287 | A    | C3'-C2'-C1' | 5.72  | 106.07      | 101.50   |
| 24  | BA    | 1884 | G    | P-O3'-C3'   | 5.71  | 126.56      | 119.70   |
| 55  | CA    | 252  | U    | C3'-C2'-C1' | 5.71  | 106.07      | 101.50   |
| 24  | DA    | 1611 | C    | P-O3'-C3'   | -5.71 | 112.84      | 119.70   |
| 24  | BA    | 1770 | G    | C5-C6-O6    | -5.71 | 125.17      | 128.60   |
| 24  | DA    | 1455 | G    | P-O3'-C3'   | -5.71 | 112.84      | 119.70   |
| 24  | DA    | 2691 | C    | O4'-C1'-N1  | 5.71  | 112.77      | 108.20   |
| 21  | AA    | 994  | A    | C3'-C2'-C1' | 5.71  | 106.07      | 101.50   |
| 24  | BA    | 871  | U    | P-O5'-C5'   | -5.71 | 111.76      | 120.90   |
| 24  | BA    | 1731 | G    | C6-C5-N7    | 5.71  | 133.83      | 130.40   |
| 21  | AA    | 251  | G    | O4'-C1'-N9  | -5.71 | 103.63      | 108.20   |
| 24  | BA    | 223  | A    | C3'-C2'-C1' | 5.71  | 106.07      | 101.50   |
| 24  | DA    | 1537 | G    | C3'-C2'-C1' | 5.71  | 106.07      | 101.50   |
| 21  | AA    | 1158 | C    | N1-C1'-C2'  | -5.71 | 105.72      | 112.00   |
| 24  | BA    | 1821 | A    | N9-C1'-C2'  | -5.71 | 105.72      | 112.00   |
| 55  | CA    | 275  | G    | C3'-C2'-C1' | 5.71  | 106.07      | 101.50   |
| 55  | CA    | 423  | G    | C3'-C2'-C1' | 5.71  | 106.07      | 101.50   |
| 55  | CA    | 1127 | G    | N9-C1'-C2'  | -5.71 | 105.72      | 112.00   |
| 24  | DA    | 1071 | G    | C3'-C2'-C1' | 5.71  | 106.07      | 101.50   |
| 21  | AA    | 1192 | C    | C3'-C2'-C1' | 5.71  | 106.06      | 101.50   |
| 24  | BA    | 2787 | C    | N1-C2-O2    | -5.71 | 115.48      | 118.90   |
| 24  | DA    | 60   | G    | C4-N9-C1'   | -5.71 | 119.08      | 126.50   |
| 24  | DA    | 1334 | G    | N9-C1'-C2'  | -5.71 | 105.72      | 112.00   |
| 24  | DA    | 1635 | A    | C3'-C2'-C1' | 5.71  | 106.06      | 101.50   |
| 24  | BA    | 2778 | A    | P-O3'-C3'   | 5.70  | 126.55      | 119.70   |
| 24  | DA    | 1315 | C    | O4'-C1'-N1  | 5.70  | 112.76      | 108.20   |
| 24  | DA    | 2324 | U    | P-O3'-C3'   | 5.70  | 126.55      | 119.70   |
| 55  | CA    | 414  | A    | C3'-C2'-C1' | 5.70  | 106.06      | 101.50   |
| 24  | DA    | 754  | U    | O4'-C1'-N1  | 5.70  | 112.76      | 108.20   |
| 24  | DA    | 2752 | C    | O4'-C1'-N1  | 5.70  | 112.76      | 108.20   |
| 24  | BA    | 866  | A    | C3'-C2'-C1' | 5.70  | 106.06      | 101.50   |
| 24  | BA    | 2249 | U    | N1-C1'-C2'  | 5.70  | 121.41      | 114.00   |
| 25  | BB    | 43   | C    | C3'-C2'-C1' | 5.70  | 106.06      | 101.50   |
| 55  | CA    | 537  | G    | N9-C1'-C2'  | -5.70 | 105.73      | 112.00   |
| 24  | DA    | 529  | A    | C5-N7-C8    | -5.70 | 101.05      | 103.90   |
| 24  | DA    | 2757 | A    | C3'-C2'-C1' | 5.70  | 106.06      | 101.50   |
| 21  | AA    | 755  | G    | C3'-C2'-C1' | 5.70  | 106.06      | 101.50   |
| 21  | AA    | 1184 | G    | C3'-C2'-C1' | 5.70  | 106.06      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 1321 | U    | C3'-C2'-C1' | 5.70  | 106.06      | 101.50   |
| 24  | DA    | 122  | G    | C3'-C2'-C1' | 5.70  | 106.06      | 101.50   |
| 24  | DA    | 491  | G    | C3'-C2'-C1' | 5.70  | 106.06      | 101.50   |
| 24  | BA    | 965  | C    | O4'-C1'-N1  | -5.70 | 103.64      | 108.20   |
| 24  | BA    | 1385 | A    | O4'-C1'-N9  | 5.70  | 112.76      | 108.20   |
| 24  | BA    | 1693 | U    | O4'-C1'-N1  | 5.70  | 112.76      | 108.20   |
| 24  | BA    | 2135 | A    | C3'-C2'-C1' | 5.69  | 106.06      | 101.50   |
| 24  | DA    | 1276 | A    | C3'-C2'-C1' | 5.69  | 106.06      | 101.50   |
| 55  | CA    | 518  | C    | O4'-C1'-N1  | 5.69  | 112.75      | 108.20   |
| 55  | CA    | 1299 | A    | O3'-P-O5'   | 5.69  | 114.82      | 104.00   |
| 24  | DA    | 93   | G    | C3'-C2'-C1' | 5.69  | 106.06      | 101.50   |
| 24  | DA    | 370  | G    | C6-C5-N7    | 5.69  | 133.81      | 130.40   |
| 24  | DA    | 1439 | A    | C6-N1-C2    | 5.69  | 122.02      | 118.60   |
| 24  | BA    | 683  | U    | O4'-C1'-N1  | 5.69  | 112.75      | 108.20   |
| 24  | BA    | 806  | C    | N1-C1'-C2'  | -5.69 | 105.74      | 112.00   |
| 24  | BA    | 2324 | U    | N1-C1'-C2'  | 5.69  | 121.40      | 114.00   |
| 55  | CA    | 276  | G    | C3'-C2'-C1' | 5.69  | 106.05      | 101.50   |
| 55  | CA    | 821  | G    | C3'-C2'-C1' | 5.69  | 106.05      | 101.50   |
| 55  | CA    | 1215 | G    | C3'-C2'-C1' | 5.69  | 106.05      | 101.50   |
| 24  | DA    | 646  | U    | O4'-C1'-N1  | -5.69 | 103.65      | 108.20   |
| 24  | DA    | 224  | U    | P-O3'-C3'   | -5.69 | 112.87      | 119.70   |
| 24  | DA    | 1700 | A    | C3'-C2'-C1' | 5.69  | 106.05      | 101.50   |
| 21  | AA    | 985  | C    | C6-N1-C2    | -5.69 | 118.03      | 120.30   |
| 24  | BA    | 2226 | C    | C3'-C2'-C1' | 5.69  | 106.05      | 101.50   |
| 24  | DA    | 2215 | C    | O4'-C1'-N1  | 5.69  | 112.75      | 108.20   |
| 24  | DA    | 2752 | C    | N1-C1'-C2'  | -5.69 | 105.74      | 112.00   |
| 24  | DA    | 1713 | A    | P-O3'-C3'   | 5.69  | 126.52      | 119.70   |
| 21  | AA    | 684  | U    | O4'-C1'-N1  | 5.68  | 112.75      | 108.20   |
| 21  | AA    | 1401 | G    | N9-C1'-C2'  | -5.68 | 105.75      | 112.00   |
| 24  | BA    | 272  | A    | C3'-C2'-C1' | 5.68  | 106.05      | 101.50   |
| 24  | BA    | 435  | C    | C3'-C2'-C1' | 5.68  | 106.05      | 101.50   |
| 24  | DA    | 656  | G    | P-O3'-C3'   | -5.68 | 112.88      | 119.70   |
| 24  | DA    | 2272 | U    | N3-C2-O2    | 5.68  | 126.18      | 122.20   |
| 21  | AA    | 813  | U    | C3'-C2'-C1' | 5.68  | 106.05      | 101.50   |
| 55  | CA    | 87   | C    | O4'-C1'-N1  | 5.68  | 112.75      | 108.20   |
| 55  | CA    | 317  | U    | C3'-C2'-C1' | 5.68  | 106.05      | 101.50   |
| 55  | CA    | 485  | U    | O4'-C1'-N1  | -5.68 | 103.65      | 108.20   |
| 21  | AA    | 597  | G    | N9-C1'-C2'  | -5.68 | 105.75      | 112.00   |
| 24  | BA    | 1798 | U    | C5-C4-O4    | 5.68  | 129.31      | 125.90   |
| 55  | CA    | 509  | A    | C3'-C2'-C1' | 5.68  | 106.05      | 101.50   |
| 55  | CA    | 1336 | C    | N1-C1'-C2'  | 5.68  | 121.39      | 114.00   |
| 24  | DA    | 777  | G    | C3'-C2'-C1' | 5.68  | 106.05      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 1778 | U    | C2-N3-C4    | -5.68 | 123.59      | 127.00   |
| 55  | CA    | 184  | G    | N9-C1'-C2'  | -5.68 | 105.75      | 112.00   |
| 24  | DA    | 1674 | G    | C4-C5-N7    | 5.68  | 113.07      | 110.80   |
| 55  | CA    | 482  | A    | P-O3'-C3'   | -5.68 | 112.89      | 119.70   |
| 21  | AA    | 162  | A    | P-O3'-C3'   | 5.68  | 126.51      | 119.70   |
| 21  | AA    | 414  | A    | C3'-C2'-C1' | 5.68  | 106.04      | 101.50   |
| 24  | BA    | 1254 | A    | P-O5'-C5'   | -5.68 | 111.82      | 120.90   |
| 24  | BA    | 2710 | C    | O4'-C1'-N1  | 5.68  | 112.74      | 108.20   |
| 21  | AA    | 511  | C    | P-O3'-C3'   | 5.67  | 126.51      | 119.70   |
| 24  | BA    | 1133 | A    | P-O5'-C5'   | -5.67 | 111.82      | 120.90   |
| 24  | BA    | 1617 | C    | N1-C2-O2    | -5.67 | 115.50      | 118.90   |
| 24  | BA    | 2860 | A    | C8-N9-C1'   | -5.67 | 117.49      | 127.70   |
| 24  | DA    | 788  | A    | P-O3'-C3'   | 5.67  | 126.51      | 119.70   |
| 24  | BA    | 2035 | G    | O5'-P-OP2   | -5.67 | 100.59      | 105.70   |
| 55  | CA    | 418  | C    | O4'-C1'-N1  | 5.67  | 112.74      | 108.20   |
| 21  | AA    | 518  | C    | O4'-C1'-N1  | 5.67  | 112.74      | 108.20   |
| 21  | AA    | 891  | U    | P-O3'-C3'   | -5.67 | 112.89      | 119.70   |
| 21  | AA    | 1197 | A    | O5'-P-OP2   | -5.67 | 100.60      | 105.70   |
| 24  | BA    | 1009 | A    | P-O3'-C3'   | -5.67 | 112.89      | 119.70   |
| 24  | DA    | 1568 | G    | C3'-C2'-C1' | 5.67  | 106.04      | 101.50   |
| 24  | DA    | 2267 | A    | C4-N9-C1'   | 5.67  | 136.51      | 126.30   |
| 27  | BD    | 10   | GLY  | N-CA-C      | 5.67  | 127.27      | 113.10   |
| 24  | DA    | 1313 | U    | C3'-C2'-C1' | 5.67  | 106.03      | 101.50   |
| 24  | DA    | 2458 | G    | O4'-C1'-N9  | 5.67  | 112.73      | 108.20   |
| 24  | DA    | 2875 | C    | O4'-C1'-N1  | 5.67  | 112.73      | 108.20   |
| 24  | BA    | 1027 | A    | N9-C1'-C2'  | -5.67 | 105.77      | 112.00   |
| 24  | DA    | 1649 | G    | C3'-C2'-C1' | 5.67  | 106.03      | 101.50   |
| 24  | BA    | 2517 | C    | C6-N1-C2    | 5.67  | 122.57      | 120.30   |
| 36  | BM    | 41   | LEU  | CA-CB-CG    | 5.67  | 128.33      | 115.30   |
| 24  | DA    | 1027 | A    | C3'-C2'-C1' | 5.67  | 106.03      | 101.50   |
| 24  | DA    | 1511 | G    | C3'-C2'-C1' | 5.67  | 106.03      | 101.50   |
| 21  | AA    | 701  | U    | N1-C1'-C2'  | 5.66  | 121.36      | 114.00   |
| 24  | BA    | 1119 | U    | N1-C1'-C2'  | -5.66 | 105.77      | 112.00   |
| 24  | DA    | 672  | C    | P-O3'-C3'   | -5.66 | 112.90      | 119.70   |
| 55  | CA    | 61   | G    | C3'-C2'-C1' | 5.66  | 106.03      | 101.50   |
| 24  | BA    | 765  | C    | N1-C1'-C2'  | -5.66 | 105.77      | 112.00   |
| 55  | CA    | 1300 | G    | P-O5'-C5'   | 5.66  | 129.96      | 120.90   |
| 55  | CA    | 1452 | C    | O4'-C1'-N1  | 5.66  | 112.73      | 108.20   |
| 55  | CA    | 174  | A    | C3'-C2'-C1' | 5.66  | 106.03      | 101.50   |
| 55  | CA    | 239  | U    | O4'-C1'-N1  | -5.66 | 103.67      | 108.20   |
| 55  | CA    | 1086 | U    | C3'-C2'-C1' | 5.66  | 106.03      | 101.50   |
| 55  | CA    | 1284 | C    | N3-C2-O2    | -5.66 | 117.94      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | CA    | 1453 | G    | C3'-C2'-C1' | 5.66  | 106.03      | 101.50   |
| 21  | AA    | 252  | U    | P-O3'-C3'   | -5.66 | 112.91      | 119.70   |
| 21  | AA    | 414  | A    | P-O3'-C3'   | -5.66 | 112.91      | 119.70   |
| 24  | BA    | 19   | A    | P-O5'-C5'   | -5.66 | 111.85      | 120.90   |
| 24  | BA    | 858  | G    | C5-C6-O6    | 5.66  | 131.99      | 128.60   |
| 24  | DA    | 575  | A    | C3'-C2'-C1' | 5.66  | 106.03      | 101.50   |
| 24  | DA    | 2714 | G    | P-O3'-C3'   | -5.66 | 112.91      | 119.70   |
| 21  | AA    | 587  | G    | P-O3'-C3'   | 5.66  | 126.49      | 119.70   |
| 55  | CA    | 735  | C    | C3'-C2'-C1' | 5.66  | 106.03      | 101.50   |
| 24  | DA    | 225  | C    | C3'-C2'-C1' | 5.66  | 106.02      | 101.50   |
| 24  | DA    | 699  | A    | O4'-C1'-N9  | -5.66 | 103.67      | 108.20   |
| 24  | DA    | 1327 | A    | C3'-C2'-C1' | 5.66  | 106.03      | 101.50   |
| 24  | BA    | 2575 | C    | C4-C5-C6    | 5.65  | 120.23      | 117.40   |
| 55  | CA    | 353  | A    | C3'-C2'-C1' | 5.65  | 106.02      | 101.50   |
| 24  | DA    | 1462 | C    | C3'-C2'-C1' | 5.65  | 106.02      | 101.50   |
| 24  | BA    | 2023 | C    | O4'-C1'-N1  | 5.65  | 112.72      | 108.20   |
| 24  | DA    | 2603 | G    | C3'-C2'-C1' | 5.65  | 106.02      | 101.50   |
| 24  | BA    | 412  | A    | P-O3'-C3'   | -5.65 | 112.92      | 119.70   |
| 55  | CA    | 832  | G    | O4'-C1'-N9  | 5.65  | 112.72      | 108.20   |
| 24  | DA    | 1634 | A    | P-O3'-C3'   | 5.65  | 126.48      | 119.70   |
| 24  | BA    | 1782 | U    | O4'-C1'-N1  | 5.65  | 112.72      | 108.20   |
| 24  | BA    | 1125 | G    | C6-C5-N7    | -5.65 | 127.01      | 130.40   |
| 24  | BA    | 2297 | A    | C3'-C2'-C1' | 5.65  | 106.02      | 101.50   |
| 24  | DA    | 628  | G    | P-O3'-C3'   | 5.65  | 126.48      | 119.70   |
| 24  | DA    | 1512 | C    | O4'-C1'-N1  | 5.65  | 112.72      | 108.20   |
| 55  | CA    | 1054 | C    | O4'-C1'-N1  | 5.64  | 112.72      | 108.20   |
| 24  | BA    | 922  | C    | P-O3'-C3'   | -5.64 | 112.93      | 119.70   |
| 24  | BA    | 1663 | G    | C4-C5-N7    | -5.64 | 108.54      | 110.80   |
| 24  | BA    | 2385 | C    | C3'-C2'-C1' | 5.64  | 106.01      | 101.50   |
| 55  | CA    | 277  | C    | O4'-C1'-N1  | 5.64  | 112.71      | 108.20   |
| 24  | DA    | 637  | A    | P-O3'-C3'   | 5.64  | 126.47      | 119.70   |
| 24  | BA    | 2629 | U    | N1-C1'-C2'  | 5.64  | 121.33      | 114.00   |
| 24  | DA    | 2251 | G    | P-O3'-C3'   | -5.64 | 112.93      | 119.70   |
| 24  | DA    | 2313 | C    | C3'-C2'-C1' | 5.64  | 106.01      | 101.50   |
| 24  | DA    | 192  | C    | P-O3'-C3'   | 5.64  | 126.47      | 119.70   |
| 24  | DA    | 1159 | U    | O4'-C1'-N1  | 5.64  | 112.71      | 108.20   |
| 24  | BA    | 2480 | C    | O4'-C1'-N1  | 5.64  | 112.71      | 108.20   |
| 24  | DA    | 442  | G    | P-O3'-C3'   | 5.64  | 126.47      | 119.70   |
| 21  | AA    | 879  | C    | O4'-C1'-N1  | 5.64  | 112.71      | 108.20   |
| 24  | BA    | 1525 | A    | N1-C6-N6    | -5.64 | 115.22      | 118.60   |
| 55  | CA    | 389  | A    | C4-C5-N7    | -5.64 | 107.88      | 110.70   |
| 55  | CA    | 1184 | G    | P-O3'-C3'   | -5.64 | 112.94      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | CA    | 1425 | U    | O4'-C1'-N1  | 5.64  | 112.71      | 108.20   |
| 24  | DA    | 2189 | U    | O4'-C1'-N1  | 5.64  | 112.71      | 108.20   |
| 24  | BA    | 1637 | A    | P-O5'-C5'   | -5.63 | 111.88      | 120.90   |
| 55  | CA    | 276  | G    | N9-C1'-C2'  | -5.63 | 105.80      | 112.00   |
| 55  | CA    | 452  | A    | C3'-C2'-C1' | 5.63  | 106.01      | 101.50   |
| 24  | DA    | 103  | A    | C3'-C2'-C1' | 5.63  | 106.01      | 101.50   |
| 24  | DA    | 313  | G    | N9-C1'-C2'  | -5.63 | 105.80      | 112.00   |
| 24  | DA    | 646  | U    | N1-C1'-C2'  | 5.63  | 121.33      | 114.00   |
| 24  | BA    | 197  | A    | C3'-C2'-C1' | 5.63  | 106.01      | 101.50   |
| 24  | BA    | 1143 | A    | P-O3'-C3'   | 5.63  | 126.46      | 119.70   |
| 24  | DA    | 461  | C    | C6-N1-C1'   | -5.63 | 114.04      | 120.80   |
| 24  | DA    | 546  | U    | P-O3'-C3'   | 5.63  | 126.46      | 119.70   |
| 24  | DA    | 671  | C    | O5'-P-OP2   | -5.63 | 100.63      | 105.70   |
| 24  | BA    | 233  | A    | C3'-C2'-C1' | 5.63  | 106.00      | 101.50   |
| 24  | BA    | 2716 | C    | O4'-C1'-N1  | 5.63  | 112.70      | 108.20   |
| 55  | CA    | 803  | G    | C3'-C2'-C1' | 5.63  | 106.00      | 101.50   |
| 24  | DA    | 2312 | U    | N3-C4-C5    | -5.63 | 111.22      | 114.60   |
| 56  | DB    | 43   | C    | C3'-C2'-C1' | 5.63  | 106.00      | 101.50   |
| 24  | BA    | 1184 | U    | N1-C1'-C2'  | 5.63  | 121.32      | 114.00   |
| 24  | BA    | 2846 | G    | C8-N9-C4    | -5.63 | 104.15      | 106.40   |
| 21  | AA    | 91   | U    | C2-N3-C4    | -5.62 | 123.62      | 127.00   |
| 21  | AA    | 430  | A    | C3'-C2'-C1' | 5.62  | 106.00      | 101.50   |
| 21  | AA    | 497  | G    | C3'-C2'-C1' | 5.62  | 106.00      | 101.50   |
| 24  | BA    | 1082 | U    | N1-C2-O2    | -5.62 | 118.86      | 122.80   |
| 24  | BA    | 2589 | A    | C5-C6-N6    | 5.62  | 128.20      | 123.70   |
| 55  | CA    | 510  | A    | N9-C1'-C2'  | -5.62 | 105.81      | 112.00   |
| 24  | DA    | 77   | G    | N9-C1'-C2'  | -5.62 | 105.81      | 112.00   |
| 24  | DA    | 964  | C    | P-O5'-C5'   | -5.62 | 111.90      | 120.90   |
| 24  | BA    | 2197 | U    | P-O3'-C3'   | 5.62  | 126.45      | 119.70   |
| 24  | BA    | 2733 | A    | N1-C6-N6    | 5.62  | 121.97      | 118.60   |
| 55  | CA    | 206  | C    | N1-C1'-C2'  | -5.62 | 105.82      | 112.00   |
| 24  | DA    | 2283 | C    | C3'-C2'-C1' | 5.62  | 106.00      | 101.50   |
| 21  | AA    | 29   | U    | O4'-C1'-N1  | 5.62  | 112.69      | 108.20   |
| 24  | BA    | 1045 | C    | N1-C1'-C2'  | 5.62  | 121.30      | 114.00   |
| 24  | BA    | 2747 | G    | C2-N3-C4    | -5.62 | 109.09      | 111.90   |
| 24  | DA    | 621  | A    | C3'-C2'-C1' | 5.62  | 106.00      | 101.50   |
| 24  | DA    | 2380 | C    | O4'-C1'-N1  | 5.62  | 112.69      | 108.20   |
| 24  | DA    | 2409 | G    | N9-C1'-C2'  | -5.62 | 105.82      | 112.00   |
| 21  | AA    | 752  | G    | P-O3'-C3'   | 5.62  | 126.44      | 119.70   |
| 24  | BA    | 676  | A    | N1-C6-N6    | 5.62  | 121.97      | 118.60   |
| 21  | AA    | 340  | U    | O4'-C1'-N1  | 5.62  | 112.69      | 108.20   |
| 21  | AA    | 1103 | C    | C3'-C2'-C1' | 5.62  | 105.99      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | CA    | 892  | A    | N9-C1'-C2'  | -5.62 | 105.82      | 112.00   |
| 24  | DA    | 164  | C    | C3'-C2'-C1' | 5.62  | 105.99      | 101.50   |
| 24  | DA    | 763  | G    | C6-C5-N7    | -5.62 | 127.03      | 130.40   |
| 24  | DA    | 2638 | G    | N1-C2-N2    | 5.62  | 121.25      | 116.20   |
| 21  | AA    | 519  | C    | C3'-C2'-C1' | 5.61  | 105.99      | 101.50   |
| 24  | BA    | 2200 | C    | C3'-C2'-C1' | 5.61  | 105.99      | 101.50   |
| 24  | BA    | 528  | A    | O4'-C1'-N9  | -5.61 | 103.71      | 108.20   |
| 55  | CA    | 961  | U    | C3'-C2'-C1' | 5.61  | 105.99      | 101.50   |
| 21  | AA    | 245  | U    | C3'-C2'-C1' | 5.61  | 105.99      | 101.50   |
| 24  | BA    | 2689 | U    | C2-N1-C1'   | -5.61 | 110.97      | 117.70   |
| 55  | CA    | 369  | G    | C3'-C2'-C1' | 5.61  | 105.98      | 101.50   |
| 55  | CA    | 1338 | G    | P-O3'-C3'   | -5.61 | 112.97      | 119.70   |
| 24  | DA    | 1277 | G    | P-O3'-C3'   | -5.61 | 112.97      | 119.70   |
| 21  | AA    | 1202 | U    | C3'-C2'-C1' | 5.61  | 105.98      | 101.50   |
| 24  | DA    | 1074 | G    | P-O3'-C3'   | 5.61  | 126.42      | 119.70   |
| 21  | AA    | 1032 | G    | N9-C1'-C2'  | -5.60 | 105.84      | 112.00   |
| 24  | BA    | 1817 | G    | C3'-C2'-C1' | 5.60  | 105.98      | 101.50   |
| 24  | BA    | 604  | G    | P-O3'-C3'   | -5.60 | 112.98      | 119.70   |
| 24  | BA    | 1476 | U    | C2-N3-C4    | -5.60 | 123.64      | 127.00   |
| 24  | BA    | 2214 | C    | C3'-C2'-C1' | 5.60  | 105.98      | 101.50   |
| 24  | BA    | 2287 | A    | P-O3'-C3'   | 5.60  | 126.42      | 119.70   |
| 55  | CA    | 915  | A    | C3'-C2'-C1' | 5.60  | 105.98      | 101.50   |
| 24  | BA    | 1669 | A    | N9-C4-C5    | 5.60  | 108.04      | 105.80   |
| 24  | BA    | 468  | G    | C5-C6-N1    | 5.60  | 114.30      | 111.50   |
| 21  | AA    | 1138 | G    | P-O3'-C3'   | -5.60 | 112.98      | 119.70   |
| 21  | AA    | 1242 | G    | P-O5'-C5'   | -5.60 | 111.94      | 120.90   |
| 24  | BA    | 1034 | G    | N9-C1'-C2'  | -5.60 | 105.84      | 112.00   |
| 24  | BA    | 2656 | U    | N3-C2-O2    | -5.60 | 118.28      | 122.20   |
| 55  | CA    | 885  | G    | C3'-C2'-C1' | 5.60  | 105.98      | 101.50   |
| 24  | DA    | 2063 | C    | C3'-C2'-C1' | 5.60  | 105.98      | 101.50   |
| 24  | BA    | 763  | G    | C4-C5-N7    | 5.59  | 113.04      | 110.80   |
| 24  | BA    | 1131 | G    | O4'-C1'-N9  | -5.59 | 103.72      | 108.20   |
| 24  | BA    | 2798 | U    | O4'-C1'-N1  | 5.59  | 112.68      | 108.20   |
| 24  | BA    | 2894 | G    | C4-N9-C1'   | 5.59  | 133.77      | 126.50   |
| 55  | CA    | 1128 | C    | P-O3'-C3'   | -5.59 | 112.99      | 119.70   |
| 21  | AA    | 889  | A    | P-O3'-C3'   | 5.59  | 126.41      | 119.70   |
| 24  | BA    | 373  | U    | C3'-C2'-C1' | 5.59  | 105.97      | 101.50   |
| 55  | CA    | 465  | A    | N9-C1'-C2'  | -5.59 | 105.85      | 112.00   |
| 24  | DA    | 1676 | A    | P-O3'-C3'   | -5.59 | 112.99      | 119.70   |
| 21  | AA    | 54   | C    | O4'-C1'-N1  | 5.59  | 112.67      | 108.20   |
| 24  | BA    | 2220 | U    | N1-C1'-C2'  | -5.59 | 105.85      | 112.00   |
| 24  | BA    | 2397 | G    | P-O3'-C3'   | -5.59 | 112.99      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | CA    | 129  | A    | P-O3'-C3'   | 5.59  | 126.41      | 119.70   |
| 24  | DA    | 301  | G    | C6-C5-N7    | 5.59  | 133.75      | 130.40   |
| 24  | DA    | 1136 | G    | C3'-C2'-C1' | 5.59  | 105.97      | 101.50   |
| 21  | AA    | 991  | U    | P-O3'-C3'   | 5.59  | 126.41      | 119.70   |
| 55  | CA    | 1176 | A    | O4'-C1'-N9  | 5.59  | 112.67      | 108.20   |
| 24  | DA    | 2215 | C    | C3'-C2'-C1' | 5.59  | 105.97      | 101.50   |
| 21  | AA    | 274  | A    | P-O3'-C3'   | 5.59  | 126.41      | 119.70   |
| 21  | AA    | 977  | A    | C3'-C2'-C1' | 5.59  | 105.97      | 101.50   |
| 24  | BA    | 783  | A    | C4-C5-N7    | 5.59  | 113.49      | 110.70   |
| 24  | BA    | 30   | G    | P-O5'-C5'   | -5.58 | 111.97      | 120.90   |
| 55  | CA    | 131  | A    | C6-N1-C2    | 5.58  | 121.95      | 118.60   |
| 24  | DA    | 1027 | A    | P-O3'-C3'   | -5.58 | 113.00      | 119.70   |
| 21  | AA    | 935  | A    | P-O5'-C5'   | -5.58 | 111.97      | 120.90   |
| 21  | AA    | 976  | G    | C3'-C2'-C1' | 5.58  | 105.97      | 101.50   |
| 24  | BA    | 676  | A    | C4-C5-N7    | 5.58  | 113.49      | 110.70   |
| 24  | BA    | 1820 | U    | O4'-C1'-N1  | 5.58  | 112.67      | 108.20   |
| 24  | DA    | 1136 | G    | P-O3'-C3'   | -5.58 | 113.00      | 119.70   |
| 55  | CA    | 463  | U    | P-O3'-C3'   | -5.58 | 113.00      | 119.70   |
| 55  | CA    | 1499 | A    | N9-C1'-C2'  | -5.58 | 105.86      | 112.00   |
| 24  | DA    | 2520 | C    | C3'-C2'-C1' | 5.58  | 105.96      | 101.50   |
| 55  | CA    | 453  | G    | C3'-C2'-C1' | 5.58  | 105.96      | 101.50   |
| 55  | CA    | 961  | U    | P-O3'-C3'   | -5.58 | 113.01      | 119.70   |
| 24  | DA    | 1698 | A    | P-O3'-C3'   | 5.58  | 126.39      | 119.70   |
| 24  | BA    | 2273 | A    | P-O3'-C3'   | -5.58 | 113.01      | 119.70   |
| 24  | DA    | 510  | C    | C3'-C2'-C1' | 5.58  | 105.96      | 101.50   |
| 21  | AA    | 95   | C    | N1-C1'-C2'  | -5.58 | 105.87      | 112.00   |
| 21  | AA    | 874  | G    | N9-C1'-C2'  | -5.58 | 105.87      | 112.00   |
| 24  | BA    | 85   | G    | N9-C1'-C2'  | -5.58 | 105.87      | 112.00   |
| 24  | BA    | 2136 | G    | N9-C1'-C2'  | -5.58 | 105.87      | 112.00   |
| 24  | DA    | 2518 | A    | P-O3'-C3'   | 5.58  | 126.39      | 119.70   |
| 24  | DA    | 139  | U    | P-O3'-C3'   | 5.57  | 126.39      | 119.70   |
| 24  | BA    | 2003 | A    | C6-N1-C2    | -5.57 | 115.26      | 118.60   |
| 21  | AA    | 169  | C    | C2-N1-C1'   | -5.57 | 112.67      | 118.80   |
| 21  | AA    | 856  | C    | P-O3'-C3'   | -5.57 | 113.02      | 119.70   |
| 55  | CA    | 935  | A    | C3'-C2'-C1' | 5.57  | 105.96      | 101.50   |
| 21  | AA    | 96   | U    | O4'-C1'-N1  | 5.57  | 112.66      | 108.20   |
| 21  | AA    | 486  | U    | C3'-C2'-C1' | 5.57  | 105.95      | 101.50   |
| 21  | AA    | 547  | A    | O4'-C1'-N9  | 5.57  | 112.65      | 108.20   |
| 21  | AA    | 1499 | A    | C3'-C2'-C1' | 5.57  | 105.95      | 101.50   |
| 24  | BA    | 1128 | G    | P-O3'-C3'   | 5.57  | 126.38      | 119.70   |
| 24  | BA    | 1154 | G    | C8-N9-C4    | -5.57 | 104.17      | 106.40   |
| 24  | BA    | 2189 | U    | O4'-C1'-N1  | 5.57  | 112.66      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | CA    | 733  | G    | C4-N9-C1'   | -5.57 | 119.26      | 126.50   |
| 56  | DB    | 75   | G    | P-O3'-C3'   | -5.57 | 113.02      | 119.70   |
| 21  | AA    | 793  | U    | O4'-C1'-N1  | 5.57  | 112.65      | 108.20   |
| 24  | BA    | 2894 | G    | C3'-C2'-C1' | 5.57  | 105.95      | 101.50   |
| 55  | CA    | 1054 | C    | P-O5'-C5'   | -5.57 | 112.00      | 120.90   |
| 24  | DA    | 915  | C    | C3'-C2'-C1' | 5.57  | 105.95      | 101.50   |
| 24  | BA    | 1524 | G    | P-O3'-C3'   | -5.56 | 113.02      | 119.70   |
| 25  | BB    | 13   | G    | C3'-C2'-C1' | 5.56  | 105.95      | 101.50   |
| 25  | BB    | 67   | G    | P-O5'-C5'   | -5.56 | 112.00      | 120.90   |
| 24  | DA    | 705  | A    | N1-C6-N6    | 5.56  | 121.94      | 118.60   |
| 21  | AA    | 1046 | A    | N1-C6-N6    | -5.56 | 115.26      | 118.60   |
| 24  | BA    | 325  | G    | P-O3'-C3'   | -5.56 | 113.03      | 119.70   |
| 24  | BA    | 1495 | A    | C3'-C2'-C1' | 5.56  | 105.95      | 101.50   |
| 24  | BA    | 2541 | A    | C8-N9-C4    | 5.56  | 108.03      | 105.80   |
| 24  | DA    | 548  | G    | N9-C1'-C2'  | -5.56 | 105.88      | 112.00   |
| 24  | DA    | 806  | C    | C6-N1-C2    | 5.56  | 122.53      | 120.30   |
| 21  | AA    | 875  | U    | C3'-C2'-C1' | 5.56  | 105.95      | 101.50   |
| 24  | BA    | 2631 | G    | N1-C6-O6    | -5.56 | 116.56      | 119.90   |
| 21  | AA    | 859  | G    | P-O5'-C5'   | -5.56 | 112.01      | 120.90   |
| 24  | BA    | 1759 | A    | C3'-C2'-C1' | 5.56  | 105.95      | 101.50   |
| 55  | CA    | 67   | C    | N3-C4-C5    | -5.56 | 119.68      | 121.90   |
| 55  | CA    | 962  | C    | O4'-C1'-N1  | 5.56  | 112.65      | 108.20   |
| 24  | DA    | 2450 | A    | C3'-C2'-C1' | 5.56  | 105.95      | 101.50   |
| 24  | DA    | 2891 | U    | O4'-C1'-N1  | 5.56  | 112.65      | 108.20   |
| 55  | CA    | 519  | C    | P-O3'-C3'   | -5.56 | 113.03      | 119.70   |
| 21  | AA    | 1414 | U    | N1-C2-O2    | 5.55  | 126.69      | 122.80   |
| 24  | BA    | 1206 | G    | C3'-C2'-C1' | 5.55  | 105.94      | 101.50   |
| 24  | BA    | 1695 | G    | C3'-C2'-C1' | 5.55  | 105.94      | 101.50   |
| 55  | CA    | 29   | U    | O4'-C1'-N1  | 5.55  | 112.64      | 108.20   |
| 55  | CA    | 1303 | C    | C6-N1-C1'   | -5.55 | 114.13      | 120.80   |
| 24  | DA    | 1213 | A    | P-O3'-C3'   | -5.55 | 113.03      | 119.70   |
| 24  | DA    | 2056 | G    | N1-C6-O6    | -5.55 | 116.57      | 119.90   |
| 24  | DA    | 2613 | U    | O4'-C1'-N1  | 5.55  | 112.64      | 108.20   |
| 21  | AA    | 879  | C    | N1-C1'-C2'  | -5.55 | 105.89      | 112.00   |
| 21  | AA    | 1168 | U    | N1-C1'-C2'  | 5.55  | 121.22      | 114.00   |
| 21  | AA    | 982  | U    | N1-C1'-C2'  | 5.55  | 121.22      | 114.00   |
| 21  | AA    | 1182 | G    | C8-N9-C1'   | 5.55  | 134.22      | 127.00   |
| 24  | BA    | 1373 | A    | N1-C6-N6    | 5.55  | 121.93      | 118.60   |
| 24  | BA    | 2273 | A    | P-O5'-C5'   | -5.55 | 112.02      | 120.90   |
| 24  | DA    | 1673 | G    | P-O3'-C3'   | 5.55  | 126.36      | 119.70   |
| 24  | DA    | 2240 | U    | P-O3'-C3'   | -5.55 | 113.04      | 119.70   |
| 12  | AM    | 74   | MET  | CG-SD-CE    | 5.55  | 109.08      | 100.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 73   | A    | P-O3'-C3'   | -5.55 | 113.04      | 119.70   |
| 24  | BA    | 1428 | C    | P-O3'-C3'   | 5.55  | 126.36      | 119.70   |
| 24  | DA    | 548  | G    | C4-N9-C1'   | 5.55  | 133.72      | 126.50   |
| 24  | BA    | 1158 | C    | N3-C4-C5    | -5.55 | 119.68      | 121.90   |
| 24  | BA    | 1499 | C    | C3'-C2'-C1' | 5.55  | 105.94      | 101.50   |
| 24  | DA    | 2302 | U    | O4'-C1'-N1  | 5.55  | 112.64      | 108.20   |
| 21  | AA    | 465  | A    | N9-C1'-C2'  | -5.55 | 105.90      | 112.00   |
| 24  | BA    | 980  | A    | C8-N9-C4    | -5.55 | 103.58      | 105.80   |
| 24  | BA    | 1663 | G    | N1-C6-O6    | -5.55 | 116.57      | 119.90   |
| 55  | CA    | 1493 | A    | P-O3'-C3'   | 5.55  | 126.36      | 119.70   |
| 24  | BA    | 1022 | G    | C2-N3-C4    | -5.54 | 109.13      | 111.90   |
| 55  | CA    | 657  | U    | O4'-C1'-N1  | 5.54  | 112.64      | 108.20   |
| 24  | DA    | 92   | U    | O4'-C1'-N1  | 5.54  | 112.63      | 108.20   |
| 24  | BA    | 2339 | C    | O4'-C1'-N1  | 5.54  | 112.63      | 108.20   |
| 55  | CA    | 243  | A    | C5-C6-N6    | 5.54  | 128.13      | 123.70   |
| 55  | CA    | 1128 | C    | C3'-C2'-C1' | 5.54  | 105.93      | 101.50   |
| 24  | DA    | 630  | G    | C2-N3-C4    | -5.54 | 109.13      | 111.90   |
| 24  | BA    | 544  | C    | P-O3'-C3'   | 5.54  | 126.35      | 119.70   |
| 24  | BA    | 2224 | G    | C2-N3-C4    | -5.54 | 109.13      | 111.90   |
| 21  | AA    | 72   | A    | P-O3'-C3'   | -5.54 | 113.05      | 119.70   |
| 21  | AA    | 994  | A    | P-O3'-C3'   | -5.54 | 113.05      | 119.70   |
| 55  | CA    | 475  | C    | P-O3'-C3'   | -5.54 | 113.05      | 119.70   |
| 24  | BA    | 753  | A    | N1-C6-N6    | -5.54 | 115.28      | 118.60   |
| 24  | BA    | 1568 | G    | C3'-C2'-C1' | 5.54  | 105.93      | 101.50   |
| 24  | BA    | 2809 | A    | P-O3'-C3'   | -5.54 | 113.06      | 119.70   |
| 24  | DA    | 1305 | C    | O4'-C1'-N1  | 5.54  | 112.63      | 108.20   |
| 24  | DA    | 1611 | C    | C3'-C2'-C1' | 5.54  | 105.93      | 101.50   |
| 21  | AA    | 1055 | A    | P-O3'-C3'   | -5.53 | 113.06      | 119.70   |
| 24  | BA    | 1386 | C    | C6-N1-C2    | -5.53 | 118.09      | 120.30   |
| 24  | BA    | 2023 | C    | C3'-C2'-C1' | 5.53  | 105.93      | 101.50   |
| 24  | DA    | 1916 | A    | N9-C1'-C2'  | -5.53 | 105.91      | 112.00   |
| 21  | AA    | 181  | A    | P-O3'-C3'   | 5.53  | 126.34      | 119.70   |
| 24  | BA    | 831  | G    | P-O5'-C5'   | -5.53 | 112.05      | 120.90   |
| 24  | BA    | 1457 | U    | N1-C1'-C2'  | 5.53  | 121.19      | 114.00   |
| 24  | BA    | 2578 | G    | C4-C5-N7    | -5.53 | 108.59      | 110.80   |
| 24  | BA    | 85   | G    | C3'-C2'-C1' | 5.53  | 105.92      | 101.50   |
| 24  | BA    | 271  | G    | C4-N9-C1'   | -5.53 | 119.31      | 126.50   |
| 24  | BA    | 846  | U    | O4'-C1'-N1  | 5.53  | 112.62      | 108.20   |
| 24  | BA    | 2799 | A    | C3'-C2'-C1' | 5.53  | 105.92      | 101.50   |
| 24  | DA    | 1267 | U    | P-O3'-C3'   | -5.53 | 113.06      | 119.70   |
| 24  | DA    | 1330 | C    | C3'-C2'-C1' | 5.53  | 105.92      | 101.50   |
| 24  | DA    | 2874 | C    | C3'-C2'-C1' | 5.53  | 105.92      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 794  | A    | C3'-C2'-C1' | 5.53  | 105.92      | 101.50   |
| 24  | BA    | 1021 | A    | C3'-C2'-C1' | 5.53  | 105.92      | 101.50   |
| 24  | BA    | 312  | G    | P-O3'-C3'   | -5.53 | 113.07      | 119.70   |
| 24  | BA    | 2551 | C    | O4'-C1'-N1  | 5.53  | 112.62      | 108.20   |
| 55  | CA    | 655  | A    | C3'-C2'-C1' | 5.53  | 105.92      | 101.50   |
| 55  | CA    | 1170 | A    | N9-C1'-C2'  | -5.53 | 105.92      | 112.00   |
| 24  | DA    | 2896 | C    | C3'-C2'-C1' | 5.53  | 105.92      | 101.50   |
| 24  | DA    | 2902 | C    | P-O3'-C3'   | 5.53  | 126.33      | 119.70   |
| 24  | BA    | 2857 | G    | N1-C2-N3    | 5.52  | 127.21      | 123.90   |
| 24  | DA    | 2568 | U    | O4'-C1'-N1  | 5.52  | 112.62      | 108.20   |
| 24  | BA    | 1408 | G    | P-O3'-C3'   | 5.52  | 126.33      | 119.70   |
| 24  | DA    | 445  | C    | C3'-C2'-C1' | 5.52  | 105.92      | 101.50   |
| 24  | DA    | 2572 | A    | O4'-C1'-N9  | 5.52  | 112.62      | 108.20   |
| 21  | AA    | 1052 | U    | P-O3'-C3'   | 5.52  | 126.33      | 119.70   |
| 24  | BA    | 1127 | A    | C3'-C2'-C1' | 5.52  | 105.92      | 101.50   |
| 24  | BA    | 1537 | G    | C3'-C2'-C1' | 5.52  | 105.92      | 101.50   |
| 24  | BA    | 1838 | C    | N1-C1'-C2'  | 5.52  | 121.18      | 114.00   |
| 24  | BA    | 2361 | G    | P-O3'-C3'   | -5.52 | 113.08      | 119.70   |
| 24  | BA    | 2452 | C    | O4'-C1'-N1  | -5.52 | 103.78      | 108.20   |
| 24  | DA    | 1931 | U    | C3'-C2'-C1' | 5.52  | 105.92      | 101.50   |
| 56  | DB    | 43   | C    | N1-C1'-C2'  | -5.52 | 105.93      | 112.00   |
| 24  | BA    | 1144 | A    | P-O3'-C3'   | -5.52 | 113.08      | 119.70   |
| 24  | DA    | 2498 | C    | P-O3'-C3'   | -5.52 | 113.08      | 119.70   |
| 21  | AA    | 14   | U    | C3'-C2'-C1' | 5.52  | 105.92      | 101.50   |
| 24  | BA    | 762  | U    | P-O3'-C3'   | 5.52  | 126.32      | 119.70   |
| 25  | BB    | 23   | G    | N3-C4-N9    | 5.52  | 129.31      | 126.00   |
| 24  | DA    | 963  | U    | P-O3'-C3'   | -5.52 | 113.08      | 119.70   |
| 24  | DA    | 1023 | U    | P-O3'-C3'   | -5.52 | 113.08      | 119.70   |
| 24  | BA    | 1309 | G    | P-O3'-C3'   | -5.52 | 113.08      | 119.70   |
| 24  | BA    | 1865 | U    | N3-C4-C5    | 5.52  | 117.91      | 114.60   |
| 21  | AA    | 96   | U    | N1-C1'-C2'  | -5.51 | 105.93      | 112.00   |
| 55  | CA    | 1333 | A    | O4'-C1'-N9  | 5.51  | 112.61      | 108.20   |
| 24  | DA    | 460  | A    | P-O5'-C5'   | -5.51 | 112.08      | 120.90   |
| 21  | AA    | 169  | C    | C6-N1-C1'   | 5.51  | 127.42      | 120.80   |
| 24  | DA    | 388  | G    | P-O3'-C3'   | -5.51 | 113.08      | 119.70   |
| 55  | CA    | 538  | G    | P-O3'-C3'   | -5.51 | 113.09      | 119.70   |
| 55  | CA    | 1064 | G    | P-O3'-C3'   | 5.51  | 126.31      | 119.70   |
| 24  | DA    | 1510 | G    | C3'-C2'-C1' | 5.51  | 105.91      | 101.50   |
| 21  | AA    | 389  | A    | C3'-C2'-C1' | 5.51  | 105.91      | 101.50   |
| 21  | AA    | 686  | U    | P-O3'-C3'   | 5.51  | 126.31      | 119.70   |
| 24  | DA    | 1551 | A    | C6-N1-C2    | 5.51  | 121.91      | 118.60   |
| 21  | AA    | 373  | A    | C3'-C2'-C1' | 5.51  | 105.91      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 2255 | G    | P-O3'-C3'   | -5.51 | 113.09      | 119.70   |
| 55  | CA    | 934  | C    | C5-C4-N4    | 5.51  | 124.06      | 120.20   |
| 24  | BA    | 674  | G    | P-O3'-C3'   | -5.51 | 113.09      | 119.70   |
| 24  | BA    | 1206 | G    | P-O3'-C3'   | -5.51 | 113.09      | 119.70   |
| 24  | BA    | 1478 | G    | N1-C6-O6    | -5.51 | 116.60      | 119.90   |
| 24  | BA    | 2337 | G    | P-O3'-C3'   | -5.51 | 113.09      | 119.70   |
| 24  | BA    | 2630 | G    | N9-C1'-C2'  | -5.50 | 105.94      | 112.00   |
| 55  | CA    | 513  | C    | C3'-C2'-C1' | 5.50  | 105.90      | 101.50   |
| 24  | BA    | 2283 | C    | C3'-C2'-C1' | 5.50  | 105.90      | 101.50   |
| 55  | CA    | 817  | C    | P-O3'-C3'   | 5.50  | 126.31      | 119.70   |
| 55  | CA    | 1160 | G    | C3'-C2'-C1' | 5.50  | 105.90      | 101.50   |
| 24  | DA    | 406  | G    | C3'-C2'-C1' | 5.50  | 105.90      | 101.50   |
| 24  | DA    | 2338 | C    | N1-C1'-C2'  | -5.50 | 105.95      | 112.00   |
| 21  | AA    | 466  | A    | P-O3'-C3'   | 5.50  | 126.30      | 119.70   |
| 24  | DA    | 1648 | U    | C3'-C2'-C1' | 5.50  | 105.90      | 101.50   |
| 29  | DF    | 78   | ILE  | CB-CA-C     | -5.50 | 100.60      | 111.60   |
| 21  | AA    | 72   | A    | C3'-C2'-C1' | 5.50  | 105.90      | 101.50   |
| 24  | BA    | 250  | G    | C3'-C2'-C1' | 5.50  | 105.90      | 101.50   |
| 24  | BA    | 1090 | A    | O4'-C1'-N9  | 5.50  | 112.60      | 108.20   |
| 24  | BA    | 2460 | U    | O4'-C1'-N1  | 5.50  | 112.60      | 108.20   |
| 55  | CA    | 1241 | G    | N9-C1'-C2'  | -5.50 | 105.95      | 112.00   |
| 24  | DA    | 1558 | C    | P-O3'-C3'   | 5.50  | 126.30      | 119.70   |
| 21  | AA    | 403  | C    | O4'-C1'-N1  | 5.50  | 112.60      | 108.20   |
| 24  | BA    | 2266 | A    | C5-N7-C8    | -5.50 | 101.15      | 103.90   |
| 24  | DA    | 1113 | U    | P-O3'-C3'   | -5.50 | 113.10      | 119.70   |
| 21  | AA    | 984  | C    | C3'-C2'-C1' | 5.50  | 105.90      | 101.50   |
| 21  | AA    | 1068 | G    | P-O3'-C3'   | -5.50 | 113.11      | 119.70   |
| 24  | BA    | 1022 | G    | C8-N9-C1'   | 5.50  | 134.14      | 127.00   |
| 24  | DA    | 207  | A    | C3'-C2'-C1' | 5.50  | 105.90      | 101.50   |
| 21  | AA    | 610  | U    | N3-C2-O2    | -5.49 | 118.36      | 122.20   |
| 24  | BA    | 312  | G    | N9-C1'-C2'  | -5.49 | 105.96      | 112.00   |
| 24  | BA    | 1019 | U    | O4'-C1'-N1  | 5.49  | 112.59      | 108.20   |
| 24  | BA    | 1143 | A    | N1-C6-N6    | 5.49  | 121.90      | 118.60   |
| 24  | BA    | 1411 | U    | O4'-C1'-N1  | 5.49  | 112.59      | 108.20   |
| 24  | DA    | 1669 | A    | C3'-C2'-C1' | 5.49  | 105.89      | 101.50   |
| 24  | DA    | 1733 | G    | C3'-C2'-C1' | 5.49  | 105.89      | 101.50   |
| 24  | DA    | 2837 | A    | C3'-C2'-C1' | 5.49  | 105.89      | 101.50   |
| 21  | AA    | 1103 | C    | P-O3'-C3'   | -5.49 | 113.11      | 119.70   |
| 24  | BA    | 861  | A    | C3'-C2'-C1' | 5.49  | 105.89      | 101.50   |
| 55  | CA    | 53   | A    | C3'-C2'-C1' | 5.49  | 105.89      | 101.50   |
| 55  | CA    | 84   | U    | N1-C1'-C2'  | 5.49  | 121.14      | 114.00   |
| 24  | DA    | 2148 | G    | C3'-C2'-C1' | 5.49  | 105.89      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 2372 | U    | P-O5'-C5'   | -5.49 | 112.12      | 120.90   |
| 55  | CA    | 71   | A    | P-O3'-C3'   | -5.49 | 113.11      | 119.70   |
| 55  | CA    | 534  | U    | C3'-C2'-C1' | 5.49  | 105.89      | 101.50   |
| 24  | DA    | 373  | U    | N1-C1'-C2'  | -5.49 | 105.96      | 112.00   |
| 24  | DA    | 1558 | C    | N1-C1'-C2'  | 5.49  | 121.14      | 114.00   |
| 24  | DA    | 2383 | G    | P-O3'-C3'   | -5.49 | 113.11      | 119.70   |
| 24  | BA    | 1129 | A    | C3'-C2'-C1' | 5.49  | 105.89      | 101.50   |
| 24  | BA    | 1027 | A    | C3'-C2'-C1' | 5.49  | 105.89      | 101.50   |
| 55  | CA    | 974  | A    | P-O3'-C3'   | 5.49  | 126.28      | 119.70   |
| 24  | DA    | 2135 | A    | C3'-C2'-C1' | 5.49  | 105.89      | 101.50   |
| 24  | DA    | 2311 | A    | C3'-C2'-C1' | 5.49  | 105.89      | 101.50   |
| 24  | BA    | 1112 | G    | C3'-C2'-C1' | 5.48  | 105.89      | 101.50   |
| 24  | BA    | 2625 | G    | C8-N9-C4    | -5.48 | 104.21      | 106.40   |
| 24  | BA    | 2656 | U    | C3'-C2'-C1' | 5.48  | 105.89      | 101.50   |
| 24  | BA    | 944  | C    | C6-N1-C2    | 5.48  | 122.49      | 120.30   |
| 24  | BA    | 2295 | C    | N1-C1'-C2'  | 5.48  | 121.12      | 114.00   |
| 24  | DA    | 2573 | C    | C3'-C2'-C1' | 5.48  | 105.88      | 101.50   |
| 24  | BA    | 1091 | G    | C3'-C2'-C1' | 5.48  | 105.88      | 101.50   |
| 24  | BA    | 1343 | G    | C3'-C2'-C1' | 5.48  | 105.88      | 101.50   |
| 24  | BA    | 1876 | A    | O4'-C1'-N9  | 5.48  | 112.58      | 108.20   |
| 24  | BA    | 1316 | U    | O4'-C1'-N1  | -5.48 | 103.82      | 108.20   |
| 24  | BA    | 2494 | G    | C4-C5-N7    | -5.48 | 108.61      | 110.80   |
| 21  | AA    | 122  | G    | N9-C1'-C2'  | -5.47 | 105.98      | 112.00   |
| 24  | BA    | 765  | C    | P-O3'-C3'   | -5.47 | 113.13      | 119.70   |
| 24  | BA    | 1491 | G    | N9-C1'-C2'  | -5.47 | 105.98      | 112.00   |
| 24  | BA    | 1804 | C    | P-O3'-C3'   | -5.47 | 113.13      | 119.70   |
| 24  | BA    | 2574 | G    | N1-C6-O6    | -5.47 | 116.62      | 119.90   |
| 25  | BB    | 29   | A    | P-O5'-C5'   | -5.47 | 112.14      | 120.90   |
| 55  | CA    | 283  | U    | C3'-C2'-C1' | 5.47  | 105.88      | 101.50   |
| 55  | CA    | 1168 | U    | P-O3'-C3'   | 5.47  | 126.27      | 119.70   |
| 55  | CA    | 1284 | C    | C3'-C2'-C1' | 5.47  | 105.88      | 101.50   |
| 23  | CW    | 5    | U    | O4'-C1'-N1  | 5.47  | 112.58      | 108.20   |
| 21  | AA    | 500  | G    | N9-C1'-C2'  | -5.47 | 105.98      | 112.00   |
| 21  | AA    | 1090 | U    | O4'-C1'-N1  | 5.47  | 112.58      | 108.20   |
| 24  | BA    | 500  | G    | N3-C4-C5    | 5.47  | 131.34      | 128.60   |
| 24  | BA    | 1295 | C    | C5-C4-N4    | 5.47  | 124.03      | 120.20   |
| 24  | DA    | 510  | C    | P-O3'-C3'   | -5.47 | 113.13      | 119.70   |
| 24  | DA    | 2505 | G    | N9-C1'-C2'  | -5.47 | 105.98      | 112.00   |
| 21  | AA    | 131  | A    | N1-C6-N6    | -5.47 | 115.32      | 118.60   |
| 55  | CA    | 53   | A    | N9-C1'-C2'  | -5.47 | 105.98      | 112.00   |
| 24  | DA    | 754  | U    | C3'-C2'-C1' | 5.47  | 105.88      | 101.50   |
| 24  | DA    | 1695 | G    | C3'-C2'-C1' | 5.47  | 105.88      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 1838 | C    | P-O3'-C3'   | 5.47  | 126.27      | 119.70   |
| 21  | AA    | 465  | A    | P-O5'-C5'   | -5.47 | 112.15      | 120.90   |
| 21  | AA    | 874  | G    | C3'-C2'-C1' | 5.47  | 105.87      | 101.50   |
| 21  | AA    | 1242 | G    | C3'-C2'-C1' | 5.47  | 105.87      | 101.50   |
| 21  | AA    | 857  | C    | O4'-C1'-N1  | 5.47  | 112.57      | 108.20   |
| 24  | BA    | 503  | A    | O4'-C1'-N9  | 5.47  | 112.57      | 108.20   |
| 24  | BA    | 819  | A    | P-O3'-C3'   | -5.47 | 113.14      | 119.70   |
| 24  | BA    | 1288 | G    | O5'-P-OP2   | -5.47 | 100.78      | 105.70   |
| 24  | BA    | 1430 | G    | C6-N1-C2    | 5.47  | 128.38      | 125.10   |
| 24  | BA    | 1560 | G    | N9-C1'-C2'  | -5.47 | 105.99      | 112.00   |
| 24  | BA    | 1881 | C    | O4'-C1'-N1  | 5.47  | 112.57      | 108.20   |
| 24  | BA    | 2407 | A    | N1-C6-N6    | -5.47 | 115.32      | 118.60   |
| 25  | BB    | 57   | A    | O5'-P-OP2   | -5.47 | 100.78      | 105.70   |
| 25  | BB    | 75   | G    | P-O3'-C3'   | -5.47 | 113.14      | 119.70   |
| 55  | CA    | 1302 | C    | C3'-C2'-C1' | 5.47  | 105.87      | 101.50   |
| 21  | AA    | 12   | U    | N1-C2-O2    | 5.46  | 126.62      | 122.80   |
| 21  | AA    | 1153 | G    | C3'-C2'-C1' | 5.46  | 105.87      | 101.50   |
| 24  | BA    | 434  | U    | N1-C1'-C2'  | 5.46  | 121.10      | 114.00   |
| 24  | BA    | 1682 | G    | C3'-C2'-C1' | 5.46  | 105.87      | 101.50   |
| 24  | DA    | 374  | A    | P-O3'-C3'   | -5.46 | 113.14      | 119.70   |
| 24  | DA    | 741  | U    | C3'-C2'-C1' | 5.46  | 105.87      | 101.50   |
| 21  | AA    | 754  | C    | N1-C1'-C2'  | -5.46 | 105.99      | 112.00   |
| 24  | BA    | 228  | C    | O4'-C1'-N1  | 5.46  | 112.57      | 108.20   |
| 24  | BA    | 2482 | A    | N1-C6-N6    | 5.46  | 121.88      | 118.60   |
| 24  | DA    | 1662 | U    | O4'-C1'-N1  | 5.46  | 112.57      | 108.20   |
| 24  | DA    | 2875 | C    | C3'-C2'-C1' | 5.46  | 105.87      | 101.50   |
| 55  | CA    | 1055 | A    | C3'-C2'-C1' | 5.46  | 105.87      | 101.50   |
| 21  | AA    | 187  | G    | C2-N3-C4    | -5.46 | 109.17      | 111.90   |
| 21  | AA    | 1287 | A    | C3'-C2'-C1' | 5.46  | 105.87      | 101.50   |
| 24  | BA    | 533  | G    | C3'-C2'-C1' | 5.46  | 105.87      | 101.50   |
| 24  | BA    | 777  | G    | P-O3'-C3'   | -5.46 | 113.15      | 119.70   |
| 24  | BA    | 1525 | A    | C5-C6-N6    | 5.46  | 128.07      | 123.70   |
| 24  | BA    | 2894 | G    | P-O3'-C3'   | -5.46 | 113.15      | 119.70   |
| 24  | DA    | 2034 | U    | C3'-C2'-C1' | 5.46  | 105.87      | 101.50   |
| 24  | BA    | 746  | U    | N1-C1'-C2'  | 5.46  | 121.09      | 114.00   |
| 55  | CA    | 735  | C    | O4'-C1'-N1  | 5.46  | 112.56      | 108.20   |
| 24  | BA    | 1805 | A    | C8-N9-C4    | -5.45 | 103.62      | 105.80   |
| 24  | BA    | 2061 | G    | N3-C4-C5    | -5.45 | 125.87      | 128.60   |
| 24  | BA    | 2386 | A    | P-O5'-C5'   | -5.45 | 112.18      | 120.90   |
| 24  | DA    | 1560 | G    | P-O3'-C3'   | -5.45 | 113.16      | 119.70   |
| 56  | DB    | 72   | G    | C2-N3-C4    | -5.45 | 109.17      | 111.90   |
| 24  | BA    | 114  | U    | O4'-C1'-N1  | -5.45 | 103.84      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 1661 | G    | P-O5'-C5'   | -5.45 | 112.18      | 120.90   |
| 24  | BA    | 2063 | C    | C3'-C2'-C1' | 5.45  | 105.86      | 101.50   |
| 55  | CA    | 1365 | G    | C3'-C2'-C1' | 5.45  | 105.86      | 101.50   |
| 24  | DA    | 2197 | U    | P-O3'-C3'   | 5.45  | 126.24      | 119.70   |
| 21  | AA    | 815  | A    | P-O3'-C3'   | 5.45  | 126.24      | 119.70   |
| 24  | BA    | 22   | C    | C2-N3-C4    | -5.45 | 117.17      | 119.90   |
| 24  | BA    | 1946 | U    | C5-C4-O4    | 5.45  | 129.17      | 125.90   |
| 24  | DA    | 1144 | A    | C3'-C2'-C1' | 5.45  | 105.86      | 101.50   |
| 21  | AA    | 431  | A    | C3'-C2'-C1' | 5.45  | 105.86      | 101.50   |
| 21  | AA    | 1181 | G    | P-O3'-C3'   | 5.45  | 126.24      | 119.70   |
| 24  | BA    | 2791 | G    | C3'-C2'-C1' | 5.45  | 105.86      | 101.50   |
| 24  | DA    | 1239 | G    | N9-C1'-C2'  | -5.45 | 106.01      | 112.00   |
| 21  | AA    | 467  | U    | O4'-C1'-N1  | 5.45  | 112.56      | 108.20   |
| 24  | BA    | 1885 | A    | N1-C6-N6    | -5.45 | 115.33      | 118.60   |
| 25  | BB    | 74   | U    | P-O5'-C5'   | -5.45 | 112.19      | 120.90   |
| 24  | DA    | 791  | C    | P-O5'-C5'   | -5.45 | 112.19      | 120.90   |
| 24  | DA    | 1026 | G    | P-O3'-C3'   | -5.45 | 113.17      | 119.70   |
| 24  | DA    | 1816 | C    | C3'-C2'-C1' | 5.45  | 105.86      | 101.50   |
| 24  | BA    | 1427 | A    | O4'-C1'-N9  | 5.44  | 112.56      | 108.20   |
| 24  | BA    | 2589 | A    | P-O5'-C5'   | -5.44 | 112.19      | 120.90   |
| 56  | DB    | 90   | C    | C3'-C2'-C1' | 5.44  | 105.86      | 101.50   |
| 21  | AA    | 81   | A    | C5-C6-N6    | 5.44  | 128.05      | 123.70   |
| 21  | AA    | 935  | A    | N9-C1'-C2'  | -5.44 | 106.02      | 112.00   |
| 24  | BA    | 137  | U    | P-O3'-C3'   | 5.44  | 126.23      | 119.70   |
| 24  | BA    | 907  | G    | C2-N3-C4    | -5.44 | 109.18      | 111.90   |
| 55  | CA    | 422  | C    | O4'-C1'-N1  | -5.44 | 103.85      | 108.20   |
| 21  | AA    | 1032 | G    | C3'-C2'-C1' | 5.44  | 105.85      | 101.50   |
| 24  | BA    | 421  | C    | N1-C1'-C2'  | 5.44  | 121.07      | 114.00   |
| 24  | BA    | 693  | A    | P-O3'-C3'   | -5.44 | 113.17      | 119.70   |
| 24  | BA    | 1875 | G    | P-O3'-C3'   | -5.44 | 113.18      | 119.70   |
| 24  | DA    | 514  | A    | N1-C6-N6    | 5.44  | 121.86      | 118.60   |
| 24  | DA    | 1779 | U    | O4'-C1'-N1  | 5.44  | 112.55      | 108.20   |
| 24  | DA    | 1888 | G    | O4'-C1'-N9  | 5.44  | 112.55      | 108.20   |
| 25  | BB    | 25   | U    | C3'-C2'-C1' | 5.44  | 105.85      | 101.50   |
| 55  | CA    | 1394 | A    | P-O3'-C3'   | 5.44  | 126.22      | 119.70   |
| 24  | DA    | 1183 | U    | O4'-C1'-N1  | 5.44  | 112.55      | 108.20   |
| 21  | AA    | 1153 | G    | N9-C1'-C2'  | -5.43 | 106.02      | 112.00   |
| 24  | BA    | 103  | A    | C3'-C2'-C1' | 5.43  | 105.85      | 101.50   |
| 24  | BA    | 670  | A    | C8-N9-C4    | 5.43  | 107.97      | 105.80   |
| 24  | BA    | 1956 | U    | P-O3'-C3'   | -5.43 | 113.18      | 119.70   |
| 24  | BA    | 1965 | C    | C2-N1-C1'   | 5.43  | 124.78      | 118.80   |
| 24  | DA    | 2385 | C    | P-O3'-C3'   | -5.43 | 113.18      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 887  | G    | P-O3'-C3'   | -5.43 | 113.18      | 119.70   |
| 24  | BA    | 1091 | G    | O4'-C1'-N9  | 5.43  | 112.55      | 108.20   |
| 24  | DA    | 629  | G    | C3'-C2'-C1' | 5.43  | 105.85      | 101.50   |
| 24  | DA    | 1829 | A    | P-O3'-C3'   | 5.43  | 126.22      | 119.70   |
| 24  | BA    | 765  | C    | C3'-C2'-C1' | 5.43  | 105.84      | 101.50   |
| 24  | DA    | 334  | C    | N1-C1'-C2'  | -5.43 | 106.03      | 112.00   |
| 55  | CA    | 352  | C    | C3'-C2'-C1' | 5.43  | 105.84      | 101.50   |
| 24  | DA    | 2798 | U    | O4'-C1'-N1  | -5.43 | 103.86      | 108.20   |
| 24  | BA    | 1872 | A    | C3'-C2'-C1' | 5.43  | 105.84      | 101.50   |
| 21  | AA    | 213  | G    | C3'-C2'-C1' | 5.43  | 105.84      | 101.50   |
| 24  | BA    | 302  | C    | P-O3'-C3'   | -5.43 | 113.19      | 119.70   |
| 24  | BA    | 1320 | C    | P-O3'-C3'   | 5.43  | 126.21      | 119.70   |
| 24  | BA    | 2217 | G    | P-O3'-C3'   | -5.43 | 113.19      | 119.70   |
| 24  | DA    | 2096 | C    | O4'-C1'-N1  | 5.43  | 112.54      | 108.20   |
| 21  | AA    | 6    | G    | C3'-C2'-C1' | 5.42  | 105.84      | 101.50   |
| 24  | BA    | 653  | U    | O4'-C1'-N1  | -5.42 | 103.86      | 108.20   |
| 24  | BA    | 1452 | G    | O4'-C1'-N9  | -5.42 | 103.86      | 108.20   |
| 24  | BA    | 2582 | G    | N1-C6-O6    | -5.42 | 116.64      | 119.90   |
| 24  | DA    | 1963 | U    | P-O3'-C3'   | -5.42 | 113.19      | 119.70   |
| 55  | CA    | 701  | U    | P-O3'-C3'   | 5.42  | 126.21      | 119.70   |
| 21  | AA    | 1215 | G    | C3'-C2'-C1' | 5.42  | 105.84      | 101.50   |
| 24  | BA    | 2585 | U    | N1-C1'-C2'  | 5.42  | 121.05      | 114.00   |
| 24  | DA    | 139  | U    | N1-C1'-C2'  | 5.42  | 121.05      | 114.00   |
| 24  | DA    | 616  | A    | P-O3'-C3'   | -5.42 | 113.19      | 119.70   |
| 56  | DB    | 118  | C    | O4'-C1'-N1  | 5.42  | 112.54      | 108.20   |
| 21  | AA    | 1303 | C    | C3'-C2'-C1' | 5.42  | 105.84      | 101.50   |
| 24  | BA    | 480  | A    | C2-N3-C4    | 5.42  | 113.31      | 110.60   |
| 55  | CA    | 373  | A    | C3'-C2'-C1' | 5.42  | 105.84      | 101.50   |
| 24  | DA    | 1181 | U    | P-O3'-C3'   | -5.42 | 113.20      | 119.70   |
| 24  | DA    | 1063 | G    | N9-C1'-C2'  | -5.42 | 106.04      | 112.00   |
| 24  | DA    | 1498 | C    | C3'-C2'-C1' | 5.42  | 105.83      | 101.50   |
| 24  | DA    | 2067 | G    | P-O3'-C3'   | 5.42  | 126.20      | 119.70   |
| 21  | AA    | 577  | G    | C3'-C2'-C1' | 5.42  | 105.83      | 101.50   |
| 24  | BA    | 1148 | U    | C5-C4-O4    | 5.42  | 129.15      | 125.90   |
| 55  | CA    | 454  | G    | N9-C1'-C2'  | -5.42 | 106.04      | 112.00   |
| 24  | DA    | 967  | U    | O4'-C1'-N1  | 5.42  | 112.53      | 108.20   |
| 24  | DA    | 2800 | A    | N9-C1'-C2'  | -5.42 | 106.04      | 112.00   |
| 21  | AA    | 52   | C    | O4'-C1'-N1  | 5.42  | 112.53      | 108.20   |
| 24  | BA    | 752  | A    | OP2-P-O3'   | 5.42  | 117.11      | 105.20   |
| 24  | DA    | 476  | G    | C3'-C2'-C1' | 5.42  | 105.83      | 101.50   |
| 24  | BA    | 829  | A    | N7-C8-N9    | -5.41 | 111.09      | 113.80   |
| 55  | CA    | 1442 | G    | P-O3'-C3'   | -5.41 | 113.21      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 487  | A    | N9-C1'-C2'  | -5.41 | 106.05      | 112.00   |
| 21  | AA    | 575  | G    | C6-C5-N7    | 5.41  | 133.65      | 130.40   |
| 55  | CA    | 513  | C    | P-O5'-C5'   | -5.41 | 112.24      | 120.90   |
| 24  | DA    | 916  | G    | N9-C1'-C2'  | -5.41 | 106.05      | 112.00   |
| 24  | DA    | 991  | C    | O4'-C1'-N1  | 5.41  | 112.53      | 108.20   |
| 24  | DA    | 1734 | G    | C3'-C2'-C1' | 5.41  | 105.83      | 101.50   |
| 21  | AA    | 1158 | C    | C3'-C2'-C1' | 5.41  | 105.83      | 101.50   |
| 24  | BA    | 677  | A    | C6-N1-C2    | -5.41 | 115.36      | 118.60   |
| 24  | BA    | 1359 | A    | C8-N9-C4    | -5.41 | 103.64      | 105.80   |
| 55  | CA    | 114  | U    | O4'-C1'-N1  | 5.41  | 112.53      | 108.20   |
| 21  | AA    | 291  | U    | O4'-C1'-N1  | 5.41  | 112.53      | 108.20   |
| 24  | BA    | 2210 | U    | N1-C1'-C2'  | 5.41  | 121.03      | 114.00   |
| 55  | CA    | 1158 | C    | N1-C1'-C2'  | -5.41 | 106.05      | 112.00   |
| 24  | BA    | 563  | A    | P-O3'-C3'   | -5.40 | 113.22      | 119.70   |
| 24  | BA    | 1062 | G    | C3'-C2'-C1' | 5.40  | 105.82      | 101.50   |
| 55  | CA    | 733  | G    | N3-C4-N9    | -5.40 | 122.76      | 126.00   |
| 21  | AA    | 816  | A    | P-O5'-C5'   | -5.40 | 112.26      | 120.90   |
| 24  | DA    | 752  | A    | P-O3'-C3'   | 5.40  | 126.18      | 119.70   |
| 24  | DA    | 763  | G    | C3'-C2'-C1' | 5.40  | 105.82      | 101.50   |
| 24  | DA    | 2521 | C    | C3'-C2'-C1' | 5.40  | 105.82      | 101.50   |
| 25  | BB    | 94   | A    | P-O5'-C5'   | -5.40 | 112.26      | 120.90   |
| 24  | DA    | 783  | A    | O4'-C1'-N9  | 5.40  | 112.52      | 108.20   |
| 21  | AA    | 14   | U    | P-O5'-C5'   | -5.40 | 112.26      | 120.90   |
| 55  | CA    | 90   | C    | C3'-C2'-C1' | 5.40  | 105.82      | 101.50   |
| 24  | DA    | 2322 | A    | N9-C1'-C2'  | -5.40 | 106.06      | 112.00   |
| 21  | AA    | 1224 | U    | C5-C4-O4    | -5.40 | 122.66      | 125.90   |
| 24  | BA    | 144  | A    | C6-N1-C2    | -5.40 | 115.36      | 118.60   |
| 24  | BA    | 530  | G    | C8-N9-C1'   | -5.40 | 119.98      | 127.00   |
| 21  | AA    | 1050 | G    | P-O3'-C3'   | -5.39 | 113.23      | 119.70   |
| 24  | DA    | 475  | C    | P-O3'-C3'   | -5.39 | 113.23      | 119.70   |
| 24  | DA    | 2567 | G    | P-O3'-C3'   | 5.39  | 126.17      | 119.70   |
| 24  | DA    | 2576 | G    | P-O3'-C3'   | 5.39  | 126.17      | 119.70   |
| 24  | BA    | 1841 | U    | C2-N3-C4    | 5.39  | 130.23      | 127.00   |
| 55  | CA    | 414  | A    | P-O3'-C3'   | -5.39 | 113.23      | 119.70   |
| 24  | DA    | 509  | C    | N1-C2-O2    | 5.39  | 122.14      | 118.90   |
| 24  | DA    | 616  | A    | C3'-C2'-C1' | 5.39  | 105.81      | 101.50   |
| 24  | BA    | 1009 | A    | P-O5'-C5'   | -5.39 | 112.28      | 120.90   |
| 24  | BA    | 1455 | G    | N9-C1'-C2'  | -5.39 | 106.07      | 112.00   |
| 24  | BA    | 1964 | G    | C4-C5-N7    | -5.39 | 108.64      | 110.80   |
| 55  | CA    | 89   | U    | C3'-C2'-C1' | 5.39  | 105.81      | 101.50   |
| 55  | CA    | 370  | C    | C5-C4-N4    | 5.39  | 123.97      | 120.20   |
| 24  | DA    | 800  | A    | P-O3'-C3'   | 5.39  | 126.17      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 56  | DB    | 16   | G    | C3'-C2'-C1' | 5.39  | 105.81      | 101.50   |
| 21  | AA    | 369  | G    | C3'-C2'-C1' | 5.39  | 105.81      | 101.50   |
| 21  | AA    | 420  | U    | O4'-C1'-N1  | 5.39  | 112.51      | 108.20   |
| 24  | BA    | 752  | A    | C5-N7-C8    | -5.39 | 101.21      | 103.90   |
| 24  | BA    | 1621 | U    | N1-C1'-C2'  | 5.39  | 121.00      | 114.00   |
| 21  | AA    | 819  | A    | P-O3'-C3'   | 5.38  | 126.16      | 119.70   |
| 21  | AA    | 1127 | G    | P-O3'-C3'   | -5.38 | 113.24      | 119.70   |
| 21  | AA    | 1469 | C    | O4'-C1'-N1  | -5.38 | 103.89      | 108.20   |
| 24  | BA    | 1004 | U    | O4'-C1'-N1  | 5.38  | 112.51      | 108.20   |
| 24  | DA    | 1551 | A    | C5-C6-N6    | 5.38  | 128.01      | 123.70   |
| 24  | BA    | 1311 | G    | N3-C4-C5    | 5.38  | 131.29      | 128.60   |
| 24  | DA    | 1395 | A    | O4'-C1'-N9  | 5.38  | 112.51      | 108.20   |
| 24  | BA    | 703  | U    | C5-C6-N1    | -5.38 | 120.01      | 122.70   |
| 24  | BA    | 1557 | C    | C3'-C2'-C1' | 5.38  | 105.81      | 101.50   |
| 55  | CA    | 1246 | A    | C3'-C2'-C1' | 5.38  | 105.81      | 101.50   |
| 24  | DA    | 1508 | A    | P-O3'-C3'   | 5.38  | 126.16      | 119.70   |
| 24  | DA    | 1612 | C    | C3'-C2'-C1' | 5.38  | 105.80      | 101.50   |
| 24  | DA    | 1865 | U    | O4'-C1'-N1  | 5.38  | 112.50      | 108.20   |
| 21  | AA    | 717  | U    | N1-C1'-C2'  | 5.38  | 120.99      | 114.00   |
| 24  | BA    | 491  | G    | N9-C1'-C2'  | -5.38 | 106.08      | 112.00   |
| 24  | BA    | 1109 | C    | C6-N1-C2    | -5.38 | 118.15      | 120.30   |
| 23  | CW    | 4    | U    | O5'-P-OP2   | -5.38 | 100.86      | 105.70   |
| 24  | DA    | 217  | A    | N9-C1'-C2'  | -5.38 | 106.08      | 112.00   |
| 21  | AA    | 132  | C    | C3'-C2'-C1' | 5.38  | 105.80      | 101.50   |
| 24  | BA    | 791  | C    | N1-C2-O2    | 5.38  | 122.13      | 118.90   |
| 24  | DA    | 272  | A    | P-O3'-C3'   | -5.38 | 113.25      | 119.70   |
| 24  | DA    | 1023 | U    | C3'-C2'-C1' | 5.38  | 105.80      | 101.50   |
| 24  | DA    | 1914 | C    | C3'-C2'-C1' | 5.38  | 105.80      | 101.50   |
| 21  | AA    | 351  | G    | C8-N9-C1'   | -5.38 | 120.01      | 127.00   |
| 24  | BA    | 2874 | C    | P-O3'-C3'   | -5.38 | 113.25      | 119.70   |
| 55  | CA    | 425  | G    | N9-C1'-C2'  | -5.38 | 106.08      | 112.00   |
| 55  | CA    | 1531 | A    | P-O3'-C3'   | -5.38 | 113.25      | 119.70   |
| 24  | DA    | 1029 | A    | N1-C6-N6    | 5.38  | 121.83      | 118.60   |
| 21  | AA    | 1001 | C    | O4'-C1'-N1  | 5.38  | 112.50      | 108.20   |
| 24  | BA    | 2679 | A    | C5-C6-N6    | 5.38  | 128.00      | 123.70   |
| 25  | BB    | 45   | A    | C3'-C2'-C1' | 5.38  | 105.80      | 101.50   |
| 55  | CA    | 1338 | G    | N9-C1'-C2'  | -5.38 | 106.09      | 112.00   |
| 21  | AA    | 305  | G    | P-O3'-C3'   | 5.37  | 126.15      | 119.70   |
| 21  | AA    | 1131 | G    | N9-C1'-C2'  | -5.37 | 106.09      | 112.00   |
| 24  | BA    | 2883 | A    | C5-C6-N1    | -5.37 | 115.01      | 117.70   |
| 24  | DA    | 1009 | A    | P-O3'-C3'   | -5.37 | 113.25      | 119.70   |
| 21  | AA    | 891  | U    | C3'-C2'-C1' | 5.37  | 105.80      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 638  | G    | C3'-C2'-C1' | 5.37  | 105.80      | 101.50   |
| 24  | DA    | 1345 | C    | C3'-C2'-C1' | 5.37  | 105.80      | 101.50   |
| 55  | CA    | 816  | A    | C3'-C2'-C1' | 5.37  | 105.80      | 101.50   |
| 55  | CA    | 1507 | A    | N9-C1'-C2'  | -5.37 | 106.09      | 112.00   |
| 56  | DB    | 76   | G    | N3-C4-C5    | 5.37  | 131.28      | 128.60   |
| 21  | AA    | 210  | C    | N1-C1'-C2'  | 5.37  | 120.98      | 114.00   |
| 21  | AA    | 795  | C    | P-O3'-C3'   | -5.37 | 113.26      | 119.70   |
| 24  | BA    | 2619 | C    | C5-C4-N4    | 5.37  | 123.96      | 120.20   |
| 55  | CA    | 210  | C    | C2-N1-C1'   | 5.37  | 124.70      | 118.80   |
| 24  | BA    | 676  | A    | C5-N7-C8    | -5.37 | 101.22      | 103.90   |
| 24  | BA    | 1635 | A    | C3'-C2'-C1' | 5.37  | 105.79      | 101.50   |
| 24  | BA    | 2454 | G    | P-O3'-C3'   | -5.37 | 113.26      | 119.70   |
| 55  | CA    | 875  | U    | C3'-C2'-C1' | 5.37  | 105.79      | 101.50   |
| 55  | CA    | 1101 | A    | P-O3'-C3'   | 5.37  | 126.14      | 119.70   |
| 24  | DA    | 121  | G    | C3'-C2'-C1' | 5.37  | 105.79      | 101.50   |
| 21  | AA    | 1132 | C    | P-O5'-C5'   | 5.36  | 129.48      | 120.90   |
| 24  | BA    | 2474 | U    | O4'-C1'-N1  | 5.36  | 112.49      | 108.20   |
| 55  | CA    | 1401 | G    | N9-C1'-C2'  | -5.36 | 106.10      | 112.00   |
| 21  | AA    | 1296 | C    | O4'-C1'-N1  | 5.36  | 112.49      | 108.20   |
| 55  | CA    | 724  | G    | C3'-C2'-C1' | 5.36  | 105.79      | 101.50   |
| 24  | DA    | 73   | A    | C3'-C2'-C1' | 5.36  | 105.79      | 101.50   |
| 24  | DA    | 1480 | C    | O4'-C1'-N1  | 5.36  | 112.49      | 108.20   |
| 24  | DA    | 2699 | C    | O4'-C1'-N1  | 5.36  | 112.49      | 108.20   |
| 21  | AA    | 97   | G    | C3'-C2'-C1' | 5.36  | 105.79      | 101.50   |
| 21  | AA    | 1094 | G    | P-O3'-C3'   | 5.36  | 126.13      | 119.70   |
| 24  | BA    | 1947 | C    | P-O3'-C3'   | -5.36 | 113.27      | 119.70   |
| 24  | BA    | 2337 | G    | C3'-C2'-C1' | 5.36  | 105.79      | 101.50   |
| 24  | BA    | 2450 | A    | N1-C2-N3    | -5.36 | 126.62      | 129.30   |
| 24  | DA    | 140  | C    | O4'-C1'-N1  | -5.36 | 103.91      | 108.20   |
| 24  | DA    | 1256 | G    | C3'-C2'-C1' | 5.36  | 105.79      | 101.50   |
| 24  | DA    | 1561 | C    | C3'-C2'-C1' | 5.36  | 105.79      | 101.50   |
| 24  | BA    | 725  | G    | P-O3'-C3'   | 5.36  | 126.13      | 119.70   |
| 24  | BA    | 962  | G    | N3-C4-C5    | 5.36  | 131.28      | 128.60   |
| 55  | CA    | 793  | U    | P-O3'-C3'   | -5.35 | 113.28      | 119.70   |
| 24  | DA    | 929  | U    | O4'-C1'-N1  | 5.35  | 112.48      | 108.20   |
| 24  | DA    | 2868 | A    | N9-C1'-C2'  | -5.35 | 106.11      | 112.00   |
| 21  | AA    | 1483 | A    | C5-C6-N6    | -5.35 | 119.42      | 123.70   |
| 24  | BA    | 277  | G    | P-O3'-C3'   | 5.35  | 126.12      | 119.70   |
| 24  | BA    | 2260 | C    | P-O3'-C3'   | -5.35 | 113.28      | 119.70   |
| 24  | BA    | 2498 | C    | C3'-C2'-C1' | 5.35  | 105.78      | 101.50   |
| 25  | BB    | 17   | C    | O4'-C1'-N1  | 5.35  | 112.48      | 108.20   |
| 24  | DA    | 365  | U    | C5-C4-O4    | -5.35 | 122.69      | 125.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 2147 | A    | P-O3'-C3'   | -5.35 | 113.28      | 119.70   |
| 24  | BA    | 2305 | U    | P-O3'-C3'   | -5.35 | 113.28      | 119.70   |
| 55  | CA    | 1325 | C    | O4'-C1'-N1  | 5.35  | 112.48      | 108.20   |
| 24  | DA    | 2499 | C    | C2-N1-C1'   | 5.35  | 124.68      | 118.80   |
| 24  | DA    | 2610 | C    | P-O3'-C3'   | 5.35  | 126.12      | 119.70   |
| 24  | BA    | 783  | A    | O5'-P-OP2   | -5.35 | 100.89      | 105.70   |
| 24  | BA    | 2751 | G    | P-O5'-C5'   | -5.35 | 112.34      | 120.90   |
| 55  | CA    | 102  | G    | C5-C6-O6    | 5.35  | 131.81      | 128.60   |
| 24  | DA    | 86   | G    | C3'-C2'-C1' | 5.35  | 105.78      | 101.50   |
| 24  | DA    | 1882 | U    | O4'-C1'-N1  | 5.35  | 112.48      | 108.20   |
| 24  | BA    | 521  | U    | P-O3'-C3'   | -5.35 | 113.28      | 119.70   |
| 24  | BA    | 2650 | U    | C6-N1-C2    | 5.35  | 124.21      | 121.00   |
| 55  | CA    | 9    | G    | C3'-C2'-C1' | 5.35  | 105.78      | 101.50   |
| 24  | BA    | 809  | G    | P-O5'-C5'   | -5.34 | 112.35      | 120.90   |
| 24  | BA    | 1871 | A    | C3'-C2'-C1' | 5.34  | 105.78      | 101.50   |
| 24  | DA    | 763  | G    | C4-C5-N7    | 5.34  | 112.94      | 110.80   |
| 24  | BA    | 2489 | U    | C2-N3-C4    | -5.34 | 123.79      | 127.00   |
| 21  | AA    | 71   | A    | P-O3'-C3'   | 5.34  | 126.11      | 119.70   |
| 24  | BA    | 727  | A    | N1-C6-N6    | 5.34  | 121.81      | 118.60   |
| 24  | BA    | 1606 | C    | O4'-C1'-N1  | -5.34 | 103.93      | 108.20   |
| 24  | DA    | 509  | C    | C3'-C2'-C1' | 5.34  | 105.77      | 101.50   |
| 24  | DA    | 2507 | C    | O4'-C1'-N1  | 5.34  | 112.47      | 108.20   |
| 24  | BA    | 979  | A    | P-O5'-C5'   | -5.34 | 112.36      | 120.90   |
| 55  | CA    | 81   | A    | N9-C4-C5    | 5.34  | 107.94      | 105.80   |
| 55  | CA    | 1410 | A    | C5-C6-N6    | 5.34  | 127.97      | 123.70   |
| 24  | DA    | 391  | A    | P-O3'-C3'   | -5.34 | 113.30      | 119.70   |
| 24  | DA    | 1636 | U    | C3'-C2'-C1' | 5.34  | 105.77      | 101.50   |
| 24  | BA    | 2639 | A    | C4-C5-N7    | 5.33  | 113.37      | 110.70   |
| 55  | CA    | 496  | A    | P-O3'-C3'   | -5.33 | 113.30      | 119.70   |
| 55  | CA    | 817  | C    | O4'-C1'-N1  | 5.33  | 112.47      | 108.20   |
| 21  | AA    | 754  | C    | N1-C2-O2    | 5.33  | 122.10      | 118.90   |
| 24  | BA    | 505  | A    | P-O5'-C5'   | -5.33 | 112.37      | 120.90   |
| 55  | CA    | 533  | A    | P-O3'-C3'   | 5.33  | 126.10      | 119.70   |
| 24  | DA    | 103  | A    | P-O3'-C3'   | -5.33 | 113.30      | 119.70   |
| 55  | CA    | 1137 | C    | P-O3'-C3'   | 5.33  | 126.10      | 119.70   |
| 24  | DA    | 1135 | C    | P-O3'-C3'   | -5.33 | 113.30      | 119.70   |
| 24  | DA    | 1558 | C    | O4'-C1'-N1  | 5.33  | 112.47      | 108.20   |
| 24  | DA    | 2493 | U    | C3'-C2'-C1' | 5.33  | 105.77      | 101.50   |
| 24  | BA    | 1970 | A    | P-O3'-C3'   | 5.33  | 126.10      | 119.70   |
| 24  | DA    | 2850 | A    | C3'-C2'-C1' | 5.33  | 105.76      | 101.50   |
| 24  | BA    | 19   | A    | P-O3'-C3'   | -5.33 | 113.31      | 119.70   |
| 24  | BA    | 2756 | U    | C6-N1-C2    | 5.33  | 124.20      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 1429 | G    | C3'-C2'-C1' | 5.33  | 105.76      | 101.50   |
| 24  | DA    | 1669 | A    | N1-C2-N3    | -5.33 | 126.64      | 129.30   |
| 24  | DA    | 2689 | U    | N1-C1'-C2'  | 5.33  | 120.93      | 114.00   |
| 21  | AA    | 754  | C    | P-O3'-C3'   | -5.33 | 113.31      | 119.70   |
| 24  | DA    | 401  | A    | O4'-C1'-N9  | 5.33  | 112.46      | 108.20   |
| 24  | BA    | 1261 | C    | N1-C2-O2    | -5.33 | 115.70      | 118.90   |
| 24  | BA    | 1304 | A    | C6-N1-C2    | 5.33  | 121.80      | 118.60   |
| 24  | BA    | 2062 | A    | C5-C6-N6    | -5.33 | 119.44      | 123.70   |
| 55  | CA    | 724  | G    | N9-C1'-C2'  | -5.33 | 106.14      | 112.00   |
| 55  | CA    | 1066 | C    | O4'-C1'-N1  | 5.33  | 112.46      | 108.20   |
| 24  | DA    | 1783 | A    | C3'-C2'-C1' | 5.33  | 105.76      | 101.50   |
| 21  | AA    | 704  | A    | C3'-C2'-C1' | 5.32  | 105.76      | 101.50   |
| 21  | AA    | 1123 | U    | O4'-C1'-N1  | 5.32  | 112.46      | 108.20   |
| 55  | CA    | 1440 | U    | N1-C1'-C2'  | 5.32  | 120.92      | 114.00   |
| 24  | BA    | 56   | A    | P-O3'-C3'   | -5.32 | 113.31      | 119.70   |
| 24  | BA    | 958  | U    | C3'-C2'-C1' | 5.32  | 105.76      | 101.50   |
| 21  | AA    | 654  | G    | P-O3'-C3'   | -5.32 | 113.31      | 119.70   |
| 21  | AA    | 884  | U    | N1-C1'-C2'  | 5.32  | 120.92      | 114.00   |
| 24  | BA    | 558  | U    | P-O3'-C3'   | -5.32 | 113.32      | 119.70   |
| 24  | BA    | 984  | A    | N1-C6-N6    | 5.32  | 121.79      | 118.60   |
| 55  | CA    | 577  | G    | P-O3'-C3'   | -5.32 | 113.32      | 119.70   |
| 21  | AA    | 194  | C    | N3-C4-C5    | -5.32 | 119.77      | 121.90   |
| 24  | BA    | 312  | G    | C3'-C2'-C1' | 5.32  | 105.75      | 101.50   |
| 55  | CA    | 430  | A    | C3'-C2'-C1' | 5.32  | 105.75      | 101.50   |
| 55  | CA    | 500  | G    | C3'-C2'-C1' | 5.32  | 105.75      | 101.50   |
| 24  | BA    | 178  | G    | P-O3'-C3'   | -5.32 | 113.32      | 119.70   |
| 24  | BA    | 1293 | C    | P-O5'-C5'   | -5.32 | 112.39      | 120.90   |
| 55  | CA    | 992  | U    | N1-C1'-C2'  | 5.32  | 120.91      | 114.00   |
| 55  | CA    | 1505 | G    | C3'-C2'-C1' | 5.32  | 105.75      | 101.50   |
| 24  | DA    | 1167 | C    | O4'-C1'-N1  | 5.31  | 112.45      | 108.20   |
| 24  | DA    | 1787 | A    | P-O3'-C3'   | -5.31 | 113.32      | 119.70   |
| 24  | BA    | 1960 | A    | P-O3'-C3'   | -5.31 | 113.33      | 119.70   |
| 24  | DA    | 2036 | C    | N1-C1'-C2'  | -5.31 | 106.16      | 112.00   |
| 24  | DA    | 26   | G    | C2-N3-C4    | -5.31 | 109.24      | 111.90   |
| 24  | DA    | 2830 | C    | O4'-C1'-N1  | 5.31  | 112.45      | 108.20   |
| 21  | AA    | 1508 | A    | P-O5'-C5'   | -5.31 | 112.41      | 120.90   |
| 24  | BA    | 964  | C    | O4'-C1'-N1  | -5.31 | 103.95      | 108.20   |
| 24  | BA    | 2902 | C    | C6-N1-C2    | 5.31  | 122.42      | 120.30   |
| 55  | CA    | 1410 | A    | N1-C6-N6    | -5.31 | 115.41      | 118.60   |
| 55  | CA    | 1483 | A    | N1-C6-N6    | 5.31  | 121.78      | 118.60   |
| 24  | DA    | 586  | A    | P-O3'-C3'   | 5.31  | 126.07      | 119.70   |
| 21  | AA    | 312  | C    | P-O3'-C3'   | 5.31  | 126.07      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 1512 | U    | P-O3'-C3'   | 5.31  | 126.07      | 119.70   |
| 24  | BA    | 459  | U    | C3'-C2'-C1' | 5.31  | 105.75      | 101.50   |
| 24  | BA    | 1313 | U    | N1-C1'-C2'  | -5.31 | 106.16      | 112.00   |
| 24  | BA    | 1416 | G    | P-O3'-C3'   | 5.31  | 126.07      | 119.70   |
| 24  | BA    | 1521 | G    | C4-N9-C1'   | 5.31  | 133.40      | 126.50   |
| 24  | BA    | 2068 | U    | C3'-C2'-C1' | 5.31  | 105.75      | 101.50   |
| 55  | CA    | 1140 | C    | N1-C1'-C2'  | -5.31 | 106.16      | 112.00   |
| 24  | DA    | 480  | A    | N9-C1'-C2'  | -5.31 | 106.16      | 112.00   |
| 21  | AA    | 97   | G    | P-O5'-C5'   | -5.31 | 112.41      | 120.90   |
| 24  | BA    | 2282 | G    | N9-C4-C5    | 5.31  | 107.52      | 105.40   |
| 24  | BA    | 339  | U    | C2-N3-C4    | -5.30 | 123.82      | 127.00   |
| 24  | BA    | 1979 | U    | P-O5'-C5'   | -5.30 | 112.41      | 120.90   |
| 24  | BA    | 2574 | G    | P-O3'-C3'   | -5.30 | 113.34      | 119.70   |
| 25  | BB    | 17   | C    | P-O3'-C3'   | -5.30 | 113.33      | 119.70   |
| 24  | DA    | 1655 | A    | C3'-C2'-C1' | 5.30  | 105.74      | 101.50   |
| 24  | DA    | 2782 | G    | N9-C1'-C2'  | -5.30 | 106.17      | 112.00   |
| 21  | AA    | 185  | U    | O4'-C1'-N1  | 5.30  | 112.44      | 108.20   |
| 21  | AA    | 998  | C    | O4'-C1'-N1  | 5.30  | 112.44      | 108.20   |
| 24  | BA    | 1492 | G    | O4'-C1'-N9  | 5.30  | 112.44      | 108.20   |
| 55  | CA    | 815  | A    | P-O3'-C3'   | 5.30  | 126.06      | 119.70   |
| 21  | AA    | 353  | A    | C3'-C2'-C1' | 5.30  | 105.74      | 101.50   |
| 24  | BA    | 2391 | G    | P-O3'-C3'   | 5.30  | 126.06      | 119.70   |
| 55  | CA    | 891  | U    | P-O3'-C3'   | -5.30 | 113.34      | 119.70   |
| 24  | BA    | 2389 | G    | P-O5'-C5'   | -5.30 | 112.42      | 120.90   |
| 24  | BA    | 2679 | A    | C6-N1-C2    | 5.30  | 121.78      | 118.60   |
| 24  | DA    | 533  | G    | C3'-C2'-C1' | 5.30  | 105.74      | 101.50   |
| 24  | DA    | 2580 | U    | P-O3'-C3'   | 5.30  | 126.06      | 119.70   |
| 24  | BA    | 829  | A    | C8-N9-C4    | 5.30  | 107.92      | 105.80   |
| 24  | BA    | 1206 | G    | N9-C1'-C2'  | -5.30 | 106.17      | 112.00   |
| 24  | BA    | 2025 | C    | N1-C1'-C2'  | 5.30  | 120.89      | 114.00   |
| 24  | BA    | 1659 | G    | P-O5'-C5'   | -5.30 | 112.42      | 120.90   |
| 24  | BA    | 2354 | C    | N3-C2-O2    | -5.30 | 118.19      | 121.90   |
| 24  | BA    | 2430 | A    | O4'-C1'-N9  | 5.30  | 112.44      | 108.20   |
| 21  | AA    | 465  | A    | C3'-C2'-C1' | 5.29  | 105.74      | 101.50   |
| 55  | CA    | 245  | U    | C3'-C2'-C1' | 5.29  | 105.74      | 101.50   |
| 21  | AA    | 1197 | A    | C3'-C2'-C1' | 5.29  | 105.73      | 101.50   |
| 24  | BA    | 933  | A    | C3'-C2'-C1' | 5.29  | 105.73      | 101.50   |
| 24  | BA    | 962  | G    | C6-N1-C2    | 5.29  | 128.28      | 125.10   |
| 24  | DA    | 530  | G    | C3'-C2'-C1' | 5.29  | 105.73      | 101.50   |
| 24  | BA    | 1362 | C    | O4'-C1'-N1  | -5.29 | 103.97      | 108.20   |
| 24  | BA    | 1978 | A    | C8-N9-C4    | 5.29  | 107.92      | 105.80   |
| 55  | CA    | 1033 | G    | P-O5'-C5'   | -5.29 | 112.43      | 120.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 29  | DF    | 109  | ARG  | CB-CA-C     | 5.29  | 120.98      | 110.40   |
| 24  | BA    | 1292 | G    | P-O3'-C3'   | -5.29 | 113.35      | 119.70   |
| 24  | BA    | 1313 | U    | C3'-C2'-C1' | 5.29  | 105.73      | 101.50   |
| 55  | CA    | 397  | A    | C6-N1-C2    | -5.29 | 115.43      | 118.60   |
| 24  | BA    | 206  | U    | C3'-C2'-C1' | 5.29  | 105.73      | 101.50   |
| 24  | DA    | 2631 | G    | C3'-C2'-C1' | 5.29  | 105.73      | 101.50   |
| 24  | BA    | 1144 | A    | P-O5'-C5'   | -5.29 | 112.44      | 120.90   |
| 21  | AA    | 733  | G    | P-O3'-C3'   | 5.29  | 126.04      | 119.70   |
| 24  | BA    | 1905 | C    | O4'-C1'-N1  | 5.29  | 112.43      | 108.20   |
| 24  | BA    | 1946 | U    | O4'-C1'-N1  | -5.29 | 103.97      | 108.20   |
| 24  | DA    | 437  | U    | C3'-C2'-C1' | 5.29  | 105.73      | 101.50   |
| 24  | BA    | 749  | A    | C3'-C2'-C1' | 5.28  | 105.73      | 101.50   |
| 24  | BA    | 1731 | G    | C4-C5-N7    | -5.28 | 108.69      | 110.80   |
| 24  | BA    | 1882 | U    | O4'-C1'-N1  | 5.28  | 112.42      | 108.20   |
| 24  | BA    | 2823 | A    | P-O5'-C5'   | -5.28 | 112.45      | 120.90   |
| 24  | BA    | 919  | U    | P-O5'-C5'   | 5.28  | 129.35      | 120.90   |
| 24  | BA    | 1769 | U    | O4'-C1'-N1  | 5.28  | 112.42      | 108.20   |
| 55  | CA    | 97   | G    | C3'-C2'-C1' | 5.28  | 105.72      | 101.50   |
| 55  | CA    | 439  | U    | C3'-C2'-C1' | 5.28  | 105.72      | 101.50   |
| 24  | DA    | 76   | C    | C3'-C2'-C1' | 5.28  | 105.72      | 101.50   |
| 24  | DA    | 1062 | G    | P-O3'-C3'   | -5.28 | 113.36      | 119.70   |
| 24  | DA    | 1080 | A    | C3'-C2'-C1' | 5.28  | 105.72      | 101.50   |
| 21  | AA    | 1216 | A    | C3'-C2'-C1' | 5.28  | 105.72      | 101.50   |
| 24  | DA    | 1011 | G    | C8-N9-C1'   | 5.28  | 133.86      | 127.00   |
| 24  | DA    | 2555 | U    | O4'-C1'-N1  | 5.28  | 112.42      | 108.20   |
| 21  | AA    | 496  | A    | C3'-C2'-C1' | 5.28  | 105.72      | 101.50   |
| 24  | BA    | 107  | G    | N9-C4-C5    | 5.28  | 107.51      | 105.40   |
| 24  | BA    | 945  | A    | N9-C1'-C2'  | 5.28  | 120.86      | 114.00   |
| 24  | BA    | 1521 | G    | N3-C4-N9    | 5.28  | 129.17      | 126.00   |
| 55  | CA    | 210  | C    | O4'-C1'-N1  | -5.28 | 103.98      | 108.20   |
| 24  | BA    | 25   | U    | P-O3'-C3'   | -5.28 | 113.37      | 119.70   |
| 24  | BA    | 481  | G    | O4'-C1'-N9  | 5.28  | 112.42      | 108.20   |
| 24  | BA    | 388  | G    | P-O5'-C5'   | -5.27 | 112.46      | 120.90   |
| 24  | BA    | 2713 | U    | N1-C1'-C2'  | 5.27  | 120.86      | 114.00   |
| 24  | DA    | 63   | A    | P-O3'-C3'   | -5.27 | 113.37      | 119.70   |
| 24  | DA    | 492  | A    | N9-C1'-C2'  | -5.27 | 106.20      | 112.00   |
| 24  | BA    | 588  | U    | C3'-C2'-C1' | 5.27  | 105.72      | 101.50   |
| 24  | BA    | 2511 | U    | C6-N1-C1'   | -5.27 | 113.82      | 121.20   |
| 55  | CA    | 909  | A    | P-O3'-C3'   | 5.27  | 126.03      | 119.70   |
| 24  | DA    | 481  | G    | N3-C4-C5    | -5.27 | 125.96      | 128.60   |
| 24  | DA    | 782  | A    | P-O3'-C3'   | 5.27  | 126.03      | 119.70   |
| 55  | CA    | 886  | G    | N9-C1'-C2'  | -5.27 | 106.20      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | AA    | 247  | G    | C3'-C2'-C1' | 5.27  | 105.72      | 101.50   |
| 24  | BA    | 2777 | G    | C3'-C2'-C1' | 5.27  | 105.72      | 101.50   |
| 55  | CA    | 876  | C    | P-O5'-C5'   | 5.27  | 129.33      | 120.90   |
| 24  | DA    | 224  | U    | C3'-C2'-C1' | 5.27  | 105.72      | 101.50   |
| 24  | DA    | 1049 | C    | P-O3'-C3'   | -5.27 | 113.38      | 119.70   |
| 24  | BA    | 396  | G    | P-O5'-C5'   | -5.27 | 112.47      | 120.90   |
| 25  | BB    | 114  | C    | C6-N1-C2    | 5.27  | 122.41      | 120.30   |
| 55  | CA    | 9    | G    | N9-C1'-C2'  | -5.27 | 106.21      | 112.00   |
| 24  | DA    | 101  | A    | C3'-C2'-C1' | 5.27  | 105.72      | 101.50   |
| 24  | DA    | 243  | U    | C3'-C2'-C1' | 5.27  | 105.71      | 101.50   |
| 24  | DA    | 589  | U    | C3'-C2'-C1' | 5.27  | 105.72      | 101.50   |
| 24  | DA    | 657  | U    | N1-C1'-C2'  | -5.27 | 106.21      | 112.00   |
| 24  | DA    | 1430 | G    | C3'-C2'-C1' | 5.27  | 105.71      | 101.50   |
| 24  | DA    | 2726 | A    | O4'-C1'-N9  | 5.27  | 112.42      | 108.20   |
| 21  | AA    | 1453 | G    | C3'-C2'-C1' | 5.27  | 105.71      | 101.50   |
| 24  | BA    | 806  | C    | N1-C2-O2    | -5.27 | 115.74      | 118.90   |
| 55  | CA    | 935  | A    | N9-C1'-C2'  | -5.27 | 106.21      | 112.00   |
| 55  | CA    | 1102 | A    | P-O3'-C3'   | -5.27 | 113.38      | 119.70   |
| 24  | DA    | 1799 | G    | N9-C4-C5    | 5.27  | 107.51      | 105.40   |
| 24  | DA    | 2297 | A    | C3'-C2'-C1' | 5.27  | 105.71      | 101.50   |
| 24  | BA    | 1156 | A    | O3'-P-O5'   | -5.26 | 94.00       | 104.00   |
| 24  | BA    | 2812 | G    | N3-C4-N9    | 5.26  | 129.16      | 126.00   |
| 55  | CA    | 1139 | G    | C3'-C2'-C1' | 5.26  | 105.71      | 101.50   |
| 24  | DA    | 2262 | U    | O4'-C1'-N1  | 5.26  | 112.41      | 108.20   |
| 21  | AA    | 82   | G    | N9-C1'-C2'  | -5.26 | 106.21      | 112.00   |
| 24  | BA    | 2809 | A    | C3'-C2'-C1' | 5.26  | 105.71      | 101.50   |
| 21  | AA    | 1528 | U    | O4'-C1'-N1  | 5.26  | 112.41      | 108.20   |
| 24  | BA    | 415  | A    | N1-C2-N3    | -5.26 | 126.67      | 129.30   |
| 24  | DA    | 2199 | A    | C3'-C2'-C1' | 5.26  | 105.71      | 101.50   |
| 21  | AA    | 1107 | C    | O4'-C1'-N1  | 5.26  | 112.41      | 108.20   |
| 24  | BA    | 1700 | A    | C3'-C2'-C1' | 5.26  | 105.71      | 101.50   |
| 24  | DA    | 406  | G    | N9-C1'-C2'  | -5.26 | 106.22      | 112.00   |
| 21  | AA    | 174  | A    | C3'-C2'-C1' | 5.26  | 105.70      | 101.50   |
| 24  | BA    | 1941 | C    | C3'-C2'-C1' | 5.26  | 105.71      | 101.50   |
| 24  | DA    | 15   | G    | C3'-C2'-C1' | 5.26  | 105.70      | 101.50   |
| 24  | BA    | 475  | C    | C3'-C2'-C1' | 5.25  | 105.70      | 101.50   |
| 55  | CA    | 381  | C    | O4'-C1'-N1  | 5.25  | 112.40      | 108.20   |
| 55  | CA    | 1319 | A    | P-O3'-C3'   | 5.25  | 126.01      | 119.70   |
| 24  | BA    | 1051 | G    | C5-C6-O6    | -5.25 | 125.45      | 128.60   |
| 24  | BA    | 1112 | G    | N9-C1'-C2'  | -5.25 | 106.22      | 112.00   |
| 24  | BA    | 1289 | C    | P-O3'-C3'   | -5.25 | 113.40      | 119.70   |
| 24  | BA    | 1694 | C    | O4'-C1'-N1  | 5.25  | 112.40      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 1759 | A    | N9-C1'-C2'  | -5.25 | 106.22      | 112.00   |
| 24  | BA    | 2382 | G    | N3-C4-C5    | 5.25  | 131.23      | 128.60   |
| 55  | CA    | 211  | G    | C3'-C2'-C1' | 5.25  | 105.70      | 101.50   |
| 55  | CA    | 652  | U    | P-O3'-C3'   | 5.25  | 126.00      | 119.70   |
| 55  | CA    | 1315 | U    | O4'-C1'-N1  | 5.25  | 112.40      | 108.20   |
| 24  | DA    | 1267 | U    | C3'-C2'-C1' | 5.25  | 105.70      | 101.50   |
| 24  | BA    | 1022 | G    | C4-N9-C1'   | -5.25 | 119.67      | 126.50   |
| 24  | DA    | 2727 | A    | C3'-C2'-C1' | 5.25  | 105.70      | 101.50   |
| 55  | CA    | 1132 | C    | O4'-C1'-N1  | 5.25  | 112.40      | 108.20   |
| 24  | BA    | 1510 | G    | N9-C1'-C2'  | -5.25 | 106.23      | 112.00   |
| 55  | CA    | 1051 | C    | P-O3'-C3'   | -5.25 | 113.40      | 119.70   |
| 24  | DA    | 324  | A    | C3'-C2'-C1' | 5.25  | 105.70      | 101.50   |
| 24  | DA    | 1551 | A    | C5-C6-N1    | -5.25 | 115.08      | 117.70   |
| 55  | CA    | 934  | C    | C2-N1-C1'   | -5.25 | 113.03      | 118.80   |
| 55  | CA    | 1066 | C    | C3'-C2'-C1' | 5.25  | 105.70      | 101.50   |
| 24  | DA    | 787  | C    | C5-C4-N4    | 5.25  | 123.87      | 120.20   |
| 24  | BA    | 1311 | G    | N3-C4-N9    | -5.25 | 122.85      | 126.00   |
| 24  | DA    | 120  | U    | P-O5'-C5'   | -5.25 | 112.51      | 120.90   |
| 55  | CA    | 212  | G    | C3'-C2'-C1' | 5.24  | 105.69      | 101.50   |
| 55  | CA    | 482  | A    | C3'-C2'-C1' | 5.24  | 105.70      | 101.50   |
| 24  | DA    | 529  | A    | C4-C5-C6    | -5.24 | 114.38      | 117.00   |
| 24  | BA    | 907  | G    | C5-C6-O6    | 5.24  | 131.75      | 128.60   |
| 55  | CA    | 1236 | A    | C6-N1-C2    | -5.24 | 115.45      | 118.60   |
| 24  | BA    | 918  | A    | N1-C6-N6    | 5.24  | 121.74      | 118.60   |
| 24  | BA    | 2899 | A    | P-O5'-C5'   | -5.24 | 112.52      | 120.90   |
| 55  | CA    | 874  | G    | C3'-C2'-C1' | 5.24  | 105.69      | 101.50   |
| 55  | CA    | 960  | U    | C2-N1-C1'   | 5.24  | 123.99      | 117.70   |
| 55  | CA    | 991  | U    | P-O3'-C3'   | 5.24  | 125.99      | 119.70   |
| 24  | DA    | 104  | A    | N9-C1'-C2'  | -5.24 | 106.23      | 112.00   |
| 24  | BA    | 1276 | A    | C8-N9-C4    | -5.24 | 103.70      | 105.80   |
| 24  | BA    | 2241 | A    | P-O3'-C3'   | -5.24 | 113.41      | 119.70   |
| 55  | CA    | 95   | C    | C3'-C2'-C1' | 5.24  | 105.69      | 101.50   |
| 55  | CA    | 832  | G    | N3-C4-N9    | -5.24 | 122.86      | 126.00   |
| 21  | AA    | 1160 | G    | N9-C1'-C2'  | -5.24 | 106.24      | 112.00   |
| 55  | CA    | 536  | C    | C3'-C2'-C1' | 5.24  | 105.69      | 101.50   |
| 24  | BA    | 509  | C    | C6-N1-C2    | -5.24 | 118.21      | 120.30   |
| 24  | BA    | 544  | C    | O4'-C1'-N1  | -5.24 | 104.01      | 108.20   |
| 24  | DA    | 272  | A    | C3'-C2'-C1' | 5.24  | 105.69      | 101.50   |
| 24  | DA    | 503  | A    | N1-C6-N6    | -5.24 | 115.46      | 118.60   |
| 24  | DA    | 778  | G    | C3'-C2'-C1' | 5.24  | 105.69      | 101.50   |
| 24  | DA    | 2386 | A    | C3'-C2'-C1' | 5.24  | 105.69      | 101.50   |
| 24  | DA    | 750  | A    | P-O3'-C3'   | -5.23 | 113.42      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 1027 | A    | P-O3'-C3'   | -5.23 | 113.42      | 119.70   |
| 55  | CA    | 436  | C    | N1-C2-O2    | 5.23  | 122.04      | 118.90   |
| 24  | DA    | 150  | U    | O4'-C1'-N1  | 5.23  | 112.39      | 108.20   |
| 24  | DA    | 753  | A    | C3'-C2'-C1' | 5.23  | 105.69      | 101.50   |
| 24  | DA    | 1818 | U    | N1-C1'-C2'  | 5.23  | 120.80      | 114.00   |
| 21  | AA    | 641  | U    | N1-C1'-C2'  | 5.23  | 120.80      | 114.00   |
| 24  | BA    | 2369 | A    | N9-C4-C5    | 5.23  | 107.89      | 105.80   |
| 24  | BA    | 2615 | U    | C3'-C2'-C1' | 5.23  | 105.68      | 101.50   |
| 24  | DA    | 412  | A    | C3'-C2'-C1' | 5.23  | 105.68      | 101.50   |
| 24  | DA    | 963  | U    | N1-C1'-C2'  | -5.23 | 106.25      | 112.00   |
| 24  | DA    | 2613 | U    | N1-C1'-C2'  | 5.23  | 120.80      | 114.00   |
| 24  | DA    | 2675 | A    | P-O3'-C3'   | -5.23 | 113.43      | 119.70   |
| 21  | AA    | 119  | A    | O4'-C1'-N9  | 5.23  | 112.38      | 108.20   |
| 21  | AA    | 724  | G    | C3'-C2'-C1' | 5.23  | 105.68      | 101.50   |
| 25  | BB    | 42   | C    | C3'-C2'-C1' | 5.23  | 105.68      | 101.50   |
| 55  | CA    | 305  | G    | P-O3'-C3'   | 5.23  | 125.97      | 119.70   |
| 55  | CA    | 376  | G    | C5-C6-O6    | 5.23  | 131.74      | 128.60   |
| 21  | AA    | 117  | G    | P-O5'-C5'   | -5.23 | 112.54      | 120.90   |
| 24  | BA    | 2268 | A    | C8-N9-C4    | -5.23 | 103.71      | 105.80   |
| 24  | BA    | 2491 | U    | O4'-C1'-N1  | 5.23  | 112.38      | 108.20   |
| 24  | DA    | 229  | C    | C3'-C2'-C1' | 5.23  | 105.68      | 101.50   |
| 24  | DA    | 2024 | G    | C3'-C2'-C1' | 5.23  | 105.68      | 101.50   |
| 21  | AA    | 88   | U    | C5-C4-O4    | 5.22  | 129.03      | 125.90   |
| 21  | AA    | 654  | G    | N9-C1'-C2'  | -5.22 | 106.25      | 112.00   |
| 24  | BA    | 142  | A    | C3'-C2'-C1' | 5.22  | 105.68      | 101.50   |
| 24  | BA    | 2054 | A    | N9-C4-C5    | 5.22  | 107.89      | 105.80   |
| 24  | BA    | 682  | G    | O4'-C1'-N9  | -5.22 | 104.02      | 108.20   |
| 24  | BA    | 1228 | G    | C2-N3-C4    | -5.22 | 109.29      | 111.90   |
| 24  | BA    | 2383 | G    | N9-C1'-C2'  | -5.22 | 106.26      | 112.00   |
| 24  | DA    | 492  | A    | P-O5'-C5'   | -5.22 | 112.55      | 120.90   |
| 24  | DA    | 2611 | C    | O4'-C1'-N1  | 5.22  | 112.38      | 108.20   |
| 21  | AA    | 915  | A    | O4'-C1'-N9  | 5.22  | 112.38      | 108.20   |
| 24  | BA    | 529  | A    | C8-N9-C4    | 5.22  | 107.89      | 105.80   |
| 24  | BA    | 753  | A    | P-O5'-C5'   | -5.22 | 112.55      | 120.90   |
| 24  | BA    | 1007 | C    | O4'-C1'-N1  | 5.22  | 112.38      | 108.20   |
| 24  | BA    | 1971 | U    | C3'-C2'-C1' | 5.22  | 105.68      | 101.50   |
| 25  | BB    | 109  | A    | N9-C1'-C2'  | -5.22 | 106.26      | 112.00   |
| 55  | CA    | 701  | U    | N1-C1'-C2'  | 5.22  | 120.79      | 114.00   |
| 55  | CA    | 1068 | G    | N9-C1'-C2'  | -5.22 | 106.26      | 112.00   |
| 24  | DA    | 77   | G    | C3'-C2'-C1' | 5.22  | 105.67      | 101.50   |
| 24  | BA    | 2250 | G    | P-O3'-C3'   | 5.22  | 125.96      | 119.70   |
| 24  | DA    | 1865 | U    | C5-C4-O4    | -5.22 | 122.77      | 125.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 56  | DB    | 104  | A    | N3-C4-C5    | -5.22 | 123.15      | 126.80   |
| 21  | AA    | 466  | A    | O3'-P-O5'   | -5.22 | 94.09       | 104.00   |
| 24  | BA    | 2652 | C    | O4'-C1'-N1  | 5.22  | 112.37      | 108.20   |
| 24  | BA    | 2757 | A    | N1-C6-N6    | 5.22  | 121.73      | 118.60   |
| 55  | CA    | 121  | U    | N1-C1'-C2'  | -5.22 | 106.26      | 112.00   |
| 21  | AA    | 1051 | C    | C3'-C2'-C1' | 5.21  | 105.67      | 101.50   |
| 24  | BA    | 509  | C    | C2-N1-C1'   | 5.21  | 124.53      | 118.80   |
| 24  | BA    | 651  | G    | P-O3'-C3'   | -5.21 | 113.44      | 119.70   |
| 24  | BA    | 1521 | G    | C6-C5-N7    | -5.21 | 127.27      | 130.40   |
| 55  | CA    | 248  | C    | C3'-C2'-C1' | 5.21  | 105.67      | 101.50   |
| 24  | DA    | 747  | U    | O4'-C1'-N1  | -5.21 | 104.03      | 108.20   |
| 24  | DA    | 1048 | A    | C3'-C2'-C1' | 5.21  | 105.67      | 101.50   |
| 24  | DA    | 2428 | G    | C3'-C2'-C1' | 5.21  | 105.67      | 101.50   |
| 24  | DA    | 2714 | G    | C3'-C2'-C1' | 5.21  | 105.67      | 101.50   |
| 24  | BA    | 806  | C    | C6-N1-C2    | -5.21 | 118.22      | 120.30   |
| 24  | BA    | 1967 | C    | C3'-C2'-C1' | 5.21  | 105.67      | 101.50   |
| 24  | DA    | 403  | U    | P-O3'-C3'   | 5.21  | 125.95      | 119.70   |
| 24  | DA    | 959  | A    | C3'-C2'-C1' | 5.21  | 105.67      | 101.50   |
| 24  | DA    | 1112 | G    | C3'-C2'-C1' | 5.21  | 105.67      | 101.50   |
| 24  | DA    | 1239 | G    | C3'-C2'-C1' | 5.21  | 105.67      | 101.50   |
| 24  | BA    | 637  | A    | O4'-C1'-N9  | 5.21  | 112.37      | 108.20   |
| 24  | BA    | 548  | G    | P-O5'-C5'   | -5.21 | 112.57      | 120.90   |
| 24  | BA    | 1644 | C    | C6-N1-C2    | 5.21  | 122.38      | 120.30   |
| 55  | CA    | 460  | A    | C3'-C2'-C1' | 5.21  | 105.67      | 101.50   |
| 55  | CA    | 889  | A    | P-O3'-C3'   | 5.21  | 125.95      | 119.70   |
| 24  | DA    | 216  | A    | C3'-C2'-C1' | 5.21  | 105.67      | 101.50   |
| 24  | DA    | 1782 | U    | P-O3'-C3'   | -5.21 | 113.45      | 119.70   |
| 24  | BA    | 124  | G    | P-O3'-C3'   | 5.21  | 125.95      | 119.70   |
| 24  | BA    | 391  | A    | N9-C1'-C2'  | -5.21 | 106.27      | 112.00   |
| 24  | BA    | 570  | G    | P-O3'-C3'   | 5.21  | 125.95      | 119.70   |
| 56  | DB    | 44   | G    | N3-C4-N9    | -5.21 | 122.88      | 126.00   |
| 21  | AA    | 1366 | C    | C3'-C2'-C1' | 5.21  | 105.66      | 101.50   |
| 24  | BA    | 858  | G    | C6-N1-C2    | -5.21 | 121.98      | 125.10   |
| 24  | BA    | 1180 | U    | N1-C1'-C2'  | 5.20  | 120.77      | 114.00   |
| 24  | BA    | 1476 | U    | C5-C4-O4    | -5.20 | 122.78      | 125.90   |
| 24  | BA    | 2639 | A    | C5-N7-C8    | -5.20 | 101.30      | 103.90   |
| 55  | CA    | 67   | C    | P-O5'-C5'   | -5.20 | 112.58      | 120.90   |
| 24  | DA    | 479  | A    | P-O3'-C3'   | 5.20  | 125.94      | 119.70   |
| 56  | DB    | 41   | G    | C3'-C2'-C1' | 5.20  | 105.66      | 101.50   |
| 24  | BA    | 575  | A    | P-O3'-C3'   | -5.20 | 113.46      | 119.70   |
| 24  | BA    | 2714 | G    | N9-C1'-C2'  | -5.20 | 106.28      | 112.00   |
| 55  | CA    | 110  | C    | P-O3'-C3'   | -5.20 | 113.46      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | CA    | 930  | C    | O4'-C1'-N1  | 5.20  | 112.36      | 108.20   |
| 24  | BA    | 470  | A    | C8-N9-C4    | -5.20 | 103.72      | 105.80   |
| 24  | BA    | 2497 | A    | O3'-P-O5'   | 5.20  | 113.88      | 104.00   |
| 55  | CA    | 1282 | C    | N1-C1'-C2'  | -5.20 | 106.28      | 112.00   |
| 24  | DA    | 1144 | A    | N9-C1'-C2'  | -5.20 | 106.28      | 112.00   |
| 24  | DA    | 1247 | A    | O4'-C1'-N9  | 5.20  | 112.36      | 108.20   |
| 21  | AA    | 212  | G    | C3'-C2'-C1' | 5.20  | 105.66      | 101.50   |
| 21  | AA    | 549  | C    | O4'-C1'-N1  | 5.20  | 112.36      | 108.20   |
| 21  | AA    | 984  | C    | P-O3'-C3'   | -5.20 | 113.46      | 119.70   |
| 21  | AA    | 1296 | C    | P-O3'-C3'   | 5.20  | 125.94      | 119.70   |
| 24  | BA    | 1147 | A    | C4-C5-N7    | -5.20 | 108.10      | 110.70   |
| 24  | BA    | 2890 | G    | O4'-C1'-N9  | -5.20 | 104.04      | 108.20   |
| 24  | DA    | 1682 | G    | C3'-C2'-C1' | 5.20  | 105.66      | 101.50   |
| 24  | DA    | 1722 | A    | C3'-C2'-C1' | 5.20  | 105.66      | 101.50   |
| 24  | DA    | 2052 | A    | N9-C1'-C2'  | -5.20 | 106.28      | 112.00   |
| 24  | DA    | 2776 | A    | P-O3'-C3'   | 5.20  | 125.94      | 119.70   |
| 24  | DA    | 2781 | A    | N9-C1'-C2'  | -5.20 | 106.28      | 112.00   |
| 56  | DB    | 40   | U    | O4'-C1'-N1  | 5.20  | 112.36      | 108.20   |
| 21  | AA    | 925  | G    | C6-N1-C2    | 5.20  | 128.22      | 125.10   |
| 24  | BA    | 654  | A    | N9-C1'-C2'  | -5.20 | 106.28      | 112.00   |
| 24  | BA    | 2269 | G    | P-O5'-C5'   | -5.20 | 112.59      | 120.90   |
| 21  | AA    | 351  | G    | N9-C1'-C2'  | 5.19  | 120.75      | 114.00   |
| 24  | BA    | 1555 | G    | C3'-C2'-C1' | 5.19  | 105.66      | 101.50   |
| 24  | BA    | 2570 | G    | C5-C6-O6    | 5.19  | 131.72      | 128.60   |
| 55  | CA    | 1136 | C    | O4'-C1'-N1  | 5.19  | 112.36      | 108.20   |
| 24  | DA    | 1476 | U    | P-O3'-C3'   | 5.19  | 125.93      | 119.70   |
| 24  | BA    | 14   | A    | P-O5'-C5'   | -5.19 | 112.59      | 120.90   |
| 24  | BA    | 2543 | G    | C5-C6-O6    | 5.19  | 131.72      | 128.60   |
| 25  | BB    | 91   | C    | N3-C2-O2    | -5.19 | 118.27      | 121.90   |
| 55  | CA    | 199  | A    | P-O3'-C3'   | -5.19 | 113.47      | 119.70   |
| 24  | DA    | 234  | U    | C3'-C2'-C1' | 5.19  | 105.65      | 101.50   |
| 24  | DA    | 370  | G    | P-O3'-C3'   | 5.19  | 125.93      | 119.70   |
| 24  | DA    | 604  | G    | C3'-C2'-C1' | 5.19  | 105.65      | 101.50   |
| 21  | AA    | 352  | C    | C3'-C2'-C1' | 5.19  | 105.65      | 101.50   |
| 21  | AA    | 688  | G    | P-O3'-C3'   | -5.19 | 113.47      | 119.70   |
| 21  | AA    | 795  | C    | O4'-C1'-N1  | 5.19  | 112.35      | 108.20   |
| 21  | AA    | 821  | G    | C3'-C2'-C1' | 5.19  | 105.65      | 101.50   |
| 21  | AA    | 978  | A    | N9-C1'-C2'  | -5.19 | 106.29      | 112.00   |
| 24  | BA    | 919  | U    | N3-C4-O4    | 5.19  | 123.03      | 119.40   |
| 24  | BA    | 1663 | G    | C5-C6-O6    | 5.19  | 131.71      | 128.60   |
| 24  | BA    | 2656 | U    | N1-C2-O2    | 5.19  | 126.43      | 122.80   |
| 55  | CA    | 66   | A    | N9-C1'-C2'  | -5.19 | 106.29      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | CA    | 596  | A    | C3'-C2'-C1' | 5.19  | 105.65      | 101.50   |
| 24  | DA    | 1635 | A    | P-O5'-C5'   | -5.19 | 112.59      | 120.90   |
| 24  | DA    | 1956 | U    | C3'-C2'-C1' | 5.19  | 105.65      | 101.50   |
| 21  | AA    | 339  | C    | N1-C2-O2    | 5.19  | 122.01      | 118.90   |
| 24  | BA    | 1459 | G    | P-O3'-C3'   | -5.19 | 113.47      | 119.70   |
| 24  | BA    | 1821 | A    | C6-N1-C2    | 5.19  | 121.71      | 118.60   |
| 29  | BF    | 112  | ASP  | OD1-CG-OD2  | 5.19  | 133.16      | 123.30   |
| 55  | CA    | 1052 | U    | O4'-C1'-N1  | 5.19  | 112.35      | 108.20   |
| 24  | DA    | 964  | C    | C3'-C2'-C1' | 5.19  | 105.65      | 101.50   |
| 24  | BA    | 1669 | A    | N1-C6-N6    | -5.19 | 115.49      | 118.60   |
| 24  | BA    | 1809 | A    | P-O3'-C3'   | -5.19 | 113.47      | 119.70   |
| 24  | BA    | 1944 | U    | O4'-C1'-N1  | 5.19  | 112.35      | 108.20   |
| 24  | BA    | 1959 | G    | P-O5'-C5'   | -5.19 | 112.60      | 120.90   |
| 24  | BA    | 2691 | C    | C3'-C2'-C1' | 5.19  | 105.65      | 101.50   |
| 24  | DA    | 506  | G    | P-O3'-C3'   | -5.19 | 113.47      | 119.70   |
| 21  | AA    | 1461 | G    | C2-N3-C4    | -5.19 | 109.31      | 111.90   |
| 55  | CA    | 480  | U    | O4'-C1'-N1  | 5.19  | 112.35      | 108.20   |
| 24  | BA    | 1955 | U    | O4'-C1'-N1  | 5.18  | 112.35      | 108.20   |
| 55  | CA    | 175  | C    | C3'-C2'-C1' | 5.18  | 105.65      | 101.50   |
| 55  | CA    | 1098 | C    | O4'-C1'-N1  | 5.18  | 112.35      | 108.20   |
| 55  | CA    | 493  | A    | O4'-C1'-N9  | 5.18  | 112.35      | 108.20   |
| 24  | DA    | 2450 | A    | P-O3'-C3'   | -5.18 | 113.48      | 119.70   |
| 21  | AA    | 722  | G    | C3'-C2'-C1' | 5.18  | 105.64      | 101.50   |
| 24  | BA    | 1379 | U    | O4'-C1'-N1  | -5.18 | 104.06      | 108.20   |
| 24  | BA    | 2282 | G    | C8-N9-C1'   | 5.18  | 133.74      | 127.00   |
| 55  | CA    | 1158 | C    | C3'-C2'-C1' | 5.18  | 105.64      | 101.50   |
| 21  | AA    | 173  | U    | N1-C1'-C2'  | 5.18  | 120.73      | 114.00   |
| 24  | BA    | 333  | G    | P-O3'-C3'   | -5.18 | 113.48      | 119.70   |
| 24  | BA    | 484  | C    | O4'-C1'-N1  | -5.18 | 104.06      | 108.20   |
| 24  | BA    | 727  | A    | C3'-C2'-C1' | 5.18  | 105.64      | 101.50   |
| 24  | BA    | 1142 | A    | N9-C4-C5    | 5.18  | 107.87      | 105.80   |
| 24  | BA    | 1698 | A    | N1-C6-N6    | 5.18  | 121.71      | 118.60   |
| 55  | CA    | 1051 | C    | C3'-C2'-C1' | 5.18  | 105.64      | 101.50   |
| 24  | DA    | 2319 | G    | P-O3'-C3'   | 5.18  | 125.92      | 119.70   |
| 24  | DA    | 2610 | C    | O4'-C1'-N1  | -5.18 | 104.06      | 108.20   |
| 24  | BA    | 1821 | A    | C3'-C2'-C1' | 5.18  | 105.64      | 101.50   |
| 24  | DA    | 968  | C    | O4'-C1'-N1  | 5.18  | 112.34      | 108.20   |
| 24  | BA    | 1086 | A    | C6-N1-C2    | -5.17 | 115.50      | 118.60   |
| 24  | BA    | 2052 | A    | C6-N1-C2    | 5.17  | 121.70      | 118.60   |
| 55  | CA    | 412  | A    | P-O3'-C3'   | 5.17  | 125.91      | 119.70   |
| 55  | CA    | 1299 | A    | C3'-C2'-C1' | 5.17  | 105.64      | 101.50   |
| 24  | DA    | 333  | G    | C3'-C2'-C1' | 5.17  | 105.64      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 1915 | U    | C3'-C2'-C1' | 5.17  | 105.64      | 101.50   |
| 24  | BA    | 340  | A    | N1-C6-N6    | 5.17  | 121.70      | 118.60   |
| 24  | BA    | 655  | A    | P-O3'-C3'   | 5.17  | 125.91      | 119.70   |
| 24  | DA    | 2894 | G    | C3'-C2'-C1' | 5.17  | 105.64      | 101.50   |
| 56  | DB    | 17   | C    | C3'-C2'-C1' | 5.17  | 105.64      | 101.50   |
| 24  | BA    | 1957 | C    | N1-C2-O2    | 5.17  | 122.00      | 118.90   |
| 21  | AA    | 756  | C    | P-O3'-C3'   | -5.17 | 113.50      | 119.70   |
| 24  | BA    | 1675 | C    | C3'-C2'-C1' | 5.17  | 105.64      | 101.50   |
| 24  | DA    | 577  | G    | N7-C8-N9    | 5.17  | 115.68      | 113.10   |
| 24  | DA    | 1415 | U    | O4'-C1'-N1  | 5.17  | 112.33      | 108.20   |
| 24  | BA    | 1731 | G    | C4-N9-C1'   | -5.17 | 119.78      | 126.50   |
| 24  | BA    | 2135 | A    | P-O3'-C3'   | -5.17 | 113.50      | 119.70   |
| 24  | BA    | 2136 | G    | C3'-C2'-C1' | 5.17  | 105.63      | 101.50   |
| 24  | BA    | 2451 | A    | C6-N1-C2    | -5.17 | 115.50      | 118.60   |
| 25  | BB    | 66   | A    | P-O5'-C5'   | 5.17  | 129.17      | 120.90   |
| 55  | CA    | 52   | C    | C3'-C2'-C1' | 5.17  | 105.63      | 101.50   |
| 24  | BA    | 100  | U    | N1-C1'-C2'  | 5.17  | 120.71      | 114.00   |
| 24  | DA    | 1554 | U    | P-O3'-C3'   | 5.17  | 125.90      | 119.70   |
| 24  | DA    | 2402 | U    | C3'-C2'-C1' | 5.17  | 105.63      | 101.50   |
| 21  | AA    | 332  | G    | C3'-C2'-C1' | 5.16  | 105.63      | 101.50   |
| 21  | AA    | 934  | C    | O3'-P-O5'   | 5.16  | 113.81      | 104.00   |
| 21  | AA    | 1411 | C    | C2-N1-C1'   | 5.16  | 124.48      | 118.80   |
| 24  | BA    | 66   | C    | O4'-C1'-N1  | 5.16  | 112.33      | 108.20   |
| 55  | CA    | 183  | C    | N1-C1'-C2'  | -5.16 | 106.32      | 112.00   |
| 24  | DA    | 206  | U    | C3'-C2'-C1' | 5.16  | 105.63      | 101.50   |
| 24  | DA    | 2286 | G    | P-O3'-C3'   | 5.16  | 125.90      | 119.70   |
| 24  | BA    | 299  | A    | C8-N9-C4    | -5.16 | 103.73      | 105.80   |
| 24  | DA    | 2589 | A    | N1-C6-N6    | -5.16 | 115.50      | 118.60   |
| 24  | BA    | 791  | C    | N3-C2-O2    | -5.16 | 118.29      | 121.90   |
| 24  | BA    | 813  | U    | O5'-P-OP2   | -5.16 | 101.06      | 105.70   |
| 55  | CA    | 1202 | U    | C3'-C2'-C1' | 5.16  | 105.63      | 101.50   |
| 24  | DA    | 105  | C    | O4'-C1'-N1  | 5.16  | 112.33      | 108.20   |
| 24  | DA    | 832  | U    | C3'-C2'-C1' | 5.16  | 105.63      | 101.50   |
| 21  | AA    | 1504 | G    | C4-C5-N7    | -5.16 | 108.74      | 110.80   |
| 24  | BA    | 752  | A    | N9-C4-C5    | -5.16 | 103.74      | 105.80   |
| 24  | DA    | 589  | U    | P-O3'-C3'   | -5.16 | 113.51      | 119.70   |
| 24  | DA    | 1386 | C    | P-O3'-C3'   | -5.16 | 113.51      | 119.70   |
| 24  | DA    | 1560 | G    | C3'-C2'-C1' | 5.16  | 105.63      | 101.50   |
| 24  | BA    | 324  | A    | C3'-C2'-C1' | 5.16  | 105.63      | 101.50   |
| 24  | BA    | 2071 | A    | P-O3'-C3'   | 5.16  | 125.89      | 119.70   |
| 24  | BA    | 2322 | A    | C3'-C2'-C1' | 5.16  | 105.62      | 101.50   |
| 24  | BA    | 2513 | A    | C8-N9-C4    | -5.16 | 103.74      | 105.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 12   | U    | C2-N1-C1'   | 5.16  | 123.89      | 117.70   |
| 24  | BA    | 1925 | C    | O4'-C1'-N1  | 5.16  | 112.32      | 108.20   |
| 24  | DA    | 2427 | C    | C3'-C2'-C1' | 5.16  | 105.62      | 101.50   |
| 21  | AA    | 1421 | G    | P-O3'-C3'   | -5.15 | 113.52      | 119.70   |
| 24  | BA    | 1144 | A    | N9-C1'-C2'  | -5.15 | 106.33      | 112.00   |
| 55  | CA    | 977  | A    | C3'-C2'-C1' | 5.15  | 105.62      | 101.50   |
| 24  | DA    | 230  | G    | N9-C1'-C2'  | -5.15 | 106.33      | 112.00   |
| 24  | DA    | 533  | G    | N9-C1'-C2'  | -5.15 | 106.33      | 112.00   |
| 21  | AA    | 1322 | C    | P-O3'-C3'   | 5.15  | 125.88      | 119.70   |
| 24  | BA    | 663  | G    | C5-C6-O6    | 5.15  | 131.69      | 128.60   |
| 24  | BA    | 2363 | G    | C8-N9-C4    | -5.15 | 104.34      | 106.40   |
| 55  | CA    | 173  | U    | P-O3'-C3'   | 5.15  | 125.88      | 119.70   |
| 55  | CA    | 425  | G    | C3'-C2'-C1' | 5.15  | 105.62      | 101.50   |
| 24  | DA    | 483  | A    | N9-C1'-C2'  | -5.15 | 106.34      | 112.00   |
| 24  | DA    | 1606 | C    | P-O3'-C3'   | 5.15  | 125.88      | 119.70   |
| 21  | AA    | 549  | C    | C3'-C2'-C1' | 5.15  | 105.62      | 101.50   |
| 21  | AA    | 577  | G    | N9-C4-C5    | 5.15  | 107.46      | 105.40   |
| 21  | AA    | 1259 | C    | O4'-C1'-N1  | 5.15  | 112.32      | 108.20   |
| 24  | BA    | 1058 | U    | O4'-C1'-N1  | 5.15  | 112.32      | 108.20   |
| 24  | BA    | 1370 | C    | N1-C2-O2    | -5.15 | 115.81      | 118.90   |
| 24  | BA    | 2822 | G    | C4-C5-N7    | 5.15  | 112.86      | 110.80   |
| 24  | DA    | 87   | U    | C3'-C2'-C1' | 5.15  | 105.62      | 101.50   |
| 24  | DA    | 975  | A    | C3'-C2'-C1' | 5.15  | 105.62      | 101.50   |
| 24  | DA    | 997  | G    | N9-C1'-C2'  | -5.15 | 106.34      | 112.00   |
| 24  | DA    | 2477 | U    | O4'-C1'-N1  | 5.15  | 112.32      | 108.20   |
| 24  | DA    | 2267 | A    | C4-C5-C6    | 5.15  | 119.57      | 117.00   |
| 21  | AA    | 930  | C    | O4'-C1'-N1  | 5.14  | 112.31      | 108.20   |
| 21  | AA    | 995  | C    | C3'-C2'-C1' | 5.14  | 105.61      | 101.50   |
| 55  | CA    | 239  | U    | P-O3'-C3'   | 5.14  | 125.87      | 119.70   |
| 55  | CA    | 723  | U    | C2-N1-C1'   | 5.14  | 123.87      | 117.70   |
| 55  | CA    | 1440 | U    | P-O3'-C3'   | 5.14  | 125.87      | 119.70   |
| 21  | AA    | 819  | A    | O4'-C1'-N9  | -5.14 | 104.09      | 108.20   |
| 24  | BA    | 1867 | G    | C3'-C2'-C1' | 5.14  | 105.61      | 101.50   |
| 55  | CA    | 120  | A    | C3'-C2'-C1' | 5.14  | 105.61      | 101.50   |
| 55  | CA    | 567  | G    | N9-C1'-C2'  | -5.14 | 106.34      | 112.00   |
| 24  | DA    | 1155 | A    | O4'-C1'-N9  | 5.14  | 112.31      | 108.20   |
| 24  | DA    | 2272 | U    | C5-C4-O4    | -5.14 | 122.81      | 125.90   |
| 24  | BA    | 753  | A    | C3'-C2'-C1' | 5.14  | 105.61      | 101.50   |
| 55  | CA    | 984  | C    | C3'-C2'-C1' | 5.14  | 105.61      | 101.50   |
| 24  | DA    | 92   | U    | C3'-C2'-C1' | 5.14  | 105.61      | 101.50   |
| 21  | AA    | 1169 | A    | P-O5'-C5'   | -5.14 | 112.68      | 120.90   |
| 21  | AA    | 1215 | G    | N9-C1'-C2'  | -5.14 | 106.35      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 86   | G    | C3'-C2'-C1' | 5.14  | 105.61      | 101.50   |
| 24  | BA    | 2676 | C    | N1-C2-O2    | -5.14 | 115.82      | 118.90   |
| 24  | BA    | 2894 | G    | C8-N9-C1'   | -5.14 | 120.32      | 127.00   |
| 55  | CA    | 1170 | A    | C3'-C2'-C1' | 5.14  | 105.61      | 101.50   |
| 24  | DA    | 2053 | G    | N1-C6-O6    | -5.14 | 116.82      | 119.90   |
| 24  | DA    | 2408 | U    | P-O3'-C3'   | -5.14 | 113.53      | 119.70   |
| 21  | AA    | 1203 | C    | P-O5'-C5'   | -5.14 | 112.68      | 120.90   |
| 24  | DA    | 1963 | U    | C3'-C2'-C1' | 5.14  | 105.61      | 101.50   |
| 24  | BA    | 1249 | U    | O4'-C1'-N1  | -5.14 | 104.09      | 108.20   |
| 55  | CA    | 88   | U    | O4'-C1'-N1  | 5.14  | 112.31      | 108.20   |
| 24  | BA    | 645  | C    | C6-N1-C1'   | -5.13 | 114.64      | 120.80   |
| 24  | BA    | 1247 | A    | C1'-O4'-C4' | -5.13 | 105.79      | 109.90   |
| 24  | BA    | 2273 | A    | C5-N7-C8    | -5.13 | 101.33      | 103.90   |
| 55  | CA    | 1051 | C    | O4'-C1'-N1  | 5.13  | 112.31      | 108.20   |
| 21  | AA    | 1504 | G    | N9-C4-C5    | 5.13  | 107.45      | 105.40   |
| 24  | BA    | 727  | A    | N9-C1'-C2'  | -5.13 | 106.35      | 112.00   |
| 24  | BA    | 752  | A    | C5-C6-N6    | -5.13 | 119.59      | 123.70   |
| 24  | BA    | 271  | G    | C8-N9-C1'   | 5.13  | 133.67      | 127.00   |
| 55  | CA    | 1371 | G    | P-O3'-C3'   | -5.13 | 113.54      | 119.70   |
| 24  | DA    | 1334 | G    | C3'-C2'-C1' | 5.13  | 105.61      | 101.50   |
| 24  | BA    | 43   | G    | P-O5'-C5'   | -5.13 | 112.69      | 120.90   |
| 24  | BA    | 2513 | A    | C4-C5-N7    | -5.13 | 108.14      | 110.70   |
| 55  | CA    | 32   | A    | N9-C1'-C2'  | -5.13 | 106.36      | 112.00   |
| 21  | AA    | 1420 | U    | P-O3'-C3'   | -5.13 | 113.55      | 119.70   |
| 24  | DA    | 162  | U    | N1-C1'-C2'  | 5.13  | 120.67      | 114.00   |
| 24  | BA    | 1952 | A    | N9-C4-C5    | 5.13  | 107.85      | 105.80   |
| 24  | BA    | 2225 | A    | N1-C6-N6    | 5.13  | 121.68      | 118.60   |
| 24  | DA    | 480  | A    | C3'-C2'-C1' | 5.13  | 105.60      | 101.50   |
| 24  | DA    | 1569 | A    | N9-C1'-C2'  | -5.13 | 106.36      | 112.00   |
| 24  | DA    | 1957 | C    | N3-C2-O2    | -5.13 | 118.31      | 121.90   |
| 24  | DA    | 2603 | G    | N9-C1'-C2'  | -5.13 | 106.36      | 112.00   |
| 24  | BA    | 1681 | G    | O4'-C1'-N9  | 5.12  | 112.30      | 108.20   |
| 24  | BA    | 1183 | U    | N1-C2-O2    | 5.12  | 126.39      | 122.80   |
| 24  | BA    | 1476 | U    | C3'-C2'-C1' | 5.12  | 105.60      | 101.50   |
| 24  | BA    | 1554 | U    | O3'-P-O5'   | -5.12 | 94.26       | 104.00   |
| 24  | BA    | 2211 | A    | P-O5'-C5'   | 5.12  | 129.10      | 120.90   |
| 24  | DA    | 179  | C    | C3'-C2'-C1' | 5.12  | 105.60      | 101.50   |
| 24  | DA    | 656  | G    | N9-C1'-C2'  | -5.12 | 106.36      | 112.00   |
| 24  | DA    | 391  | A    | C3'-C2'-C1' | 5.12  | 105.60      | 101.50   |
| 24  | DA    | 831  | G    | C3'-C2'-C1' | 5.12  | 105.60      | 101.50   |
| 24  | DA    | 1696 | G    | C3'-C2'-C1' | 5.12  | 105.60      | 101.50   |
| 24  | DA    | 2459 | A    | N9-C1'-C2'  | -5.12 | 106.37      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 1033 | U    | N1-C1'-C2'  | 5.12  | 120.66      | 114.00   |
| 24  | BA    | 2250 | G    | N7-C8-N9    | 5.12  | 115.66      | 113.10   |
| 24  | DA    | 444  | C    | C3'-C2'-C1' | 5.12  | 105.60      | 101.50   |
| 24  | BA    | 1294 | U    | O4'-C1'-N1  | -5.12 | 104.11      | 108.20   |
| 24  | BA    | 1693 | U    | O3'-P-O5'   | -5.12 | 94.28       | 104.00   |
| 24  | BA    | 2371 | G    | N3-C2-N2    | -5.12 | 116.32      | 119.90   |
| 24  | BA    | 2631 | G    | C5-C6-O6    | 5.12  | 131.67      | 128.60   |
| 55  | CA    | 170  | U    | O4'-C1'-N1  | 5.12  | 112.30      | 108.20   |
| 55  | CA    | 529  | G    | P-O3'-C3'   | -5.12 | 113.56      | 119.70   |
| 24  | DA    | 577  | G    | N3-C4-N9    | 5.12  | 129.07      | 126.00   |
| 21  | AA    | 66   | A    | C3'-C2'-C1' | 5.12  | 105.59      | 101.50   |
| 24  | DA    | 867  | C    | C3'-C2'-C1' | 5.12  | 105.59      | 101.50   |
| 24  | BA    | 800  | A    | N9-C4-C5    | 5.12  | 107.85      | 105.80   |
| 24  | BA    | 1313 | U    | P-O3'-C3'   | -5.12 | 113.56      | 119.70   |
| 24  | BA    | 1657 | U    | P-O3'-C3'   | -5.12 | 113.56      | 119.70   |
| 55  | CA    | 989  | U    | O4'-C1'-N1  | 5.12  | 112.29      | 108.20   |
| 55  | CA    | 1322 | C    | P-O3'-C3'   | 5.12  | 125.84      | 119.70   |
| 21  | AA    | 978  | A    | C3'-C2'-C1' | 5.11  | 105.59      | 101.50   |
| 24  | BA    | 688  | U    | C3'-C2'-C1' | 5.11  | 105.59      | 101.50   |
| 24  | BA    | 1566 | A    | O4'-C1'-N9  | -5.11 | 104.11      | 108.20   |
| 24  | BA    | 1865 | U    | C5-C6-N1    | -5.11 | 120.14      | 122.70   |
| 24  | BA    | 2812 | G    | C8-N9-C1'   | -5.11 | 120.35      | 127.00   |
| 24  | DA    | 1111 | A    | P-O3'-C3'   | -5.11 | 113.56      | 119.70   |
| 24  | BA    | 1521 | G    | C8-N9-C1'   | -5.11 | 120.35      | 127.00   |
| 55  | CA    | 1158 | C    | P-O3'-C3'   | -5.11 | 113.57      | 119.70   |
| 24  | DA    | 64   | A    | N1-C6-N6    | -5.11 | 115.53      | 118.60   |
| 24  | BA    | 763  | G    | C8-N9-C1'   | -5.11 | 120.36      | 127.00   |
| 24  | BA    | 2451 | A    | N9-C4-C5    | 5.11  | 107.84      | 105.80   |
| 24  | DA    | 1390 | U    | O4'-C1'-N1  | 5.11  | 112.29      | 108.20   |
| 24  | BA    | 1681 | G    | O3'-P-O5'   | -5.11 | 94.29       | 104.00   |
| 21  | AA    | 1224 | U    | P-O3'-C3'   | 5.11  | 125.83      | 119.70   |
| 24  | BA    | 2262 | U    | O4'-C1'-N1  | 5.11  | 112.29      | 108.20   |
| 24  | BA    | 2752 | C    | O4'-C1'-N1  | 5.11  | 112.28      | 108.20   |
| 24  | BA    | 2893 | A    | N7-C8-N9    | -5.11 | 111.25      | 113.80   |
| 24  | DA    | 60   | G    | N9-C4-C5    | 5.11  | 107.44      | 105.40   |
| 24  | DA    | 503  | A    | O4'-C1'-N9  | 5.11  | 112.29      | 108.20   |
| 56  | DB    | 42   | C    | C3'-C2'-C1' | 5.11  | 105.59      | 101.50   |
| 21  | AA    | 519  | C    | P-O3'-C3'   | -5.11 | 113.57      | 119.70   |
| 21  | AA    | 562  | U    | P-O3'-C3'   | 5.11  | 125.83      | 119.70   |
| 21  | AA    | 858  | G    | P-O3'-C3'   | 5.11  | 125.83      | 119.70   |
| 24  | BA    | 763  | G    | N7-C8-N9    | 5.11  | 115.65      | 113.10   |
| 24  | BA    | 962  | G    | C3'-C2'-C1' | 5.11  | 105.58      | 101.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 1649 | G    | N9-C1'-C2'  | -5.11 | 106.39      | 112.00   |
| 21  | AA    | 198  | G    | P-O3'-C3'   | -5.10 | 113.58      | 119.70   |
| 21  | AA    | 1063 | C    | C6-N1-C2    | 5.10  | 122.34      | 120.30   |
| 24  | BA    | 1915 | U    | C3'-C2'-C1' | 5.10  | 105.58      | 101.50   |
| 24  | DA    | 1634 | A    | O3'-P-O5'   | -5.10 | 94.30       | 104.00   |
| 24  | BA    | 241  | A    | O4'-C1'-N9  | 5.10  | 112.28      | 108.20   |
| 24  | BA    | 1375 | U    | C5-C4-O4    | 5.10  | 128.96      | 125.90   |
| 24  | BA    | 1915 | U    | C2-N1-C1'   | 5.10  | 123.82      | 117.70   |
| 24  | BA    | 2294 | G    | C4-C5-N7    | 5.10  | 112.84      | 110.80   |
| 25  | BB    | 87   | U    | N1-C1'-C2'  | 5.10  | 120.63      | 114.00   |
| 24  | DA    | 1075 | C    | P-O3'-C3'   | -5.10 | 113.58      | 119.70   |
| 24  | DA    | 1677 | A    | P-O3'-C3'   | -5.10 | 113.58      | 119.70   |
| 24  | BA    | 1682 | G    | N9-C1'-C2'  | -5.10 | 106.39      | 112.00   |
| 55  | CA    | 51   | A    | P-O3'-C3'   | 5.10  | 125.82      | 119.70   |
| 24  | DA    | 783  | A    | P-O3'-C3'   | -5.10 | 113.58      | 119.70   |
| 21  | AA    | 190  | A    | C5-C6-N6    | -5.10 | 119.62      | 123.70   |
| 24  | BA    | 1019 | U    | P-O3'-C3'   | 5.10  | 125.82      | 119.70   |
| 24  | BA    | 1332 | G    | C4-N9-C1'   | 5.10  | 133.13      | 126.50   |
| 24  | BA    | 2603 | G    | N9-C1'-C2'  | -5.10 | 106.39      | 112.00   |
| 41  | BR    | 9    | GLY  | N-CA-C      | -5.10 | 100.35      | 113.10   |
| 24  | DA    | 318  | C    | O4'-C1'-N1  | 5.10  | 112.28      | 108.20   |
| 21  | AA    | 253  | A    | P-O5'-C5'   | -5.10 | 112.74      | 120.90   |
| 24  | BA    | 444  | C    | P-O3'-C3'   | -5.10 | 113.58      | 119.70   |
| 24  | BA    | 446  | G    | P-O3'-C3'   | 5.10  | 125.82      | 119.70   |
| 24  | DA    | 482  | A    | C3'-C2'-C1' | 5.10  | 105.58      | 101.50   |
| 24  | BA    | 984  | A    | O4'-C1'-N9  | -5.10 | 104.12      | 108.20   |
| 56  | DB    | 77   | U    | O4'-C1'-N1  | 5.10  | 112.28      | 108.20   |
| 24  | BA    | 985  | C    | C2-N1-C1'   | 5.09  | 124.40      | 118.80   |
| 24  | BA    | 1245 | G    | N9-C4-C5    | 5.09  | 107.44      | 105.40   |
| 24  | BA    | 2650 | U    | C5-C6-N1    | -5.09 | 120.15      | 122.70   |
| 55  | CA    | 424  | G    | C3'-C2'-C1' | 5.09  | 105.58      | 101.50   |
| 24  | BA    | 1787 | A    | N9-C1'-C2'  | -5.09 | 106.40      | 112.00   |
| 24  | BA    | 919  | U    | N1-C2-N3    | -5.09 | 111.84      | 114.90   |
| 24  | BA    | 2075 | U    | C2-N3-C4    | 5.09  | 130.06      | 127.00   |
| 24  | DA    | 2440 | C    | O4'-C1'-N1  | 5.09  | 112.27      | 108.20   |
| 24  | BA    | 548  | G    | C4-N9-C1'   | 5.09  | 133.12      | 126.50   |
| 24  | BA    | 1442 | U    | P-O3'-C3'   | -5.09 | 113.59      | 119.70   |
| 55  | CA    | 347  | G    | C3'-C2'-C1' | 5.09  | 105.57      | 101.50   |
| 55  | CA    | 965  | U    | N1-C1'-C2'  | 5.09  | 120.62      | 114.00   |
| 24  | BA    | 222  | A    | N1-C6-N6    | 5.09  | 121.65      | 118.60   |
| 24  | BA    | 1003 | G    | C8-N9-C4    | -5.09 | 104.36      | 106.40   |
| 24  | BA    | 1957 | C    | N3-C2-O2    | -5.09 | 118.34      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 1208 | C    | C5-C6-N1    | -5.09 | 118.46      | 121.00   |
| 24  | BA    | 1344 | U    | O4'-C1'-N1  | 5.09  | 112.27      | 108.20   |
| 24  | DA    | 142  | A    | C3'-C2'-C1' | 5.09  | 105.57      | 101.50   |
| 24  | DA    | 1063 | G    | C3'-C2'-C1' | 5.08  | 105.57      | 101.50   |
| 24  | DA    | 1268 | A    | N9-C1'-C2'  | -5.08 | 106.41      | 112.00   |
| 24  | DA    | 2492 | U    | O4'-C1'-N1  | 5.08  | 112.27      | 108.20   |
| 24  | BA    | 988  | A    | P-O3'-C3'   | 5.08  | 125.80      | 119.70   |
| 24  | BA    | 2312 | U    | P-O3'-C3'   | -5.08 | 113.60      | 119.70   |
| 21  | AA    | 90   | C    | C3'-C2'-C1' | 5.08  | 105.56      | 101.50   |
| 21  | AA    | 131  | A    | N9-C4-C5    | 5.08  | 107.83      | 105.80   |
| 24  | BA    | 604  | G    | C3'-C2'-C1' | 5.08  | 105.57      | 101.50   |
| 24  | BA    | 2066 | C    | N1-C2-N3    | -5.08 | 115.64      | 119.20   |
| 24  | BA    | 122  | G    | C3'-C2'-C1' | 5.08  | 105.56      | 101.50   |
| 24  | BA    | 1171 | G    | N9-C4-C5    | 5.08  | 107.43      | 105.40   |
| 24  | DA    | 1942 | C    | C3'-C2'-C1' | 5.08  | 105.56      | 101.50   |
| 24  | BA    | 1029 | A    | N9-C4-C5    | -5.08 | 103.77      | 105.80   |
| 24  | BA    | 2259 | U    | C2-N3-C4    | -5.08 | 123.95      | 127.00   |
| 55  | CA    | 1162 | C    | C3'-C2'-C1' | 5.08  | 105.56      | 101.50   |
| 24  | DA    | 164  | C    | P-O3'-C3'   | -5.08 | 113.61      | 119.70   |
| 24  | BA    | 1380 | G    | N1-C6-O6    | -5.08 | 116.85      | 119.90   |
| 24  | BA    | 2224 | G    | N9-C4-C5    | -5.08 | 103.37      | 105.40   |
| 24  | BA    | 2792 | A    | C3'-C2'-C1' | 5.08  | 105.56      | 101.50   |
| 24  | BA    | 434  | U    | C5-C6-N1    | -5.08 | 120.16      | 122.70   |
| 24  | BA    | 1669 | A    | C3'-C2'-C1' | 5.08  | 105.56      | 101.50   |
| 24  | BA    | 1865 | U    | N1-C1'-C2'  | 5.08  | 120.60      | 114.00   |
| 24  | BA    | 2359 | C    | C5-C6-N1    | -5.08 | 118.46      | 121.00   |
| 24  | DA    | 74   | A    | C3'-C2'-C1' | 5.08  | 105.56      | 101.50   |
| 24  | DA    | 1941 | C    | C3'-C2'-C1' | 5.08  | 105.56      | 101.50   |
| 24  | DA    | 1965 | C    | C3'-C2'-C1' | 5.08  | 105.56      | 101.50   |
| 56  | DB    | 103  | U    | N1-C1'-C2'  | 5.08  | 120.60      | 114.00   |
| 24  | BA    | 1286 | A    | C5-N7-C8    | 5.07  | 106.44      | 103.90   |
| 24  | DA    | 312  | G    | C3'-C2'-C1' | 5.07  | 105.56      | 101.50   |
| 24  | DA    | 1019 | U    | N1-C2-N3    | 5.07  | 117.94      | 114.90   |
| 24  | BA    | 1648 | U    | C3'-C2'-C1' | 5.07  | 105.56      | 101.50   |
| 24  | DA    | 388  | G    | C3'-C2'-C1' | 5.07  | 105.56      | 101.50   |
| 24  | DA    | 687  | C    | P-O3'-C3'   | -5.07 | 113.61      | 119.70   |
| 24  | DA    | 1048 | A    | P-O3'-C3'   | -5.07 | 113.61      | 119.70   |
| 24  | DA    | 1957 | C    | C3'-C2'-C1' | 5.07  | 105.56      | 101.50   |
| 24  | DA    | 2337 | G    | C3'-C2'-C1' | 5.07  | 105.56      | 101.50   |
| 24  | BA    | 2311 | A    | P-O3'-C3'   | 5.07  | 125.78      | 119.70   |
| 24  | BA    | 2326 | C    | C6-N1-C2    | 5.07  | 122.33      | 120.30   |
| 24  | DA    | 1767 | G    | N1-C6-O6    | -5.07 | 116.86      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 2778 | A    | C3'-C2'-C1' | 5.07  | 105.55      | 101.50   |
| 21  | AA    | 43   | C    | C6-N1-C2    | 5.07  | 122.33      | 120.30   |
| 21  | AA    | 1382 | C    | P-O3'-C3'   | -5.07 | 113.62      | 119.70   |
| 24  | DA    | 2425 | A    | O4'-C1'-N9  | 5.07  | 112.25      | 108.20   |
| 24  | DA    | 2832 | U    | O4'-C1'-N1  | 5.07  | 112.25      | 108.20   |
| 24  | DA    | 323  | C    | O4'-C1'-N1  | 5.06  | 112.25      | 108.20   |
| 21  | AA    | 1055 | A    | N1-C6-N6    | 5.06  | 121.64      | 118.60   |
| 21  | AA    | 1486 | G    | C6-N1-C2    | -5.06 | 122.06      | 125.10   |
| 24  | BA    | 1809 | A    | N9-C1'-C2'  | -5.06 | 106.43      | 112.00   |
| 25  | BB    | 88   | C    | C6-N1-C2    | 5.06  | 122.33      | 120.30   |
| 24  | DA    | 1972 | G    | C3'-C2'-C1' | 5.06  | 105.55      | 101.50   |
| 21  | AA    | 1144 | G    | P-O3'-C3'   | 5.06  | 125.77      | 119.70   |
| 24  | BA    | 2093 | G    | C3'-C2'-C1' | 5.06  | 105.55      | 101.50   |
| 55  | CA    | 1033 | G    | C3'-C2'-C1' | 5.06  | 105.55      | 101.50   |
| 24  | DA    | 2616 | C    | C3'-C2'-C1' | 5.06  | 105.55      | 101.50   |
| 24  | DA    | 1082 | U    | C2-N3-C4    | -5.06 | 123.96      | 127.00   |
| 24  | DA    | 2770 | G    | C6-C5-N7    | -5.06 | 127.36      | 130.40   |
| 56  | DB    | 13   | G    | C3'-C2'-C1' | 5.06  | 105.55      | 101.50   |
| 21  | AA    | 1304 | G    | C8-N9-C4    | -5.06 | 104.38      | 106.40   |
| 24  | BA    | 1782 | U    | C3'-C2'-C1' | 5.06  | 105.55      | 101.50   |
| 55  | CA    | 96   | U    | C3'-C2'-C1' | 5.06  | 105.55      | 101.50   |
| 24  | BA    | 58   | G    | N9-C4-C5    | 5.05  | 107.42      | 105.40   |
| 24  | BA    | 463  | G    | O4'-C1'-N9  | 5.05  | 112.24      | 108.20   |
| 24  | BA    | 807  | U    | P-O5'-C5'   | -5.05 | 112.81      | 120.90   |
| 24  | BA    | 1406 | U    | N1-C1'-C2'  | 5.05  | 120.57      | 114.00   |
| 24  | BA    | 1796 | U    | O4'-C1'-N1  | 5.05  | 112.24      | 108.20   |
| 24  | BA    | 2520 | C    | N3-C4-C5    | -5.05 | 119.88      | 121.90   |
| 24  | DA    | 1378 | A    | P-O3'-C3'   | 5.05  | 125.77      | 119.70   |
| 24  | BA    | 1029 | A    | O4'-C1'-N9  | -5.05 | 104.16      | 108.20   |
| 25  | BB    | 53   | A    | N9-C1'-C2'  | -5.05 | 106.44      | 112.00   |
| 24  | DA    | 1439 | A    | C6-C5-N7    | -5.05 | 128.76      | 132.30   |
| 56  | DB    | 44   | G    | C6-C5-N7    | 5.05  | 133.43      | 130.40   |
| 21  | AA    | 331  | G    | C3'-C2'-C1' | 5.05  | 105.54      | 101.50   |
| 24  | BA    | 729  | G    | P-O3'-C3'   | -5.05 | 113.64      | 119.70   |
| 55  | CA    | 30   | U    | P-O3'-C3'   | 5.05  | 125.76      | 119.70   |
| 24  | DA    | 26   | G    | P-O3'-C3'   | 5.05  | 125.76      | 119.70   |
| 24  | DA    | 1865 | U    | N1-C1'-C2'  | 5.05  | 120.57      | 114.00   |
| 24  | DA    | 2210 | U    | O3'-P-O5'   | 5.05  | 113.60      | 104.00   |
| 21  | AA    | 960  | U    | C2-N1-C1'   | 5.05  | 123.76      | 117.70   |
| 24  | BA    | 1070 | A    | P-O3'-C3'   | 5.05  | 125.76      | 119.70   |
| 24  | BA    | 1777 | U    | C2-N3-C4    | 5.05  | 130.03      | 127.00   |
| 24  | BA    | 2849 | U    | C5'-C4'-O4' | -5.05 | 103.04      | 109.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | CA    | 169  | C    | C5-C4-N4    | 5.05  | 123.73      | 120.20   |
| 56  | DB    | 43   | C    | C6-N1-C2    | -5.05 | 118.28      | 120.30   |
| 21  | AA    | 253  | A    | C3'-C2'-C1' | 5.05  | 105.54      | 101.50   |
| 24  | BA    | 1958 | C    | C6-N1-C2    | 5.05  | 122.32      | 120.30   |
| 24  | BA    | 2818 | U    | P-O3'-C3'   | -5.05 | 113.64      | 119.70   |
| 24  | DA    | 1507 | C    | C2-N3-C4    | 5.05  | 122.42      | 119.90   |
| 24  | DA    | 2036 | C    | P-O3'-C3'   | -5.05 | 113.64      | 119.70   |
| 21  | AA    | 1210 | C    | P-O3'-C3'   | -5.04 | 113.65      | 119.70   |
| 24  | BA    | 2213 | U    | P-O3'-C3'   | -5.04 | 113.65      | 119.70   |
| 24  | BA    | 2822 | G    | C6-C5-N7    | -5.04 | 127.37      | 130.40   |
| 24  | BA    | 105  | C    | N1-C2-O2    | 5.04  | 121.93      | 118.90   |
| 24  | BA    | 1947 | C    | N1-C2-O2    | -5.04 | 115.87      | 118.90   |
| 24  | BA    | 2491 | U    | O5'-P-OP2   | -5.04 | 101.16      | 105.70   |
| 24  | DA    | 2260 | C    | C6-N1-C2    | -5.04 | 118.28      | 120.30   |
| 21  | AA    | 9    | G    | C3'-C2'-C1' | 5.04  | 105.53      | 101.50   |
| 24  | BA    | 1497 | U    | P-O3'-C3'   | 5.04  | 125.75      | 119.70   |
| 24  | BA    | 2494 | G    | P-O3'-C3'   | -5.04 | 113.65      | 119.70   |
| 24  | DA    | 657  | U    | C3'-C2'-C1' | 5.04  | 105.53      | 101.50   |
| 24  | DA    | 783  | A    | N9-C1'-C2'  | -5.04 | 106.45      | 112.00   |
| 55  | CA    | 1508 | A    | N9-C1'-C2'  | -5.04 | 106.46      | 112.00   |
| 24  | DA    | 2239 | G    | C3'-C2'-C1' | 5.04  | 105.53      | 101.50   |
| 24  | BA    | 2219 | U    | O4'-C1'-N1  | 5.04  | 112.23      | 108.20   |
| 25  | BB    | 25   | U    | N1-C1'-C2'  | -5.04 | 106.46      | 112.00   |
| 24  | DA    | 1900 | A    | P-O3'-C3'   | 5.04  | 125.75      | 119.70   |
| 21  | AA    | 279  | A    | O4'-C1'-N9  | -5.04 | 104.17      | 108.20   |
| 21  | AA    | 520  | A    | C3'-C2'-C1' | 5.04  | 105.53      | 101.50   |
| 24  | DA    | 1439 | A    | N1-C6-N6    | 5.04  | 121.62      | 118.60   |
| 21  | AA    | 30   | U    | N1-C1'-C2'  | 5.04  | 120.55      | 114.00   |
| 24  | BA    | 12   | U    | N1-C2-O2    | 5.04  | 126.33      | 122.80   |
| 24  | BA    | 1511 | G    | C3'-C2'-C1' | 5.04  | 105.53      | 101.50   |
| 24  | BA    | 1844 | C    | O4'-C1'-N1  | -5.04 | 104.17      | 108.20   |
| 24  | DA    | 813  | U    | O4'-C1'-N1  | 5.04  | 112.23      | 108.20   |
| 24  | DA    | 1062 | G    | C8-N9-C4    | -5.04 | 104.39      | 106.40   |
| 24  | DA    | 2586 | U    | C3'-C2'-C1' | 5.04  | 105.53      | 101.50   |
| 24  | BA    | 8    | C    | P-O5'-C5'   | -5.03 | 112.85      | 120.90   |
| 24  | BA    | 1695 | G    | C8-N9-C4    | -5.03 | 104.39      | 106.40   |
| 25  | BB    | 26   | C    | C3'-C2'-C1' | 5.03  | 105.53      | 101.50   |
| 25  | BB    | 53   | A    | C3'-C2'-C1' | 5.03  | 105.53      | 101.50   |
| 55  | CA    | 1454 | G    | P-O3'-C3'   | -5.03 | 113.66      | 119.70   |
| 24  | DA    | 2616 | C    | C6-N1-C2    | -5.03 | 118.29      | 120.30   |
| 24  | BA    | 461  | C    | C2-N3-C4    | -5.03 | 117.38      | 119.90   |
| 24  | BA    | 2246 | G    | C6-C5-N7    | -5.03 | 127.38      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 1204 | A    | P-O3'-C3'   | 5.03  | 125.74      | 119.70   |
| 21  | AA    | 509  | A    | P-O3'-C3'   | -5.03 | 113.66      | 119.70   |
| 24  | BA    | 628  | G    | C3'-C2'-C1' | 5.03  | 105.52      | 101.50   |
| 21  | AA    | 754  | C    | O4'-C1'-N1  | 5.03  | 112.22      | 108.20   |
| 24  | BA    | 1781 | U    | P-O5'-C5'   | -5.03 | 112.85      | 120.90   |
| 21  | AA    | 116  | A    | P-O3'-C3'   | -5.03 | 113.67      | 119.70   |
| 24  | BA    | 2268 | A    | P-O3'-C3'   | -5.03 | 113.67      | 119.70   |
| 55  | CA    | 83   | C    | N1-C1'-C2'  | 5.03  | 120.54      | 114.00   |
| 55  | CA    | 794  | A    | N9-C1'-C2'  | -5.03 | 106.47      | 112.00   |
| 55  | CA    | 1139 | G    | N9-C1'-C2'  | -5.03 | 106.47      | 112.00   |
| 24  | DA    | 6    | A    | C6-N1-C2    | 5.03  | 121.62      | 118.60   |
| 24  | DA    | 373  | U    | O4'-C1'-N1  | 5.03  | 112.22      | 108.20   |
| 24  | DA    | 2312 | U    | N1-C2-O2    | 5.03  | 126.32      | 122.80   |
| 24  | BA    | 754  | U    | P-O3'-C3'   | -5.03 | 113.67      | 119.70   |
| 25  | BB    | 53   | A    | P-O3'-C3'   | -5.03 | 113.67      | 119.70   |
| 55  | CA    | 36   | C    | P-O3'-C3'   | -5.03 | 113.67      | 119.70   |
| 55  | CA    | 91   | U    | C3'-C2'-C1' | 5.03  | 105.52      | 101.50   |
| 24  | DA    | 2241 | A    | O4'-C1'-N9  | 5.03  | 112.22      | 108.20   |
| 56  | DB    | 104  | A    | C2-N3-C4    | 5.03  | 113.11      | 110.60   |
| 21  | AA    | 1483 | A    | N9-C4-C5    | -5.02 | 103.79      | 105.80   |
| 24  | BA    | 2451 | A    | C8-N9-C1'   | 5.02  | 136.74      | 127.70   |
| 24  | BA    | 2801 | G    | P-O3'-C3'   | -5.02 | 113.67      | 119.70   |
| 55  | CA    | 1216 | A    | C3'-C2'-C1' | 5.02  | 105.52      | 101.50   |
| 24  | DA    | 2496 | C    | O4'-C1'-N1  | 5.02  | 112.22      | 108.20   |
| 24  | BA    | 60   | G    | OP1-P-O3'   | 5.02  | 116.25      | 105.20   |
| 24  | BA    | 1782 | U    | P-O5'-C5'   | -5.02 | 112.86      | 120.90   |
| 24  | BA    | 1872 | A    | N9-C1'-C2'  | -5.02 | 106.47      | 112.00   |
| 24  | BA    | 2867 | G    | C8-N9-C1'   | 5.02  | 133.53      | 127.00   |
| 55  | CA    | 971  | G    | P-O3'-C3'   | 5.02  | 125.73      | 119.70   |
| 24  | DA    | 41   | C    | O4'-C1'-N1  | 5.02  | 112.22      | 108.20   |
| 24  | BA    | 1779 | U    | O4'-C1'-N1  | 5.02  | 112.22      | 108.20   |
| 55  | CA    | 962  | C    | C3'-C2'-C1' | 5.02  | 105.52      | 101.50   |
| 24  | DA    | 1838 | C    | N1-C1'-C2'  | 5.02  | 120.53      | 114.00   |
| 21  | AA    | 500  | G    | C3'-C2'-C1' | 5.02  | 105.52      | 101.50   |
| 24  | BA    | 69   | C    | C2-N3-C4    | 5.02  | 122.41      | 119.90   |
| 24  | BA    | 71   | A    | O5'-P-OP2   | -5.02 | 101.18      | 105.70   |
| 55  | CA    | 1055 | A    | N9-C1'-C2'  | -5.02 | 106.48      | 112.00   |
| 24  | BA    | 468  | G    | C6-N1-C2    | -5.02 | 122.09      | 125.10   |
| 24  | BA    | 682  | G    | C4-N9-C1'   | 5.02  | 133.02      | 126.50   |
| 24  | BA    | 1667 | G    | O4'-C1'-N9  | 5.02  | 112.21      | 108.20   |
| 24  | DA    | 353  | C    | N1-C1'-C2'  | 5.02  | 120.52      | 114.00   |
| 24  | DA    | 1799 | G    | C4-C5-N7    | -5.02 | 108.79      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | DA    | 2322 | A    | C3'-C2'-C1' | 5.02  | 105.51      | 101.50   |
| 55  | CA    | 274  | A    | O4'-C1'-N9  | 5.02  | 112.21      | 108.20   |
| 24  | DA    | 1507 | C    | N1-C2-O2    | 5.02  | 121.91      | 118.90   |
| 24  | BA    | 514  | A    | P-O5'-C5'   | -5.01 | 112.88      | 120.90   |
| 24  | BA    | 1539 | U    | O4'-C1'-N1  | 5.01  | 112.21      | 108.20   |
| 55  | CA    | 238  | A    | P-O3'-C3'   | 5.01  | 125.72      | 119.70   |
| 55  | CA    | 520  | A    | C3'-C2'-C1' | 5.01  | 105.51      | 101.50   |
| 23  | CW    | 5    | U    | C3'-C2'-C1' | 5.01  | 105.51      | 101.50   |
| 24  | DA    | 1738 | G    | O4'-C1'-N9  | 5.01  | 112.21      | 108.20   |
| 55  | CA    | 688  | G    | C3'-C2'-C1' | 5.01  | 105.51      | 101.50   |
| 21  | AA    | 972  | C    | O4'-C1'-N1  | 5.01  | 112.21      | 108.20   |
| 24  | BA    | 141  | G    | C3'-C2'-C1' | 5.01  | 105.51      | 101.50   |
| 24  | BA    | 334  | C    | O4'-C1'-N1  | 5.01  | 112.21      | 108.20   |
| 24  | BA    | 415  | A    | C6-N1-C2    | 5.01  | 121.61      | 118.60   |
| 24  | BA    | 2589 | A    | N1-C6-N6    | -5.01 | 115.59      | 118.60   |
| 55  | CA    | 1044 | A    | P-O3'-C3'   | 5.01  | 125.71      | 119.70   |
| 55  | CA    | 1338 | G    | C3'-C2'-C1' | 5.01  | 105.51      | 101.50   |
| 24  | DA    | 1061 | U    | P-O3'-C3'   | -5.01 | 113.69      | 119.70   |
| 24  | BA    | 200  | U    | C3'-C2'-C1' | 5.01  | 105.51      | 101.50   |
| 24  | BA    | 623  | C    | C6-N1-C2    | 5.01  | 122.30      | 120.30   |
| 24  | BA    | 783  | A    | N9-C1'-C2'  | -5.01 | 106.49      | 112.00   |
| 24  | BA    | 1496 | A    | P-O5'-C5'   | -5.01 | 112.89      | 120.90   |
| 55  | CA    | 719  | C    | O4'-C1'-N1  | 5.01  | 112.21      | 108.20   |
| 55  | CA    | 1168 | U    | C2-N1-C1'   | 5.01  | 123.71      | 117.70   |
| 24  | DA    | 83   | A    | P-O3'-C3'   | 5.01  | 125.71      | 119.70   |
| 24  | DA    | 2277 | G    | C3'-C2'-C1' | 5.01  | 105.51      | 101.50   |
| 24  | DA    | 335  | C    | C3'-C2'-C1' | 5.01  | 105.51      | 101.50   |
| 21  | AA    | 723  | U    | O4'-C1'-N1  | -5.01 | 104.19      | 108.20   |
| 21  | AA    | 1138 | G    | C3'-C2'-C1' | 5.01  | 105.50      | 101.50   |
| 24  | BA    | 2076 | U    | P-O3'-C3'   | -5.01 | 113.69      | 119.70   |
| 24  | DA    | 483  | A    | C3'-C2'-C1' | 5.01  | 105.51      | 101.50   |
| 24  | DA    | 812  | C    | C6-N1-C2    | 5.01  | 122.30      | 120.30   |
| 24  | DA    | 1061 | U    | C5-C6-N1    | 5.01  | 125.20      | 122.70   |
| 24  | DA    | 2033 | A    | P-O3'-C3'   | 5.01  | 125.71      | 119.70   |
| 24  | DA    | 2064 | C    | C3'-C2'-C1' | 5.01  | 105.51      | 101.50   |
| 24  | DA    | 2312 | U    | C3'-C2'-C1' | 5.01  | 105.50      | 101.50   |
| 24  | BA    | 1908 | C    | O4'-C1'-N1  | 5.00  | 112.20      | 108.20   |
| 24  | BA    | 2249 | U    | C4'-C3'-C2' | 5.00  | 107.61      | 102.60   |
| 24  | DA    | 1238 | G    | P-O3'-C3'   | 5.00  | 125.71      | 119.70   |
| 24  | DA    | 2339 | C    | P-O5'-C5'   | -5.00 | 112.89      | 120.90   |
| 24  | BA    | 684  | G    | C4-C5-N7    | 5.00  | 112.80      | 110.80   |
| 24  | BA    | 1082 | U    | P-O3'-C3'   | 5.00  | 125.70      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | BA    | 1565 | C    | O4'-C1'-N1  | 5.00  | 112.20      | 108.20   |
| 24  | BA    | 2770 | G    | C2-N3-C4    | -5.00 | 109.40      | 111.90   |
| 24  | DA    | 1311 | G    | P-O3'-C3'   | 5.00  | 125.70      | 119.70   |
| 24  | DA    | 1400 | U    | C3'-C2'-C1' | 5.00  | 105.50      | 101.50   |
| 24  | DA    | 2441 | U    | C3'-C2'-C1' | 5.00  | 105.50      | 101.50   |
| 24  | DA    | 2645 | G    | N3-C4-C5    | 5.00  | 131.10      | 128.60   |
| 24  | BA    | 686  | U    | O5'-P-OP2   | -5.00 | 101.20      | 105.70   |
| 24  | BA    | 1985 | C    | P-O5'-C5'   | -5.00 | 112.90      | 120.90   |
| 24  | DA    | 1078 | U    | P-O3'-C3'   | 5.00  | 125.70      | 119.70   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 12  | AM    | 70  | ARG  | Peptide   |
| 27  | BD    | 10  | GLY  | Peptide   |
| 31  | BH    | 48  | GLU  | Mainchain |
| 31  | BH    | 49  | ALA  | Mainchain |
| 37  | BN    | 101 | GLY  | Peptide   |
| 31  | DH    | 47  | PHE  | Peptide   |
| 31  | DH    | 48  | GLU  | Peptide   |
| 31  | DH    | 49  | ALA  | Mainchain |

## 5.2 Too-close contacts [i](#)

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   | AB    | 1704  | 0        | 1732     | 253     | 0            |
| 1   | CB    | 1704  | 0        | 1732     | 203     | 0            |
| 2   | AC    | 1624  | 0        | 1699     | 133     | 0            |
| 2   | CC    | 1624  | 0        | 1699     | 149     | 0            |
| 3   | AD    | 1643  | 0        | 1710     | 139     | 0            |
| 3   | CD    | 1643  | 0        | 1710     | 139     | 0            |
| 4   | AE    | 1105  | 0        | 1148     | 196     | 0            |
| 4   | CE    | 1105  | 0        | 1148     | 127     | 0            |
| 5   | AF    | 817   | 0        | 808      | 91      | 0            |
| 5   | CF    | 817   | 0        | 808      | 76      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | AG    | 1181  | 0        | 1240     | 100     | 0            |
| 6   | CG    | 1174  | 0        | 1230     | 154     | 0            |
| 7   | AH    | 979   | 0        | 1034     | 107     | 0            |
| 7   | CH    | 979   | 0        | 1034     | 95      | 0            |
| 8   | AI    | 1022  | 0        | 1070     | 122     | 0            |
| 8   | CI    | 1022  | 0        | 1070     | 108     | 0            |
| 9   | AJ    | 786   | 0        | 828      | 69      | 0            |
| 9   | CJ    | 786   | 0        | 828      | 114     | 0            |
| 10  | AK    | 877   | 0        | 887      | 103     | 0            |
| 10  | CK    | 877   | 0        | 887      | 82      | 0            |
| 11  | AL    | 955   | 0        | 1019     | 97      | 0            |
| 11  | CL    | 955   | 0        | 1019     | 101     | 0            |
| 12  | AM    | 883   | 0        | 944      | 69      | 0            |
| 12  | CM    | 876   | 0        | 937      | 123     | 0            |
| 13  | AN    | 774   | 0        | 827      | 72      | 0            |
| 13  | CN    | 769   | 0        | 822      | 83      | 0            |
| 14  | AO    | 714   | 0        | 737      | 50      | 0            |
| 14  | CO    | 714   | 0        | 737      | 40      | 0            |
| 15  | AP    | 649   | 0        | 666      | 63      | 0            |
| 15  | CP    | 638   | 0        | 656      | 56      | 0            |
| 16  | AQ    | 648   | 0        | 691      | 70      | 0            |
| 16  | CQ    | 648   | 0        | 691      | 59      | 0            |
| 17  | AR    | 455   | 0        | 478      | 36      | 0            |
| 17  | CR    | 455   | 0        | 478      | 41      | 0            |
| 18  | AS    | 637   | 0        | 665      | 42      | 0            |
| 18  | CS    | 637   | 0        | 665      | 79      | 0            |
| 19  | AT    | 665   | 0        | 714      | 56      | 0            |
| 19  | CT    | 665   | 0        | 714      | 58      | 0            |
| 20  | AU    | 425   | 0        | 449      | 65      | 0            |
| 20  | CU    | 425   | 0        | 449      | 70      | 0            |
| 21  | AA    | 32895 | 0        | 16553    | 1800    | 0            |
| 22  | AV    | 365   | 0        | 185      | 24      | 0            |
| 22  | AX    | 365   | 0        | 185      | 20      | 0            |
| 22  | CV    | 365   | 0        | 185      | 26      | 0            |
| 22  | CX    | 365   | 0        | 185      | 11      | 0            |
| 23  | AW    | 120   | 0        | 61       | 8       | 0            |
| 23  | CW    | 120   | 0        | 61       | 4       | 0            |
| 24  | BA    | 61274 | 0        | 30819    | 3133    | 0            |
| 24  | DA    | 60995 | 0        | 30679    | 3843    | 0            |
| 25  | BB    | 2529  | 0        | 1281     | 109     | 0            |
| 26  | BC    | 2082  | 0        | 2157     | 226     | 0            |
| 26  | DC    | 2082  | 0        | 2157     | 230     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 27  | BD    | 1565  | 0        | 1616     | 200     | 0            |
| 27  | DD    | 1565  | 0        | 1616     | 162     | 0            |
| 28  | BE    | 1552  | 0        | 1619     | 158     | 0            |
| 28  | DE    | 1552  | 0        | 1619     | 170     | 0            |
| 29  | BF    | 1410  | 0        | 1447     | 144     | 0            |
| 29  | DF    | 1420  | 0        | 1460     | 183     | 0            |
| 30  | BG    | 1323  | 0        | 1374     | 149     | 0            |
| 30  | DG    | 1323  | 0        | 1374     | 116     | 0            |
| 31  | BH    | 1111  | 0        | 1148     | 108     | 0            |
| 31  | DH    | 1111  | 0        | 1148     | 100     | 0            |
| 32  | BI    | 1032  | 0        | 1088     | 116     | 0            |
| 32  | DI    | 1032  | 0        | 1088     | 69      | 0            |
| 33  | BJ    | 1129  | 0        | 1162     | 160     | 0            |
| 33  | DJ    | 1129  | 0        | 1162     | 122     | 0            |
| 34  | BK    | 938   | 0        | 1012     | 102     | 0            |
| 34  | DK    | 938   | 0        | 1012     | 114     | 0            |
| 35  | BL    | 1045  | 0        | 1117     | 133     | 0            |
| 35  | DL    | 1045  | 0        | 1117     | 130     | 0            |
| 36  | BM    | 1074  | 0        | 1157     | 129     | 0            |
| 36  | DM    | 1074  | 0        | 1157     | 96      | 0            |
| 37  | BN    | 960   | 0        | 1000     | 102     | 0            |
| 37  | DN    | 960   | 0        | 1000     | 107     | 0            |
| 38  | BO    | 892   | 0        | 923      | 82      | 0            |
| 38  | DO    | 892   | 0        | 923      | 90      | 0            |
| 39  | BP    | 917   | 0        | 965      | 120     | 0            |
| 39  | DP    | 917   | 0        | 965      | 87      | 0            |
| 40  | BQ    | 947   | 0        | 1022     | 147     | 0            |
| 40  | DQ    | 947   | 0        | 1022     | 120     | 0            |
| 41  | BR    | 816   | 0        | 839      | 102     | 0            |
| 41  | DR    | 816   | 0        | 839      | 90      | 0            |
| 42  | BS    | 857   | 0        | 922      | 89      | 0            |
| 42  | DS    | 857   | 0        | 922      | 83      | 0            |
| 43  | BT    | 738   | 0        | 807      | 103     | 0            |
| 43  | DT    | 738   | 0        | 807      | 96      | 0            |
| 44  | BU    | 779   | 0        | 834      | 65      | 0            |
| 44  | DU    | 779   | 0        | 834      | 93      | 0            |
| 45  | BV    | 753   | 0        | 780      | 54      | 0            |
| 45  | DV    | 753   | 0        | 780      | 98      | 0            |
| 46  | BW    | 596   | 0        | 610      | 179     | 0            |
| 46  | DW    | 596   | 0        | 610      | 105     | 0            |
| 47  | BX    | 625   | 0        | 655      | 68      | 0            |
| 47  | DX    | 625   | 0        | 655      | 76      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 48  | BY    | 509   | 0        | 543      | 45      | 0            |
| 48  | DY    | 509   | 0        | 543      | 55      | 0            |
| 49  | BZ    | 449   | 0        | 491      | 41      | 0            |
| 49  | DZ    | 449   | 0        | 491      | 40      | 0            |
| 50  | B0    | 444   | 0        | 461      | 36      | 0            |
| 50  | D0    | 444   | 0        | 461      | 63      | 0            |
| 51  | B1    | 409   | 0        | 440      | 43      | 0            |
| 51  | D1    | 409   | 0        | 440      | 33      | 0            |
| 52  | B2    | 377   | 0        | 418      | 28      | 0            |
| 52  | D2    | 377   | 0        | 418      | 42      | 0            |
| 53  | B3    | 504   | 0        | 574      | 41      | 0            |
| 53  | D3    | 504   | 0        | 574      | 54      | 0            |
| 54  | B4    | 302   | 0        | 340      | 40      | 0            |
| 54  | D4    | 302   | 0        | 340      | 27      | 0            |
| 55  | CA    | 32831 | 0        | 16521    | 2003    | 0            |
| 56  | DB    | 2507  | 0        | 1270     | 160     | 0            |
| 57  | AA    | 43    | 0        | 0        | 0       | 0            |
| 57  | BA    | 136   | 0        | 0        | 0       | 0            |
| 57  | BB    | 4     | 0        | 0        | 0       | 0            |
| 57  | BD    | 1     | 0        | 0        | 0       | 0            |
| 57  | CA    | 42    | 0        | 0        | 0       | 0            |
| 57  | D4    | 1     | 0        | 0        | 0       | 0            |
| 57  | DA    | 132   | 0        | 0        | 0       | 0            |
| 57  | DB    | 1     | 0        | 0        | 0       | 0            |
| 57  | DC    | 2     | 0        | 0        | 0       | 0            |
| 57  | DJ    | 1     | 0        | 0        | 0       | 0            |
| 58  | B4    | 1     | 0        | 0        | 0       | 0            |
| 58  | D4    | 1     | 0        | 0        | 0       | 0            |
| 59  | AA    | 196   | 0        | 0        | 7       | 0            |
| 59  | AE    | 1     | 0        | 0        | 0       | 0            |
| 59  | AL    | 3     | 0        | 0        | 0       | 0            |
| 59  | AN    | 6     | 0        | 0        | 1       | 0            |
| 59  | AT    | 1     | 0        | 0        | 0       | 0            |
| 59  | AU    | 1     | 0        | 0        | 0       | 0            |
| 59  | B2    | 1     | 0        | 0        | 0       | 0            |
| 59  | B3    | 3     | 0        | 0        | 0       | 0            |
| 59  | B4    | 2     | 0        | 0        | 0       | 0            |
| 59  | BA    | 615   | 0        | 0        | 21      | 0            |
| 59  | BB    | 20    | 0        | 0        | 1       | 0            |
| 59  | BC    | 8     | 0        | 0        | 1       | 0            |
| 59  | BD    | 3     | 0        | 0        | 4       | 0            |
| 59  | BE    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 59  | BL    | 3      | 0        | 0        | 0       | 0            |
| 59  | BN    | 3      | 0        | 0        | 0       | 0            |
| 59  | BT    | 1      | 0        | 0        | 1       | 0            |
| 59  | CA    | 195    | 0        | 0        | 6       | 0            |
| 59  | CE    | 4      | 0        | 0        | 0       | 0            |
| 59  | CI    | 1      | 0        | 0        | 0       | 0            |
| 59  | CL    | 1      | 0        | 0        | 0       | 0            |
| 59  | CN    | 2      | 0        | 0        | 0       | 0            |
| 59  | CT    | 2      | 0        | 0        | 0       | 0            |
| 59  | CU    | 2      | 0        | 0        | 0       | 0            |
| 59  | D2    | 1      | 0        | 0        | 0       | 0            |
| 59  | D3    | 1      | 0        | 0        | 0       | 0            |
| 59  | D4    | 5      | 0        | 0        | 0       | 0            |
| 59  | DA    | 600    | 0        | 0        | 17      | 0            |
| 59  | DB    | 4      | 0        | 0        | 0       | 0            |
| 59  | DC    | 12     | 0        | 0        | 0       | 0            |
| 59  | DD    | 2      | 0        | 0        | 0       | 0            |
| 59  | DE    | 3      | 0        | 0        | 0       | 0            |
| 59  | DJ    | 3      | 0        | 0        | 0       | 0            |
| 59  | DL    | 6      | 0        | 0        | 0       | 0            |
| 59  | DN    | 2      | 0        | 0        | 1       | 0            |
| 59  | DT    | 2      | 0        | 0        | 0       | 0            |
| 59  | DU    | 1      | 0        | 0        | 0       | 0            |
| 59  | DV    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 286150 | 0        | 191700   | 19249   | 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 41.

All (19249) 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) |
|------------------|--------------------|--------------------------|-------------------|
| 12:AM:67:ASP:O   | 12:AM:70:ARG:HD2   | 1.23                     | 1.31              |
| 55:CA:1213:A:O2' | 55:CA:1214:C:H5'   | 1.29                     | 1.25              |
| 24:DA:604:G:O2'  | 24:DA:605:G:H5'    | 1.40                     | 1.19              |
| 40:BQ:63:ARG:NH1 | 40:BQ:96:ASP:HA    | 1.56                     | 1.18              |
| 24:DA:297:G:H5'' | 44:DU:84:PHE:HB2   | 1.26                     | 1.18              |
| 24:BA:2197:U:O2' | 24:BA:2198:A:H2'   | 1.44                     | 1.17              |
| 26:BC:68:ARG:HD3 | 26:BC:103:ILE:HD11 | 1.22                     | 1.15              |
| 24:DA:1439:A:N1  | 24:DA:1552:A:C5    | 2.13                     | 1.15              |
| 29:BF:35:LEU:HB3 | 29:BF:153:ILE:HG22 | 1.24                     | 1.14              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:AM:74:MET:HA   | 12:AM:74:MET:CE   | 1.76                     | 1.13              |
| 52:B2:3:ARG:HH21  | 52:B2:3:ARG:HG2   | 1.14                     | 1.12              |
| 24:DA:1537:G:H2'  | 24:DA:1538:G:H4'  | 1.29                     | 1.11              |
| 33:BJ:44:TYR:HB2  | 40:BQ:63:ARG:HB3  | 1.31                     | 1.11              |
| 55:CA:453:G:H2'   | 55:CA:454:G:H8    | 1.11                     | 1.11              |
| 11:CL:43:LYS:HB3  | 11:CL:44:PRO:HD2  | 1.11                     | 1.11              |
| 4:AE:81:GLN:HG2   | 4:AE:149:PRO:HG3  | 1.28                     | 1.11              |
| 24:DA:1669:A:H2'  | 24:DA:1669:A:N3   | 1.59                     | 1.11              |
| 24:DA:197:A:H62   | 24:DA:2430:A:H2'  | 1.01                     | 1.11              |
| 55:CA:1031:C:H5'  | 55:CA:1032:G:H5'' | 1.31                     | 1.11              |
| 29:DF:109:ARG:HB2 | 29:DF:109:ARG:CZ  | 1.50                     | 1.11              |
| 35:BL:74:THR:HG22 | 35:BL:107:PHE:HB2 | 1.28                     | 1.10              |
| 40:DQ:61:ILE:HD11 | 40:DQ:92:LYS:HD3  | 1.31                     | 1.10              |
| 12:CM:2:ARG:CG    | 12:CM:8:ILE:HG12  | 1.81                     | 1.10              |
| 40:BQ:43:GLN:NE2  | 41:BR:77:PHE:HB3  | 1.67                     | 1.10              |
| 55:CA:974:A:H5''  | 55:CA:975:A:H5'   | 1.24                     | 1.09              |
| 24:DA:2313:C:O2'  | 24:DA:2314:A:H5'  | 1.52                     | 1.09              |
| 6:CG:45:ALA:HB1   | 6:CG:120:ALA:HB2  | 1.33                     | 1.09              |
| 24:DA:216:A:O2'   | 24:DA:217:A:H8    | 1.34                     | 1.09              |
| 24:DA:391:A:O2'   | 24:DA:392:U:H5'   | 1.52                     | 1.08              |
| 46:DW:40:ARG:HG2  | 46:DW:40:ARG:HH11 | 0.99                     | 1.08              |
| 33:BJ:73:VAL:HG23 | 33:BJ:74:TYR:H    | 1.16                     | 1.08              |
| 38:BO:31:THR:HG22 | 38:BO:34:HIS:H    | 1.13                     | 1.08              |
| 12:AM:74:MET:HE2  | 12:AM:74:MET:HA   | 1.13                     | 1.07              |
| 24:DA:1062:G:O2'  | 24:DA:1063:G:H8   | 1.37                     | 1.07              |
| 24:DA:2092:U:H4'  | 24:DA:2093:G:H5'' | 1.28                     | 1.07              |
| 4:AE:96:GLN:O     | 4:AE:122:VAL:HB   | 1.55                     | 1.07              |
| 6:CG:118:ARG:HH22 | 55:CA:1239:A:H3'  | 1.13                     | 1.07              |
| 12:CM:2:ARG:HG3   | 12:CM:8:ILE:CG1   | 1.85                     | 1.06              |
| 18:CS:40:PHE:HB3  | 18:CS:41:PRO:HD2  | 1.37                     | 1.06              |
| 55:CA:82:G:H2'    | 55:CA:83:C:H4'    | 1.35                     | 1.06              |
| 19:AT:43:LYS:HB3  | 19:AT:86:ALA:HB1  | 1.38                     | 1.06              |
| 34:DK:71:ARG:HB3  | 34:DK:72:PRO:HD3  | 1.33                     | 1.06              |
| 55:CA:1054:C:O2'  | 55:CA:1055:A:H5'' | 1.56                     | 1.05              |
| 24:BA:1179:G:H3'  | 24:BA:1180:U:H4'  | 1.36                     | 1.05              |
| 24:DA:2287:A:O2'  | 24:DA:2288:A:H3'  | 1.55                     | 1.05              |
| 24:BA:459:U:O2'   | 24:BA:460:A:H5'   | 1.56                     | 1.05              |
| 5:AF:16:GLU:HG2   | 3:CD:191:SER:HB2  | 1.37                     | 1.05              |
| 27:DD:124:ARG:HD3 | 27:DD:125:TRP:CD1 | 1.91                     | 1.05              |
| 55:CA:453:G:H2'   | 55:CA:454:G:C8    | 1.92                     | 1.05              |
| 24:DA:740:C:H5'   | 24:DA:1784:A:H3'  | 1.34                     | 1.05              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:AK:87:GLY:H    | 10:AK:113:THR:HG22 | 1.20                     | 1.04              |
| 5:AF:3:HIS:H      | 5:AF:92:THR:HG23   | 1.21                     | 1.04              |
| 29:DF:109:ARG:CZ  | 29:DF:109:ARG:CB   | 2.34                     | 1.04              |
| 12:CM:2:ARG:HG3   | 12:CM:8:ILE:HG12   | 1.05                     | 1.03              |
| 12:AM:67:ASP:O    | 12:AM:70:ARG:CD    | 2.05                     | 1.03              |
| 47:DX:53:LYS:HA   | 47:DX:56:ARG:HB3   | 1.37                     | 1.03              |
| 21:AA:414:A:O2'   | 21:AA:415:A:H5'    | 1.56                     | 1.03              |
| 35:BL:27:LEU:HD12 | 35:BL:27:LEU:H     | 1.20                     | 1.03              |
| 40:BQ:63:ARG:HH12 | 40:BQ:96:ASP:HA    | 1.10                     | 1.03              |
| 24:DA:2517:C:O2'  | 24:DA:2518:A:H3'   | 1.58                     | 1.03              |
| 24:DA:740:C:O2'   | 24:DA:741:U:H5'    | 1.57                     | 1.03              |
| 56:DB:58:A:H2'    | 56:DB:59:A:C8      | 1.93                     | 1.03              |
| 11:AL:33:CYS:HA   | 11:AL:54:VAL:HA    | 1.35                     | 1.03              |
| 39:BP:4:ILE:HG22  | 39:BP:5:LYS:H      | 1.20                     | 1.03              |
| 46:BW:17:ALA:HA   | 46:BW:35:ILE:HG23  | 1.40                     | 1.03              |
| 21:AA:1238:A:H5'  | 21:AA:1336:C:H41   | 1.24                     | 1.02              |
| 1:AB:137:THR:HA   | 1:AB:140:LEU:HD13  | 1.41                     | 1.02              |
| 40:DQ:87:VAL:HG21 | 41:DR:52:PRO:HD3   | 1.38                     | 1.02              |
| 24:DA:996:A:H4'   | 40:DQ:91:ARG:HD2   | 1.40                     | 1.02              |
| 39:BP:50:ARG:HB3  | 39:BP:57:ALA:H     | 1.24                     | 1.02              |
| 30:BG:84:LYS:HG3  | 30:BG:132:LEU:H    | 1.25                     | 1.01              |
| 6:CG:101:ARG:HH21 | 55:CA:940:C:H5'    | 1.20                     | 1.01              |
| 12:CM:2:ARG:HD3   | 12:CM:2:ARG:N      | 1.75                     | 1.01              |
| 24:DA:302:C:O2'   | 24:DA:303:G:H8     | 1.42                     | 1.01              |
| 24:BA:825:A:H1'   | 35:BL:54:GLN:NE2   | 1.76                     | 1.01              |
| 14:CO:63:ARG:HH22 | 24:DA:715:A:H5'    | 1.21                     | 1.01              |
| 39:BP:50:ARG:CB   | 39:BP:57:ALA:H     | 1.73                     | 1.01              |
| 43:BT:50:LEU:HD12 | 43:BT:50:LEU:H     | 1.22                     | 1.01              |
| 55:CA:1450:U:H4'  | 55:CA:1451:U:H5    | 1.25                     | 1.01              |
| 32:BI:79:LEU:HA   | 32:BI:83:ALA:HB3   | 1.36                     | 1.01              |
| 24:DA:271:G:O2'   | 24:DA:272:A:H5''   | 1.59                     | 1.01              |
| 24:DA:1439:A:C2   | 24:DA:1552:A:C6    | 2.48                     | 1.01              |
| 24:DA:2746:U:H1'  | 30:DG:138:GLN:HE21 | 1.25                     | 1.01              |
| 36:DM:27:SER:H    | 36:DM:66:ARG:NH2   | 1.59                     | 1.01              |
| 46:BW:37:VAL:HG12 | 46:BW:38:ARG:H     | 1.19                     | 1.00              |
| 9:CJ:79:PRO:HA    | 9:CJ:84:VAL:HG11   | 1.39                     | 1.00              |
| 54:B4:36:ARG:HG2  | 54:B4:37:GLN:H     | 1.22                     | 1.00              |
| 36:DM:136:MET:OXT | 36:DM:136:MET:HG2  | 1.59                     | 1.00              |
| 24:BA:2725:A:O2'  | 24:BA:2726:A:H2'   | 1.58                     | 1.00              |
| 33:BJ:6:ALA:HB3   | 33:BJ:45:THR:HG21  | 1.41                     | 1.00              |
| 33:BJ:21:THR:HG22 | 33:BJ:22:GLY:N     | 1.76                     | 0.99              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:DC:15:VAL:HG22  | 26:DC:205:GLY:HA3 | 1.43                     | 0.99              |
| 55:CA:211:G:H2'    | 55:CA:211:G:N3    | 1.74                     | 0.99              |
| 27:BD:106:LYS:HB3  | 27:BD:206:ALA:HB3 | 1.41                     | 0.99              |
| 26:DC:144:GLU:HA   | 26:DC:151:GLY:HA2 | 1.42                     | 0.99              |
| 27:DD:124:ARG:HD3  | 27:DD:125:TRP:NE1 | 1.77                     | 0.99              |
| 2:AC:76:ILE:HA     | 2:AC:83:VAL:HG23  | 1.43                     | 0.99              |
| 24:DA:2886:A:H62   | 50:D0:39:ARG:HD3  | 1.25                     | 0.99              |
| 12:CM:102:LYS:HA   | 55:CA:1226:C:H5   | 1.24                     | 0.99              |
| 24:DA:1439:A:C2    | 24:DA:1552:A:C5   | 2.50                     | 0.99              |
| 24:DA:197:A:N6     | 24:DA:2430:A:H2'  | 1.77                     | 0.99              |
| 8:AI:129:ARG:NH2   | 21:AA:966:G:H21   | 1.59                     | 0.99              |
| 46:DW:13:ARG:HG3   | 46:DW:14:ASP:H    | 1.28                     | 0.99              |
| 11:CL:43:LYS:HB3   | 11:CL:44:PRO:CD   | 1.91                     | 0.99              |
| 21:AA:982:U:H4'    | 21:AA:983:A:O5'   | 1.61                     | 0.99              |
| 55:CA:1278:G:H4'   | 55:CA:1279:G:O5'  | 1.60                     | 0.99              |
| 18:CS:38:THR:HG1   | 18:CS:40:PHE:HD1  | 1.04                     | 0.99              |
| 24:BA:855:G:H21    | 46:BW:23:LYS:HG2  | 1.26                     | 0.98              |
| 28:DE:170:ARG:HH22 | 28:DE:176:ASP:HB2 | 1.25                     | 0.98              |
| 21:AA:1349:A:H2'   | 21:AA:1350:A:H8   | 1.25                     | 0.98              |
| 13:AN:20:PHE:HA    | 13:AN:24:ALA:HB3  | 1.45                     | 0.98              |
| 21:AA:1050:G:HO2'  | 21:AA:1051:C:H6   | 1.01                     | 0.98              |
| 4:AE:156:ARG:HG2   | 7:AH:63:LYS:HZ1   | 1.24                     | 0.98              |
| 42:BS:96:ILE:HG13  | 42:BS:96:ILE:O    | 1.62                     | 0.98              |
| 24:DA:1311:G:H21   | 24:DA:1603:A:H62  | 1.04                     | 0.98              |
| 37:DN:37:THR:HG22  | 37:DN:39:PRO:HD2  | 1.44                     | 0.98              |
| 55:CA:183:C:O2'    | 55:CA:184:G:H5'   | 1.63                     | 0.98              |
| 36:BM:35:ALA:O     | 36:BM:36:VAL:HB   | 1.64                     | 0.98              |
| 24:DA:2748:A:H1'   | 30:DG:66:THR:HG22 | 1.45                     | 0.98              |
| 21:AA:6:G:N3       | 21:AA:6:G:H2'     | 1.79                     | 0.98              |
| 55:CA:282:A:H2'    | 55:CA:283:U:C6    | 1.97                     | 0.98              |
| 24:BA:1079:C:N4    | 24:BA:1088:A:H2   | 1.62                     | 0.98              |
| 45:BV:80:HIS:HD2   | 45:BV:83:LYS:H    | 1.11                     | 0.98              |
| 24:DA:2023:C:HO2'  | 24:DA:2024:G:H8   | 1.01                     | 0.98              |
| 6:AG:14:ASP:HB3    | 6:AG:18:GLY:H     | 1.29                     | 0.98              |
| 46:BW:9:THR:HG23   | 46:BW:10:ARG:HD3  | 1.45                     | 0.98              |
| 7:CH:52:GLY:HA3    | 7:CH:56:PRO:HA    | 1.43                     | 0.98              |
| 24:DA:2324:U:H5'   | 24:DA:2325:G:H5'' | 1.45                     | 0.98              |
| 24:BA:637:A:H4'    | 24:BA:638:G:O5'   | 1.62                     | 0.97              |
| 31:BH:31:VAL:HB    | 31:BH:32:PRO:HD2  | 1.45                     | 0.97              |
| 40:BQ:69:ARG:HB2   | 40:BQ:69:ARG:HH21 | 1.23                     | 0.97              |
| 1:AB:40:ILE:HD13   | 1:AB:201:GLY:HA2  | 1.46                     | 0.97              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BR:49:ILE:CD1   | 41:BR:52:PRO:HA    | 1.93                     | 0.97              |
| 41:BR:49:ILE:HD12  | 41:BR:52:PRO:HA    | 0.97                     | 0.97              |
| 1:CB:19:THR:HB     | 1:CB:37:VAL:HA     | 1.46                     | 0.97              |
| 24:DA:616:A:H2'    | 24:DA:617:G:C8     | 1.99                     | 0.97              |
| 8:AI:129:ARG:HH21  | 21:AA:966:G:H21    | 1.12                     | 0.97              |
| 24:BA:826:U:O2'    | 35:BL:53:GLY:HA3   | 1.64                     | 0.97              |
| 55:CA:372:C:H4'    | 55:CA:373:A:H5'    | 1.46                     | 0.97              |
| 24:DA:475:C:H2'    | 24:DA:476:G:C8     | 1.99                     | 0.97              |
| 24:DA:491:G:H2'    | 24:DA:492:A:C8     | 2.00                     | 0.97              |
| 27:BD:5:VAL:H      | 27:BD:32:ASN:HD21  | 1.08                     | 0.97              |
| 2:CC:2:GLN:HB3     | 55:CA:1191:A:OP1   | 1.65                     | 0.97              |
| 55:CA:282:A:H2'    | 55:CA:283:U:H6     | 1.26                     | 0.97              |
| 24:DA:2836:U:HO2'  | 24:DA:2837:A:H8    | 0.99                     | 0.97              |
| 4:AE:19:ARG:HA     | 4:AE:31:SER:O      | 1.64                     | 0.97              |
| 8:AI:6:TYR:HE2     | 8:AI:17:ARG:HB2    | 1.29                     | 0.97              |
| 29:BF:104:THR:HG22 | 29:BF:105:ILE:HG23 | 1.47                     | 0.97              |
| 24:DA:1552:A:N3    | 24:DA:1552:A:H2'   | 1.79                     | 0.97              |
| 41:BR:49:ILE:HD12  | 41:BR:52:PRO:CA    | 1.94                     | 0.97              |
| 55:CA:6:G:N3       | 55:CA:6:G:H2'      | 1.80                     | 0.97              |
| 24:DA:1429:G:O2'   | 24:DA:1430:G:H8    | 1.46                     | 0.97              |
| 21:AA:430:A:O2'    | 21:AA:431:A:H5'    | 1.63                     | 0.96              |
| 24:BA:1179:G:C5    | 24:BA:1180:U:H1'   | 2.00                     | 0.96              |
| 24:DA:1716:U:O2'   | 24:DA:1717:A:H8    | 1.46                     | 0.96              |
| 11:AL:23:LEU:HG    | 11:AL:24:GLU:H     | 1.28                     | 0.96              |
| 24:BA:2136:G:H2'   | 24:BA:2137:U:C5    | 1.99                     | 0.96              |
| 24:BA:990:A:H5'    | 24:BA:990:A:H8     | 1.30                     | 0.96              |
| 24:DA:1731:G:O2'   | 24:DA:1732:C:H5''  | 1.64                     | 0.96              |
| 40:DQ:4:LYS:NZ     | 40:DQ:6:GLY:HA3    | 1.79                     | 0.96              |
| 43:DT:39:THR:HG21  | 43:DT:42:GLU:HB2   | 1.42                     | 0.96              |
| 31:DH:97:ARG:O     | 31:DH:98:ASP:HB2   | 1.64                     | 0.96              |
| 21:AA:1258:G:O2'   | 21:AA:1259:C:H5'   | 1.64                     | 0.96              |
| 17:CR:72:ARG:H     | 17:CR:72:ARG:HE    | 1.01                     | 0.96              |
| 21:AA:1046:A:O2'   | 21:AA:1047:G:H5'   | 1.65                     | 0.96              |
| 11:AL:33:CYS:HB3   | 11:AL:54:VAL:HG22  | 1.46                     | 0.96              |
| 27:BD:13:ARG:HH12  | 39:BP:74:GLN:HE21  | 1.04                     | 0.96              |
| 8:CI:125:GLN:HE21  | 8:CI:125:GLN:H     | 1.04                     | 0.96              |
| 9:CJ:52:LEU:HB2    | 13:CN:80:ARG:HE    | 1.30                     | 0.96              |
| 24:DA:1283:G:H22   | 24:DA:1286:A:H5'   | 1.26                     | 0.96              |
| 24:DA:2631:G:H2'   | 24:DA:2632:A:H5''  | 1.48                     | 0.96              |
| 45:DV:29:ILE:HD13  | 45:DV:31:TYR:CE2   | 1.99                     | 0.96              |
| 26:BC:251:THR:HG22 | 26:BC:252:LYS:H    | 1.26                     | 0.96              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BN:33:ILE:HG23  | 37:BN:114:GLU:HB3  | 1.47                     | 0.96              |
| 6:CG:91:ARG:HG2    | 6:CG:92:PRO:HD2    | 1.47                     | 0.96              |
| 2:AC:154:GLY:HA2   | 2:AC:162:ALA:HB1   | 1.48                     | 0.95              |
| 1:CB:104:LYS:H     | 1:CB:104:LYS:HD2   | 1.31                     | 0.95              |
| 31:BH:31:VAL:HB    | 31:BH:32:PRO:CD    | 1.95                     | 0.95              |
| 1:AB:22:TRP:HA     | 1:AB:189:ASN:HA    | 1.46                     | 0.95              |
| 24:DA:1537:G:C2'   | 24:DA:1538:G:H4'   | 1.95                     | 0.95              |
| 21:AA:1054:C:C5    | 22:AX:34:G:H1'     | 2.02                     | 0.95              |
| 24:BA:2136:G:H2'   | 24:BA:2137:U:H5    | 1.28                     | 0.95              |
| 37:BN:38:LEU:O     | 37:BN:38:LEU:HD12  | 1.65                     | 0.95              |
| 10:CK:115:ILE:HD12 | 20:CU:23:GLU:HG2   | 1.47                     | 0.95              |
| 24:BA:1073:A:H2'   | 24:BA:1074:G:H5''  | 1.46                     | 0.95              |
| 8:CI:125:GLN:H     | 8:CI:125:GLN:NE2   | 1.63                     | 0.95              |
| 24:DA:1476:U:O2'   | 24:DA:1477:A:O5'   | 1.84                     | 0.95              |
| 24:DA:1931:U:H2'   | 24:DA:1932:A:H8    | 1.29                     | 0.95              |
| 34:DK:111:LYS:HE3  | 34:DK:111:LYS:H    | 1.32                     | 0.95              |
| 36:DM:19:GLY:H     | 36:DM:38:ARG:HH21  | 1.10                     | 0.95              |
| 39:DP:91:VAL:HG22  | 39:DP:109:ILE:HG21 | 1.48                     | 0.95              |
| 24:BA:2355:G:H4'   | 46:BW:20:LEU:HD13  | 1.48                     | 0.95              |
| 36:BM:40:ARG:HB2   | 36:BM:93:VAL:HG21  | 1.49                     | 0.95              |
| 24:DA:1439:A:C6    | 24:DA:1552:A:N7    | 2.35                     | 0.95              |
| 21:AA:183:C:O2'    | 21:AA:184:G:H5'    | 1.67                     | 0.95              |
| 30:BG:84:LYS:HG3   | 30:BG:132:LEU:N    | 1.80                     | 0.95              |
| 55:CA:1213:A:O2'   | 55:CA:1214:C:C5'   | 2.14                     | 0.94              |
| 20:CU:24:LYS:HG3   | 20:CU:25:ALA:H     | 1.31                     | 0.94              |
| 24:DA:1784:A:H4'   | 24:DA:1785:A:O5'   | 1.66                     | 0.94              |
| 6:AG:87:PRO:HG3    | 6:AG:148:LYS:HA    | 1.44                     | 0.94              |
| 21:AA:204:G:H3'    | 21:AA:205:A:H5''   | 1.45                     | 0.94              |
| 24:BA:639:U:H2'    | 24:BA:640:C:C6     | 2.01                     | 0.94              |
| 20:CU:36:PHE:HB3   | 20:CU:40:PRO:HD3   | 1.46                     | 0.94              |
| 46:DW:27:GLY:HA2   | 46:DW:31:LEU:HD11  | 1.47                     | 0.94              |
| 7:CH:11:THR:HG22   | 7:CH:14:ARG:HH12   | 1.28                     | 0.94              |
| 24:DA:491:G:H2'    | 24:DA:492:A:H8     | 1.31                     | 0.94              |
| 8:AI:50:PRO:HD3    | 8:AI:79:ARG:HG2    | 1.48                     | 0.94              |
| 28:BE:169:VAL:O    | 28:BE:170:ARG:HD2  | 1.67                     | 0.94              |
| 12:CM:102:LYS:HA   | 55:CA:1226:C:C5    | 2.03                     | 0.94              |
| 56:DB:42:C:H2'     | 56:DB:43:C:C6      | 2.03                     | 0.94              |
| 55:CA:1218:C:H2'   | 55:CA:1219:A:C8    | 2.03                     | 0.94              |
| 24:DA:1935:G:H1'   | 24:DA:1964:G:N2    | 1.83                     | 0.94              |
| 31:DH:3:VAL:HG12   | 31:DH:38:PRO:HA    | 1.50                     | 0.94              |
| 24:DA:96:C:H4'     | 48:DY:41:HIS:CD2   | 2.03                     | 0.94              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:AK:28:ASN:HD21  | 10:AK:47:GLY:H    | 1.11                     | 0.94              |
| 33:BJ:81:ILE:HG23  | 33:BJ:82:GLY:H    | 1.30                     | 0.94              |
| 46:BW:24:ARG:HD2   | 46:BW:25:PHE:N    | 1.81                     | 0.94              |
| 24:DA:142:A:H2'    | 24:DA:143:C:C6    | 2.03                     | 0.94              |
| 1:AB:24:PRO:HG3    | 21:AA:830:G:H5'   | 1.50                     | 0.93              |
| 24:BA:1287:A:O2'   | 24:BA:1288:G:H5'  | 1.68                     | 0.93              |
| 40:BQ:10:ARG:NH1   | 40:BQ:10:ARG:HB2  | 1.83                     | 0.93              |
| 36:BM:108:VAL:HG13 | 36:BM:109:PRO:HD2 | 1.50                     | 0.93              |
| 24:DA:1326:U:HO2'  | 24:DA:1327:A:H8   | 0.96                     | 0.93              |
| 24:DA:1915:U:H2'   | 24:DA:1916:A:C8   | 2.04                     | 0.93              |
| 29:DF:137:PHE:HB2  | 29:DF:138:PRO:HD2 | 1.49                     | 0.93              |
| 24:BA:1056:G:H5''  | 24:BA:1057:A:H5'  | 1.47                     | 0.93              |
| 9:CJ:84:VAL:HG23   | 9:CJ:85:ASP:H     | 1.34                     | 0.93              |
| 55:CA:1088:G:H21   | 55:CA:1167:A:H61  | 1.14                     | 0.93              |
| 1:AB:113:LEU:HD22  | 1:AB:143:LEU:HG   | 1.48                     | 0.93              |
| 24:DA:364:C:H2'    | 24:DA:365:U:C6    | 2.04                     | 0.93              |
| 24:DA:589:U:O2'    | 24:DA:590:A:H8    | 1.50                     | 0.93              |
| 11:AL:43:LYS:HD3   | 11:AL:43:LYS:H    | 1.32                     | 0.93              |
| 43:BT:30:ILE:HG23  | 43:BT:85:VAL:HB   | 1.51                     | 0.93              |
| 20:CU:39:LYS:H     | 20:CU:40:PRO:HD2  | 1.32                     | 0.93              |
| 46:DW:39:GLN:HE22  | 46:DW:58:LEU:HD23 | 1.34                     | 0.93              |
| 49:BZ:29:ARG:HH21  | 49:BZ:29:ARG:HG3  | 1.34                     | 0.93              |
| 21:AA:109:A:H2'    | 21:AA:326:G:H21   | 1.34                     | 0.92              |
| 35:BL:93:ASN:HD22  | 35:BL:94:THR:N    | 1.67                     | 0.92              |
| 24:DA:1469:A:H2'   | 24:DA:1470:A:C8   | 2.03                     | 0.92              |
| 55:CA:977:A:H2'    | 55:CA:1224:U:O4   | 1.69                     | 0.92              |
| 24:DA:15:G:OP1     | 50:D0:20:ALA:HB2  | 1.70                     | 0.92              |
| 24:DA:33:C:O2'     | 24:DA:34:U:H5'    | 1.68                     | 0.92              |
| 35:DL:23:ILE:HG13  | 41:DR:82:HIS:CE1  | 2.04                     | 0.92              |
| 42:BS:73:LYS:HE3   | 42:BS:74:ILE:H    | 1.34                     | 0.92              |
| 24:DA:802:A:H2'    | 24:DA:803:U:C6    | 2.03                     | 0.92              |
| 24:BA:1784:A:H4'   | 24:BA:1785:A:O5'  | 1.66                     | 0.92              |
| 24:BA:802:A:H2'    | 24:BA:803:U:C6    | 2.04                     | 0.92              |
| 34:BK:111:LYS:H    | 34:BK:111:LYS:HE2 | 1.33                     | 0.92              |
| 55:CA:1399:C:H4'   | 55:CA:1400:C:O5'  | 1.68                     | 0.92              |
| 55:CA:512:U:O2'    | 55:CA:513:C:H5'   | 1.70                     | 0.92              |
| 21:AA:1349:A:H2'   | 21:AA:1350:A:C8   | 2.05                     | 0.92              |
| 24:BA:2233:U:H2'   | 24:BA:2234:G:C8   | 2.04                     | 0.92              |
| 42:BS:18:ARG:HG2   | 42:BS:76:VAL:HG13 | 1.49                     | 0.92              |
| 35:BL:29:LYS:HG2   | 35:BL:30:THR:HG23 | 1.50                     | 0.92              |
| 38:BO:49:VAL:HG21  | 38:BO:82:ALA:HA   | 1.51                     | 0.92              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:CA:1255:G:H22  | 55:CA:1283:U:H3    | 1.18                     | 0.92              |
| 55:CA:1450:U:H4'  | 55:CA:1451:U:C5    | 2.04                     | 0.92              |
| 24:DA:445:C:O2'   | 24:DA:446:G:O4'    | 1.88                     | 0.92              |
| 32:BI:23:VAL:HB   | 32:BI:27:LEU:HB3   | 1.49                     | 0.92              |
| 33:BJ:30:THR:HG22 | 33:BJ:31:GLU:N     | 1.85                     | 0.92              |
| 38:BO:31:THR:CG2  | 38:BO:34:HIS:H     | 1.82                     | 0.92              |
| 4:CE:38:VAL:HG12  | 4:CE:39:GLY:H      | 1.32                     | 0.92              |
| 40:DQ:4:LYS:HZ2   | 40:DQ:6:GLY:HA3    | 1.29                     | 0.92              |
| 46:DW:28:GLU:H    | 46:DW:31:LEU:HD21  | 1.32                     | 0.92              |
| 24:DA:2051:A:H4'  | 24:DA:2052:A:OP1   | 1.68                     | 0.92              |
| 5:AF:50:PRO:HD2   | 17:AR:73:HIS:HD2   | 1.35                     | 0.92              |
| 30:BG:8:VAL:HG11  | 30:BG:49:LEU:HB2   | 1.50                     | 0.92              |
| 24:DA:1238:G:H2'  | 24:DA:1239:G:H8    | 1.33                     | 0.92              |
| 28:DE:130:LYS:HB3 | 28:DE:133:LEU:HB3  | 1.52                     | 0.92              |
| 24:DA:444:C:HO2'  | 24:DA:445:C:H6     | 0.98                     | 0.91              |
| 24:DA:647:G:H2'   | 24:DA:648:G:H8     | 1.32                     | 0.91              |
| 43:DT:29:THR:HB   | 43:DT:87:LEU:H     | 1.33                     | 0.91              |
| 55:CA:1215:G:O2'  | 55:CA:1216:A:H5'   | 1.69                     | 0.91              |
| 55:CA:132:C:HO2'  | 55:CA:133:U:H6     | 0.95                     | 0.91              |
| 11:CL:80:LEU:HD23 | 11:CL:97:VAL:HG21  | 1.51                     | 0.91              |
| 24:DA:1474:U:H2'  | 24:DA:1475:G:H5'   | 1.52                     | 0.91              |
| 29:BF:134:GLN:HG2 | 29:BF:135:ILE:H    | 1.36                     | 0.91              |
| 43:BT:56:GLU:HG2  | 43:BT:57:VAL:HG12  | 1.51                     | 0.91              |
| 55:CA:547:A:H4'   | 55:CA:548:G:O5'    | 1.66                     | 0.91              |
| 24:DA:915:C:H2'   | 24:DA:916:G:C8     | 2.04                     | 0.91              |
| 39:DP:63:ILE:HA   | 39:DP:68:GLY:HA2   | 1.52                     | 0.91              |
| 21:AA:94:G:H4'    | 21:AA:95:C:C5'     | 2.01                     | 0.91              |
| 21:AA:71:A:H61    | 21:AA:99:C:H1'     | 1.34                     | 0.91              |
| 24:DA:1010:A:O2'  | 24:DA:1011:G:H5''  | 1.70                     | 0.91              |
| 39:DP:20:ARG:HG2  | 39:DP:112:ARG:HH12 | 1.33                     | 0.91              |
| 8:CI:125:GLN:HE21 | 8:CI:125:GLN:N     | 1.69                     | 0.91              |
| 24:DA:1565:C:HO2' | 24:DA:1566:A:H8    | 1.05                     | 0.91              |
| 24:DA:247:G:H4'   | 24:DA:386:G:C5     | 2.05                     | 0.91              |
| 24:BA:979:A:H2'   | 24:BA:982:C:H42    | 1.33                     | 0.91              |
| 21:AA:486:U:H2'   | 21:AA:487:A:C8     | 2.05                     | 0.91              |
| 29:DF:74:ALA:HB3  | 29:DF:78:ILE:HG13  | 1.53                     | 0.91              |
| 21:AA:496:A:N3    | 21:AA:496:A:H2'    | 1.82                     | 0.91              |
| 2:AC:56:ILE:HG12  | 2:AC:65:VAL:HG22   | 1.53                     | 0.91              |
| 41:BR:42:ALA:HA   | 41:BR:46:GLU:HB2   | 1.52                     | 0.91              |
| 42:BS:73:LYS:HE3  | 42:BS:74:ILE:N     | 1.85                     | 0.91              |
| 46:BW:28:GLU:HB3  | 46:BW:31:LEU:HD21  | 1.53                     | 0.91              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DD:106:LYS:HB3  | 27:DD:206:ALA:HB3 | 1.52                     | 0.91              |
| 3:AD:68:GLU:HG3    | 21:AA:545:C:H5'   | 1.53                     | 0.90              |
| 28:DE:47:LYS:HB3   | 28:DE:51:GLU:HB2  | 1.53                     | 0.90              |
| 46:DW:40:ARG:NH1   | 46:DW:40:ARG:HG2  | 1.80                     | 0.90              |
| 24:BA:1060:U:H5''  | 24:BA:1061:U:H5'  | 1.51                     | 0.90              |
| 24:BA:1746:A:H2'   | 24:BA:1747:U:C6   | 2.05                     | 0.90              |
| 55:CA:1382:C:HO2'  | 55:CA:1383:C:H6   | 0.96                     | 0.90              |
| 24:DA:616:A:H2'    | 24:DA:617:G:H8    | 1.35                     | 0.90              |
| 34:BK:21:CYS:HB2   | 34:BK:39:ILE:HD11 | 1.53                     | 0.90              |
| 40:BQ:65:ASN:HD21  | 40:BQ:69:ARG:HH22 | 1.15                     | 0.90              |
| 24:DA:2135:A:H2'   | 24:DA:2136:G:O4'  | 1.70                     | 0.90              |
| 1:AB:108:GLN:H     | 1:AB:108:GLN:HE21 | 1.17                     | 0.90              |
| 1:AB:89:PHE:HB3    | 1:AB:149:GLY:HA2  | 1.54                     | 0.90              |
| 32:BI:15:GLY:HA2   | 32:BI:50:LYS:HB3  | 1.53                     | 0.90              |
| 21:AA:1319:A:H4'   | 21:AA:1320:C:OP1  | 1.71                     | 0.90              |
| 40:BQ:63:ARG:HH12  | 40:BQ:96:ASP:CA   | 1.83                     | 0.90              |
| 1:CB:79:VAL:HA     | 1:CB:213:LEU:HD21 | 1.51                     | 0.90              |
| 24:DA:373:U:HO2'   | 24:DA:374:A:H8    | 0.90                     | 0.90              |
| 24:BA:859:G:H8     | 24:BA:859:G:OP2   | 1.55                     | 0.90              |
| 24:DA:915:C:H2'    | 24:DA:916:G:H8    | 1.36                     | 0.90              |
| 30:DG:93:TYR:HD2   | 30:DG:93:TYR:H    | 1.16                     | 0.90              |
| 15:AP:73:ALA:O     | 15:AP:77:GLU:HB2  | 1.72                     | 0.90              |
| 41:BR:16:GLU:HA    | 41:BR:98:ILE:HG22 | 1.53                     | 0.90              |
| 24:DA:397:U:OP1    | 47:DX:30:PRO:HA   | 1.72                     | 0.90              |
| 24:DA:647:G:H2'    | 24:DA:648:G:C8    | 2.07                     | 0.90              |
| 21:AA:212:G:O2'    | 21:AA:213:G:H8    | 1.52                     | 0.90              |
| 3:AD:109:THR:HG23  | 3:AD:112:GLU:H    | 1.33                     | 0.90              |
| 24:DA:2036:C:O2'   | 24:DA:2037:A:C8   | 2.25                     | 0.90              |
| 37:DN:22:ARG:HG3   | 37:DN:70:THR:HA   | 1.52                     | 0.90              |
| 24:BA:752:A:H62    | 24:BA:2609:U:H3   | 1.17                     | 0.90              |
| 43:BT:39:THR:HB    | 43:BT:42:GLU:HB2  | 1.51                     | 0.90              |
| 24:BA:2354:C:H4'   | 46:BW:31:LEU:HD22 | 1.54                     | 0.89              |
| 24:DA:2311:A:N3    | 24:DA:2311:A:H2'  | 1.86                     | 0.89              |
| 10:AK:28:ASN:ND2   | 10:AK:47:GLY:H    | 1.70                     | 0.89              |
| 27:BD:9:VAL:HG22   | 27:BD:26:VAL:HB   | 1.54                     | 0.89              |
| 55:CA:1241:G:O2'   | 55:CA:1242:G:H8   | 1.54                     | 0.89              |
| 26:DC:128:THR:HG22 | 26:DC:188:ARG:HB3 | 1.54                     | 0.89              |
| 24:BA:1563:U:H2'   | 24:BA:1564:C:H6   | 1.38                     | 0.89              |
| 24:DA:2358:A:H61   | 35:DL:54:GLN:HE22 | 1.17                     | 0.89              |
| 21:AA:555:U:H2'    | 21:AA:556:C:H6    | 1.37                     | 0.89              |
| 4:AE:76:ASN:HB3    | 4:AE:81:GLN:HG3   | 1.54                     | 0.89              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:AE:94:PHE:HZ    | 4:AE:96:GLN:HE21   | 1.17                     | 0.89              |
| 24:DA:2308:G:O6   | 24:DA:2311:A:N6    | 2.06                     | 0.89              |
| 38:DO:115:LEU:H   | 38:DO:115:LEU:HD13 | 1.36                     | 0.89              |
| 13:AN:40:ARG:HH12 | 13:AN:44:VAL:HG21  | 1.35                     | 0.89              |
| 24:BA:2308:G:HO2' | 24:BA:2310:C:H5    | 0.93                     | 0.89              |
| 24:DA:1739:A:H2'  | 24:DA:1740:G:H8    | 1.37                     | 0.89              |
| 13:CN:89:ARG:HG3  | 13:CN:91:GLU:HG2   | 1.54                     | 0.89              |
| 21:AA:513:C:H2'   | 21:AA:514:C:H6     | 1.37                     | 0.89              |
| 27:BD:53:GLY:HA3  | 27:BD:77:ARG:H     | 1.38                     | 0.89              |
| 6:AG:3:ARG:HG3    | 6:AG:4:ARG:H       | 1.38                     | 0.89              |
| 6:AG:74:VAL:HG21  | 6:AG:143:MET:HG2   | 1.51                     | 0.89              |
| 5:AF:50:PRO:HD2   | 17:AR:73:HIS:CD2   | 2.08                     | 0.89              |
| 24:BA:197:A:H62   | 24:BA:2430:A:H2'   | 1.33                     | 0.89              |
| 24:BA:860:U:O2'   | 24:BA:861:A:H5'    | 1.73                     | 0.89              |
| 24:DA:1739:A:H2'  | 24:DA:1740:G:C8    | 2.08                     | 0.89              |
| 4:AE:76:ASN:HB3   | 4:AE:81:GLN:CG     | 2.03                     | 0.89              |
| 24:BA:118:A:C8    | 24:BA:119:A:C8     | 2.61                     | 0.89              |
| 40:BQ:43:GLN:HE21 | 41:BR:77:PHE:HB3   | 1.24                     | 0.89              |
| 21:AA:1530:G:O2'  | 21:AA:1531:A:H8    | 1.56                     | 0.89              |
| 26:BC:12:ARG:HH11 | 26:BC:12:ARG:CG    | 1.86                     | 0.89              |
| 55:CA:181:A:HO2'  | 55:CA:182:A:H2     | 0.94                     | 0.89              |
| 7:CH:73:SER:HB2   | 7:CH:129:ALA:HB3   | 1.52                     | 0.89              |
| 27:BD:97:SER:HB3  | 27:BD:99:GLU:OE1   | 1.74                     | 0.88              |
| 55:CA:1356:G:H2'  | 55:CA:1357:A:C8    | 2.08                     | 0.88              |
| 24:DA:2259:U:O2'  | 24:DA:2260:C:H6    | 1.54                     | 0.88              |
| 48:DY:20:ASN:HD22 | 48:DY:50:VAL:HG22  | 1.35                     | 0.88              |
| 24:DA:2056:G:H21  | 50:D0:1:ALA:H3     | 1.19                     | 0.88              |
| 24:DA:946:C:HO2'  | 24:DA:947:A:H8     | 0.89                     | 0.88              |
| 6:CG:118:ARG:NH2  | 55:CA:1239:A:H3'   | 1.88                     | 0.88              |
| 7:CH:106:SER:HA   | 55:CA:642:A:N7     | 1.88                     | 0.88              |
| 1:CB:67:LEU:HB2   | 1:CB:160:LEU:HG    | 1.56                     | 0.88              |
| 28:BE:79:ARG:HG2  | 28:BE:80:SER:H     | 1.38                     | 0.88              |
| 2:CC:106:ARG:HD3  | 2:CC:106:ARG:H     | 1.37                     | 0.88              |
| 30:BG:122:ALA:HB2 | 30:BG:132:LEU:HB3  | 1.54                     | 0.88              |
| 55:CA:151:A:H2'   | 55:CA:152:A:O4'    | 1.74                     | 0.88              |
| 55:CA:499:A:O2'   | 55:CA:500:G:C8     | 2.25                     | 0.88              |
| 1:CB:114:LYS:HA   | 1:CB:117:GLU:HG2   | 1.55                     | 0.88              |
| 24:DA:637:A:H4'   | 24:DA:638:G:O5'    | 1.69                     | 0.88              |
| 24:DA:668:A:H2'   | 24:DA:670:A:H62    | 1.37                     | 0.88              |
| 51:B1:47:ILE:H    | 51:B1:47:ILE:HD12  | 1.38                     | 0.88              |
| 24:BA:1509:A:O2'  | 24:BA:1510:G:O5'   | 1.92                     | 0.88              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:109:C:H4'   | 24:DA:348:A:H4'    | 1.55                     | 0.88              |
| 24:DA:575:A:O2'   | 24:DA:576:U:H5'    | 1.73                     | 0.88              |
| 33:BJ:44:TYR:CD1  | 40:BQ:59:LEU:HD11  | 2.08                     | 0.88              |
| 46:BW:51:GLY:HA3  | 46:BW:59:PHE:CE2   | 2.08                     | 0.88              |
| 55:CA:113:G:H1'   | 55:CA:354:G:H5'    | 1.56                     | 0.88              |
| 24:BA:869:G:H4'   | 36:BM:8:LYS:HE2    | 1.56                     | 0.88              |
| 55:CA:960:U:O2'   | 55:CA:1223:C:H5''  | 1.72                     | 0.88              |
| 51:D1:7:LYS:HD3   | 53:D3:33:THR:HG21  | 1.55                     | 0.88              |
| 36:DM:35:ALA:HB3  | 36:DM:99:GLY:H     | 1.38                     | 0.88              |
| 24:DA:83:A:H61    | 24:DA:101:A:H5'    | 1.37                     | 0.88              |
| 24:DA:2838:G:H1'  | 37:DN:45:ARG:HH22  | 1.38                     | 0.88              |
| 15:CP:20:VAL:HG21 | 15:CP:32:PHE:HB2   | 1.53                     | 0.88              |
| 24:DA:2385:C:HO2' | 24:DA:2386:A:H8    | 1.22                     | 0.88              |
| 41:DR:39:LEU:HA   | 41:DR:49:ILE:HG21  | 1.54                     | 0.88              |
| 24:BA:2197:U:OP1  | 3:CD:150:LYS:HG3   | 1.74                     | 0.87              |
| 24:BA:954:G:C5    | 24:BA:955:U:C5     | 2.61                     | 0.87              |
| 55:CA:1300:G:H22  | 55:CA:1334:G:H2'   | 1.37                     | 0.87              |
| 55:CA:654:G:H2'   | 55:CA:655:A:C8     | 2.09                     | 0.87              |
| 24:DA:2024:G:H2'  | 24:DA:2025:C:C6    | 2.09                     | 0.87              |
| 24:DA:2415:G:H4'  | 35:DL:66:PHE:HB2   | 1.53                     | 0.87              |
| 7:AH:29:SER:HB3   | 7:AH:32:LYS:HG3    | 1.56                     | 0.87              |
| 39:BP:20:ARG:HD2  | 39:BP:112:ARG:NH1  | 1.89                     | 0.87              |
| 10:AK:87:GLY:N    | 10:AK:113:THR:HG22 | 1.90                     | 0.87              |
| 24:BA:1817:G:O2'  | 24:BA:1818:U:H5'   | 1.74                     | 0.87              |
| 24:BA:784:G:C6    | 26:BC:227:VAL:HG11 | 2.10                     | 0.87              |
| 31:BH:45:GLU:O    | 31:BH:49:ALA:HB2   | 1.75                     | 0.87              |
| 34:BK:18:ARG:HG3  | 34:BK:18:ARG:HH11  | 1.39                     | 0.87              |
| 37:BN:73:ASN:HA   | 37:BN:76:VAL:HG12  | 1.54                     | 0.87              |
| 56:DB:38:C:H4'    | 38:DO:100:HIS:NE2  | 1.88                     | 0.87              |
| 2:AC:166:TRP:H    | 2:AC:166:TRP:HE3   | 1.16                     | 0.87              |
| 16:AQ:18:LYS:HA   | 16:AQ:47:ASP:HB2   | 1.56                     | 0.87              |
| 24:BA:370:G:O2'   | 24:BA:424:G:OP1    | 1.92                     | 0.87              |
| 24:BA:638:G:H2'   | 24:BA:639:U:C6     | 2.10                     | 0.87              |
| 55:CA:500:G:O2'   | 55:CA:501:C:H5'    | 1.74                     | 0.87              |
| 24:BA:2327:A:H2'  | 24:BA:2328:A:C8    | 2.09                     | 0.87              |
| 24:BA:2492:U:O2'  | 24:BA:2493:U:H5'   | 1.75                     | 0.87              |
| 24:BA:2602:A:H4'  | 24:BA:2603:G:OP2   | 1.74                     | 0.87              |
| 21:AA:82:G:H21    | 21:AA:84:U:H3      | 1.20                     | 0.87              |
| 7:AH:95:MET:HB2   | 7:AH:98:LEU:O      | 1.73                     | 0.87              |
| 24:BA:1026:G:H2'  | 24:BA:1027:A:C8    | 2.10                     | 0.87              |
| 24:BA:754:U:H2'   | 24:BA:755:U:H6     | 1.38                     | 0.87              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BH:32:PRO:HB3   | 47:BX:38:TRP:HB3   | 1.56                     | 0.87              |
| 55:CA:1157:A:H4'   | 55:CA:1158:C:O5'   | 1.72                     | 0.87              |
| 55:CA:994:A:HO2'   | 55:CA:995:C:H6     | 0.89                     | 0.87              |
| 8:CI:5:TYR:HB2     | 8:CI:20:ILE:HG22   | 1.54                     | 0.87              |
| 31:DH:59:ALA:HA    | 31:DH:63:ALA:HB3   | 1.55                     | 0.87              |
| 21:AA:967:C:H2'    | 21:AA:968:A:C8     | 2.10                     | 0.87              |
| 24:BA:860:U:H6     | 24:BA:860:U:H5'    | 1.38                     | 0.87              |
| 29:BF:132:ARG:O    | 29:BF:133:GLU:HB3  | 1.75                     | 0.87              |
| 4:CE:148:SER:H     | 4:CE:151:MET:HE3   | 1.38                     | 0.87              |
| 1:CB:11:ALA:HB1    | 1:CB:211:LEU:HD21  | 1.56                     | 0.87              |
| 33:DJ:64:VAL:HG22  | 33:DJ:68:LYS:HE2   | 1.57                     | 0.87              |
| 20:AU:19:LYS:HZ2   | 20:AU:19:LYS:HA    | 1.40                     | 0.86              |
| 24:DA:272:A:O2'    | 24:DA:273:G:C8     | 2.27                     | 0.86              |
| 28:BE:161:ALA:HA   | 28:BE:164:LEU:HB2  | 1.57                     | 0.86              |
| 24:DA:395:U:O2'    | 24:DA:396:G:H8     | 1.56                     | 0.86              |
| 46:BW:23:LYS:O     | 46:BW:66:VAL:HB    | 1.73                     | 0.86              |
| 55:CA:977:A:H8     | 55:CA:1223:C:C2    | 1.93                     | 0.86              |
| 17:AR:22:TYR:HB2   | 17:AR:61:ALA:HB2   | 1.56                     | 0.86              |
| 17:AR:63:TYR:HE1   | 21:AA:734:G:H21    | 1.18                     | 0.86              |
| 55:CA:922:G:H2'    | 55:CA:923:A:C8     | 2.11                     | 0.86              |
| 24:DA:782:A:OP1    | 24:DA:782:A:H8     | 1.57                     | 0.86              |
| 21:AA:82:G:N2      | 21:AA:84:U:H3      | 1.71                     | 0.86              |
| 21:AA:946:A:H2'    | 21:AA:947:G:C8     | 2.10                     | 0.86              |
| 30:DG:120:ILE:HG13 | 30:DG:140:ILE:HG22 | 1.57                     | 0.86              |
| 46:DW:37:VAL:HG12  | 46:DW:55:ASP:HB2   | 1.56                     | 0.86              |
| 3:AD:187:ARG:HH12  | 3:AD:191:SER:HB2   | 1.36                     | 0.86              |
| 39:BP:61:ARG:HG2   | 39:BP:70:GLU:HG2   | 1.57                     | 0.86              |
| 8:CI:17:ARG:HB2    | 8:CI:65:THR:HB     | 1.58                     | 0.86              |
| 31:DH:115:VAL:HG12 | 31:DH:132:PHE:HB2  | 1.57                     | 0.86              |
| 21:AA:94:G:H4'     | 21:AA:95:C:O5'     | 1.73                     | 0.86              |
| 55:CA:1322:C:O2'   | 55:CA:1323:G:H5'   | 1.74                     | 0.86              |
| 1:CB:53:LEU:HG     | 1:CB:219:THR:HG21  | 1.58                     | 0.86              |
| 24:DA:1312:U:O2'   | 24:DA:1314:C:N4    | 2.08                     | 0.86              |
| 24:DA:2458:G:H2'   | 24:DA:2490:G:H1    | 1.38                     | 0.86              |
| 24:BA:2023:C:O2'   | 24:BA:2024:G:H5'   | 1.75                     | 0.86              |
| 46:BW:9:THR:CG2    | 46:BW:10:ARG:HD3   | 2.05                     | 0.86              |
| 24:DA:1391:U:H4'   | 43:DT:19:LYS:HZ1   | 1.41                     | 0.86              |
| 24:DA:206:U:O2'    | 24:DA:207:A:H5'    | 1.76                     | 0.86              |
| 24:DA:250:G:H2'    | 24:DA:251:A:C8     | 2.10                     | 0.86              |
| 37:DN:62:ASN:O     | 37:DN:63:ARG:HB2   | 1.74                     | 0.86              |
| 45:DV:31:TYR:OH    | 45:DV:90:ASP:HB3   | 1.75                     | 0.86              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:198:G:O2'   | 21:AA:199:A:H8     | 1.57                     | 0.86              |
| 21:AA:484:G:H4'   | 21:AA:485:U:O5'    | 1.73                     | 0.86              |
| 24:BA:459:U:HO2'  | 24:BA:460:A:H5'    | 1.40                     | 0.86              |
| 24:BA:636:G:C6    | 35:BL:111:ILE:HD11 | 2.11                     | 0.86              |
| 6:CG:101:ARG:HH12 | 55:CA:1375:A:H4'   | 1.40                     | 0.86              |
| 55:CA:197:A:C6    | 55:CA:221:C:H4'    | 2.11                     | 0.86              |
| 7:CH:106:SER:HA   | 55:CA:642:A:C5     | 2.11                     | 0.86              |
| 24:DA:1639:C:H2'  | 24:DA:1640:A:H5''  | 1.58                     | 0.86              |
| 45:DV:77:VAL:HA   | 45:DV:89:ILE:HG22  | 1.58                     | 0.86              |
| 24:DA:1931:U:H2'  | 24:DA:1932:A:C8    | 2.11                     | 0.86              |
| 35:DL:47:ARG:HG2  | 35:DL:47:ARG:HH21  | 1.38                     | 0.86              |
| 21:AA:702:A:O2'   | 21:AA:703:G:OP1    | 1.91                     | 0.85              |
| 6:AG:147:ASN:H    | 6:AG:147:ASN:HD22  | 1.24                     | 0.85              |
| 24:BA:1063:G:H2'  | 24:BA:1064:C:O4'   | 1.76                     | 0.85              |
| 24:BA:271:G:O2'   | 24:BA:272:A:H5''   | 1.76                     | 0.85              |
| 30:BG:33:THR:HA   | 30:BG:34:ARG:HH11  | 1.40                     | 0.85              |
| 24:DA:1508:A:H4'  | 24:DA:1509:A:OP1   | 1.73                     | 0.85              |
| 26:BC:52:HIS:NE2  | 26:BC:218:THR:HG23 | 1.91                     | 0.85              |
| 55:CA:555:U:H2'   | 55:CA:556:C:H6     | 1.41                     | 0.85              |
| 32:DI:91:LYS:HB3  | 32:DI:94:LYS:HB2   | 1.57                     | 0.85              |
| 34:DK:13:ASN:HD21 | 34:DK:97:THR:H     | 1.24                     | 0.85              |
| 20:AU:19:LYS:NZ   | 20:AU:19:LYS:HA    | 1.91                     | 0.85              |
| 55:CA:197:A:H4'   | 55:CA:198:G:O5'    | 1.72                     | 0.85              |
| 55:CA:346:G:H2'   | 55:CA:346:G:N3     | 1.88                     | 0.85              |
| 24:DA:1245:G:H4'  | 28:DE:33:VAL:HG11  | 1.58                     | 0.85              |
| 24:DA:1857:G:H1'  | 24:DA:1884:G:H22   | 1.41                     | 0.85              |
| 4:AE:96:GLN:OE1   | 4:AE:97:PRO:HD2    | 1.74                     | 0.85              |
| 8:AI:59:LYS:HD2   | 8:AI:60:LEU:HD22   | 1.55                     | 0.85              |
| 24:BA:669:G:N3    | 24:BA:669:G:H2'    | 1.90                     | 0.85              |
| 28:BE:44:ARG:HG3  | 28:BE:44:ARG:NH2   | 1.90                     | 0.85              |
| 6:CG:101:ARG:NH2  | 55:CA:940:C:H5'    | 1.90                     | 0.85              |
| 24:DA:1654:A:O2'  | 24:DA:1655:A:H8    | 1.59                     | 0.85              |
| 21:AA:423:G:H2'   | 21:AA:423:G:N3     | 1.88                     | 0.85              |
| 21:AA:486:U:H5''  | 21:AA:486:U:C6     | 2.12                     | 0.85              |
| 13:AN:44:VAL:HG23 | 13:AN:45:LEU:H     | 1.41                     | 0.85              |
| 9:CJ:11:LYS:NZ    | 9:CJ:99:GLN:HB3    | 1.91                     | 0.85              |
| 24:DA:1819:A:H1'  | 24:DA:1821:A:C6    | 2.11                     | 0.85              |
| 21:AA:51:A:H3'    | 21:AA:51:A:OP1     | 1.76                     | 0.85              |
| 21:AA:631:C:H5''  | 21:AA:632:U:H5'    | 1.57                     | 0.85              |
| 24:BA:1560:G:H2'  | 24:BA:1561:C:H6    | 1.39                     | 0.85              |
| 24:BA:1847:A:H8   | 24:BA:1848:A:N7    | 1.74                     | 0.85              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BE:146:VAL:HG23 | 28:BE:167:VAL:HG23 | 1.57                     | 0.85              |
| 30:BG:7:PRO:O      | 30:BG:8:VAL:HB     | 1.74                     | 0.85              |
| 24:DA:2385:C:O2'   | 24:DA:2386:A:H8    | 1.60                     | 0.85              |
| 24:DA:604:G:HO2'   | 24:DA:605:G:H8     | 0.86                     | 0.85              |
| 46:DW:40:ARG:CG    | 46:DW:40:ARG:HH11  | 1.88                     | 0.85              |
| 21:AA:566:G:H4'    | 21:AA:567:G:OP1    | 1.76                     | 0.85              |
| 24:BA:762:U:H4'    | 24:BA:763:G:O5'    | 1.77                     | 0.85              |
| 26:BC:14:HIS:O     | 26:BC:203:VAL:HG11 | 1.74                     | 0.85              |
| 33:BJ:31:GLU:HG3   | 33:BJ:142:ILE:HG21 | 1.59                     | 0.85              |
| 54:D4:16:ILE:HG12  | 54:D4:25:VAL:HG22  | 1.56                     | 0.85              |
| 24:DA:9:G:H1       | 24:DA:2629:U:H2'   | 1.42                     | 0.85              |
| 46:DW:17:ALA:O     | 46:DW:18:LYS:HB3   | 1.74                     | 0.85              |
| 24:BA:13:A:O2'     | 24:BA:15:G:N7      | 2.10                     | 0.85              |
| 24:BA:181:A:H2'    | 24:BA:182:A:C8     | 2.11                     | 0.85              |
| 24:BA:581:C:H2'    | 24:BA:582:A:H8     | 1.40                     | 0.85              |
| 11:CL:2:THR:HB     | 11:CL:5:GLN:HB2    | 1.56                     | 0.85              |
| 12:CM:12:LYS:HE3   | 12:CM:12:LYS:HA    | 1.56                     | 0.85              |
| 24:DA:373:U:O2'    | 24:DA:374:A:H8     | 1.59                     | 0.85              |
| 30:DG:124:CYS:HB3  | 30:DG:130:ILE:HA   | 1.57                     | 0.85              |
| 21:AA:575:G:H4'    | 21:AA:576:C:C5'    | 2.07                     | 0.85              |
| 21:AA:889:A:H4'    | 21:AA:890:G:OP1    | 1.77                     | 0.85              |
| 21:AA:79:G:H2'     | 21:AA:80:A:H8      | 1.40                     | 0.85              |
| 24:BA:459:U:H2'    | 24:BA:460:A:H8     | 1.40                     | 0.85              |
| 34:BK:71:ARG:HB2   | 34:BK:72:PRO:HD3   | 1.58                     | 0.85              |
| 24:DA:1635:A:O2'   | 24:DA:1636:U:H5'   | 1.75                     | 0.85              |
| 24:DA:2408:U:O2'   | 24:DA:2409:G:H8    | 1.57                     | 0.85              |
| 24:BA:931:U:O4     | 24:BA:1166:G:N2    | 2.09                     | 0.84              |
| 48:BY:56:LEU:O     | 48:BY:57:LEU:HB3   | 1.73                     | 0.84              |
| 24:DA:2837:A:H2'   | 24:DA:2838:G:C8    | 2.12                     | 0.84              |
| 24:DA:510:C:H2'    | 24:DA:511:U:C6     | 2.12                     | 0.84              |
| 27:DD:34:VAL:HG12  | 27:DD:48:ILE:HD11  | 1.59                     | 0.84              |
| 37:BN:79:LEU:O     | 37:BN:80:PHE:HB2   | 1.76                     | 0.84              |
| 55:CA:1203:C:H2'   | 55:CA:1204:A:C8    | 2.11                     | 0.84              |
| 24:DA:1062:G:O4'   | 24:DA:1088:A:N7    | 2.10                     | 0.84              |
| 34:DK:38:ILE:HG12  | 34:DK:61:VAL:HG12  | 1.60                     | 0.84              |
| 21:AA:1157:A:H4'   | 21:AA:1158:C:O5'   | 1.76                     | 0.84              |
| 21:AA:486:U:H6     | 21:AA:486:U:H5''   | 1.41                     | 0.84              |
| 21:AA:548:G:O2'    | 21:AA:549:C:H5'    | 1.77                     | 0.84              |
| 10:CK:110:THR:HG22 | 20:CU:4:LYS:HA     | 1.60                     | 0.84              |
| 24:DA:1996:C:H4'   | 24:DA:1997:C:OP1   | 1.75                     | 0.84              |
| 21:AA:1236:A:H4'   | 21:AA:1304:G:H4'   | 1.57                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:1140:C:P    | 33:BJ:68:LYS:HZ3  | 1.99                     | 0.84              |
| 24:BA:335:C:H5''  | 44:BU:81:ARG:HD3  | 1.59                     | 0.84              |
| 47:BX:5:GLN:NE2   | 47:BX:49:ARG:H    | 1.75                     | 0.84              |
| 55:CA:1299:A:N3   | 55:CA:1299:A:H2'  | 1.91                     | 0.84              |
| 55:CA:374:A:H5''  | 55:CA:452:A:N1    | 1.91                     | 0.84              |
| 5:CF:92:THR:HG22  | 5:CF:94:HIS:H     | 1.42                     | 0.84              |
| 24:DA:2460:U:H2'  | 24:DA:2461:A:C8   | 2.12                     | 0.84              |
| 27:DD:119:ALA:HB3 | 27:DD:163:GLY:H   | 1.41                     | 0.84              |
| 55:CA:576:C:H3'   | 55:CA:577:G:H3'   | 1.59                     | 0.84              |
| 30:DG:1:SER:HB2   | 30:DG:61:TRP:HB3  | 1.60                     | 0.84              |
| 24:DA:2757:A:N1   | 30:DG:66:THR:HG21 | 1.93                     | 0.84              |
| 42:DS:8:ARG:O     | 42:DS:9:HIS:HB2   | 1.76                     | 0.84              |
| 19:AT:6:ALA:HB1   | 19:AT:9:ARG:HB2   | 1.58                     | 0.84              |
| 22:AX:27:G:H8     | 22:AX:27:G:H5''   | 1.42                     | 0.84              |
| 24:BA:279:A:O2'   | 24:BA:280:U:H5'   | 1.77                     | 0.84              |
| 24:BA:320:A:HO2'  | 24:BA:322:A:H8    | 1.24                     | 0.84              |
| 55:CA:834:U:H2'   | 55:CA:835:U:C6    | 2.12                     | 0.84              |
| 24:DA:2520:C:O2'  | 24:DA:2521:C:H6   | 1.59                     | 0.84              |
| 24:DA:607:U:OP1   | 28:DE:98:LYS:HB3  | 1.78                     | 0.84              |
| 21:AA:1138:G:H2'  | 21:AA:1138:G:N3   | 1.92                     | 0.84              |
| 24:BA:545:U:H2'   | 24:BA:546:U:H4'   | 1.58                     | 0.84              |
| 40:BQ:4:LYS:HG3   | 40:BQ:5:ARG:H     | 1.42                     | 0.84              |
| 24:DA:1069:A:O2'  | 24:DA:1070:A:H5'  | 1.76                     | 0.84              |
| 24:DA:2825:G:H3'  | 24:DA:2826:A:H8   | 1.41                     | 0.84              |
| 24:BA:860:U:C6    | 24:BA:860:U:H5'   | 2.12                     | 0.84              |
| 39:BP:33:GLU:HB2  | 39:BP:38:ARG:HH11 | 1.43                     | 0.84              |
| 24:BA:855:G:N2    | 46:BW:23:LYS:HG2  | 1.91                     | 0.84              |
| 55:CA:913:A:O2'   | 55:CA:914:A:H5''  | 1.78                     | 0.84              |
| 1:CB:206:ILE:HA   | 1:CB:209:VAL:HG22 | 1.59                     | 0.84              |
| 32:DI:104:GLN:HA  | 32:DI:107:GLU:HB2 | 1.60                     | 0.84              |
| 21:AA:390:U:H2'   | 21:AA:391:G:H8    | 1.42                     | 0.84              |
| 9:AJ:35:GLN:HA    | 9:AJ:35:GLN:HE21  | 1.43                     | 0.84              |
| 29:BF:35:LEU:HB3  | 29:BF:153:ILE:CG2 | 2.07                     | 0.84              |
| 55:CA:704:A:H2'   | 55:CA:705:G:H8    | 1.42                     | 0.84              |
| 2:CC:150:VAL:HG12 | 2:CC:199:VAL:HG12 | 1.59                     | 0.84              |
| 24:DA:1662:U:H2'  | 24:DA:1663:G:H5'' | 1.57                     | 0.84              |
| 24:DA:919:U:H2'   | 24:DA:920:A:C8    | 2.12                     | 0.84              |
| 24:BA:2197:U:HO2' | 24:BA:2198:A:H8   | 1.25                     | 0.84              |
| 24:BA:2305:U:H2'  | 24:BA:2306:C:O4'  | 1.77                     | 0.84              |
| 24:BA:796:C:H2'   | 24:BA:797:G:H8    | 1.43                     | 0.84              |
| 55:CA:496:A:N3    | 55:CA:496:A:H2'   | 1.91                     | 0.84              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:1563:U:H2'   | 24:DA:1564:C:C6    | 2.13                     | 0.84              |
| 24:DA:787:C:H3'    | 24:DA:791:C:H41    | 1.43                     | 0.84              |
| 34:DK:69:VAL:HG11  | 34:DK:106:GLU:HG2  | 1.58                     | 0.84              |
| 24:DA:922:C:H1'    | 46:DW:22:VAL:HG21  | 1.59                     | 0.84              |
| 21:AA:473:U:H2'    | 21:AA:474:G:H8     | 1.42                     | 0.83              |
| 13:AN:50:LEU:HB3   | 13:AN:51:PRO:HD2   | 1.60                     | 0.83              |
| 24:BA:1392:A:H2'   | 24:BA:1393:A:C8    | 2.13                     | 0.83              |
| 24:BA:945:A:H5'    | 24:BA:946:C:OP2    | 1.78                     | 0.83              |
| 36:BM:40:ARG:HB2   | 36:BM:93:VAL:CG2   | 2.08                     | 0.83              |
| 55:CA:1255:G:N2    | 55:CA:1283:U:H3    | 1.75                     | 0.83              |
| 1:CB:162:VAL:HG13  | 1:CB:184:ALA:HB2   | 1.59                     | 0.83              |
| 22:AX:30:G:H2'     | 22:AX:31:A:H8      | 1.43                     | 0.83              |
| 39:BP:3:ILE:HD13   | 39:BP:3:ILE:O      | 1.78                     | 0.83              |
| 24:DA:1439:A:N1    | 24:DA:1552:A:N7    | 2.24                     | 0.83              |
| 28:DE:148:ILE:HD13 | 28:DE:187:VAL:HG21 | 1.61                     | 0.83              |
| 43:DT:44:LYS:O     | 43:DT:48:GLN:HG2   | 1.78                     | 0.83              |
| 21:AA:94:G:H4'     | 21:AA:95:C:H5''    | 1.60                     | 0.83              |
| 27:BD:107:VAL:H    | 27:BD:206:ALA:H    | 1.23                     | 0.83              |
| 55:CA:1054:C:N4    | 22:CX:34:G:H1'     | 1.93                     | 0.83              |
| 26:DC:146:LYS:HB2  | 26:DC:149:LYS:HB2  | 1.58                     | 0.83              |
| 24:DA:1324:G:O2'   | 24:DA:1616:A:C6    | 2.31                     | 0.83              |
| 24:DA:2287:A:HO2'  | 24:DA:2288:A:H3'   | 1.41                     | 0.83              |
| 24:DA:654:A:H2'    | 24:DA:655:A:H5''   | 1.61                     | 0.83              |
| 21:AA:1224:U:H4'   | 21:AA:1225:A:OP2   | 1.77                     | 0.83              |
| 4:AE:37:VAL:HG21   | 4:AE:113:VAL:HG12  | 1.58                     | 0.83              |
| 20:AU:52:VAL:HG13  | 20:AU:53:LYS:H     | 1.41                     | 0.83              |
| 24:BA:404:A:O2'    | 24:BA:405:U:OP2    | 1.96                     | 0.83              |
| 40:BQ:65:ASN:ND2   | 40:BQ:69:ARG:HH22  | 1.75                     | 0.83              |
| 12:CM:25:GLY:N     | 55:CA:1329:A:H5''  | 1.92                     | 0.83              |
| 9:CJ:11:LYS:HZ1    | 9:CJ:99:GLN:HB3    | 1.44                     | 0.83              |
| 24:DA:16:C:H2'     | 24:DA:17:G:H8      | 1.43                     | 0.83              |
| 24:DA:2273:A:H2'   | 24:DA:2274:A:C8    | 2.12                     | 0.83              |
| 5:AF:53:LYS:NZ     | 21:AA:710:G:H5''   | 1.94                     | 0.83              |
| 24:BA:74:A:H4'     | 24:BA:75:G:O5'     | 1.77                     | 0.83              |
| 38:BO:51:ALA:HB3   | 38:BO:78:VAL:HG13  | 1.60                     | 0.83              |
| 43:BT:29:THR:HB    | 43:BT:86:THR:HG22  | 1.58                     | 0.83              |
| 24:DA:2776:A:H4'   | 24:DA:2777:G:O5'   | 1.77                     | 0.83              |
| 27:DD:105:LYS:HA   | 27:DD:177:VAL:HG22 | 1.60                     | 0.83              |
| 46:BW:39:GLN:HG2   | 46:BW:41:GLY:H     | 1.43                     | 0.83              |
| 55:CA:116:A:H2'    | 55:CA:117:G:C8     | 2.14                     | 0.83              |
| 55:CA:724:G:H2'    | 55:CA:725:G:H8     | 1.40                     | 0.83              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AB:113:LEU:HB2   | 1:AB:143:LEU:HD11 | 1.60                     | 0.83              |
| 24:BA:2297:A:N1    | 24:BA:2321:U:H5   | 1.75                     | 0.83              |
| 55:CA:519:C:H2'    | 55:CA:520:A:C8    | 2.13                     | 0.83              |
| 24:DA:1676:A:C2    | 24:DA:1993:U:H5'  | 2.12                     | 0.83              |
| 46:DW:27:GLY:CA    | 46:DW:31:LEU:HD11 | 2.08                     | 0.83              |
| 24:BA:2756:U:H4'   | 24:BA:2757:A:O5'  | 1.78                     | 0.83              |
| 46:BW:37:VAL:HG12  | 46:BW:38:ARG:N    | 1.94                     | 0.83              |
| 55:CA:274:A:HO2'   | 55:CA:275:G:H8    | 1.25                     | 0.83              |
| 4:CE:41:GLY:O      | 4:CE:118:GLY:HA3  | 1.77                     | 0.83              |
| 24:DA:1283:G:N2    | 24:DA:1286:A:H5'  | 1.93                     | 0.83              |
| 24:DA:2024:G:H2'   | 24:DA:2025:C:H6   | 1.43                     | 0.83              |
| 6:AG:147:ASN:HD22  | 6:AG:147:ASN:N    | 1.75                     | 0.83              |
| 27:BD:16:THR:HG23  | 27:BD:18:ASP:OD1  | 1.78                     | 0.83              |
| 43:BT:44:LYS:HG3   | 43:BT:55:VAL:HG11 | 1.61                     | 0.83              |
| 20:CU:16:ARG:HG3   | 20:CU:19:LYS:HG2  | 1.57                     | 0.83              |
| 24:DA:1674:G:H21   | 24:DA:1677:A:H61  | 1.24                     | 0.83              |
| 24:BA:1509:A:O2'   | 24:BA:1510:G:P    | 2.36                     | 0.82              |
| 31:BH:2:GLN:O      | 31:BH:3:VAL:HG22  | 1.79                     | 0.82              |
| 9:CJ:57:VAL:HG22   | 9:CJ:58:ASN:H     | 1.41                     | 0.82              |
| 24:BA:2148:G:H2'   | 24:BA:2149:U:O4'  | 1.79                     | 0.82              |
| 26:BC:246:PRO:HG2  | 26:BC:247:TRP:CZ3 | 2.14                     | 0.82              |
| 24:DA:2682:A:H61   | 24:DA:2728:U:H1'  | 1.44                     | 0.82              |
| 24:DA:2798:U:H5'   | 24:DA:2800:A:C5   | 2.13                     | 0.82              |
| 26:DC:144:GLU:HB3  | 26:DC:187:CYS:HB2 | 1.60                     | 0.82              |
| 35:DL:124:GLY:H    | 35:DL:143:GLU:HG3 | 1.44                     | 0.82              |
| 39:DP:50:ARG:HB3   | 39:DP:56:SER:HB3  | 1.61                     | 0.82              |
| 21:AA:1386:G:H2'   | 21:AA:1387:G:H8   | 1.44                     | 0.82              |
| 21:AA:96:U:HO2'    | 21:AA:97:G:H8     | 1.27                     | 0.82              |
| 3:AD:172:VAL:HG22  | 3:AD:173:ASP:H    | 1.43                     | 0.82              |
| 5:AF:46:GLN:HA     | 5:AF:56:LYS:HG2   | 1.61                     | 0.82              |
| 9:AJ:57:VAL:HG22   | 9:AJ:58:ASN:H     | 1.45                     | 0.82              |
| 53:B3:22:LYS:HA    | 53:B3:47:ALA:O    | 1.80                     | 0.82              |
| 30:BG:96:ALA:HB3   | 30:BG:103:ASN:HB3 | 1.61                     | 0.82              |
| 32:BI:100:ILE:HG22 | 32:BI:101:SER:H   | 1.45                     | 0.82              |
| 55:CA:82:G:C2'     | 55:CA:83:C:H4'    | 2.08                     | 0.82              |
| 13:CN:89:ARG:HG3   | 13:CN:91:GLU:CG   | 2.09                     | 0.82              |
| 19:CT:2:ASN:N      | 19:CT:7:LYS:HZ3   | 1.77                     | 0.82              |
| 24:DA:1204:A:H4'   | 24:DA:1205:A:O5'  | 1.79                     | 0.82              |
| 21:AA:654:G:H2'    | 21:AA:655:A:C8    | 2.15                     | 0.82              |
| 21:AA:792:A:H4'    | 21:AA:793:U:O5'   | 1.79                     | 0.82              |
| 21:AA:984:C:HO2'   | 21:AA:985:C:H6    | 0.85                     | 0.82              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AC:86:LEU:O     | 2:AC:90:VAL:HG23   | 1.78                     | 0.82              |
| 24:BA:1673:G:H2'  | 24:BA:1674:G:H5'   | 1.61                     | 0.82              |
| 32:BI:78:LEU:HD13 | 32:BI:108:ILE:HG23 | 1.60                     | 0.82              |
| 8:CI:75:ALA:HA    | 8:CI:78:ILE:HD12   | 1.60                     | 0.82              |
| 24:DA:656:G:H2'   | 24:DA:657:U:C6     | 2.13                     | 0.82              |
| 56:DB:5:U:H2'     | 56:DB:6:G:C8       | 2.14                     | 0.82              |
| 39:DP:88:ARG:HE   | 39:DP:112:ARG:HH21 | 1.25                     | 0.82              |
| 21:AA:306:A:H2'   | 21:AA:307:C:C6     | 2.13                     | 0.82              |
| 39:BP:50:ARG:CD   | 39:BP:51:ASN:H     | 1.93                     | 0.82              |
| 46:BW:51:GLY:HA3  | 46:BW:59:PHE:CZ    | 2.14                     | 0.82              |
| 55:CA:94:G:H4'    | 55:CA:95:C:OP1     | 1.79                     | 0.82              |
| 14:CO:16:ARG:HB2  | 14:CO:23:SER:HB2   | 1.61                     | 0.82              |
| 17:CR:72:ARG:H    | 17:CR:72:ARG:NE    | 1.78                     | 0.82              |
| 24:DA:1809:A:O2'  | 24:DA:1810:A:H8    | 1.62                     | 0.82              |
| 37:DN:2:ARG:HD2   | 37:DN:5:LYS:HB3    | 1.61                     | 0.82              |
| 21:AA:558:G:OP1   | 59:AA:1841:HOH:O   | 1.98                     | 0.82              |
| 7:AH:22:ALA:HA    | 7:AH:62:LEU:HB2    | 1.59                     | 0.82              |
| 7:AH:6:ILE:HB     | 7:AH:76:ARG:HH12   | 1.41                     | 0.82              |
| 35:BL:29:LYS:O    | 35:BL:31:GLY:N     | 2.12                     | 0.82              |
| 55:CA:518:C:H4'   | 55:CA:519:C:H5''   | 1.61                     | 0.82              |
| 31:DH:90:LEU:HB2  | 31:DH:123:ARG:HB3  | 1.61                     | 0.82              |
| 32:DI:113:ALA:HB1 | 32:DI:124:MET:SD   | 2.18                     | 0.82              |
| 21:AA:1240:U:H3'  | 21:AA:1241:G:H5'   | 1.59                     | 0.82              |
| 11:AL:62:VAL:HG21 | 11:AL:94:TYR:HE2   | 1.44                     | 0.82              |
| 24:BA:1932:A:H2'  | 24:BA:1933:G:O4'   | 1.80                     | 0.82              |
| 30:BG:82:PHE:CE2  | 30:BG:137:LYS:HB2  | 2.13                     | 0.82              |
| 46:BW:72:GLY:O    | 46:BW:74:LYS:N     | 2.13                     | 0.82              |
| 50:D0:12:ARG:HG3  | 50:D0:15:ARG:HH11  | 1.44                     | 0.82              |
| 24:DA:833:A:H2'   | 24:DA:834:G:C8     | 2.14                     | 0.82              |
| 44:DU:14:THR:HG23 | 44:DU:15:GLY:H     | 1.45                     | 0.82              |
| 21:AA:198:G:HO2'  | 21:AA:199:A:H8     | 0.85                     | 0.82              |
| 10:AK:121:ARG:HE  | 20:AU:35:GLU:HG3   | 1.45                     | 0.82              |
| 24:BA:1073:A:C2'  | 24:BA:1074:G:H5''  | 2.08                     | 0.82              |
| 24:BA:1799:G:H4'  | 24:BA:1800:C:O5'   | 1.79                     | 0.82              |
| 24:BA:1867:G:O2'  | 24:BA:1868:C:H5'   | 1.78                     | 0.82              |
| 11:CL:34:THR:HG22 | 11:CL:35:ARG:HG2   | 1.62                     | 0.82              |
| 18:CS:42:ASN:HB2  | 18:CS:43:MET:HE2   | 1.60                     | 0.82              |
| 24:DA:2753:A:O2'  | 24:DA:2754:U:H5'   | 1.78                     | 0.82              |
| 24:DA:2819:G:H2'  | 24:DA:2821:A:N7    | 1.95                     | 0.82              |
| 35:DL:79:LEU:HB2  | 35:DL:113:ALA:H    | 1.42                     | 0.82              |
| 1:AB:108:GLN:HA   | 1:AB:111:LYS:HB3   | 1.61                     | 0.82              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:1454:C:H41   | 37:BN:73:ASN:HD21  | 1.24                     | 0.82              |
| 24:DA:2460:U:H2'   | 24:DA:2461:A:H8    | 1.43                     | 0.82              |
| 36:DM:42:THR:HG22  | 36:DM:44:ARG:H     | 1.44                     | 0.82              |
| 37:DN:28:LEU:HD21  | 37:DN:115:LEU:HD21 | 1.61                     | 0.82              |
| 19:CT:81:GLN:NE2   | 55:CA:258:G:H5'    | 1.95                     | 0.82              |
| 34:DK:61:VAL:HG11  | 34:DK:112:PHE:HE2  | 1.45                     | 0.82              |
| 21:AA:1007:U:H2'   | 21:AA:1008:U:H5''  | 1.61                     | 0.81              |
| 4:AE:83:PRO:HB3    | 4:AE:97:PRO:HD3    | 1.62                     | 0.81              |
| 31:BH:8:LYS:O      | 31:BH:9:VAL:HB     | 1.80                     | 0.81              |
| 37:BN:23:ASN:HD22  | 37:BN:23:ASN:N     | 1.77                     | 0.81              |
| 38:BO:31:THR:HG22  | 38:BO:34:HIS:N     | 1.93                     | 0.81              |
| 55:CA:1038:C:H2'   | 55:CA:1039:G:C8    | 2.15                     | 0.81              |
| 55:CA:9:G:H2'      | 55:CA:10:A:H8      | 1.45                     | 0.81              |
| 55:CA:78:A:H2'     | 55:CA:79:G:C8      | 2.14                     | 0.81              |
| 24:DA:2421:G:N7    | 53:D3:30:HIS:HD2   | 1.78                     | 0.81              |
| 24:DA:1965:C:H5'   | 24:DA:1966:A:H5''  | 1.60                     | 0.81              |
| 24:DA:249:C:H5''   | 24:DA:2394:C:O2'   | 1.80                     | 0.81              |
| 21:AA:946:A:H2'    | 21:AA:947:G:H8     | 1.43                     | 0.81              |
| 3:AD:115:GLN:HE21  | 3:AD:115:GLN:HA    | 1.44                     | 0.81              |
| 19:AT:82:ILE:O     | 19:AT:86:ALA:HB3   | 1.80                     | 0.81              |
| 24:BA:947:A:H2'    | 24:BA:948:C:C6     | 2.15                     | 0.81              |
| 26:BC:244:VAL:HG12 | 26:BC:250:GLN:HA   | 1.61                     | 0.81              |
| 24:BA:1998:A:OP2   | 27:BD:141:ARG:NH2  | 2.13                     | 0.81              |
| 4:CE:98:ALA:HB2    | 4:CE:123:LEU:HG    | 1.62                     | 0.81              |
| 6:CG:24:LYS:O      | 6:CG:28:ILE:HG12   | 1.80                     | 0.81              |
| 24:DA:1780:A:H4'   | 24:DA:1781:U:OP2   | 1.79                     | 0.81              |
| 24:DA:2189:U:H2'   | 24:DA:2190:G:H5''  | 1.61                     | 0.81              |
| 42:DS:6:LYS:NZ     | 42:DS:104:THR:HG23 | 1.95                     | 0.81              |
| 21:AA:243:A:H4'    | 21:AA:244:U:H5''   | 1.62                     | 0.81              |
| 16:AQ:12:VAL:HG13  | 16:AQ:13:SER:H     | 1.45                     | 0.81              |
| 24:BA:1013:C:H2'   | 24:BA:1014:A:H8    | 1.45                     | 0.81              |
| 24:BA:1368:G:H2'   | 24:BA:1369:G:H8    | 1.44                     | 0.81              |
| 26:BC:80:LEU:HD11  | 26:BC:109:LEU:HG   | 1.62                     | 0.81              |
| 1:CB:116:LEU:HA    | 1:CB:119:GLN:HB2   | 1.62                     | 0.81              |
| 4:CE:104:ILE:HD13  | 4:CE:120:HIS:HA    | 1.62                     | 0.81              |
| 8:CI:112:ARG:HH22  | 9:CJ:64:GLN:HE21   | 1.24                     | 0.81              |
| 32:DI:45:THR:HG23  | 32:DI:54:ILE:HD13  | 1.61                     | 0.81              |
| 38:DO:30:ARG:HG3   | 38:DO:30:ARG:HH11  | 1.46                     | 0.81              |
| 2:AC:184:ASN:HD22  | 2:AC:185:THR:H     | 1.29                     | 0.81              |
| 24:BA:1469:A:H2'   | 24:BA:1470:A:C8    | 2.15                     | 0.81              |
| 24:BA:2472:G:H2'   | 24:BA:2475:C:H42   | 1.46                     | 0.81              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:BA:990:A:H5'    | 24:BA:990:A:C8    | 2.15                     | 0.81              |
| 45:BV:10:LYS:H     | 45:BV:10:LYS:HD3  | 1.45                     | 0.81              |
| 13:CN:63:CYS:HB3   | 13:CN:67:GLY:H    | 1.46                     | 0.81              |
| 26:DC:62:ARG:HG2   | 26:DC:62:ARG:HH21 | 1.44                     | 0.81              |
| 29:DF:64:PRO:HA    | 29:DF:88:VAL:HG22 | 1.60                     | 0.81              |
| 26:BC:109:LEU:HD23 | 26:BC:110:LYS:H   | 1.44                     | 0.81              |
| 55:CA:820:U:H4'    | 55:CA:821:G:OP2   | 1.79                     | 0.81              |
| 53:D3:41:ARG:HH21  | 53:D3:41:ARG:HG3  | 1.45                     | 0.81              |
| 24:DA:1558:C:H4'   | 24:DA:1559:U:H5'  | 1.62                     | 0.81              |
| 24:DA:794:A:H2'    | 24:DA:795:C:C6    | 2.15                     | 0.81              |
| 28:DE:108:ILE:HD11 | 28:DE:181:ILE:HB  | 1.61                     | 0.81              |
| 21:AA:1050:G:O2'   | 21:AA:1051:C:H6   | 1.64                     | 0.81              |
| 21:AA:1197:A:O2'   | 21:AA:1198:G:H5'  | 1.79                     | 0.81              |
| 27:BD:106:LYS:O    | 27:BD:107:VAL:HB  | 1.79                     | 0.81              |
| 29:BF:35:LEU:HD13  | 29:BF:56:LEU:HD22 | 1.62                     | 0.81              |
| 41:BR:49:ILE:HB    | 41:BR:51:VAL:O    | 1.81                     | 0.81              |
| 46:BW:47:GLY:H     | 46:BW:80:SER:HB3  | 1.46                     | 0.81              |
| 9:CJ:82:LYS:HA     | 9:CJ:86:ALA:HB3   | 1.63                     | 0.81              |
| 24:DA:2756:U:O2'   | 24:DA:2757:A:H5'  | 1.81                     | 0.81              |
| 24:DA:762:U:H4'    | 24:DA:763:G:O5'   | 1.81                     | 0.81              |
| 24:BA:1730:C:H1'   | 24:BA:1731:G:N2   | 1.95                     | 0.81              |
| 24:BA:839:U:H2'    | 24:BA:840:C:C6    | 2.15                     | 0.81              |
| 28:BE:44:ARG:HH21  | 28:BE:44:ARG:HG3  | 1.44                     | 0.81              |
| 29:BF:114:ARG:H    | 29:BF:114:ARG:HD2 | 1.46                     | 0.81              |
| 55:CA:960:U:O2'    | 55:CA:1223:C:C5'  | 2.29                     | 0.81              |
| 34:DK:35:VAL:HG23  | 34:DK:36:GLY:H    | 1.46                     | 0.81              |
| 41:DR:27:ILE:HG22  | 41:DR:28:ALA:H    | 1.45                     | 0.81              |
| 55:CA:654:G:H2'    | 55:CA:655:A:H8    | 1.45                     | 0.81              |
| 15:CP:54:LEU:HG    | 15:CP:55:ASP:H    | 1.46                     | 0.81              |
| 20:CU:25:ALA:HA    | 20:CU:28:LEU:HB3  | 1.62                     | 0.81              |
| 24:BA:1560:G:H2'   | 24:BA:1561:C:C6   | 2.15                     | 0.81              |
| 24:BA:2135:A:H2'   | 24:BA:2136:G:C8   | 2.16                     | 0.81              |
| 44:BU:97:SER:O     | 44:BU:98:ASN:HB3  | 1.80                     | 0.81              |
| 5:CF:11:HIS:CE1    | 5:CF:54:LEU:HD21  | 2.15                     | 0.81              |
| 24:DA:1060:U:H4'   | 24:DA:1061:U:C5'  | 2.11                     | 0.81              |
| 24:DA:1287:A:O2'   | 24:DA:1288:G:H5'  | 1.81                     | 0.81              |
| 38:DO:67:ASN:H     | 38:DO:70:ALA:HB3  | 1.46                     | 0.81              |
| 21:AA:939:G:H2'    | 21:AA:940:C:H6    | 1.45                     | 0.81              |
| 24:BA:1430:G:H2'   | 24:BA:1431:A:H8   | 1.45                     | 0.81              |
| 24:BA:2756:U:H1'   | 24:BA:2757:A:H5'' | 1.62                     | 0.81              |
| 40:BQ:63:ARG:HD2   | 40:BQ:64:ILE:N    | 1.95                     | 0.81              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CC:196:GLY:H    | 55:CA:1057:G:H4'   | 1.46                     | 0.81              |
| 24:DA:2056:G:N2   | 50:D0:1:ALA:H3     | 1.79                     | 0.81              |
| 24:DA:2461:A:H1'  | 24:DA:2492:U:H3    | 1.45                     | 0.81              |
| 29:DF:74:ALA:HB1  | 29:DF:76:PHE:CD2   | 2.15                     | 0.81              |
| 44:DU:92:VAL:HB   | 44:DU:101:THR:HG21 | 1.63                     | 0.81              |
| 49:DZ:16:LEU:H    | 49:DZ:16:LEU:HD22  | 1.46                     | 0.81              |
| 1:AB:71:THR:HG22  | 1:AB:72:LYS:H      | 1.45                     | 0.81              |
| 26:BC:166:ARG:HG3 | 26:BC:166:ARG:O    | 1.81                     | 0.81              |
| 37:BN:73:ASN:HD22 | 37:BN:76:VAL:HG11  | 1.46                     | 0.81              |
| 26:DC:43:ASN:ND2  | 26:DC:44:ASN:H     | 1.78                     | 0.81              |
| 7:AH:17:GLN:HE21  | 7:AH:71:VAL:HG23   | 1.46                     | 0.80              |
| 24:BA:1073:A:H3'  | 24:BA:1074:G:C5'   | 2.10                     | 0.80              |
| 24:BA:2292:U:H2'  | 24:BA:2293:G:H8    | 1.46                     | 0.80              |
| 24:BA:994:C:H1'   | 41:BR:10:LYS:NZ    | 1.97                     | 0.80              |
| 40:BQ:91:ARG:NH2  | 40:BQ:93:ILE:HD13  | 1.95                     | 0.80              |
| 55:CA:994:A:O2'   | 55:CA:995:C:H6     | 1.63                     | 0.80              |
| 24:DA:946:C:O2'   | 24:DA:947:A:H8     | 1.63                     | 0.80              |
| 21:AA:1135:U:H3   | 21:AA:1140:C:H42   | 1.25                     | 0.80              |
| 21:AA:968:A:H4'   | 21:AA:969:A:OP2    | 1.82                     | 0.80              |
| 54:B4:33:HIS:O    | 54:B4:35:GLN:HG3   | 1.80                     | 0.80              |
| 24:BA:1062:G:H1'  | 32:BI:134:SER:HB3  | 1.62                     | 0.80              |
| 24:BA:1973:G:H2'  | 24:BA:1974:C:H6    | 1.46                     | 0.80              |
| 33:BJ:21:THR:HG22 | 33:BJ:22:GLY:H     | 1.45                     | 0.80              |
| 55:CA:559:A:H4'   | 55:CA:560:A:H5''   | 1.64                     | 0.80              |
| 12:CM:102:LYS:HG2 | 55:CA:1226:C:H41   | 1.44                     | 0.80              |
| 21:AA:841:C:C2    | 21:AA:843:U:H5'    | 2.17                     | 0.80              |
| 24:BA:1872:A:H2'  | 24:BA:1873:G:O4'   | 1.81                     | 0.80              |
| 24:BA:243:U:O2'   | 24:BA:244:A:H5'    | 1.80                     | 0.80              |
| 39:BP:59:THR:HG23 | 39:BP:72:VAL:HG12  | 1.64                     | 0.80              |
| 55:CA:1135:U:H2'  | 55:CA:1137:C:O2    | 1.81                     | 0.80              |
| 55:CA:373:A:O2'   | 55:CA:374:A:H5'    | 1.82                     | 0.80              |
| 55:CA:792:A:O2'   | 55:CA:794:A:N7     | 2.15                     | 0.80              |
| 24:DA:2493:U:H2'  | 24:DA:2494:G:H5''  | 1.64                     | 0.80              |
| 35:DL:79:LEU:HA   | 35:DL:82:LEU:HD11  | 1.61                     | 0.80              |
| 21:AA:1288:A:O2'  | 21:AA:1289:A:O4'   | 1.99                     | 0.80              |
| 24:BA:2058:A:H5'' | 24:BA:2059:A:OP2   | 1.81                     | 0.80              |
| 24:BA:2104:C:H2'  | 24:BA:2105:U:O4'   | 1.81                     | 0.80              |
| 39:BP:4:ILE:HG22  | 39:BP:5:LYS:N      | 1.97                     | 0.80              |
| 39:BP:67:GLU:HG3  | 39:BP:68:GLY:H     | 1.44                     | 0.80              |
| 2:CC:136:ALA:HA   | 2:CC:139:ASN:HD21  | 1.46                     | 0.80              |
| 15:CP:48:GLU:HG3  | 15:CP:51:ARG:HH21  | 1.46                     | 0.80              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:449:A:O2'    | 24:DA:450:G:H5'    | 1.81                     | 0.80              |
| 26:DC:119:VAL:HG13 | 26:DC:133:ASN:HD21 | 1.45                     | 0.80              |
| 21:AA:1067:A:H1'   | 21:AA:1068:G:C8    | 2.17                     | 0.80              |
| 21:AA:575:G:C6     | 21:AA:821:G:N7     | 2.49                     | 0.80              |
| 21:AA:984:C:O2'    | 21:AA:985:C:H6     | 1.64                     | 0.80              |
| 8:AI:6:TYR:CE2     | 8:AI:17:ARG:HB2    | 2.17                     | 0.80              |
| 24:BA:1746:A:H2'   | 24:BA:1747:U:H6    | 1.45                     | 0.80              |
| 25:BB:53:A:O2'     | 25:BB:54:G:H5'     | 1.81                     | 0.80              |
| 24:DA:1951:U:H2'   | 24:DA:1953:A:OP2   | 1.80                     | 0.80              |
| 24:DA:2574:G:O2'   | 27:DD:148:GLN:HB2  | 1.81                     | 0.80              |
| 24:DA:787:C:H3'    | 24:DA:791:C:N4     | 1.96                     | 0.80              |
| 56:DB:45:A:H2'     | 56:DB:46:A:C8      | 2.17                     | 0.80              |
| 35:DL:92:LEU:HD22  | 35:DL:124:GLY:HA3  | 1.63                     | 0.80              |
| 24:BA:2787:C:O2'   | 24:BA:2788:C:H5'   | 1.80                     | 0.80              |
| 27:BD:114:LYS:NZ   | 27:BD:116:LYS:HE2  | 1.97                     | 0.80              |
| 55:CA:983:A:O2'    | 55:CA:984:C:H5'    | 1.82                     | 0.80              |
| 24:DA:1238:G:H2'   | 24:DA:1239:G:C8    | 2.16                     | 0.80              |
| 24:DA:783:A:O2'    | 24:DA:784:G:H4'    | 1.81                     | 0.80              |
| 24:DA:915:C:O2'    | 24:DA:916:G:H5'    | 1.80                     | 0.80              |
| 26:DC:147:PRO:HD3  | 26:DC:184:GLU:HG3  | 1.63                     | 0.80              |
| 41:DR:1:MET:HG3    | 41:DR:101:ILE:HD12 | 1.62                     | 0.80              |
| 42:DS:73:LYS:HB2   | 42:DS:106:VAL:HB   | 1.63                     | 0.80              |
| 21:AA:939:G:H2'    | 21:AA:940:C:C6     | 2.17                     | 0.80              |
| 1:AB:163:ILE:HG23  | 1:AB:164:ASP:H     | 1.47                     | 0.80              |
| 24:BA:2320:U:H4'   | 24:BA:2321:U:H5''  | 1.64                     | 0.80              |
| 24:BA:2796:U:H3    | 24:BA:2799:A:H61   | 1.28                     | 0.80              |
| 27:BD:140:HIS:NE2  | 59:BD:402:HOH:O    | 2.13                     | 0.80              |
| 35:BL:4:ASN:HD22   | 35:BL:4:ASN:H      | 1.30                     | 0.80              |
| 20:CU:24:LYS:CG    | 20:CU:25:ALA:H     | 1.95                     | 0.80              |
| 27:DD:8:LYS:HB2    | 27:DD:201:LEU:HD11 | 1.62                     | 0.80              |
| 24:BA:1059:G:H5''  | 24:BA:1060:U:H3'   | 1.63                     | 0.80              |
| 55:CA:1086:U:O2'   | 55:CA:1087:G:H5'   | 1.82                     | 0.80              |
| 55:CA:404:G:H2'    | 55:CA:405:U:H6     | 1.47                     | 0.80              |
| 1:CB:119:GLN:HG2   | 1:CB:124:THR:HG21  | 1.64                     | 0.80              |
| 1:CB:47:PRO:HA     | 1:CB:50:ASN:HB2    | 1.64                     | 0.80              |
| 4:CE:22:LYS:HD2    | 55:CA:1081:A:H5'   | 1.64                     | 0.80              |
| 24:DA:1464:G:H2'   | 24:DA:1465:G:C8    | 2.16                     | 0.80              |
| 24:DA:533:G:H21    | 40:DQ:44:TYR:HD1   | 1.29                     | 0.80              |
| 56:DB:90:C:H6      | 56:DB:90:C:H5''    | 1.46                     | 0.80              |
| 31:DH:72:ILE:HD11  | 31:DH:141:LYS:H    | 1.47                     | 0.80              |
| 8:AI:23:GLY:H      | 8:AI:60:LEU:HA     | 1.46                     | 0.80              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:636:G:C5     | 35:BL:111:ILE:HD11 | 2.17                     | 0.80              |
| 24:BA:86:G:O2'     | 24:BA:87:U:H5'     | 1.81                     | 0.80              |
| 27:BD:140:HIS:HE1  | 59:BD:403:HOH:O    | 1.62                     | 0.80              |
| 30:BG:22:VAL:HG22  | 30:BG:36:LEU:HD11  | 1.63                     | 0.80              |
| 46:BW:41:GLY:HA2   | 46:BW:44:PHE:CE2   | 2.16                     | 0.80              |
| 3:CD:25:ARG:HH11   | 3:CD:30:LYS:HE2    | 1.46                     | 0.80              |
| 52:D2:19:ARG:HB3   | 52:D2:19:ARG:HH21  | 1.47                     | 0.80              |
| 24:DA:2406:A:H4'   | 24:DA:2407:A:O5'   | 1.81                     | 0.80              |
| 24:DA:547:A:H3'    | 24:DA:548:G:H5'    | 1.62                     | 0.80              |
| 26:DC:122:ALA:HB3  | 26:DC:127:ASN:ND2  | 1.96                     | 0.80              |
| 44:DU:54:PRO:HG2   | 44:DU:55:GLY:H     | 1.47                     | 0.80              |
| 21:AA:1322:C:O2'   | 21:AA:1323:G:H5'   | 1.82                     | 0.80              |
| 24:BA:2093:G:C6    | 24:BA:2225:A:C8    | 2.70                     | 0.80              |
| 24:BA:2757:A:N1    | 30:BG:66:THR:HG21  | 1.98                     | 0.80              |
| 24:BA:705:A:N6     | 24:BA:726:G:H1'    | 1.97                     | 0.80              |
| 30:BG:120:ILE:HD11 | 30:BG:132:LEU:HB2  | 1.64                     | 0.80              |
| 32:BI:115:ASP:O    | 32:BI:116:MET:HG2  | 1.82                     | 0.80              |
| 39:BP:105:LYS:HA   | 39:BP:108:ARG:HH21 | 1.46                     | 0.80              |
| 55:CA:1455:G:H2'   | 55:CA:1456:A:C8    | 2.17                     | 0.80              |
| 20:CU:39:LYS:N     | 20:CU:40:PRO:HD2   | 1.96                     | 0.80              |
| 24:DA:1438:U:H2'   | 24:DA:1439:A:O4'   | 1.82                     | 0.80              |
| 24:DA:1819:A:H1'   | 24:DA:1821:A:N6    | 1.97                     | 0.80              |
| 24:DA:959:A:H2'    | 24:DA:960:A:C8     | 2.17                     | 0.80              |
| 24:DA:2275:C:O2'   | 36:DM:84:LYS:HA    | 1.82                     | 0.80              |
| 24:BA:1269:A:OP2   | 59:BA:3388:HOH:O   | 2.00                     | 0.79              |
| 35:BL:100:ILE:HD12 | 35:BL:101:ILE:HD13 | 1.65                     | 0.79              |
| 55:CA:90:C:O2'     | 55:CA:91:U:H5'     | 1.82                     | 0.79              |
| 9:CJ:47:GLU:HB2    | 9:CJ:67:ILE:HG13   | 1.63                     | 0.79              |
| 24:DA:127:A:N7     | 52:D2:46:LYS:HE3   | 1.97                     | 0.79              |
| 25:BB:62:C:H2'     | 25:BB:63:C:H6      | 1.46                     | 0.79              |
| 9:CJ:66:GLU:HB2    | 13:CN:100:TRP:CZ3  | 2.17                     | 0.79              |
| 19:CT:24:ARG:HD3   | 19:CT:28:ARG:HH21  | 1.47                     | 0.79              |
| 24:BA:2328:A:H2'   | 24:BA:2329:U:C6    | 2.17                     | 0.79              |
| 34:BK:21:CYS:HB2   | 34:BK:39:ILE:CD1   | 2.11                     | 0.79              |
| 9:CJ:52:LEU:HB2    | 13:CN:80:ARG:NE    | 1.98                     | 0.79              |
| 10:CK:28:ASN:OD1   | 10:CK:46:ALA:HB3   | 1.82                     | 0.79              |
| 24:DA:1131:G:O2'   | 24:DA:1133:A:N7    | 2.15                     | 0.79              |
| 24:DA:1802:A:H2'   | 24:DA:1803:A:C8    | 2.16                     | 0.79              |
| 24:DA:2149:U:H2'   | 24:DA:2150:C:C6    | 2.17                     | 0.79              |
| 34:DK:2:ILE:HB     | 34:DK:33:ALA:HB3   | 1.63                     | 0.79              |
| 20:CU:3:ILE:HG21   | 20:CU:18:PHE:HB3   | 1.63                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:DX:52:ALA:O    | 47:DX:53:LYS:HB3  | 1.83                     | 0.79              |
| 21:AA:1021:A:H2'  | 21:AA:1022:A:H5'' | 1.64                     | 0.79              |
| 4:AE:79:THR:HA    | 4:AE:119:VAL:HG12 | 1.64                     | 0.79              |
| 24:BA:1060:U:H4'  | 24:BA:1061:U:H5'  | 1.65                     | 0.79              |
| 55:CA:120:A:C2'   | 55:CA:121:U:H5''  | 2.13                     | 0.79              |
| 2:CC:18:ASN:HD21  | 2:CC:53:ARG:NH1   | 1.80                     | 0.79              |
| 8:CI:30:ASN:HD21  | 8:CI:66:VAL:H     | 1.27                     | 0.79              |
| 1:AB:43:GLU:O     | 1:AB:47:PRO:HG2   | 1.82                     | 0.79              |
| 10:AK:19:VAL:HB   | 10:AK:34:THR:HG23 | 1.65                     | 0.79              |
| 24:BA:1794:A:H2'  | 24:BA:1795:C:H6   | 1.45                     | 0.79              |
| 24:BA:1255:U:H5   | 28:BE:68:ALA:HA   | 1.47                     | 0.79              |
| 40:BQ:6:GLY:HA2   | 40:BQ:9:ALA:HB3   | 1.65                     | 0.79              |
| 3:CD:106:PHE:CD1  | 3:CD:144:ILE:HD11 | 2.18                     | 0.79              |
| 24:DA:604:G:O2'   | 24:DA:605:G:H8    | 1.64                     | 0.79              |
| 16:AQ:28:VAL:O    | 16:AQ:37:ILE:HD12 | 1.82                     | 0.79              |
| 24:BA:2502:G:H5'  | 24:BA:2503:A:H5'' | 1.63                     | 0.79              |
| 24:BA:1783:A:C2   | 24:BA:2587:A:C4   | 2.70                     | 0.79              |
| 2:CC:18:ASN:HD21  | 2:CC:53:ARG:HH11  | 1.28                     | 0.79              |
| 11:CL:49:ARG:NH2  | 55:CA:522:C:H41   | 1.81                     | 0.79              |
| 24:DA:2582:G:O2'  | 24:DA:2583:G:H5'  | 1.83                     | 0.79              |
| 28:DE:128:ALA:HB1 | 28:DE:129:PRO:HD2 | 1.65                     | 0.79              |
| 34:DK:71:ARG:HB3  | 34:DK:72:PRO:CD   | 2.08                     | 0.79              |
| 36:DM:27:SER:H    | 36:DM:66:ARG:HH22 | 1.29                     | 0.79              |
| 21:AA:1395:C:H5'  | 21:AA:1401:G:H21  | 1.48                     | 0.79              |
| 7:AH:6:ILE:HB     | 7:AH:76:ARG:NH1   | 1.98                     | 0.79              |
| 24:BA:1062:G:H2'  | 24:BA:1063:G:C8   | 2.16                     | 0.79              |
| 55:CA:1348:U:H2'  | 55:CA:1349:A:H8   | 1.48                     | 0.79              |
| 55:CA:61:G:H2'    | 55:CA:62:U:C6     | 2.17                     | 0.79              |
| 29:DF:49:LEU:H    | 29:DF:49:LEU:HD22 | 1.46                     | 0.79              |
| 40:BQ:78:PHE:CZ   | 40:BQ:82:LEU:HD11 | 2.17                     | 0.79              |
| 46:BW:67:LYS:O    | 46:BW:68:PHE:HB2  | 1.83                     | 0.79              |
| 55:CA:555:U:H2'   | 55:CA:556:C:C6    | 2.17                     | 0.79              |
| 1:CB:9:LEU:HG     | 1:CB:10:LYS:H     | 1.46                     | 0.79              |
| 4:CE:29:ILE:HG23  | 4:CE:30:PHE:N     | 1.98                     | 0.79              |
| 24:DA:2303:G:H2'  | 24:DA:2304:G:H8   | 1.48                     | 0.79              |
| 24:DA:670:A:O2'   | 24:DA:671:C:OP2   | 2.00                     | 0.79              |
| 29:DF:43:ILE:HG23 | 29:DF:44:ALA:H    | 1.48                     | 0.79              |
| 33:DJ:18:VAL:HG13 | 33:DJ:56:VAL:HA   | 1.65                     | 0.79              |
| 24:BA:2868:A:H2'  | 24:BA:2869:G:C8   | 2.18                     | 0.79              |
| 37:BN:31:HIS:O    | 37:BN:33:ILE:HD12 | 1.83                     | 0.79              |
| 42:BS:17:VAL:HG12 | 42:BS:76:VAL:HG11 | 1.65                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:202:G:H2'   | 55:CA:203:G:C8    | 2.18                     | 0.79              |
| 55:CA:283:U:H2'   | 55:CA:284:C:C6    | 2.17                     | 0.79              |
| 12:CM:8:ILE:N     | 12:CM:9:PRO:CD    | 2.45                     | 0.79              |
| 24:DA:1127:A:O2'  | 24:DA:1128:G:H5'  | 1.83                     | 0.79              |
| 24:DA:141:G:H3'   | 24:DA:142:A:O4'   | 1.82                     | 0.79              |
| 21:AA:1160:G:O2'  | 21:AA:1161:C:H5'  | 1.84                     | 0.78              |
| 4:AE:139:THR:O    | 4:AE:143:LEU:HG   | 1.83                     | 0.78              |
| 7:AH:78:SER:HB3   | 7:AH:124:ILE:O    | 1.83                     | 0.78              |
| 35:BL:91:ASP:H    | 35:BL:94:THR:HG21 | 1.46                     | 0.78              |
| 6:CG:148:LYS:NZ   | 6:CG:148:LYS:HB2  | 1.98                     | 0.78              |
| 10:CK:123:PRO:HB2 | 10:CK:125:LYS:HG3 | 1.65                     | 0.78              |
| 39:DP:28:LYS:HB2  | 39:DP:28:LYS:HZ2  | 1.49                     | 0.78              |
| 43:DT:3:ARG:HD2   | 43:DT:42:GLU:HG2  | 1.65                     | 0.78              |
| 21:AA:1101:A:H4'  | 21:AA:1102:A:O5'  | 1.83                     | 0.78              |
| 3:AD:173:ASP:CG   | 3:AD:174:ALA:H    | 1.85                     | 0.78              |
| 4:AE:55:VAL:N     | 4:AE:56:PRO:HD2   | 1.97                     | 0.78              |
| 55:CA:927:G:H4'   | 55:CA:1503:A:N7   | 1.98                     | 0.78              |
| 55:CA:982:U:H1'   | 55:CA:983:A:N7    | 1.98                     | 0.78              |
| 24:DA:479:A:O2'   | 24:DA:480:A:C5'   | 2.31                     | 0.78              |
| 56:DB:56:G:H4'    | 56:DB:57:A:O5'    | 1.83                     | 0.78              |
| 21:AA:1078:U:H2'  | 21:AA:1079:G:O4'  | 1.82                     | 0.78              |
| 21:AA:1234:C:H1'  | 21:AA:1364:U:H6   | 1.47                     | 0.78              |
| 21:AA:495:A:H4'   | 21:AA:496:A:O5'   | 1.84                     | 0.78              |
| 13:AN:60:ARG:O    | 13:AN:61:ASN:HB2  | 1.81                     | 0.78              |
| 24:BA:1309:G:OP1  | 52:B2:9:VAL:HG12  | 1.83                     | 0.78              |
| 24:BA:2813:A:H2   | 24:BA:2887:A:N6   | 1.80                     | 0.78              |
| 33:BJ:73:VAL:HG23 | 33:BJ:74:TYR:N    | 1.96                     | 0.78              |
| 55:CA:1119:C:H2'  | 55:CA:1120:C:H6   | 1.47                     | 0.78              |
| 3:CD:2:ARG:HH21   | 3:CD:114:ARG:HD3  | 1.48                     | 0.78              |
| 20:CU:39:LYS:H    | 20:CU:40:PRO:CD   | 1.96                     | 0.78              |
| 21:AA:677:U:H3    | 21:AA:713:G:H22   | 1.30                     | 0.78              |
| 2:AC:39:ARG:CD    | 2:AC:54:ILE:HD11  | 2.13                     | 0.78              |
| 13:AN:20:PHE:C    | 13:AN:22:LYS:H    | 1.85                     | 0.78              |
| 24:BA:653:U:H3'   | 24:BA:654:A:C5'   | 2.12                     | 0.78              |
| 24:DA:1178:C:H2'  | 24:DA:1179:G:O4'  | 1.83                     | 0.78              |
| 24:DA:1391:U:H4'  | 43:DT:19:LYS:NZ   | 1.97                     | 0.78              |
| 24:DA:826:U:H5''  | 24:DA:2429:G:OP1  | 1.82                     | 0.78              |
| 33:DJ:99:ARG:HA   | 33:DJ:102:GLU:HB3 | 1.64                     | 0.78              |
| 45:DV:61:LEU:HD23 | 45:DV:61:LEU:H    | 1.47                     | 0.78              |
| 15:AP:54:LEU:HD22 | 15:AP:80:LYS:HG3  | 1.64                     | 0.78              |
| 24:BA:2733:A:O5'  | 24:BA:2733:A:H8   | 1.66                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:603:A:H4'   | 24:BA:604:G:O5'   | 1.83                     | 0.78              |
| 28:BE:3:LEU:O     | 28:BE:11:ALA:HA   | 1.82                     | 0.78              |
| 36:BM:13:HIS:O    | 36:BM:14:LYS:HB2  | 1.82                     | 0.78              |
| 40:BQ:86:SER:HB2  | 41:BR:50:GLY:O    | 1.83                     | 0.78              |
| 44:BU:73:ASN:ND2  | 44:BU:76:THR:HG23 | 1.98                     | 0.78              |
| 3:CD:144:ILE:HD12 | 3:CD:177:MET:HB3  | 1.64                     | 0.78              |
| 24:DA:83:A:N6     | 24:DA:101:A:H5'   | 1.99                     | 0.78              |
| 24:DA:1464:G:H2'  | 24:DA:1465:G:H8   | 1.48                     | 0.78              |
| 24:DA:923:G:H1'   | 46:DW:23:LYS:NZ   | 1.97                     | 0.78              |
| 21:AA:654:G:H2'   | 21:AA:655:A:H8    | 1.48                     | 0.78              |
| 24:BA:1997:C:O2'  | 24:BA:1998:A:H5'  | 1.84                     | 0.78              |
| 25:BB:90:C:H6     | 25:BB:90:C:H5''   | 1.46                     | 0.78              |
| 40:BQ:91:ARG:HD3  | 41:BR:11:GLN:HG3  | 1.66                     | 0.78              |
| 55:CA:482:A:O2'   | 55:CA:483:C:H5'   | 1.84                     | 0.78              |
| 55:CA:890:G:O2'   | 55:CA:906:A:N6    | 2.17                     | 0.78              |
| 24:DA:1060:U:H4'  | 24:DA:1061:U:H5'' | 1.63                     | 0.78              |
| 24:DA:1912:A:N6   | 24:DA:1918:A:H1'  | 1.98                     | 0.78              |
| 24:DA:1965:C:H5'' | 24:DA:1966:A:H2'  | 1.66                     | 0.78              |
| 24:DA:2386:A:O2'  | 24:DA:2387:U:C6   | 2.36                     | 0.78              |
| 1:AB:165:ALA:HB3  | 1:AB:190:SER:HB3  | 1.65                     | 0.78              |
| 24:BA:996:A:N6    | 24:BA:1160:G:C6   | 2.51                     | 0.78              |
| 24:BA:2391:G:O6   | 24:BA:2425:A:H8   | 1.66                     | 0.78              |
| 46:BW:19:ARG:HA   | 46:BW:34:SER:HA   | 1.65                     | 0.78              |
| 55:CA:1157:A:H1'  | 55:CA:1181:G:N2   | 1.98                     | 0.78              |
| 55:CA:451:A:H4'   | 55:CA:452:A:O5'   | 1.84                     | 0.78              |
| 24:DA:1785:A:H2'  | 24:DA:1787:A:N7   | 1.99                     | 0.78              |
| 21:AA:1144:G:H21  | 21:AA:1146:A:H62  | 1.31                     | 0.78              |
| 4:AE:87:VAL:HG12  | 4:AE:92:ARG:HA    | 1.65                     | 0.78              |
| 11:AL:45:ASN:ND2  | 21:AA:528:C:H41   | 1.82                     | 0.78              |
| 24:BA:1327:A:C2'  | 24:BA:1328:A:H5'  | 2.12                     | 0.78              |
| 24:BA:704:G:H1'   | 24:BA:727:A:N6    | 1.99                     | 0.78              |
| 24:BA:729:G:H5'   | 26:BC:206:LYS:NZ  | 1.99                     | 0.78              |
| 55:CA:1054:C:C4   | 22:CX:34:G:H1'    | 2.18                     | 0.78              |
| 10:CK:118:ASN:OD1 | 55:CA:718:A:H5'   | 1.83                     | 0.78              |
| 55:CA:764:C:H3'   | 55:CA:765:G:H21   | 1.46                     | 0.78              |
| 12:CM:104:ASN:HB3 | 55:CA:948:C:H5''  | 1.66                     | 0.78              |
| 9:CJ:39:PRO:HA    | 9:CJ:74:VAL:H     | 1.49                     | 0.78              |
| 28:DE:149:ILE:O   | 28:DE:188:MET:HA  | 1.82                     | 0.78              |
| 56:DB:77:U:OP1    | 45:DV:18:ARG:HG3  | 1.83                     | 0.78              |
| 45:BV:80:HIS:HD2  | 45:BV:83:LYS:N    | 1.81                     | 0.78              |
| 52:D2:5:PHE:HZ    | 52:D2:12:ARG:HH11 | 1.28                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DE:6:LYS:HB2    | 28:DE:121:VAL:HG12 | 1.66                     | 0.78              |
| 29:DF:41:GLU:HG2   | 29:DF:42:ALA:H     | 1.49                     | 0.78              |
| 30:DG:48:THR:O     | 30:DG:49:LEU:HB2   | 1.83                     | 0.78              |
| 21:AA:1016:A:C8    | 21:AA:1017:U:H1'   | 2.19                     | 0.78              |
| 21:AA:596:A:H2'    | 21:AA:597:G:H8     | 1.48                     | 0.78              |
| 10:AK:22:ILE:HD11  | 10:AK:85:VAL:HG22  | 1.66                     | 0.78              |
| 27:BD:108:ASP:OD2  | 27:BD:173:GLN:HA   | 1.83                     | 0.78              |
| 55:CA:120:A:C3'    | 55:CA:121:U:H5''   | 2.14                     | 0.78              |
| 6:CG:9:ARG:HH12    | 55:CA:1346:A:N6    | 1.81                     | 0.78              |
| 55:CA:1481:U:H2'   | 55:CA:1482:G:H8    | 1.49                     | 0.78              |
| 24:DA:532:A:N1     | 24:DA:2020:A:H1'   | 1.99                     | 0.78              |
| 24:DA:2429:G:H3'   | 24:DA:2429:G:OP2   | 1.83                     | 0.78              |
| 45:DV:29:ILE:HD13  | 45:DV:31:TYR:HE2   | 1.47                     | 0.78              |
| 12:AM:67:ASP:O     | 12:AM:70:ARG:HB3   | 1.82                     | 0.77              |
| 52:B2:43:THR:O     | 52:B2:44:VAL:HB    | 1.81                     | 0.77              |
| 24:BA:646:U:H3'    | 24:BA:647:G:H5''   | 1.65                     | 0.77              |
| 24:BA:1818:U:O2'   | 26:BC:152:GLN:O    | 1.99                     | 0.77              |
| 18:CS:68:HIS:HB3   | 18:CS:72:GLU:HG3   | 1.66                     | 0.77              |
| 24:DA:1809:A:O2'   | 24:DA:1810:A:C8    | 2.36                     | 0.77              |
| 24:DA:632:A:H2'    | 24:DA:633:A:C8     | 2.19                     | 0.77              |
| 24:DA:979:A:H2'    | 24:DA:982:C:H41    | 1.46                     | 0.77              |
| 24:BA:529:A:H4'    | 24:BA:530:G:OP1    | 1.82                     | 0.77              |
| 55:CA:495:A:H4'    | 55:CA:496:A:O5'    | 1.83                     | 0.77              |
| 2:CC:152:VAL:HA    | 2:CC:197:VAL:HG22  | 1.66                     | 0.77              |
| 9:CJ:42:LEU:HD22   | 9:CJ:71:LEU:HD23   | 1.65                     | 0.77              |
| 13:CN:52:ARG:HA    | 13:CN:52:ARG:NH1   | 1.99                     | 0.77              |
| 24:DA:1563:U:H2'   | 24:DA:1564:C:H6    | 1.49                     | 0.77              |
| 29:DF:136:ILE:HD13 | 29:DF:145:VAL:HG11 | 1.66                     | 0.77              |
| 24:DA:855:G:H21    | 46:DW:23:LYS:HZ2   | 1.32                     | 0.77              |
| 21:AA:96:U:O2'     | 21:AA:97:G:H8      | 1.67                     | 0.77              |
| 8:AI:128:LYS:CD    | 8:AI:129:ARG:H     | 1.97                     | 0.77              |
| 24:BA:2253:G:H2'   | 24:BA:2254:C:H6    | 1.47                     | 0.77              |
| 24:BA:2352:A:C6    | 46:BW:30:VAL:HG11  | 2.19                     | 0.77              |
| 4:CE:80:LEU:HD12   | 4:CE:97:PRO:HD3    | 1.64                     | 0.77              |
| 6:CG:74:VAL:HG13   | 6:CG:140:VAL:HG13  | 1.67                     | 0.77              |
| 24:DA:2015:A:C2    | 50:D0:2:VAL:HG11   | 2.20                     | 0.77              |
| 24:DA:1432:G:H2'   | 24:DA:1433:A:C8    | 2.19                     | 0.77              |
| 56:DB:100:G:H2'    | 56:DB:101:A:O4'    | 1.84                     | 0.77              |
| 56:DB:58:A:H2'     | 56:DB:59:A:H8      | 1.46                     | 0.77              |
| 21:AA:182:A:C6     | 21:AA:194:C:N4     | 2.51                     | 0.77              |
| 24:BA:1181:U:HO2'  | 24:BA:1182:G:H8    | 1.29                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:2305:U:H5'' | 29:BF:130:GLY:HA3 | 1.66                     | 0.77              |
| 24:BA:709:U:H2'   | 24:BA:710:U:C6    | 2.19                     | 0.77              |
| 40:BQ:65:ASN:HD21 | 40:BQ:69:ARG:NH2  | 1.81                     | 0.77              |
| 55:CA:1523:G:H2'  | 55:CA:1524:C:H6   | 1.49                     | 0.77              |
| 36:DM:72:PRO:O    | 36:DM:73:ILE:HB   | 1.83                     | 0.77              |
| 40:DQ:57:ARG:NH1  | 40:DQ:92:LYS:HE2  | 1.99                     | 0.77              |
| 21:AA:1305:G:HO2' | 21:AA:1306:A:H8   | 1.33                     | 0.77              |
| 21:AA:1361:G:H2'  | 21:AA:1362:A:H5'  | 1.65                     | 0.77              |
| 24:BA:1584:U:H2'  | 24:BA:1585:C:H5'  | 1.67                     | 0.77              |
| 24:BA:859:G:C8    | 24:BA:859:G:OP2   | 2.38                     | 0.77              |
| 31:BH:94:ILE:HG21 | 31:BH:99:ILE:HG12 | 1.67                     | 0.77              |
| 55:CA:1203:C:H2'  | 55:CA:1204:A:H8   | 1.48                     | 0.77              |
| 55:CA:563:A:N3    | 55:CA:563:A:H2'   | 1.99                     | 0.77              |
| 55:CA:915:A:O2'   | 55:CA:916:U:H5'   | 1.85                     | 0.77              |
| 4:CE:29:ILE:HG23  | 4:CE:30:PHE:H     | 1.49                     | 0.77              |
| 29:DF:39:VAL:HA   | 29:DF:49:LEU:HG   | 1.67                     | 0.77              |
| 21:AA:1218:C:H2'  | 21:AA:1219:A:C8   | 2.20                     | 0.77              |
| 21:AA:41:G:H2'    | 21:AA:42:G:H8     | 1.48                     | 0.77              |
| 1:AB:160:LEU:HG   | 1:AB:161:PHE:H    | 1.48                     | 0.77              |
| 24:BA:2233:U:H2'  | 24:BA:2234:G:H8   | 1.48                     | 0.77              |
| 24:BA:319:G:H2'   | 24:BA:320:A:O4'   | 1.83                     | 0.77              |
| 29:BF:134:GLN:HG2 | 29:BF:135:ILE:N   | 1.99                     | 0.77              |
| 30:BG:3:VAL:O     | 30:BG:68:ARG:HG3  | 1.83                     | 0.77              |
| 55:CA:1048:G:H21  | 55:CA:1214:C:H5   | 1.32                     | 0.77              |
| 55:CA:1508:A:O2'  | 55:CA:1509:C:O4'  | 2.02                     | 0.77              |
| 55:CA:664:G:H22   | 55:CA:741:G:H1    | 1.29                     | 0.77              |
| 3:CD:109:THR:HG22 | 3:CD:111:ALA:H    | 1.48                     | 0.77              |
| 18:CS:54:ARG:HG2  | 18:CS:55:GLN:H    | 1.48                     | 0.77              |
| 1:AB:107:ARG:HE   | 1:AB:108:GLN:NE2  | 1.82                     | 0.77              |
| 14:AO:27:GLN:HA   | 14:AO:30:LEU:HD12 | 1.66                     | 0.77              |
| 24:BA:1069:A:O2'  | 24:BA:1070:A:H5'' | 1.84                     | 0.77              |
| 24:BA:1886:U:H2'  | 24:BA:1887:C:H6   | 1.49                     | 0.77              |
| 24:BA:734:A:C5    | 24:BA:735:A:C8    | 2.73                     | 0.77              |
| 27:BD:12:THR:HG22 | 27:BD:13:ARG:N    | 2.00                     | 0.77              |
| 1:CB:14:HIS:CE1   | 1:CB:42:LEU:HD21  | 2.19                     | 0.77              |
| 17:CR:72:ARG:HE   | 17:CR:72:ARG:N    | 1.82                     | 0.77              |
| 24:DA:1429:G:HO2' | 24:DA:1430:G:H8   | 0.79                     | 0.77              |
| 41:DR:89:HIS:NE2  | 41:DR:91:GLN:HB2  | 2.00                     | 0.77              |
| 44:DU:92:VAL:HB   | 44:DU:101:THR:CG2 | 2.14                     | 0.77              |
| 9:AJ:65:TYR:HB3   | 13:AN:95:LEU:HD11 | 1.66                     | 0.77              |
| 40:BQ:10:ARG:HH11 | 40:BQ:10:ARG:HB2  | 1.48                     | 0.77              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:DA:217:A:H2'    | 24:DA:218:A:C8    | 2.19                     | 0.77              |
| 24:DA:594:U:H2'    | 24:DA:595:C:C6    | 2.19                     | 0.77              |
| 2:AC:39:ARG:HD3    | 2:AC:54:ILE:HD11  | 1.66                     | 0.77              |
| 24:BA:1870:C:H4'   | 24:BA:1871:A:OP1  | 1.83                     | 0.77              |
| 24:BA:513:A:O2'    | 24:BA:514:A:H5'   | 1.85                     | 0.77              |
| 37:BN:75:ILE:O     | 37:BN:79:LEU:HD12 | 1.85                     | 0.77              |
| 55:CA:14:U:H2'     | 55:CA:16:A:OP2    | 1.83                     | 0.77              |
| 9:CJ:52:LEU:CB     | 13:CN:80:ARG:HE   | 1.98                     | 0.77              |
| 24:DA:1056:G:H21   | 24:DA:1102:C:H41  | 1.33                     | 0.77              |
| 24:DA:1079:C:N3    | 24:DA:1088:A:H2   | 1.83                     | 0.77              |
| 24:DA:1760:C:H2'   | 24:DA:1761:C:C6   | 2.19                     | 0.77              |
| 35:DL:96:LYS:HD3   | 35:DL:103:ILE:HA  | 1.66                     | 0.77              |
| 21:AA:1032:G:H2'   | 21:AA:1033:G:O4'  | 1.85                     | 0.77              |
| 2:AC:152:VAL:HG12  | 2:AC:197:VAL:HG22 | 1.67                     | 0.77              |
| 24:DA:2197:U:O2'   | 24:DA:2198:A:C8   | 2.38                     | 0.77              |
| 24:DA:2520:C:HO2'  | 24:DA:2521:C:H6   | 0.78                     | 0.77              |
| 53:B3:54:LEU:O     | 53:B3:58:ILE:HG13 | 1.85                     | 0.76              |
| 24:BA:633:A:H8     | 24:BA:633:A:O5'   | 1.67                     | 0.76              |
| 24:BA:687:C:H2'    | 24:BA:688:U:C6    | 2.19                     | 0.76              |
| 24:BA:919:U:H2'    | 24:BA:920:A:O4'   | 1.85                     | 0.76              |
| 34:BK:111:LYS:H    | 34:BK:111:LYS:CE  | 1.98                     | 0.76              |
| 9:CJ:40:ILE:HG22   | 9:CJ:42:LEU:HD12  | 1.65                     | 0.76              |
| 24:DA:1062:G:C8    | 24:DA:1088:A:C8   | 2.73                     | 0.76              |
| 24:DA:2023:C:O2'   | 24:DA:2024:G:H8   | 1.67                     | 0.76              |
| 16:AQ:12:VAL:HG13  | 16:AQ:13:SER:N    | 2.00                     | 0.76              |
| 55:CA:1194:U:H2'   | 55:CA:1195:C:C6   | 2.19                     | 0.76              |
| 3:CD:137:SER:O     | 3:CD:140:ASP:HB2  | 1.85                     | 0.76              |
| 7:CH:9:MET:HB2     | 7:CH:32:LYS:HE2   | 1.67                     | 0.76              |
| 18:CS:40:PHE:CB    | 18:CS:41:PRO:HD2  | 2.15                     | 0.76              |
| 13:CN:40:ARG:NH1   | 18:CS:6:LYS:HB2   | 2.00                     | 0.76              |
| 37:DN:35:LYS:HZ2   | 37:DN:112:TYR:HE1 | 1.32                     | 0.76              |
| 11:AL:6:LEU:HD23   | 16:AQ:33:TYR:CE2  | 2.20                     | 0.76              |
| 10:CK:127:ARG:HH21 | 55:CA:795:C:H5''  | 1.50                     | 0.76              |
| 24:DA:2516:A:C2    | 24:DA:2569:G:C2   | 2.73                     | 0.76              |
| 24:DA:918:A:C5     | 24:DA:919:U:H1'   | 2.19                     | 0.76              |
| 43:DT:29:THR:H     | 43:DT:87:LEU:HB2  | 1.50                     | 0.76              |
| 46:DW:23:LYS:HD2   | 46:DW:24:ARG:N    | 2.00                     | 0.76              |
| 12:AM:14:ALA:O     | 12:AM:18:LEU:HD23 | 1.84                     | 0.76              |
| 24:BA:1563:U:H2'   | 24:BA:1564:C:C6   | 2.20                     | 0.76              |
| 24:BA:752:A:N6     | 24:BA:2609:U:H3   | 1.83                     | 0.76              |
| 33:BJ:56:VAL:HG12  | 33:BJ:57:LEU:N    | 2.01                     | 0.76              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 44:BU:10:VAL:HB    | 44:BU:70:ALA:O    | 1.85                     | 0.76              |
| 55:CA:783:C:O2'    | 55:CA:784:A:H5'   | 1.85                     | 0.76              |
| 1:CB:69:VAL:HB     | 1:CB:162:VAL:HB   | 1.66                     | 0.76              |
| 21:AA:1399:C:H4'   | 21:AA:1400:C:O5'  | 1.85                     | 0.76              |
| 10:AK:21:HIS:CD2   | 10:AK:34:THR:HG21 | 2.21                     | 0.76              |
| 21:AA:1230:C:H5'   | 22:AV:30:G:H5''   | 1.65                     | 0.76              |
| 55:CA:974:A:C5'    | 55:CA:975:A:H5'   | 2.11                     | 0.76              |
| 7:CH:86:LYS:HB3    | 7:CH:90:GLU:HB2   | 1.67                     | 0.76              |
| 12:CM:2:ARG:CD     | 12:CM:8:ILE:HG12  | 2.15                     | 0.76              |
| 24:DA:172:A:H2'    | 24:DA:173:A:C8    | 2.20                     | 0.76              |
| 24:DA:2376:A:H2    | 38:DO:92:PHE:HB3  | 1.51                     | 0.76              |
| 5:AF:40:GLU:HB2    | 5:AF:42:TRP:HE1   | 1.51                     | 0.76              |
| 6:AG:78:ARG:HD2    | 6:AG:83:THR:HA    | 1.68                     | 0.76              |
| 24:BA:1021:A:H61   | 24:BA:1142:A:N6   | 1.83                     | 0.76              |
| 24:BA:1060:U:C5'   | 24:BA:1061:U:H5'  | 2.15                     | 0.76              |
| 24:BA:1759:A:O2'   | 24:BA:1760:C:H5'  | 1.84                     | 0.76              |
| 24:BA:2407:A:H2'   | 24:BA:2408:U:C6   | 2.21                     | 0.76              |
| 44:BU:3:LYS:HD3    | 44:BU:82:VAL:HB   | 1.67                     | 0.76              |
| 55:CA:1303:C:H3'   | 55:CA:1304:G:H8   | 1.51                     | 0.76              |
| 9:CJ:15:HIS:HA     | 9:CJ:18:ILE:HG22  | 1.67                     | 0.76              |
| 24:DA:1490:A:C8    | 26:DC:73:ILE:HD12 | 2.20                     | 0.76              |
| 24:DA:2623:G:H21   | 50:D0:18:HIS:CE1  | 2.03                     | 0.76              |
| 24:DA:532:A:H4'    | 24:DA:533:G:C8    | 2.21                     | 0.76              |
| 24:DA:673:C:H5''   | 28:DE:75:SER:HB2  | 1.68                     | 0.76              |
| 45:DV:80:HIS:HD2   | 45:DV:82:TYR:H    | 1.31                     | 0.76              |
| 21:AA:1227:A:N3    | 21:AA:1227:A:H2'  | 2.00                     | 0.76              |
| 10:AK:39:ASN:O     | 21:AA:684:U:H1'   | 1.85                     | 0.76              |
| 16:AQ:76:ARG:HG2   | 16:AQ:77:VAL:H    | 1.50                     | 0.76              |
| 24:BA:1333:G:O2'   | 24:BA:1334:G:H5'  | 1.86                     | 0.76              |
| 24:BA:1385:A:H4'   | 24:BA:1386:C:OP1  | 1.86                     | 0.76              |
| 24:BA:1965:C:H5''  | 24:BA:1965:C:H6   | 1.50                     | 0.76              |
| 24:BA:581:C:H2'    | 24:BA:582:A:C8    | 2.20                     | 0.76              |
| 28:BE:79:ARG:CG    | 28:BE:80:SER:H    | 1.95                     | 0.76              |
| 3:CD:205:LYS:HD3   | 55:CA:8:A:N6      | 2.01                     | 0.76              |
| 24:DA:2726:A:O2'   | 24:DA:2727:A:H5'  | 1.85                     | 0.76              |
| 24:DA:775:G:N2     | 24:DA:794:A:H5'   | 2.01                     | 0.76              |
| 30:DG:112:VAL:HG12 | 30:DG:114:HIS:H   | 1.50                     | 0.76              |
| 24:DA:857:G:H1'    | 46:DW:19:ARG:NE   | 2.01                     | 0.76              |
| 21:AA:251:G:N1     | 21:AA:266:G:O6    | 2.18                     | 0.76              |
| 24:BA:1091:G:O2'   | 24:BA:1092:C:C6   | 2.37                     | 0.76              |
| 24:BA:1695:G:N3    | 24:BA:1695:G:H5'' | 2.01                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:303:G:H2'    | 24:BA:304:U:H6     | 1.51                     | 0.76              |
| 25:BB:28:C:OP1     | 38:BO:31:THR:HG21  | 1.85                     | 0.76              |
| 27:BD:101:PHE:HE2  | 27:BD:203:VAL:HG22 | 1.50                     | 0.76              |
| 32:BI:33:ASN:HB3   | 32:BI:36:GLU:HB2   | 1.68                     | 0.76              |
| 2:CC:166:TRP:O     | 2:CC:167:TYR:HB2   | 1.84                     | 0.76              |
| 24:DA:1964:G:H4'   | 24:DA:1965:C:OP2   | 1.85                     | 0.76              |
| 27:DD:184:ARG:HH22 | 39:DP:6:GLN:HE21   | 1.31                     | 0.76              |
| 21:AA:486:U:H2'    | 21:AA:487:A:H8     | 1.49                     | 0.76              |
| 21:AA:519:C:H2'    | 21:AA:520:A:C8     | 2.21                     | 0.76              |
| 13:AN:82:LYS:HE2   | 13:AN:82:LYS:HA    | 1.67                     | 0.76              |
| 24:BA:1655:A:H2'   | 24:BA:1656:C:O4'   | 1.85                     | 0.76              |
| 27:BD:5:VAL:N      | 27:BD:32:ASN:HD21  | 1.83                     | 0.76              |
| 28:BE:149:ILE:HD11 | 28:BE:172:ALA:HA   | 1.68                     | 0.76              |
| 37:BN:23:ASN:H     | 37:BN:23:ASN:HD22  | 1.34                     | 0.76              |
| 55:CA:1296:C:O2'   | 55:CA:1302:C:C4    | 2.37                     | 0.76              |
| 55:CA:1465:A:H2'   | 55:CA:1466:C:C6    | 2.21                     | 0.76              |
| 55:CA:252:U:HO2'   | 55:CA:253:A:H8     | 1.33                     | 0.76              |
| 55:CA:366:A:O2'    | 55:CA:394:G:N2     | 2.19                     | 0.76              |
| 55:CA:977:A:H8     | 55:CA:1223:C:N3    | 1.84                     | 0.76              |
| 24:DA:1312:U:H4'   | 24:DA:1313:U:O5'   | 1.85                     | 0.76              |
| 24:DA:172:A:H2'    | 24:DA:173:A:H8     | 1.51                     | 0.76              |
| 21:AA:60:A:H4'     | 21:AA:61:G:O5'     | 1.86                     | 0.76              |
| 15:AP:52:LEU:HD21  | 15:AP:75:ILE:HG12  | 1.66                     | 0.76              |
| 24:BA:1079:C:N4    | 24:BA:1088:A:C2    | 2.52                     | 0.76              |
| 24:BA:1444:G:H2'   | 24:BA:1445:G:H8    | 1.49                     | 0.76              |
| 24:BA:1735:A:H2'   | 24:BA:1736:U:C6    | 2.21                     | 0.76              |
| 24:BA:2267:A:H2'   | 24:BA:2267:A:N3    | 2.00                     | 0.76              |
| 24:BA:371:A:H61    | 24:BA:401:A:H3'    | 1.49                     | 0.76              |
| 24:BA:714:U:H5'    | 24:BA:715:A:OP2    | 1.85                     | 0.76              |
| 24:BA:2680:U:P     | 27:BD:114:LYS:HE2  | 2.25                     | 0.76              |
| 29:BF:9:ASP:O      | 29:BF:10:GLU:HB2   | 1.84                     | 0.76              |
| 32:BI:74:PRO:O     | 32:BI:77:VAL:HG22  | 1.85                     | 0.76              |
| 35:BL:78:ARG:HB3   | 35:BL:113:ALA:CB   | 2.15                     | 0.76              |
| 39:BP:25:VAL:HG11  | 39:BP:46:VAL:HG23  | 1.67                     | 0.76              |
| 24:BA:996:A:O3'    | 40:BQ:91:ARG:HG2   | 1.86                     | 0.76              |
| 24:BA:994:C:H1'    | 41:BR:10:LYS:HZ1   | 1.51                     | 0.76              |
| 15:CP:20:VAL:CG2   | 15:CP:32:PHE:HB2   | 2.16                     | 0.76              |
| 52:D2:31:LEU:HA    | 52:D2:34:ARG:HB2   | 1.68                     | 0.76              |
| 46:DW:18:LYS:HD3   | 46:DW:19:ARG:N     | 2.00                     | 0.76              |
| 21:AA:499:A:O2'    | 21:AA:500:G:C8     | 2.39                     | 0.75              |
| 12:AM:70:ARG:HG2   | 12:AM:71:GLU:CA    | 2.16                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:B3:56:LEU:H     | 53:B3:56:LEU:HD22  | 1.50                     | 0.75              |
| 54:B4:3:VAL:O      | 54:B4:4:ARG:O      | 2.03                     | 0.75              |
| 24:BA:1555:G:O2'   | 24:BA:1556:C:H5'   | 1.85                     | 0.75              |
| 24:BA:1842:G:H2'   | 24:BA:1843:C:H6    | 1.51                     | 0.75              |
| 26:BC:77:VAL:HG22  | 26:BC:111:ALA:HA   | 1.69                     | 0.75              |
| 32:BI:104:GLN:O    | 32:BI:105:LEU:HB2  | 1.86                     | 0.75              |
| 34:BK:116:ILE:HD12 | 34:BK:117:SER:N    | 2.01                     | 0.75              |
| 12:CM:13:HIS:HB3   | 12:CM:16:ILE:HD13  | 1.68                     | 0.75              |
| 24:DA:142:A:H2'    | 24:DA:143:C:H6     | 1.47                     | 0.75              |
| 24:DA:232:G:H4'    | 24:DA:233:A:OP1    | 1.84                     | 0.75              |
| 24:DA:374:A:H2'    | 24:DA:375:G:C8     | 2.21                     | 0.75              |
| 24:DA:673:C:H2'    | 24:DA:674:G:H5'    | 1.66                     | 0.75              |
| 21:AA:197:A:H4'    | 21:AA:198:G:O5'    | 1.86                     | 0.75              |
| 21:AA:513:C:H2'    | 21:AA:514:C:C6     | 2.20                     | 0.75              |
| 21:AA:563:A:H2'    | 21:AA:563:A:N3     | 2.01                     | 0.75              |
| 15:AP:18:GLN:HE21  | 15:AP:35:ARG:HD2   | 1.50                     | 0.75              |
| 24:BA:1965:C:H6    | 24:BA:1965:C:C5'   | 1.99                     | 0.75              |
| 33:BJ:101:ILE:O    | 33:BJ:105:VAL:HG13 | 1.86                     | 0.75              |
| 35:BL:95:LEU:HB3   | 35:BL:100:ILE:HD11 | 1.67                     | 0.75              |
| 43:BT:29:THR:N     | 43:BT:91:GLN:HE22  | 1.83                     | 0.75              |
| 47:BX:39:VAL:HG22  | 47:BX:44:ARG:O     | 1.86                     | 0.75              |
| 14:CO:63:ARG:NH2   | 24:DA:715:A:H5'    | 1.99                     | 0.75              |
| 24:DA:983:A:N6     | 24:DA:984:A:N1     | 2.34                     | 0.75              |
| 34:DK:70:ARG:HB3   | 34:DK:76:VAL:HG22  | 1.69                     | 0.75              |
| 21:AA:89:U:O2'     | 21:AA:90:C:H5''    | 1.86                     | 0.75              |
| 4:AE:84:VAL:HG11   | 4:AE:143:LEU:HD23  | 1.67                     | 0.75              |
| 51:B1:7:LYS:HE3    | 53:B3:33:THR:HG21  | 1.68                     | 0.75              |
| 24:BA:306:U:H2'    | 24:BA:307:G:O4'    | 1.85                     | 0.75              |
| 28:BE:117:ARG:HA   | 28:BE:185:LYS:HD3  | 1.68                     | 0.75              |
| 55:CA:65:A:H2'     | 55:CA:382:A:H61    | 1.52                     | 0.75              |
| 4:CE:131:ASN:O     | 4:CE:135:VAL:HG23  | 1.86                     | 0.75              |
| 8:CI:6:TYR:HE2     | 8:CI:17:ARG:HA     | 1.52                     | 0.75              |
| 24:DA:2285:C:H5    | 51:D1:5:ARG:NH2    | 1.85                     | 0.75              |
| 24:DA:479:A:O2'    | 24:DA:480:A:H5'    | 1.86                     | 0.75              |
| 24:DA:480:A:H3'    | 24:DA:481:G:C5'    | 2.15                     | 0.75              |
| 56:DB:16:G:O2'     | 56:DB:17:C:H5'     | 1.86                     | 0.75              |
| 41:DR:39:LEU:O     | 41:DR:40:MET:HB2   | 1.87                     | 0.75              |
| 21:AA:1533:C:H3'   | 21:AA:1534:A:H5''  | 1.67                     | 0.75              |
| 21:AA:64:G:H4'     | 21:AA:65:A:O5'     | 1.86                     | 0.75              |
| 4:AE:105:ILE:HG13  | 4:AE:105:ILE:O     | 1.86                     | 0.75              |
| 7:AH:105:THR:HG21  | 7:AH:120:LEU:HD13  | 1.67                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:754:U:H2'    | 24:BA:755:U:C6     | 2.21                     | 0.75              |
| 33:BJ:25:LEU:HD22  | 33:BJ:26:GLY:N     | 2.02                     | 0.75              |
| 55:CA:1102:A:H2'   | 55:CA:1103:C:H6    | 1.51                     | 0.75              |
| 8:CI:9:GLY:HA3     | 8:CI:16:ALA:HB3    | 1.66                     | 0.75              |
| 12:CM:95:PRO:HD3   | 12:CM:108:ARG:HG2  | 1.67                     | 0.75              |
| 24:DA:713:G:H21    | 24:DA:718:A:H2     | 1.34                     | 0.75              |
| 32:DI:55:PRO:HG2   | 32:DI:70:THR:HG23  | 1.66                     | 0.75              |
| 43:DT:14:PRO:O     | 43:DT:15:HIS:HB2   | 1.87                     | 0.75              |
| 21:AA:47:C:H4'     | 21:AA:48:C:O5'     | 1.86                     | 0.75              |
| 21:AA:580:C:H2'    | 21:AA:581:G:C8     | 2.21                     | 0.75              |
| 24:BA:1179:G:C6    | 24:BA:1180:U:H1'   | 2.22                     | 0.75              |
| 24:BA:1585:C:H2'   | 24:BA:1586:A:O4'   | 1.87                     | 0.75              |
| 24:BA:2846:G:N2    | 24:BA:2871:U:H1'   | 2.02                     | 0.75              |
| 24:BA:363:G:H2'    | 24:BA:364:C:C6     | 2.21                     | 0.75              |
| 24:BA:62:U:H4'     | 24:BA:63:A:OP1     | 1.87                     | 0.75              |
| 28:BE:176:ASP:OD1  | 28:BE:178:VAL:HG13 | 1.87                     | 0.75              |
| 30:BG:140:ILE:HD12 | 30:BG:141:GLY:N    | 2.01                     | 0.75              |
| 38:BO:76:LYS:O     | 38:BO:80:GLU:HG2   | 1.86                     | 0.75              |
| 24:BA:2013:A:N3    | 42:BS:88:ARG:NH1   | 2.34                     | 0.75              |
| 24:DA:2056:G:N2    | 50:D0:1:ALA:N      | 2.34                     | 0.75              |
| 24:DA:2886:A:H62   | 50:D0:39:ARG:CD    | 1.98                     | 0.75              |
| 51:D1:8:ILE:HD11   | 51:D1:52:LYS:HE3   | 1.67                     | 0.75              |
| 24:DA:1714:U:H3'   | 24:DA:1715:G:C5'   | 2.17                     | 0.75              |
| 56:DB:104:A:H2'    | 56:DB:105:G:O4'    | 1.87                     | 0.75              |
| 36:DM:19:GLY:H     | 36:DM:38:ARG:NH2   | 1.83                     | 0.75              |
| 21:AA:274:A:O2'    | 21:AA:275:G:C8     | 2.39                     | 0.75              |
| 24:BA:839:U:H2'    | 24:BA:840:C:H6     | 1.51                     | 0.75              |
| 26:BC:12:ARG:HH11  | 26:BC:12:ARG:HG3   | 1.52                     | 0.75              |
| 41:BR:4:VAL:HA     | 41:BR:12:HIS:O     | 1.86                     | 0.75              |
| 55:CA:383:A:H2'    | 55:CA:384:G:O4'    | 1.86                     | 0.75              |
| 55:CA:60:A:H1'     | 55:CA:61:G:O4'     | 1.87                     | 0.75              |
| 24:DA:1071:G:O2'   | 24:DA:1072:C:H5'   | 1.87                     | 0.75              |
| 24:DA:1399:C:O2'   | 24:DA:1400:U:H5'   | 1.86                     | 0.75              |
| 24:DA:1432:G:H2'   | 24:DA:1433:A:H8    | 1.51                     | 0.75              |
| 24:DA:2214:C:O2'   | 24:DA:2215:C:H5'   | 1.87                     | 0.75              |
| 24:DA:2543:G:H2'   | 24:DA:2544:G:C8    | 2.21                     | 0.75              |
| 38:DO:53:THR:HB    | 38:DO:65:THR:HG22  | 1.67                     | 0.75              |
| 24:DA:2387:U:H1'   | 46:DW:38:ARG:HH12  | 1.51                     | 0.75              |
| 21:AA:1076:U:H2'   | 21:AA:1077:G:H8    | 1.51                     | 0.75              |
| 21:AA:547:A:H4'    | 21:AA:548:G:O5'    | 1.85                     | 0.75              |
| 50:B0:39:ARG:HH11  | 50:B0:39:ARG:HB2   | 1.51                     | 0.75              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:BA:1798:U:OP1   | 26:BC:257:ARG:HB2 | 1.87                     | 0.75              |
| 34:BK:18:ARG:H     | 34:BK:45:GLU:HB2  | 1.51                     | 0.75              |
| 27:BD:186:LEU:HD11 | 39:BP:3:ILE:HD11  | 1.68                     | 0.75              |
| 40:BQ:94:LEU:HD11  | 41:BR:4:VAL:HG11  | 1.69                     | 0.75              |
| 43:BT:13:ALA:HB1   | 43:BT:14:PRO:HD2  | 1.68                     | 0.75              |
| 55:CA:268:U:H2'    | 55:CA:269:C:C6    | 2.22                     | 0.75              |
| 9:CJ:11:LYS:HD3    | 9:CJ:11:LYS:H     | 1.52                     | 0.75              |
| 12:CM:102:LYS:HG2  | 55:CA:1226:C:N4   | 2.00                     | 0.75              |
| 12:CM:14:ALA:HB1   | 12:CM:33:LEU:HD13 | 1.68                     | 0.75              |
| 24:DA:1846:G:H5''  | 24:DA:1847:A:OP2  | 1.87                     | 0.75              |
| 24:DA:2503:A:H4'   | 24:DA:2504:U:OP1  | 1.84                     | 0.75              |
| 40:DQ:87:VAL:HG11  | 41:DR:52:PRO:HG3  | 1.66                     | 0.75              |
| 48:DY:1:MET:H3     | 48:DY:1:MET:HE2   | 1.52                     | 0.75              |
| 11:AL:87:LYS:HE2   | 21:AA:526:C:OP2   | 1.86                     | 0.75              |
| 24:BA:2144:G:H2'   | 24:BA:2148:G:O6   | 1.87                     | 0.75              |
| 31:BH:5:LEU:HD13   | 31:BH:13:GLY:HA2  | 1.69                     | 0.75              |
| 48:BY:45:GLN:O     | 48:BY:46:VAL:HB   | 1.87                     | 0.75              |
| 9:CJ:45:ARG:NH2    | 55:CA:1279:G:H5'' | 2.01                     | 0.75              |
| 55:CA:652:U:HO2'   | 55:CA:653:U:H6    | 1.33                     | 0.75              |
| 5:AF:16:GLU:CG     | 3:CD:191:SER:HB2  | 2.15                     | 0.75              |
| 24:DA:456:C:O2'    | 43:DT:73:ARG:HG3  | 1.85                     | 0.75              |
| 21:AA:297:G:H4'    | 21:AA:557:G:H4'   | 1.67                     | 0.75              |
| 1:AB:33:ALA:HA     | 1:AB:38:HIS:HA    | 1.69                     | 0.75              |
| 6:AG:88:VAL:HG22   | 6:AG:89:GLU:H     | 1.50                     | 0.75              |
| 7:AH:63:LYS:O      | 7:AH:70:VAL:HG23  | 1.87                     | 0.75              |
| 24:BA:1327:A:H2'   | 24:BA:1328:A:H5'  | 1.68                     | 0.75              |
| 49:BZ:29:ARG:HH21  | 49:BZ:29:ARG:CG   | 1.99                     | 0.75              |
| 4:CE:14:LEU:HG     | 4:CE:15:ILE:H     | 1.50                     | 0.75              |
| 18:CS:51:HIS:CD2   | 18:CS:53:GLY:H    | 2.04                     | 0.75              |
| 24:DA:2304:G:H1    | 24:DA:2312:U:H3   | 1.35                     | 0.75              |
| 29:DF:91:ARG:HB3   | 29:DF:91:ARG:HH21 | 1.51                     | 0.75              |
| 27:DD:9:VAL:O      | 39:DP:4:ILE:HD11  | 1.86                     | 0.75              |
| 31:BH:89:LYS:HG2   | 31:BH:90:LEU:H    | 1.50                     | 0.74              |
| 36:BM:133:LYS:O    | 36:BM:134:THR:HB  | 1.86                     | 0.74              |
| 40:BQ:69:ARG:CB    | 40:BQ:69:ARG:HH21 | 2.00                     | 0.74              |
| 8:CI:15:ALA:O      | 8:CI:66:VAL:HG23  | 1.87                     | 0.74              |
| 24:DA:1847:A:O2'   | 24:DA:1848:A:C8   | 2.38                     | 0.74              |
| 24:DA:92:U:H2'     | 24:DA:93:G:H8     | 1.51                     | 0.74              |
| 21:AA:428:G:H1'    | 21:AA:430:A:N7    | 2.02                     | 0.74              |
| 24:BA:2747:G:O2'   | 30:BG:66:THR:HG22 | 1.87                     | 0.74              |
| 29:BF:68:LYS:HD2   | 29:BF:68:LYS:H    | 1.49                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:1498:U:H2'  | 23:CW:2:U:OP1     | 1.87                     | 0.74              |
| 1:CB:92:ASN:H     | 1:CB:92:ASN:HD22  | 1.35                     | 0.74              |
| 7:CH:106:SER:HB2  | 55:CA:640:A:O2'   | 1.87                     | 0.74              |
| 24:DA:1458:U:O3'  | 24:DA:1459:G:H4'  | 1.86                     | 0.74              |
| 24:DA:1570:A:H2'  | 24:DA:1571:A:C8   | 2.21                     | 0.74              |
| 24:BA:2615:U:C2   | 50:B0:3:GLN:HA    | 2.22                     | 0.74              |
| 24:BA:2707:U:O2   | 37:BN:71:ARG:NH1  | 2.20                     | 0.74              |
| 24:BA:276:U:H1'   | 24:BA:278:A:H62   | 1.52                     | 0.74              |
| 24:BA:31:C:O3'    | 24:BA:1238:G:H5'' | 1.88                     | 0.74              |
| 37:BN:1:MET:O     | 37:BN:2:ARG:HB2   | 1.87                     | 0.74              |
| 48:BY:57:LEU:HA   | 48:BY:60:LYS:HB3  | 1.67                     | 0.74              |
| 21:AA:1338:G:H2'  | 21:AA:1339:A:C8   | 2.23                     | 0.74              |
| 8:AI:51:LEU:HD13  | 8:AI:56:MET:HG2   | 1.68                     | 0.74              |
| 10:AK:66:ALA:HB1  | 10:AK:99:LEU:HD13 | 1.68                     | 0.74              |
| 24:BA:2673:G:C2   | 24:BA:2674:G:C8   | 2.76                     | 0.74              |
| 24:BA:794:A:H2'   | 24:BA:795:C:C6    | 2.23                     | 0.74              |
| 27:BD:97:SER:C    | 27:BD:99:GLU:HG2  | 2.07                     | 0.74              |
| 28:BE:57:LYS:HG3  | 28:BE:58:LYS:N    | 2.01                     | 0.74              |
| 55:CA:613:C:H2'   | 55:CA:614:C:H6    | 1.51                     | 0.74              |
| 24:DA:1070:A:N6   | 32:DI:8:VAL:HG12  | 2.02                     | 0.74              |
| 24:DA:1838:C:H5'' | 24:DA:1839:G:OP1  | 1.88                     | 0.74              |
| 24:DA:241:A:H1'   | 24:DA:243:U:C5    | 2.22                     | 0.74              |
| 24:DA:2543:G:C6   | 24:DA:2765:A:C5   | 2.76                     | 0.74              |
| 56:DB:45:A:H2'    | 56:DB:46:A:H8     | 1.51                     | 0.74              |
| 28:DE:170:ARG:NH2 | 28:DE:176:ASP:HB2 | 2.02                     | 0.74              |
| 30:DG:162:ARG:H   | 30:DG:162:ARG:HD2 | 1.52                     | 0.74              |
| 32:DI:57:VAL:HG12 | 32:DI:58:ILE:H    | 1.50                     | 0.74              |
| 56:DB:50:A:OP1    | 38:DO:68:LYS:N    | 2.20                     | 0.74              |
| 21:AA:1279:G:O2'  | 21:AA:1282:C:N4   | 2.21                     | 0.74              |
| 21:AA:243:A:H4'   | 21:AA:244:U:C5'   | 2.17                     | 0.74              |
| 21:AA:748:G:H2'   | 21:AA:749:A:C8    | 2.23                     | 0.74              |
| 18:AS:62:THR:HG22 | 18:AS:63:ASP:H    | 1.52                     | 0.74              |
| 24:BA:2358:A:H61  | 35:BL:54:GLN:HE22 | 1.33                     | 0.74              |
| 24:BA:2783:U:H2'  | 24:BA:2784:U:H6   | 1.51                     | 0.74              |
| 24:BA:742:A:H2'   | 24:BA:743:A:C8    | 2.22                     | 0.74              |
| 27:BD:99:GLU:HG3  | 27:BD:100:LEU:H   | 1.52                     | 0.74              |
| 24:BA:1654:A:H4'  | 27:BD:118:PHE:CZ  | 2.23                     | 0.74              |
| 31:BH:34:GLY:O    | 31:BH:35:LYS:HG3  | 1.87                     | 0.74              |
| 43:BT:87:LEU:HB2  | 43:BT:91:GLN:HG2  | 1.67                     | 0.74              |
| 24:DA:2544:G:H5'  | 24:DA:2645:G:N7   | 2.01                     | 0.74              |
| 29:DF:76:PHE:H    | 29:DF:76:PHE:HD2  | 1.33                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DN:38:LEU:HB3   | 37:DN:39:PRO:HD3   | 1.68                     | 0.74              |
| 24:BA:243:U:OP1    | 53:B3:5:THR:HG21   | 1.88                     | 0.74              |
| 24:BA:142:A:H2'    | 24:BA:143:C:C6     | 2.22                     | 0.74              |
| 24:BA:303:G:H2'    | 24:BA:304:U:C6     | 2.22                     | 0.74              |
| 24:BA:734:A:C5     | 24:BA:735:A:N7     | 2.55                     | 0.74              |
| 30:BG:126:THR:HG22 | 30:BG:127:GLN:H    | 1.51                     | 0.74              |
| 46:BW:18:LYS:HA    | 46:BW:36:ILE:CG1   | 2.18                     | 0.74              |
| 55:CA:116:A:H2'    | 55:CA:117:G:H8     | 1.52                     | 0.74              |
| 5:CF:66:ALA:HB1    | 5:CF:70:VAL:HG23   | 1.70                     | 0.74              |
| 11:CL:45:ASN:HA    | 55:CA:529:G:O6     | 1.86                     | 0.74              |
| 24:DA:1695:G:C8    | 26:DC:7:PRO:HB2    | 2.21                     | 0.74              |
| 38:DO:11:ALA:HB2   | 38:DO:96:GLY:N     | 2.02                     | 0.74              |
| 3:AD:60:VAL:O      | 3:AD:63:ILE:HG22   | 1.88                     | 0.74              |
| 24:BA:2253:G:H2'   | 24:BA:2254:C:C6    | 2.22                     | 0.74              |
| 24:BA:571:U:H4'    | 24:BA:572:A:OP1    | 1.86                     | 0.74              |
| 30:BG:60:GLY:O     | 30:BG:61:TRP:HB2   | 1.88                     | 0.74              |
| 45:BV:80:HIS:CD2   | 45:BV:83:LYS:H     | 2.01                     | 0.74              |
| 24:DA:1565:C:H5''  | 26:DC:17:LYS:HE2   | 1.69                     | 0.74              |
| 24:DA:247:G:C5     | 24:DA:249:C:H1'    | 2.22                     | 0.74              |
| 33:DJ:17:VAL:HG23  | 33:DJ:137:PRO:HB2  | 1.70                     | 0.74              |
| 21:AA:874:G:O2'    | 21:AA:875:U:H5'    | 1.88                     | 0.74              |
| 1:AB:113:LEU:HD13  | 1:AB:143:LEU:HD21  | 1.70                     | 0.74              |
| 4:AE:82:HIS:NE2    | 4:AE:146:MET:HG3   | 2.03                     | 0.74              |
| 6:AG:73:GLU:HA     | 6:AG:140:VAL:HG12  | 1.70                     | 0.74              |
| 24:BA:1013:C:H2'   | 24:BA:1014:A:C8    | 2.22                     | 0.74              |
| 24:BA:395:U:O2'    | 24:BA:396:G:C8     | 2.40                     | 0.74              |
| 24:BA:417:C:H2'    | 24:BA:418:C:H6     | 1.53                     | 0.74              |
| 27:BD:193:VAL:HG21 | 27:BD:201:LEU:HD21 | 1.70                     | 0.74              |
| 31:BH:90:LEU:HB2   | 31:BH:123:ARG:HB3  | 1.67                     | 0.74              |
| 40:BQ:97:ILE:HD11  | 40:BQ:105:PHE:CA   | 2.17                     | 0.74              |
| 43:BT:4:GLU:OE1    | 43:BT:6:ARG:HG3    | 1.87                     | 0.74              |
| 55:CA:154:U:H2'    | 55:CA:155:A:H5'    | 1.70                     | 0.74              |
| 55:CA:459:A:O2'    | 55:CA:460:A:H5'    | 1.88                     | 0.74              |
| 6:CG:75:LYS:HE2    | 6:CG:76:SER:H      | 1.50                     | 0.74              |
| 24:DA:2311:A:N3    | 24:DA:2311:A:C2'   | 2.50                     | 0.74              |
| 24:DA:873:C:H4'    | 36:DM:64:TRP:NE1   | 2.03                     | 0.74              |
| 42:DS:17:VAL:HG11  | 42:DS:103:ILE:HG13 | 1.68                     | 0.74              |
| 24:BA:1027:A:C6    | 24:BA:1126:A:N3    | 2.56                     | 0.74              |
| 24:BA:2336:A:N6    | 46:BW:40:ARG:HD2   | 2.03                     | 0.74              |
| 26:BC:104:LEU:O    | 26:BC:105:ALA:HB2  | 1.87                     | 0.74              |
| 31:BH:97:ARG:HG2   | 31:BH:111:ALA:HB1  | 1.70                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BH:48:GLU:HA    | 31:BH:51:ARG:HG3   | 1.69                     | 0.74              |
| 24:DA:2868:A:H2'   | 24:DA:2869:G:C8    | 2.23                     | 0.74              |
| 24:DA:589:U:O2'    | 24:DA:590:A:H5'    | 1.88                     | 0.74              |
| 24:DA:828:U:H4'    | 24:DA:831:G:C6     | 2.23                     | 0.74              |
| 29:DF:74:ALA:HB3   | 29:DF:78:ILE:CG1   | 2.16                     | 0.74              |
| 37:DN:5:LYS:HG2    | 37:DN:6:SER:H      | 1.52                     | 0.74              |
| 21:AA:132:C:H2'    | 21:AA:133:U:H6     | 1.52                     | 0.74              |
| 24:BA:2353:G:H1'   | 46:BW:30:VAL:CG1   | 2.18                     | 0.74              |
| 55:CA:1508:A:H2'   | 55:CA:1509:C:C6    | 2.23                     | 0.74              |
| 55:CA:781:A:H2'    | 55:CA:782:A:H5'    | 1.70                     | 0.74              |
| 9:CJ:66:GLU:HB2    | 13:CN:100:TRP:HZ3  | 1.53                     | 0.74              |
| 54:D4:19:ARG:O     | 54:D4:20:ASP:HB2   | 1.87                     | 0.74              |
| 24:DA:2292:U:H2'   | 24:DA:2293:G:H8    | 1.53                     | 0.74              |
| 24:DA:2385:C:O2'   | 24:DA:2386:A:C8    | 2.37                     | 0.74              |
| 24:DA:665:U:H2'    | 24:DA:666:A:H8     | 1.51                     | 0.74              |
| 28:DE:126:VAL:HG21 | 28:DE:134:LEU:HD13 | 1.70                     | 0.74              |
| 29:DF:12:VAL:HA    | 29:DF:15:LEU:HB2   | 1.70                     | 0.74              |
| 43:DT:60:THR:HG22  | 43:DT:83:ALA:HA    | 1.70                     | 0.74              |
| 24:BA:204:A:H4'    | 24:BA:205:G:OP1    | 1.86                     | 0.73              |
| 24:BA:2068:U:H5''  | 24:BA:2068:U:H6    | 1.52                     | 0.73              |
| 24:BA:2654:A:H4'   | 24:BA:2655:G:OP1   | 1.86                     | 0.73              |
| 24:BA:85:G:OP1     | 44:BU:27:VAL:HG11  | 1.88                     | 0.73              |
| 34:BK:18:ARG:CG    | 34:BK:18:ARG:HH11  | 2.01                     | 0.73              |
| 36:BM:17:ASN:O     | 36:BM:38:ARG:HD3   | 1.88                     | 0.73              |
| 55:CA:977:A:N3     | 55:CA:977:A:H5''   | 2.03                     | 0.73              |
| 12:CM:8:ILE:HD13   | 29:DF:136:ILE:HG13 | 1.67                     | 0.73              |
| 24:DA:784:G:O6     | 26:DC:227:VAL:HG11 | 1.88                     | 0.73              |
| 21:AA:922:G:H2'    | 21:AA:923:A:C8     | 2.24                     | 0.73              |
| 24:BA:786:C:O2'    | 24:BA:787:C:H5'    | 1.88                     | 0.73              |
| 24:BA:856:G:H21    | 46:BW:19:ARG:HH22  | 1.35                     | 0.73              |
| 40:BQ:85:ALA:O     | 40:BQ:86:SER:C     | 2.24                     | 0.73              |
| 55:CA:1201:A:O2'   | 55:CA:1202:U:OP2   | 2.06                     | 0.73              |
| 55:CA:1239:A:H62   | 55:CA:1299:A:N6    | 1.84                     | 0.73              |
| 21:AA:903:G:H2'    | 21:AA:904:U:C6     | 2.24                     | 0.73              |
| 4:AE:155:LYS:HD2   | 4:AE:156:ARG:HG2   | 1.70                     | 0.73              |
| 4:AE:32:PHE:CD2    | 4:AE:54:GLU:HA     | 2.24                     | 0.73              |
| 51:B1:49:LYS:HG2   | 51:B1:50:GLU:H     | 1.54                     | 0.73              |
| 24:BA:1181:U:O2'   | 24:BA:1182:G:O5'   | 2.06                     | 0.73              |
| 24:BA:1286:A:O2'   | 24:BA:1288:G:OP2   | 2.05                     | 0.73              |
| 24:BA:1333:G:H2'   | 24:BA:1334:G:H8    | 1.52                     | 0.73              |
| 24:BA:2093:G:O2'   | 24:BA:2094:A:H5'   | 1.89                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:63:A:C2     | 24:BA:64:A:N7      | 2.56                     | 0.73              |
| 24:BA:802:A:H2'   | 24:BA:803:U:H6     | 1.49                     | 0.73              |
| 26:BC:180:MET:HG3 | 26:BC:268:ARG:NH1  | 2.03                     | 0.73              |
| 55:CA:1160:G:C6   | 55:CA:1181:G:O6    | 2.41                     | 0.73              |
| 55:CA:1432:G:H1'  | 55:CA:1468:A:N6    | 2.03                     | 0.73              |
| 55:CA:1446:A:H2'  | 55:CA:1447:A:H5''  | 1.68                     | 0.73              |
| 12:CM:16:ILE:H    | 12:CM:16:ILE:HD12  | 1.53                     | 0.73              |
| 18:CS:40:PHE:HB3  | 18:CS:41:PRO:CD    | 2.17                     | 0.73              |
| 24:DA:1201:U:H2'  | 24:DA:1202:G:H8    | 1.53                     | 0.73              |
| 24:DA:2895:G:HO2' | 24:DA:2896:C:H6    | 1.31                     | 0.73              |
| 24:DA:668:A:C5    | 24:DA:670:A:N7     | 2.56                     | 0.73              |
| 24:DA:95:A:H1'    | 48:DY:40:SER:HB2   | 1.69                     | 0.73              |
| 8:AI:8:THR:HG23   | 21:AA:1148:U:H5''  | 1.70                     | 0.73              |
| 34:BK:63:VAL:HG22 | 34:BK:107:LEU:HD21 | 1.68                     | 0.73              |
| 42:BS:97:LEU:HD22 | 42:BS:97:LEU:N     | 2.03                     | 0.73              |
| 55:CA:1213:A:HO2' | 55:CA:1214:C:H5'   | 1.53                     | 0.73              |
| 55:CA:250:A:H1'   | 55:CA:252:U:N3     | 2.03                     | 0.73              |
| 24:DA:1919:A:H8   | 24:DA:1919:A:O5'   | 1.69                     | 0.73              |
| 24:DA:391:A:O2'   | 24:DA:392:U:C5'    | 2.36                     | 0.73              |
| 24:DA:412:A:H2'   | 24:DA:413:C:C6     | 2.23                     | 0.73              |
| 24:DA:506:G:H4'   | 24:DA:507:A:H5'    | 1.70                     | 0.73              |
| 29:DF:28:PRO:HB2  | 29:DF:168:LEU:HD21 | 1.70                     | 0.73              |
| 21:AA:1376:U:H2'  | 21:AA:1377:A:H8    | 1.53                     | 0.73              |
| 14:AO:42:PHE:CE1  | 14:AO:55:LEU:HD22  | 2.24                     | 0.73              |
| 24:BA:1073:A:C3'  | 24:BA:1074:G:H5''  | 2.19                     | 0.73              |
| 24:BA:1328:A:H2'  | 24:BA:1330:C:C5    | 2.23                     | 0.73              |
| 24:BA:1669:A:N3   | 24:BA:1669:A:H2'   | 2.01                     | 0.73              |
| 24:BA:979:A:H2'   | 24:BA:982:C:N4     | 2.03                     | 0.73              |
| 31:BH:31:VAL:CB   | 31:BH:32:PRO:HD2   | 2.16                     | 0.73              |
| 24:BA:1082:U:H5'  | 32:BI:117:THR:O    | 1.88                     | 0.73              |
| 55:CA:1124:G:H4'  | 55:CA:1125:U:OP1   | 1.89                     | 0.73              |
| 20:CU:38:GLU:HG3  | 55:CA:1526:G:OP1   | 1.88                     | 0.73              |
| 55:CA:874:G:O2'   | 55:CA:875:U:H5'    | 1.88                     | 0.73              |
| 12:CM:77:LYS:HE3  | 12:CM:77:LYS:O     | 1.88                     | 0.73              |
| 24:DA:2063:C:O2'  | 24:DA:2064:C:H5'   | 1.89                     | 0.73              |
| 43:DT:50:LEU:HD23 | 43:DT:51:PHE:H     | 1.54                     | 0.73              |
| 48:DY:1:MET:HG2   | 48:DY:4:LYS:HZ1    | 1.52                     | 0.73              |
| 4:AE:25:LYS:HZ2   | 4:AE:25:LYS:HB3    | 1.52                     | 0.73              |
| 24:BA:1738:G:HO2' | 24:BA:1739:A:H8    | 1.37                     | 0.73              |
| 24:BA:2047:C:O2'  | 24:BA:2048:G:H5'   | 1.89                     | 0.73              |
| 24:BA:2305:U:C4   | 24:BA:2306:C:C4    | 2.76                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BH:117:LEU:HD11 | 31:BH:130:VAL:HG11 | 1.70                     | 0.73              |
| 32:BI:79:LEU:HD13  | 32:BI:135:MET:SD   | 2.29                     | 0.73              |
| 35:BL:27:LEU:N     | 35:BL:27:LEU:HD12  | 2.00                     | 0.73              |
| 43:BT:29:THR:HB    | 43:BT:86:THR:CG2   | 2.18                     | 0.73              |
| 44:BU:15:GLY:O     | 44:BU:17:ASP:N     | 2.21                     | 0.73              |
| 13:CN:62:ARG:HE    | 13:CN:69:PRO:HA    | 1.52                     | 0.73              |
| 24:DA:1333:G:HO2'  | 24:DA:1334:G:H8    | 1.35                     | 0.73              |
| 24:DA:1447:C:H2'   | 24:DA:1448:G:C8    | 2.23                     | 0.73              |
| 56:DB:98:G:H1      | 45:DV:14:LYS:CB    | 2.01                     | 0.73              |
| 26:DC:140:VAL:HG22 | 26:DC:161:VAL:O    | 1.88                     | 0.73              |
| 31:DH:78:VAL:HG22  | 31:DH:100:ALA:HA   | 1.69                     | 0.73              |
| 33:DJ:25:LEU:HD12  | 33:DJ:64:VAL:HA    | 1.71                     | 0.73              |
| 22:AV:27:G:H5''    | 22:AV:27:G:H8      | 1.54                     | 0.73              |
| 24:BA:1064:C:H4'   | 32:BI:90:GLY:H     | 1.52                     | 0.73              |
| 24:BA:2092:U:H4'   | 24:BA:2093:G:O5'   | 1.88                     | 0.73              |
| 24:BA:2275:C:O2'   | 36:BM:84:LYS:HA    | 1.88                     | 0.73              |
| 24:BA:2896:C:H2'   | 24:BA:2897:U:H6    | 1.54                     | 0.73              |
| 24:BA:1255:U:C5    | 28:BE:68:ALA:HA    | 2.23                     | 0.73              |
| 36:BM:73:ILE:HG21  | 36:BM:91:TYR:CZ    | 2.24                     | 0.73              |
| 2:CC:122:GLN:HB2   | 2:CC:127:VAL:HG21  | 1.71                     | 0.73              |
| 2:CC:190:THR:HG22  | 2:CC:192:TYR:H     | 1.53                     | 0.73              |
| 53:D3:22:LYS:H     | 53:D3:48:MET:HB3   | 1.54                     | 0.73              |
| 24:DA:1062:G:C8    | 24:DA:1088:A:H8    | 2.06                     | 0.73              |
| 24:DA:1258:U:H2'   | 24:DA:1259:G:C8    | 2.23                     | 0.73              |
| 24:DA:2291:U:H2'   | 24:DA:2292:U:C6    | 2.24                     | 0.73              |
| 31:DH:41:LYS:HA    | 31:DH:44:ILE:HG12  | 1.69                     | 0.73              |
| 18:AS:5:LYS:HD3    | 21:AA:1314:C:C5    | 2.24                     | 0.73              |
| 21:AA:1432:G:H1'   | 21:AA:1468:A:N6    | 2.03                     | 0.73              |
| 21:AA:204:G:H3'    | 21:AA:205:A:C5'    | 2.18                     | 0.73              |
| 13:AN:46:LYS:HD2   | 18:AS:12:LEU:HD21  | 1.69                     | 0.73              |
| 24:BA:1430:G:H2'   | 24:BA:1431:A:C8    | 2.23                     | 0.73              |
| 24:BA:855:G:N3     | 46:BW:23:LYS:HD3   | 2.04                     | 0.73              |
| 42:BS:13:SER:OG    | 42:BS:16:LYS:HD2   | 1.89                     | 0.73              |
| 46:BW:23:LYS:CE    | 46:BW:24:ARG:HG3   | 2.18                     | 0.73              |
| 55:CA:864:A:H2'    | 55:CA:865:A:C8     | 2.23                     | 0.73              |
| 1:CB:49:PHE:HA     | 1:CB:52:ALA:HB3    | 1.71                     | 0.73              |
| 6:CG:22:LEU:HA     | 6:CG:25:PHE:HB3    | 1.70                     | 0.73              |
| 10:CK:70:ALA:HA    | 10:CK:73:VAL:HG22  | 1.69                     | 0.73              |
| 16:CQ:13:SER:HB3   | 16:CQ:21:VAL:HB    | 1.69                     | 0.73              |
| 24:DA:1070:A:H5'   | 24:DA:1071:G:H5''  | 1.71                     | 0.73              |
| 24:DA:1522:A:H1'   | 24:DA:1524:G:C5    | 2.24                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:1313:U:C6   | 24:DA:1610:A:C8   | 2.77                     | 0.73              |
| 24:DA:2135:A:H3'  | 24:DA:2136:G:H5'' | 1.70                     | 0.73              |
| 24:DA:729:G:N3    | 24:DA:729:G:H2'   | 2.03                     | 0.73              |
| 28:DE:122:GLU:HA  | 28:DE:190:ALA:HB2 | 1.71                     | 0.73              |
| 32:DI:8:VAL:C     | 32:DI:9:LYS:HG2   | 2.08                     | 0.73              |
| 49:DZ:4:ILE:HD12  | 49:DZ:58:GLU:HA   | 1.71                     | 0.73              |
| 21:AA:1278:G:H4'  | 21:AA:1279:G:C8   | 2.23                     | 0.73              |
| 21:AA:1435:G:H2'  | 21:AA:1436:U:C6   | 2.23                     | 0.73              |
| 21:AA:205:A:H4'   | 21:AA:205:A:OP1   | 1.88                     | 0.73              |
| 3:AD:96:ARG:HB3   | 3:AD:98:ASP:OD1   | 1.89                     | 0.73              |
| 4:AE:25:LYS:HB3   | 4:AE:25:LYS:NZ    | 2.04                     | 0.73              |
| 4:AE:15:ILE:HD11  | 4:AE:37:VAL:HG23  | 1.71                     | 0.73              |
| 5:AF:38:ARG:HB3   | 5:AF:63:ASN:HB2   | 1.70                     | 0.73              |
| 24:BA:491:G:N2    | 24:BA:492:A:H1'   | 2.02                     | 0.73              |
| 40:BQ:97:ILE:HD11 | 40:BQ:105:PHE:HA  | 1.69                     | 0.73              |
| 40:BQ:39:ILE:O    | 40:BQ:43:GLN:HG3  | 1.89                     | 0.73              |
| 55:CA:1095:U:H2'  | 55:CA:1096:C:C6   | 2.24                     | 0.73              |
| 24:DA:2197:U:O2'  | 24:DA:2198:A:H8   | 1.71                     | 0.73              |
| 24:DA:274:C:H2'   | 24:DA:275:C:O4'   | 1.89                     | 0.73              |
| 24:DA:526:A:N6    | 24:DA:2626:C:H4'  | 2.04                     | 0.73              |
| 24:DA:2529:G:H4'  | 30:DG:174:LYS:HD3 | 1.70                     | 0.73              |
| 27:DD:14:ILE:HG13 | 39:DP:11:GLN:HE22 | 1.52                     | 0.73              |
| 3:AD:62:ARG:HA    | 3:AD:62:ARG:NE    | 2.03                     | 0.73              |
| 3:AD:90:LEU:HA    | 3:AD:93:LEU:HD12  | 1.70                     | 0.73              |
| 11:AL:29:LYS:O    | 11:AL:81:ILE:HG22 | 1.89                     | 0.73              |
| 24:BA:2251:G:H2'  | 24:BA:2252:G:C8   | 2.24                     | 0.73              |
| 24:BA:855:G:H1'   | 46:BW:23:LYS:HD3  | 1.69                     | 0.73              |
| 28:BE:44:ARG:HH21 | 28:BE:44:ARG:CG   | 2.02                     | 0.73              |
| 24:BA:470:A:H61   | 43:BT:72:GLN:HE22 | 1.33                     | 0.73              |
| 48:BY:39:GLN:HB2  | 48:BY:41:HIS:CD2  | 2.24                     | 0.73              |
| 55:CA:1023:U:H2'  | 55:CA:1024:G:C8   | 2.24                     | 0.73              |
| 55:CA:47:C:H4'    | 55:CA:48:C:O5'    | 1.87                     | 0.73              |
| 52:D2:19:ARG:HB3  | 52:D2:19:ARG:NH2  | 2.03                     | 0.73              |
| 24:DA:1854:A:N6   | 24:DA:1888:G:H1'  | 2.03                     | 0.73              |
| 24:DA:61:C:O2'    | 24:DA:62:U:H5'    | 1.87                     | 0.73              |
| 34:DK:60:ALA:HA   | 34:DK:87:LEU:HD23 | 1.71                     | 0.73              |
| 36:DM:41:LEU:HD23 | 36:DM:46:ILE:HG22 | 1.70                     | 0.73              |
| 27:BD:45:TYR:CD1  | 27:BD:45:TYR:N    | 2.57                     | 0.72              |
| 8:CI:56:MET:HG3   | 8:CI:57:VAL:HG23  | 1.70                     | 0.72              |
| 45:DV:9:ARG:HG2   | 45:DV:39:ALA:O    | 1.89                     | 0.72              |
| 1:AB:41:ASN:HB3   | 1:AB:44:LYS:HB3   | 1.69                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:AV:33:U:H5'    | 22:AV:34:G:OP2    | 1.89                     | 0.72              |
| 24:BA:1681:G:O2'  | 24:BA:1762:A:O2'  | 2.06                     | 0.72              |
| 24:BA:1962:C:O2'  | 24:BA:1964:G:OP2  | 2.07                     | 0.72              |
| 37:BN:74:GLU:O    | 37:BN:77:ALA:HB3  | 1.89                     | 0.72              |
| 40:BQ:63:ARG:HH22 | 40:BQ:96:ASP:HB3  | 1.54                     | 0.72              |
| 42:BS:69:LEU:HD12 | 42:BS:108:SER:O   | 1.89                     | 0.72              |
| 55:CA:533:A:C2    | 55:CA:536:C:C5    | 2.77                     | 0.72              |
| 55:CA:736:C:H2'   | 55:CA:737:C:C6    | 2.24                     | 0.72              |
| 6:CG:59:GLU:HB2   | 6:CG:62:GLU:HB2   | 1.68                     | 0.72              |
| 24:DA:2674:G:H2'  | 24:DA:2675:A:H8   | 1.53                     | 0.72              |
| 24:DA:303:G:H2'   | 24:DA:304:U:C6    | 2.24                     | 0.72              |
| 24:DA:395:U:HO2'  | 24:DA:396:G:H8    | 0.78                     | 0.72              |
| 24:DA:2529:G:H4'  | 30:DG:174:LYS:CD  | 2.19                     | 0.72              |
| 40:DQ:69:ARG:HH21 | 40:DQ:69:ARG:HB2  | 1.53                     | 0.72              |
| 45:DV:59:GLU:HG2  | 45:DV:60:VAL:H    | 1.53                     | 0.72              |
| 48:DY:18:LEU:O    | 48:DY:22:LEU:HD13 | 1.88                     | 0.72              |
| 21:AA:116:A:O2'   | 21:AA:117:G:H5'   | 1.90                     | 0.72              |
| 4:AE:156:ARG:HG2  | 7:AH:63:LYS:NZ    | 2.01                     | 0.72              |
| 24:BA:2727:A:O2'  | 24:BA:2728:U:H5'  | 1.89                     | 0.72              |
| 24:BA:395:U:O2'   | 24:BA:396:G:N7    | 2.22                     | 0.72              |
| 43:BT:11:LEU:HD11 | 43:BT:47:VAL:HG22 | 1.71                     | 0.72              |
| 24:DA:223:A:N6    | 24:DA:422:A:C6    | 2.57                     | 0.72              |
| 56:DB:42:C:H2'    | 56:DB:43:C:H6     | 1.51                     | 0.72              |
| 43:DT:20:ALA:HB1  | 43:DT:31:VAL:HG21 | 1.71                     | 0.72              |
| 44:DU:17:ASP:HB2  | 44:DU:38:ILE:HA   | 1.70                     | 0.72              |
| 47:DX:63:ILE:HD12 | 47:DX:64:ASP:H    | 1.54                     | 0.72              |
| 21:AA:753:A:H4'   | 21:AA:754:C:O5'   | 1.89                     | 0.72              |
| 1:AB:119:GLN:C    | 1:AB:119:GLN:HE21 | 1.93                     | 0.72              |
| 4:AE:84:VAL:HB    | 4:AE:146:MET:HE3  | 1.70                     | 0.72              |
| 9:AJ:52:LEU:HD21  | 9:AJ:59:LYS:HA    | 1.72                     | 0.72              |
| 44:BU:73:ASN:ND2  | 44:BU:75:ALA:HB3  | 2.05                     | 0.72              |
| 55:CA:1241:G:HO2' | 55:CA:1242:G:H8   | 0.76                     | 0.72              |
| 55:CA:1376:U:H2'  | 55:CA:1377:A:C8   | 2.24                     | 0.72              |
| 55:CA:243:A:N3    | 55:CA:245:U:H2'   | 2.04                     | 0.72              |
| 55:CA:834:U:H2'   | 55:CA:835:U:H6    | 1.51                     | 0.72              |
| 4:CE:125:LYS:HG2  | 4:CE:126:ALA:N    | 2.05                     | 0.72              |
| 19:CT:23:ARG:HB3  | 19:CT:60:GLN:HE22 | 1.53                     | 0.72              |
| 24:DA:123:G:O3'   | 24:DA:1376:C:H4'  | 1.89                     | 0.72              |
| 24:DA:1450:G:H21  | 24:DA:1452:G:H1   | 1.35                     | 0.72              |
| 24:DA:85:G:HO2'   | 24:DA:86:G:H8     | 1.35                     | 0.72              |
| 27:DD:51:THR:CG2  | 27:DD:76:GLY:HA3  | 2.20                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:1364:G:C5    | 47:DX:1:SER:HB2    | 2.25                     | 0.72              |
| 21:AA:555:U:H2'    | 21:AA:556:C:C6     | 2.24                     | 0.72              |
| 6:AG:110:ARG:HH11  | 6:AG:122:GLU:HG2   | 1.53                     | 0.72              |
| 24:BA:387:U:H4'    | 24:BA:388:G:H5''   | 1.70                     | 0.72              |
| 24:BA:515:A:H5''   | 24:BA:516:C:OP2    | 1.88                     | 0.72              |
| 24:BA:588:U:H1'    | 28:BE:85:PHE:CD1   | 2.25                     | 0.72              |
| 28:BE:95:LYS:O     | 28:BE:96:VAL:HB    | 1.89                     | 0.72              |
| 30:BG:84:LYS:CG    | 30:BG:132:LEU:H    | 2.00                     | 0.72              |
| 55:CA:372:C:H4'    | 55:CA:373:A:C5'    | 2.18                     | 0.72              |
| 1:CB:130:LYS:HA    | 1:CB:133:ALA:HB3   | 1.72                     | 0.72              |
| 2:CC:133:MET:HE2   | 2:CC:150:VAL:HG23  | 1.69                     | 0.72              |
| 4:CE:95:MET:HA     | 4:CE:124:ALA:HB2   | 1.71                     | 0.72              |
| 24:DA:1565:C:O2'   | 24:DA:1566:A:H8    | 1.71                     | 0.72              |
| 24:DA:482:A:N6     | 24:DA:506:G:C4     | 2.58                     | 0.72              |
| 24:DA:538:A:H5''   | 33:DJ:7:LYS:NZ     | 2.04                     | 0.72              |
| 24:DA:574:A:H4'    | 24:DA:575:A:H5'    | 1.71                     | 0.72              |
| 41:DR:82:HIS:O     | 41:DR:82:HIS:CG    | 2.40                     | 0.72              |
| 21:AA:415:A:H2'    | 21:AA:416:G:C8     | 2.24                     | 0.72              |
| 21:AA:895:G:C5     | 21:AA:896:C:C5     | 2.78                     | 0.72              |
| 24:BA:811:U:O2     | 24:BA:1250:G:H3'   | 1.90                     | 0.72              |
| 24:BA:1993:U:H4'   | 27:BD:133:THR:HG21 | 1.72                     | 0.72              |
| 27:BD:110:THR:HG23 | 27:BD:171:THR:HG22 | 1.70                     | 0.72              |
| 33:BJ:30:THR:CG2   | 33:BJ:31:GLU:N     | 2.53                     | 0.72              |
| 55:CA:252:U:O2'    | 55:CA:253:A:H8     | 1.71                     | 0.72              |
| 55:CA:981:U:H2'    | 55:CA:982:U:C5     | 2.24                     | 0.72              |
| 24:DA:1069:A:H4'   | 24:DA:1070:A:O5'   | 1.87                     | 0.72              |
| 24:DA:1264:A:H5'   | 50:D0:7:PRO:HG2    | 1.72                     | 0.72              |
| 24:DA:1271:G:OP2   | 59:DA:3400:HOH:O   | 2.06                     | 0.72              |
| 24:DA:1737:G:C6    | 24:DA:1738:G:N1    | 2.58                     | 0.72              |
| 27:DD:107:VAL:HG13 | 27:DD:109:VAL:HG23 | 1.71                     | 0.72              |
| 47:DX:30:PRO:HG2   | 47:DX:32:LEU:HD21  | 1.72                     | 0.72              |
| 19:AT:26:MET:HB3   | 21:AA:1457:G:O3'   | 1.89                     | 0.72              |
| 1:AB:30:ILE:HG12   | 1:AB:39:ILE:O      | 1.89                     | 0.72              |
| 24:BA:1444:G:H2'   | 24:BA:1445:G:C8    | 2.24                     | 0.72              |
| 24:BA:1820:U:H4'   | 24:BA:1821:A:OP2   | 1.90                     | 0.72              |
| 24:BA:2197:U:HO2'  | 24:BA:2198:A:H2'   | 1.53                     | 0.72              |
| 24:BA:265:A:C8     | 24:BA:428:A:C2     | 2.77                     | 0.72              |
| 24:BA:811:U:C4     | 35:BL:21:ARG:NH2   | 2.57                     | 0.72              |
| 24:BA:856:G:H21    | 46:BW:19:ARG:NH2   | 1.88                     | 0.72              |
| 26:BC:123:ILE:HG12 | 26:BC:123:ILE:O    | 1.89                     | 0.72              |
| 29:BF:112:ASP:OD1  | 29:BF:113:PHE:N    | 2.23                     | 0.72              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 55:CA:965:U:H1'    | 55:CA:969:A:C6    | 2.24                     | 0.72              |
| 24:DA:1223:G:N2    | 24:DA:1226:A:OP2  | 2.22                     | 0.72              |
| 24:DA:379:G:C6     | 24:DA:396:G:O6    | 2.43                     | 0.72              |
| 21:AA:32:A:H2'     | 21:AA:33:A:C8     | 2.24                     | 0.72              |
| 9:AJ:81:GLU:HA     | 9:AJ:84:VAL:HG12  | 1.72                     | 0.72              |
| 29:BF:134:GLN:O    | 29:BF:136:ILE:N   | 2.21                     | 0.72              |
| 55:CA:1088:G:H21   | 55:CA:1167:A:N6   | 1.88                     | 0.72              |
| 55:CA:1338:G:H2'   | 55:CA:1339:A:C8   | 2.25                     | 0.72              |
| 55:CA:198:G:H2'    | 55:CA:199:A:H8    | 1.54                     | 0.72              |
| 55:CA:599:C:H2'    | 55:CA:600:A:H8    | 1.55                     | 0.72              |
| 4:CE:93:VAL:HG21   | 4:CE:139:THR:HG22 | 1.71                     | 0.72              |
| 24:DA:783:A:H2     | 24:DA:1778:U:H4'  | 1.54                     | 0.72              |
| 24:DA:333:G:O2'    | 24:DA:334:C:H5'   | 1.89                     | 0.72              |
| 24:DA:520:G:H2'    | 24:DA:521:U:C6    | 2.25                     | 0.72              |
| 24:DA:1565:C:H5''  | 26:DC:17:LYS:CE   | 2.19                     | 0.72              |
| 21:AA:1261:A:N6    | 21:AA:1274:A:H2'  | 2.05                     | 0.72              |
| 21:AA:316:C:H41    | 21:AA:351:G:N2    | 1.88                     | 0.72              |
| 24:BA:734:A:C4     | 24:BA:735:A:C8    | 2.77                     | 0.72              |
| 27:BD:99:GLU:HG3   | 27:BD:100:LEU:N   | 2.05                     | 0.72              |
| 29:BF:134:GLN:HE22 | 29:BF:150:GLY:H   | 1.37                     | 0.72              |
| 32:BI:7:TYR:HB3    | 32:BI:58:ILE:H    | 1.55                     | 0.72              |
| 37:BN:24:MET:HG2   | 37:BN:44:LEU:HD22 | 1.70                     | 0.72              |
| 27:BD:13:ARG:NH1   | 39:BP:74:GLN:HE21 | 1.86                     | 0.72              |
| 55:CA:1051:C:O2'   | 55:CA:1052:U:H6   | 1.72                     | 0.72              |
| 55:CA:1481:U:H2'   | 55:CA:1482:G:C8   | 2.25                     | 0.72              |
| 55:CA:721:G:H4'    | 55:CA:722:G:O5'   | 1.90                     | 0.72              |
| 55:CA:815:A:OP2    | 55:CA:816:A:H8    | 1.73                     | 0.72              |
| 8:CI:35:GLU:HA     | 8:CI:39:GLY:HA3   | 1.70                     | 0.72              |
| 24:DA:2615:U:C2    | 50:D0:3:GLN:HA    | 2.24                     | 0.72              |
| 24:DA:1723:G:H2'   | 24:DA:1724:G:H8   | 1.55                     | 0.72              |
| 24:DA:67:U:H2'     | 24:DA:68:G:H8     | 1.55                     | 0.72              |
| 24:DA:975:A:O2'    | 24:DA:976:G:H5'   | 1.89                     | 0.72              |
| 26:DC:8:THR:O      | 26:DC:9:SER:HB3   | 1.89                     | 0.72              |
| 21:AA:132:C:H2'    | 21:AA:133:U:C6    | 2.25                     | 0.72              |
| 4:AE:133:ILE:H     | 4:AE:133:ILE:HD12 | 1.53                     | 0.72              |
| 6:AG:144:ALA:C     | 6:AG:146:ALA:H    | 1.92                     | 0.72              |
| 10:AK:21:HIS:CD2   | 21:AA:707:U:H4'   | 2.24                     | 0.72              |
| 26:BC:106:PRO:HA   | 26:BC:141:HIS:NE2 | 2.05                     | 0.72              |
| 32:BI:53:PRO:HD2   | 32:BI:77:VAL:HG21 | 1.72                     | 0.72              |
| 47:BX:34:SER:HA    | 47:BX:49:ARG:HA   | 1.71                     | 0.72              |
| 24:DA:1700:A:H2'   | 24:DA:1701:A:H5'  | 1.71                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:1802:A:N6    | 24:DA:1817:G:N2    | 2.38                     | 0.72              |
| 24:DA:2439:A:H4'   | 24:DA:2440:C:O5'   | 1.88                     | 0.72              |
| 24:DA:638:G:H2'    | 24:DA:639:U:C6     | 2.25                     | 0.72              |
| 26:DC:159:THR:O    | 26:DC:194:VAL:HG12 | 1.90                     | 0.72              |
| 26:DC:166:ARG:HB2  | 26:DC:171:VAL:HG22 | 1.72                     | 0.72              |
| 29:DF:49:LEU:HA    | 29:DF:52:ALA:HB3   | 1.70                     | 0.72              |
| 6:AG:100:MET:O     | 6:AG:104:VAL:HG23  | 1.90                     | 0.71              |
| 24:BA:1181:U:O2'   | 24:BA:1182:G:H8    | 1.71                     | 0.71              |
| 29:BF:131:VAL:HG22 | 29:BF:151:LEU:O    | 1.90                     | 0.71              |
| 32:BI:89:SER:HB3   | 32:BI:92:PRO:HG3   | 1.72                     | 0.71              |
| 35:BL:91:ASP:H     | 35:BL:94:THR:CG2   | 2.01                     | 0.71              |
| 14:CO:28:VAL:HG11  | 14:CO:66:LEU:HD21  | 1.71                     | 0.71              |
| 24:DA:1141:U:H4'   | 24:DA:1142:A:O4'   | 1.91                     | 0.71              |
| 24:DA:1352:U:H5    | 24:DA:1377:G:C5    | 2.08                     | 0.71              |
| 24:DA:1385:A:H4'   | 24:DA:1386:C:OP1   | 1.89                     | 0.71              |
| 24:DA:2461:A:H1'   | 24:DA:2492:U:N3    | 2.05                     | 0.71              |
| 27:DD:106:LYS:HB3  | 27:DD:206:ALA:CB   | 2.20                     | 0.71              |
| 29:DF:136:ILE:O    | 29:DF:137:PHE:O    | 2.07                     | 0.71              |
| 21:AA:1046:A:O2'   | 21:AA:1047:G:C5'   | 2.37                     | 0.71              |
| 21:AA:1064:G:O2'   | 21:AA:1190:G:N2    | 2.24                     | 0.71              |
| 20:AU:45:LYS:HA    | 20:AU:45:LYS:HE3   | 1.72                     | 0.71              |
| 24:BA:1027:A:C2    | 24:BA:1126:A:C4    | 2.78                     | 0.71              |
| 24:BA:2353:G:H1'   | 46:BW:30:VAL:HG13  | 1.71                     | 0.71              |
| 24:BA:279:A:H2'    | 24:BA:280:U:H6     | 1.55                     | 0.71              |
| 28:BE:73:ILE:HG12  | 28:BE:73:ILE:O     | 1.90                     | 0.71              |
| 31:BH:41:LYS:HA    | 31:BH:44:ILE:HG12  | 1.72                     | 0.71              |
| 55:CA:1054:C:O2'   | 55:CA:1055:A:C5'   | 2.37                     | 0.71              |
| 55:CA:1242:G:C2    | 55:CA:1243:C:H1'   | 2.25                     | 0.71              |
| 55:CA:223:A:H2'    | 55:CA:224:U:H6     | 1.53                     | 0.71              |
| 6:CG:88:VAL:HG22   | 6:CG:89:GLU:H      | 1.54                     | 0.71              |
| 35:DL:64:PHE:HD2   | 53:D3:24:LYS:HG2   | 1.53                     | 0.71              |
| 24:DA:603:A:H4'    | 24:DA:604:G:O5'    | 1.89                     | 0.71              |
| 24:DA:84:A:H4'     | 24:DA:85:G:O5'     | 1.89                     | 0.71              |
| 24:BA:924:G:H4'    | 46:BW:24:ARG:HH21  | 1.54                     | 0.71              |
| 32:BI:98:GLY:HA3   | 32:BI:137:LEU:HD23 | 1.71                     | 0.71              |
| 34:BK:47:ILE:HG13  | 34:BK:48:PRO:HD2   | 1.73                     | 0.71              |
| 24:BA:825:A:C1'    | 35:BL:54:GLN:NE2   | 2.52                     | 0.71              |
| 39:BP:4:ILE:CG2    | 39:BP:5:LYS:H      | 2.02                     | 0.71              |
| 9:CJ:59:LYS:HB2    | 9:CJ:62:ARG:HH21   | 1.54                     | 0.71              |
| 22:CV:34:G:H2'     | 22:CV:35:A:H8      | 1.55                     | 0.71              |
| 24:DA:547:A:C3'    | 24:DA:548:G:H5'    | 2.20                     | 0.71              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:DF:107:VAL:C    | 29:DF:109:ARG:H   | 1.92                     | 0.71              |
| 30:DG:126:THR:HG22 | 30:DG:127:GLN:H   | 1.55                     | 0.71              |
| 9:AJ:55:PRO:HG3    | 21:AA:1059:C:O2   | 1.89                     | 0.71              |
| 21:AA:1240:U:H3'   | 21:AA:1241:G:C5'  | 2.19                     | 0.71              |
| 21:AA:1273:C:H2'   | 21:AA:1274:A:O4'  | 1.89                     | 0.71              |
| 21:AA:1303:C:H2'   | 21:AA:1304:G:H8   | 1.54                     | 0.71              |
| 21:AA:697:U:O2     | 21:AA:798:U:H1'   | 1.91                     | 0.71              |
| 5:AF:49:TYR:CE1    | 17:AR:65:SER:HA   | 2.25                     | 0.71              |
| 55:CA:147:G:H2'    | 55:CA:148:G:C8    | 2.26                     | 0.71              |
| 55:CA:274:A:O2'    | 55:CA:275:G:H8    | 1.74                     | 0.71              |
| 55:CA:926:G:H2'    | 55:CA:1505:G:N3   | 2.05                     | 0.71              |
| 51:D1:51:ALA:O     | 51:D1:52:LYS:HB2  | 1.89                     | 0.71              |
| 24:DA:1760:C:H2'   | 24:DA:1761:C:H6   | 1.54                     | 0.71              |
| 24:DA:609:A:H2'    | 24:DA:610:C:O4'   | 1.90                     | 0.71              |
| 36:DM:61:GLY:HA2   | 36:DM:107:GLY:HA3 | 1.72                     | 0.71              |
| 21:AA:903:G:H2'    | 21:AA:904:U:H6    | 1.55                     | 0.71              |
| 1:AB:101:THR:HG23  | 1:AB:102:ASN:H    | 1.55                     | 0.71              |
| 3:AD:34:GLU:O      | 3:AD:37:PRO:HD3   | 1.90                     | 0.71              |
| 12:AM:28:ARG:O     | 12:AM:32:ILE:HG12 | 1.91                     | 0.71              |
| 54:B4:24:ARG:HG2   | 54:B4:24:ARG:HH21 | 1.53                     | 0.71              |
| 24:BA:738:G:C6     | 24:BA:739:A:C2    | 2.79                     | 0.71              |
| 28:BE:5:LEU:HD12   | 28:BE:10:SER:HB3  | 1.71                     | 0.71              |
| 24:DA:828:U:C4     | 24:DA:829:A:N6    | 2.58                     | 0.71              |
| 21:AA:1386:G:H2'   | 21:AA:1387:G:C8   | 2.26                     | 0.71              |
| 22:AV:40:C:H2'     | 22:AV:41:C:C6     | 2.25                     | 0.71              |
| 55:CA:197:A:O2'    | 55:CA:198:G:C8    | 2.44                     | 0.71              |
| 55:CA:32:A:H2'     | 55:CA:33:A:C8     | 2.25                     | 0.71              |
| 2:CC:19:SER:HB3    | 2:CC:21:TRP:NE1   | 2.05                     | 0.71              |
| 24:DA:2886:A:N6    | 50:D0:39:ARG:HD3  | 2.05                     | 0.71              |
| 24:DA:1490:A:H8    | 26:DC:73:ILE:HD12 | 1.53                     | 0.71              |
| 24:DA:1506:U:H2'   | 24:DA:1507:C:O4'  | 1.91                     | 0.71              |
| 24:DA:1652:A:H3'   | 24:DA:1653:G:C8   | 2.26                     | 0.71              |
| 24:DA:2147:A:OP1   | 24:DA:2147:A:H4'  | 1.90                     | 0.71              |
| 24:DA:764:A:H2     | 26:DC:217:PRO:HG3 | 1.55                     | 0.71              |
| 45:DV:9:ARG:HD3    | 45:DV:39:ALA:HB1  | 1.71                     | 0.71              |
| 21:AA:1234:C:HO2'  | 21:AA:1364:U:H6   | 1.38                     | 0.71              |
| 11:AL:2:THR:HG22   | 11:AL:4:ASN:N     | 2.06                     | 0.71              |
| 12:AM:74:MET:SD    | 12:AM:77:LYS:HD3  | 2.31                     | 0.71              |
| 19:AT:4:LYS:HE2    | 19:AT:5:SER:HB3   | 1.71                     | 0.71              |
| 52:B2:43:THR:O     | 52:B2:44:VAL:CB   | 2.37                     | 0.71              |
| 25:BB:15:A:O2'     | 25:BB:16:G:H5'    | 1.90                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:BJ:2:LYS:HD3   | 33:BJ:2:LYS:N      | 2.05                     | 0.71              |
| 36:BM:81:ARG:HG3  | 36:BM:82:MET:H     | 1.53                     | 0.71              |
| 40:BQ:71:ASN:HB3  | 40:BQ:109:VAL:HG11 | 1.73                     | 0.71              |
| 46:BW:23:LYS:NZ   | 46:BW:24:ARG:HG3   | 2.05                     | 0.71              |
| 55:CA:120:A:H3'   | 55:CA:121:U:H5''   | 1.71                     | 0.71              |
| 55:CA:1256:A:N1   | 55:CA:1278:G:H2'   | 2.06                     | 0.71              |
| 55:CA:407:U:H2'   | 55:CA:408:A:H8     | 1.54                     | 0.71              |
| 12:CM:85:TYR:HE2  | 12:CM:96:VAL:HG13  | 1.55                     | 0.71              |
| 24:DA:1097:U:H2'  | 24:DA:1098:A:O4'   | 1.89                     | 0.71              |
| 24:DA:1667:G:OP2  | 24:DA:1667:G:H8    | 1.73                     | 0.71              |
| 24:DA:1929:G:H4'  | 24:DA:1930:G:OP1   | 1.89                     | 0.71              |
| 24:DA:2307:G:H1'  | 24:DA:2308:G:N7    | 2.05                     | 0.71              |
| 24:DA:2757:A:O2'  | 24:DA:2758:A:H5'   | 1.90                     | 0.71              |
| 43:DT:43:ILE:HG21 | 43:DT:58:VAL:HG11  | 1.71                     | 0.71              |
| 21:AA:338:A:N1    | 21:AA:351:G:O6     | 2.23                     | 0.71              |
| 1:AB:130:LYS:NZ   | 1:AB:130:LYS:HA    | 2.06                     | 0.71              |
| 8:AI:39:GLY:O     | 8:AI:40:ARG:HB2    | 1.91                     | 0.71              |
| 24:BA:1553:A:N7   | 24:BA:1555:G:C5    | 2.59                     | 0.71              |
| 24:BA:1963:U:H6   | 24:BA:1963:U:O5'   | 1.72                     | 0.71              |
| 24:BA:729:G:H5'   | 26:BC:206:LYS:HZ3  | 1.53                     | 0.71              |
| 26:BC:229:HIS:HD2 | 26:BC:246:PRO:HB3  | 1.56                     | 0.71              |
| 32:BI:76:ALA:HB2  | 32:BI:131:THR:HG23 | 1.73                     | 0.71              |
| 24:BA:871:U:OP1   | 36:BM:5:LYS:HG3    | 1.91                     | 0.71              |
| 39:BP:105:LYS:HA  | 39:BP:108:ARG:HD3  | 1.73                     | 0.71              |
| 55:CA:890:G:O2'   | 55:CA:891:U:OP2    | 2.07                     | 0.71              |
| 24:DA:688:U:O2'   | 24:DA:689:A:H5'    | 1.90                     | 0.71              |
| 28:DE:166:LYS:HA  | 28:DE:166:LYS:HE2  | 1.73                     | 0.71              |
| 36:DM:7:THR:HG22  | 36:DM:9:PHE:H      | 1.56                     | 0.71              |
| 43:DT:1:MET:HG2   | 43:DT:4:GLU:HA     | 1.70                     | 0.71              |
| 21:AA:955:U:H2'   | 21:AA:956:U:H6     | 1.55                     | 0.71              |
| 2:AC:99:GLN:O     | 2:AC:100:ILE:HB    | 1.90                     | 0.71              |
| 13:AN:81:ILE:HG21 | 21:AA:1202:U:C4    | 2.25                     | 0.71              |
| 24:BA:975:A:H2'   | 24:BA:976:G:H8     | 1.56                     | 0.71              |
| 27:BD:93:GLY:O    | 27:BD:95:SER:N     | 2.24                     | 0.71              |
| 37:BN:71:ARG:HH21 | 37:BN:71:ARG:CG    | 2.04                     | 0.71              |
| 55:CA:1009:U:H2'  | 55:CA:1010:U:C6    | 2.26                     | 0.71              |
| 55:CA:1376:U:H2'  | 55:CA:1377:A:H8    | 1.56                     | 0.71              |
| 55:CA:317:U:H2'   | 55:CA:318:G:H8     | 1.56                     | 0.71              |
| 3:CD:121:ALA:O    | 3:CD:122:ILE:HD13  | 1.90                     | 0.71              |
| 6:CG:100:MET:HE2  | 6:CG:100:MET:H     | 1.55                     | 0.71              |
| 52:D2:34:ARG:HB3  | 52:D2:42:LEU:HD11  | 1.73                     | 0.71              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:DA:1026:G:O2'   | 24:DA:1027:A:H5'  | 1.89                     | 0.71              |
| 24:DA:1272:A:C5    | 24:DA:1618:A:H1'  | 2.24                     | 0.71              |
| 1:AB:59:ILE:HD11   | 1:AB:220:VAL:HG13 | 1.72                     | 0.71              |
| 3:AD:55:ARG:HA     | 3:AD:55:ARG:HH11  | 1.56                     | 0.71              |
| 24:BA:1062:G:O2'   | 24:BA:1063:G:O4'  | 2.08                     | 0.71              |
| 24:BA:2200:C:N4    | 24:BA:2224:G:N2   | 2.38                     | 0.71              |
| 24:BA:729:G:N3     | 24:BA:729:G:H2'   | 2.04                     | 0.71              |
| 24:BA:1993:U:H4'   | 27:BD:133:THR:CG2 | 2.20                     | 0.71              |
| 24:BA:2305:U:H1'   | 29:BF:132:ARG:H   | 1.55                     | 0.71              |
| 36:BM:132:THR:HG22 | 36:BM:133:LYS:H   | 1.55                     | 0.71              |
| 44:BU:52:ASN:C     | 44:BU:54:PRO:HD2  | 2.12                     | 0.71              |
| 55:CA:1324:A:H2'   | 55:CA:1325:C:H6   | 1.54                     | 0.71              |
| 19:CT:26:MET:HG2   | 55:CA:1457:G:O2'  | 1.91                     | 0.71              |
| 24:DA:1075:C:O2'   | 24:DA:1076:C:H5'  | 1.90                     | 0.71              |
| 24:DA:1087:G:N2    | 24:DA:1103:A:H1'  | 2.05                     | 0.71              |
| 24:DA:1515:A:H2'   | 24:DA:1516:G:O4'  | 1.91                     | 0.71              |
| 24:DA:1669:A:C2'   | 24:DA:1669:A:N3   | 2.48                     | 0.71              |
| 24:DA:1936:A:H5''  | 24:DA:1937:A:O5'  | 1.91                     | 0.71              |
| 24:DA:861:A:H2'    | 24:DA:862:G:H8    | 1.56                     | 0.71              |
| 34:DK:118:LEU:C    | 34:DK:120:PRO:HD2 | 2.11                     | 0.71              |
| 18:AS:5:LYS:HD2    | 21:AA:1314:C:OP2  | 1.90                     | 0.70              |
| 4:AE:14:LEU:HD22   | 4:AE:15:ILE:N     | 2.06                     | 0.70              |
| 24:BA:1343:G:H2'   | 24:BA:1344:U:C6   | 2.26                     | 0.70              |
| 39:BP:63:ILE:HA    | 39:BP:68:GLY:HA2  | 1.72                     | 0.70              |
| 55:CA:1292:G:H2'   | 55:CA:1293:C:C6   | 2.26                     | 0.70              |
| 24:DA:1947:C:H2'   | 24:DA:1948:G:H8   | 1.54                     | 0.70              |
| 24:DA:2441:U:O2'   | 24:DA:2442:C:H5'  | 1.90                     | 0.70              |
| 24:DA:2738:A:H2    | 24:DA:2766:A:H61  | 1.36                     | 0.70              |
| 24:DA:2867:G:N3    | 24:DA:2867:G:H2'  | 2.04                     | 0.70              |
| 26:DC:52:HIS:HA    | 26:DC:216:ARG:HB2 | 1.73                     | 0.70              |
| 30:DG:16:VAL:HG11  | 30:DG:44:HIS:CD2  | 2.26                     | 0.70              |
| 30:DG:83:THR:C     | 30:DG:84:LYS:HD3  | 2.11                     | 0.70              |
| 33:DJ:117:ALA:HA   | 33:DJ:120:ARG:HD2 | 1.72                     | 0.70              |
| 40:DQ:50:ARG:N     | 40:DQ:50:ARG:HD2  | 2.05                     | 0.70              |
| 45:DV:80:HIS:CD2   | 45:DV:82:TYR:H    | 2.08                     | 0.70              |
| 21:AA:1125:U:O2'   | 21:AA:1126:U:H2'  | 1.91                     | 0.70              |
| 10:AK:119:GLY:HA2  | 21:AA:716:A:H1'   | 1.73                     | 0.70              |
| 18:AS:6:LYS:HE2    | 18:AS:6:LYS:HA    | 1.73                     | 0.70              |
| 24:BA:394:C:H2'    | 24:BA:395:U:O4'   | 1.91                     | 0.70              |
| 24:BA:811:U:C2     | 24:BA:1251:C:C5   | 2.79                     | 0.70              |
| 26:BC:141:HIS:HB2  | 26:BC:190:THR:HB  | 1.73                     | 0.70              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BH:67:ALA:HA   | 31:BH:138:VAL:HB   | 1.74                     | 0.70              |
| 55:CA:113:G:C1'   | 55:CA:354:G:H5'    | 2.22                     | 0.70              |
| 55:CA:1088:G:N2   | 55:CA:1167:A:H61   | 1.89                     | 0.70              |
| 7:CH:11:THR:HG22  | 7:CH:14:ARG:NH1    | 2.04                     | 0.70              |
| 7:CH:1:SER:HB3    | 7:CH:3:GLN:HG3     | 1.72                     | 0.70              |
| 18:CS:35:ARG:HA   | 18:CS:70:LEU:HB2   | 1.71                     | 0.70              |
| 24:DA:2145:C:H3'  | 24:DA:2147:A:OP2   | 1.90                     | 0.70              |
| 24:DA:2285:C:OP2  | 51:D1:5:ARG:HD3    | 1.91                     | 0.70              |
| 24:DA:2497:A:H1'  | 24:DA:2498:C:C5    | 2.26                     | 0.70              |
| 24:DA:2746:U:H5'' | 30:DG:137:LYS:HG2  | 1.72                     | 0.70              |
| 24:DA:2303:G:H1'  | 29:DF:122:ASP:OD2  | 1.91                     | 0.70              |
| 21:AA:268:U:H2'   | 21:AA:269:C:C6     | 2.25                     | 0.70              |
| 21:AA:967:C:H2'   | 21:AA:968:A:N7     | 2.06                     | 0.70              |
| 1:AB:53:LEU:HA    | 1:AB:56:LEU:HB3    | 1.72                     | 0.70              |
| 18:AS:10:ILE:HD11 | 18:AS:15:LEU:HB2   | 1.74                     | 0.70              |
| 24:BA:1090:A:C2   | 24:BA:1091:G:C8    | 2.79                     | 0.70              |
| 24:BA:2532:G:C5   | 24:BA:2533:U:C5    | 2.79                     | 0.70              |
| 24:BA:2583:G:OP2  | 59:BA:3713:HOH:O   | 2.09                     | 0.70              |
| 27:BD:106:LYS:H   | 27:BD:106:LYS:HD2  | 1.56                     | 0.70              |
| 27:BD:13:ARG:HH12 | 39:BP:74:GLN:NE2   | 1.85                     | 0.70              |
| 30:BG:104:LEU:HB2 | 30:BG:112:VAL:CG2  | 2.21                     | 0.70              |
| 33:BJ:99:ARG:O    | 33:BJ:103:ILE:HG23 | 1.91                     | 0.70              |
| 34:BK:21:CYS:CB   | 34:BK:39:ILE:HD11  | 2.21                     | 0.70              |
| 36:BM:46:ILE:HG13 | 36:BM:47:GLU:H     | 1.55                     | 0.70              |
| 55:CA:110:C:H2'   | 55:CA:111:G:C8     | 2.27                     | 0.70              |
| 4:CE:103:GLY:HA3  | 4:CE:121:ASN:HA    | 1.72                     | 0.70              |
| 5:CF:91:ARG:O     | 5:CF:93:LYS:HE3    | 1.91                     | 0.70              |
| 24:DA:973:A:H1'   | 24:DA:1188:U:C6    | 2.26                     | 0.70              |
| 24:DA:704:G:H2'   | 24:DA:726:G:H22    | 1.55                     | 0.70              |
| 56:DB:30:C:H2'    | 56:DB:31:C:H5'     | 1.73                     | 0.70              |
| 36:DM:34:LYS:HD3  | 36:DM:131:VAL:HG21 | 1.74                     | 0.70              |
| 21:AA:1062:U:H2'  | 21:AA:1063:C:C6    | 2.25                     | 0.70              |
| 1:AB:110:ILE:CD1  | 1:AB:147:LEU:HD13  | 2.22                     | 0.70              |
| 3:AD:10:LEU:CD2   | 3:AD:62:ARG:HG3    | 2.21                     | 0.70              |
| 3:AD:32:LYS:HE3   | 21:AA:413:G:C6     | 2.26                     | 0.70              |
| 24:BA:1256:G:H2'  | 28:BE:77:ILE:HD11  | 1.74                     | 0.70              |
| 24:BA:2038:G:H2'  | 24:BA:2039:U:O4'   | 1.91                     | 0.70              |
| 26:BC:91:ALA:HB3  | 26:BC:103:ILE:HG22 | 1.73                     | 0.70              |
| 32:BI:20:SER:HB3  | 32:BI:21:PRO:HD3   | 1.73                     | 0.70              |
| 46:BW:39:GLN:HE21 | 46:BW:43:LYS:N     | 1.88                     | 0.70              |
| 20:CU:16:ARG:CG   | 20:CU:19:LYS:HG2   | 2.21                     | 0.70              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:1552:A:C2   | 24:DA:1553:A:C8    | 2.80                     | 0.70              |
| 24:DA:2198:A:HO2' | 24:DA:2199:A:H8    | 1.37                     | 0.70              |
| 35:DL:17:LYS:NZ   | 35:DL:19:LEU:HD22  | 2.07                     | 0.70              |
| 21:AA:1303:C:H2'  | 21:AA:1304:G:C8    | 2.27                     | 0.70              |
| 21:AA:79:G:H2'    | 21:AA:80:A:C8      | 2.24                     | 0.70              |
| 24:BA:1810:A:H2'  | 24:BA:1811:G:O4'   | 1.92                     | 0.70              |
| 24:BA:64:A:H2'    | 24:BA:65:U:C6      | 2.26                     | 0.70              |
| 39:BP:8:GLU:O     | 39:BP:11:GLN:HB2   | 1.91                     | 0.70              |
| 42:BS:73:LYS:O    | 42:BS:106:VAL:N    | 2.23                     | 0.70              |
| 55:CA:1504:G:C4'  | 55:CA:1505:G:H5'   | 2.22                     | 0.70              |
| 56:DB:77:U:OP2    | 45:DV:14:LYS:HA    | 1.91                     | 0.70              |
| 44:DU:95:PHE:H    | 44:DU:95:PHE:HD1   | 1.39                     | 0.70              |
| 21:AA:415:A:H2'   | 21:AA:416:G:H8     | 1.56                     | 0.70              |
| 21:AA:748:G:H2'   | 21:AA:749:A:H8     | 1.53                     | 0.70              |
| 1:AB:15:PHE:HB2   | 1:AB:39:ILE:HG23   | 1.72                     | 0.70              |
| 6:AG:149:ALA:HA   | 10:AK:60:PHE:HB3   | 1.73                     | 0.70              |
| 17:AR:42:ARG:HG3  | 17:AR:43:ILE:HG12  | 1.73                     | 0.70              |
| 24:BA:1253:A:N7   | 59:BA:3337:HOH:O   | 2.23                     | 0.70              |
| 32:BI:42:ASN:HA   | 32:BI:45:THR:HB    | 1.74                     | 0.70              |
| 45:BV:77:VAL:HG23 | 45:BV:89:ILE:HG12  | 1.72                     | 0.70              |
| 46:BW:8:SER:O     | 46:BW:9:THR:HB     | 1.92                     | 0.70              |
| 55:CA:1234:C:H1'  | 55:CA:1364:U:C6    | 2.26                     | 0.70              |
| 55:CA:87:C:O2'    | 55:CA:88:U:H4'     | 1.91                     | 0.70              |
| 24:DA:684:G:H5'   | 52:D2:16:HIS:CE1   | 2.26                     | 0.70              |
| 24:DA:1439:A:C6   | 24:DA:1552:A:C5    | 2.80                     | 0.70              |
| 24:DA:202:U:C4    | 24:DA:203:A:C6     | 2.79                     | 0.70              |
| 24:DA:2337:G:N3   | 24:DA:2337:G:H2'   | 2.04                     | 0.70              |
| 24:DA:571:U:H4'   | 24:DA:573:U:H5     | 1.57                     | 0.70              |
| 26:DC:173:LEU:H   | 26:DC:173:LEU:HD22 | 1.56                     | 0.70              |
| 49:DZ:16:LEU:HD23 | 49:DZ:19:HIS:CD2   | 2.26                     | 0.70              |
| 21:AA:367:U:O2'   | 21:AA:368:U:H4'    | 1.91                     | 0.70              |
| 21:AA:766:A:H2'   | 21:AA:767:A:C8     | 2.26                     | 0.70              |
| 10:AK:21:HIS:HB2  | 10:AK:32:THR:O     | 1.92                     | 0.70              |
| 24:BA:825:A:H1'   | 35:BL:54:GLN:HE21  | 1.55                     | 0.70              |
| 24:BA:923:G:H1'   | 46:BW:23:LYS:HE2   | 1.74                     | 0.70              |
| 30:BG:10:VAL:O    | 30:BG:10:VAL:HG23  | 1.90                     | 0.70              |
| 42:BS:4:ILE:HG22  | 42:BS:106:VAL:HG13 | 1.74                     | 0.70              |
| 46:BW:39:GLN:NE2  | 46:BW:43:LYS:H     | 1.87                     | 0.70              |
| 48:BY:9:LYS:HA    | 48:BY:9:LYS:NZ     | 2.05                     | 0.70              |
| 7:CH:26:MET:HB2   | 7:CH:27:PRO:HD2    | 1.72                     | 0.70              |
| 10:CK:30:ILE:HG12 | 10:CK:45:THR:HB    | 1.74                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:1552:A:O2'   | 24:DA:1553:A:H5'   | 1.92                     | 0.70              |
| 24:DA:2285:C:H2'   | 24:DA:2286:G:H5''  | 1.74                     | 0.70              |
| 27:DD:141:ARG:HH11 | 27:DD:141:ARG:HB3  | 1.56                     | 0.70              |
| 45:DV:70:ILE:HD13  | 45:DV:70:ILE:N     | 2.07                     | 0.70              |
| 21:AA:1306:A:N6    | 21:AA:1331:G:H1'   | 2.06                     | 0.70              |
| 21:AA:450:G:N7     | 21:AA:481:G:O6     | 2.24                     | 0.70              |
| 21:AA:549:C:O2'    | 21:AA:550:G:O4'    | 2.09                     | 0.70              |
| 21:AA:765:G:N2     | 21:AA:812:G:HO2'   | 1.88                     | 0.70              |
| 21:AA:858:G:C2'    | 21:AA:859:G:H5'    | 2.21                     | 0.70              |
| 2:AC:148:ILE:HA    | 2:AC:200:TRP:O     | 1.92                     | 0.70              |
| 24:BA:1210:G:O2'   | 24:BA:1211:C:OP2   | 2.07                     | 0.70              |
| 24:BA:1339:G:H21   | 24:BA:1603:A:H1'   | 1.57                     | 0.70              |
| 24:BA:1789:A:OP2   | 26:BC:220:ARG:NH1  | 2.25                     | 0.70              |
| 24:BA:1956:U:H2'   | 24:BA:1957:C:H6    | 1.56                     | 0.70              |
| 24:BA:90:U:C2      | 24:BA:91:A:N7      | 2.60                     | 0.70              |
| 24:BA:811:U:N3     | 35:BL:21:ARG:NH2   | 2.40                     | 0.70              |
| 35:BL:23:ILE:HD12  | 41:BR:84:ARG:HG2   | 1.74                     | 0.70              |
| 40:BQ:48:ASP:HA    | 40:BQ:51:GLN:HB2   | 1.74                     | 0.70              |
| 55:CA:1235:U:H2'   | 55:CA:1236:A:C8    | 2.26                     | 0.70              |
| 55:CA:260:G:H2'    | 55:CA:261:U:C6     | 2.27                     | 0.70              |
| 24:DA:1807:G:H2'   | 24:DA:1808:A:H5'   | 1.74                     | 0.70              |
| 24:DA:2233:U:H2'   | 24:DA:2234:G:H8    | 1.57                     | 0.70              |
| 24:DA:91:A:H1'     | 24:DA:92:U:C5      | 2.27                     | 0.70              |
| 49:DZ:23:LEU:HD21  | 49:DZ:53:MET:HE1   | 1.72                     | 0.70              |
| 21:AA:332:G:O2'    | 21:AA:333:U:H5'    | 1.90                     | 0.70              |
| 21:AA:455:G:H2'    | 21:AA:456:A:H8     | 1.57                     | 0.70              |
| 21:AA:858:G:O2'    | 21:AA:859:G:H5'    | 1.91                     | 0.70              |
| 1:AB:165:ALA:HB2   | 1:AB:186:VAL:HG12  | 1.74                     | 0.70              |
| 24:BA:1278:C:H2'   | 24:BA:1279:G:H8    | 1.56                     | 0.70              |
| 26:BC:145:MET:SD   | 26:BC:153:LEU:HD21 | 2.31                     | 0.70              |
| 30:BG:84:LYS:HB3   | 30:BG:132:LEU:O    | 1.92                     | 0.70              |
| 36:BM:14:LYS:O     | 36:BM:15:GLY:O     | 2.09                     | 0.70              |
| 55:CA:1137:C:H4'   | 55:CA:1138:G:C2    | 2.26                     | 0.70              |
| 55:CA:1269:A:H2    | 55:CA:1312:G:H21   | 1.39                     | 0.70              |
| 1:CB:195:VAL:HG12  | 1:CB:197:PHE:H     | 1.57                     | 0.70              |
| 3:CD:2:ARG:HH21    | 3:CD:114:ARG:CD    | 2.05                     | 0.70              |
| 4:CE:75:LEU:HD21   | 4:CE:80:LEU:HA     | 1.74                     | 0.70              |
| 24:DA:2423:U:H1'   | 24:DA:2425:A:C5    | 2.26                     | 0.70              |
| 24:DA:2866:U:H4'   | 24:DA:2867:G:O5'   | 1.89                     | 0.70              |
| 28:DE:46:GLN:HB3   | 28:DE:86:ALA:HB1   | 1.72                     | 0.70              |
| 32:DI:51:GLY:O     | 32:DI:52:LEU:HB2   | 1.91                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:DJ:106:LYS:HB2 | 33:DJ:119:PHE:HE2 | 1.56                     | 0.70              |
| 42:DS:70:LYS:H    | 42:DS:70:LYS:HE3  | 1.56                     | 0.70              |
| 4:AE:100:GLU:HB3  | 4:AE:121:ASN:HA   | 1.72                     | 0.70              |
| 10:AK:30:ILE:HG22 | 10:AK:45:THR:HG22 | 1.73                     | 0.70              |
| 24:BA:2333:A:H4'  | 24:BA:2334:U:O5'  | 1.92                     | 0.70              |
| 24:BA:747:U:C4    | 24:BA:2613:U:C5   | 2.79                     | 0.70              |
| 26:BC:144:GLU:HA  | 26:BC:151:GLY:HA2 | 1.72                     | 0.70              |
| 27:BD:69:ALA:HA   | 27:BD:73:VAL:HG13 | 1.74                     | 0.70              |
| 30:BG:8:VAL:HG12  | 30:BG:49:LEU:H    | 1.56                     | 0.70              |
| 34:BK:71:ARG:CB   | 34:BK:72:PRO:HD3  | 2.21                     | 0.70              |
| 38:BO:67:ASN:O    | 38:BO:69:ASP:N    | 2.24                     | 0.70              |
| 46:BW:39:GLN:HE21 | 46:BW:43:LYS:H    | 1.40                     | 0.70              |
| 55:CA:301:G:H2'   | 55:CA:302:G:H8    | 1.57                     | 0.70              |
| 4:CE:39:GLY:HA2   | 4:CE:44:ARG:O     | 1.91                     | 0.70              |
| 7:CH:13:ILE:HG23  | 7:CH:62:LEU:HD11  | 1.73                     | 0.70              |
| 12:CM:2:ARG:HD2   | 12:CM:8:ILE:CG2   | 2.21                     | 0.70              |
| 24:DA:1012:U:O4   | 33:DJ:30:THR:HG21 | 1.91                     | 0.70              |
| 24:DA:576:U:H2'   | 24:DA:577:G:C8    | 2.26                     | 0.70              |
| 24:DA:685:A:H5'   | 24:DA:686:U:OP1   | 1.92                     | 0.70              |
| 24:DA:2392:A:H2   | 35:DL:55:MET:SD   | 2.14                     | 0.70              |
| 56:DB:51:G:O6     | 38:DO:32:PRO:HB3  | 1.92                     | 0.70              |
| 40:DQ:91:ARG:NH1  | 41:DR:10:LYS:HB3  | 2.07                     | 0.70              |
| 24:DA:2356:U:H4'  | 46:DW:16:GLU:HG3  | 1.73                     | 0.70              |
| 21:AA:631:C:C5'   | 21:AA:632:U:H5'   | 2.21                     | 0.69              |
| 21:AA:792:A:N3    | 21:AA:794:A:C5    | 2.60                     | 0.69              |
| 4:AE:81:GLN:CG    | 4:AE:149:PRO:HG3  | 2.17                     | 0.69              |
| 24:BA:1060:U:H4'  | 24:BA:1061:U:C5'  | 2.22                     | 0.69              |
| 24:BA:1708:C:O2'  | 24:BA:1709:U:H5'  | 1.91                     | 0.69              |
| 24:BA:1735:A:H2'  | 24:BA:1736:U:H6   | 1.55                     | 0.69              |
| 24:BA:2503:A:H4'  | 24:BA:2504:U:OP1  | 1.91                     | 0.69              |
| 24:BA:742:A:H2'   | 24:BA:743:A:H8    | 1.56                     | 0.69              |
| 24:BA:868:U:C4    | 24:BA:869:G:N7    | 2.60                     | 0.69              |
| 24:BA:528:A:OP2   | 33:BJ:116:ARG:NH2 | 2.24                     | 0.69              |
| 42:BS:25:ARG:HE   | 42:BS:73:LYS:NZ   | 1.88                     | 0.69              |
| 49:BZ:4:ILE:HG23  | 49:BZ:37:ARG:O    | 1.92                     | 0.69              |
| 4:CE:103:GLY:O    | 4:CE:104:ILE:HG22 | 1.91                     | 0.69              |
| 24:DA:1201:U:H2'  | 24:DA:1202:G:C8   | 2.27                     | 0.69              |
| 24:DA:1331:G:O2'  | 24:DA:1332:G:H5'  | 1.92                     | 0.69              |
| 24:DA:379:G:C6    | 24:DA:396:G:C6    | 2.80                     | 0.69              |
| 56:DB:5:U:H2'     | 56:DB:6:G:H8      | 1.56                     | 0.69              |
| 56:DB:75:G:C2'    | 56:DB:76:G:H5'    | 2.22                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:DK:6:THR:O     | 34:DK:8:LEU:HD12  | 1.91                     | 0.69              |
| 47:DX:58:ILE:HA   | 47:DX:66:VAL:HG21 | 1.74                     | 0.69              |
| 21:AA:143:A:N3    | 21:AA:143:A:H2'   | 2.05                     | 0.69              |
| 4:AE:152:VAL:O    | 4:AE:156:ARG:HG3  | 1.93                     | 0.69              |
| 4:AE:82:HIS:HB2   | 7:AH:95:MET:SD    | 2.32                     | 0.69              |
| 11:AL:28:GLN:HB2  | 11:AL:81:ILE:O    | 1.92                     | 0.69              |
| 24:BA:646:U:C4    | 24:BA:2368:C:H1'  | 2.26                     | 0.69              |
| 24:BA:2204:G:O5'  | 26:BC:149:LYS:HE3 | 1.92                     | 0.69              |
| 36:BM:21:ALA:HB1  | 36:BM:100:LYS:HG2 | 1.74                     | 0.69              |
| 43:BT:50:LEU:HD12 | 43:BT:50:LEU:N    | 2.04                     | 0.69              |
| 55:CA:589:U:O2'   | 55:CA:590:U:H5'   | 1.92                     | 0.69              |
| 55:CA:708:C:H2'   | 55:CA:709:U:H6    | 1.56                     | 0.69              |
| 8:CI:24:ASN:HB2   | 8:CI:26:LYS:NZ    | 2.07                     | 0.69              |
| 18:CS:38:THR:OG1  | 18:CS:40:PHE:HD1  | 1.74                     | 0.69              |
| 24:DA:1788:C:O2'  | 24:DA:1789:A:O4'  | 2.10                     | 0.69              |
| 33:DJ:25:LEU:HD22 | 33:DJ:26:GLY:N    | 2.07                     | 0.69              |
| 21:AA:512:U:H2'   | 21:AA:513:C:H6    | 1.58                     | 0.69              |
| 21:AA:68:G:C5     | 21:AA:69:G:H1'    | 2.28                     | 0.69              |
| 4:AE:19:ARG:HD2   | 4:AE:30:PHE:HB3   | 1.73                     | 0.69              |
| 6:AG:78:ARG:HH22  | 6:AG:81:GLY:HA2   | 1.57                     | 0.69              |
| 24:BA:1538:G:N2   | 24:BA:1539:U:C2   | 2.61                     | 0.69              |
| 24:BA:532:A:N7    | 24:BA:2021:C:H2'  | 2.06                     | 0.69              |
| 35:BL:77:ILE:O    | 35:BL:110:VAL:O   | 2.10                     | 0.69              |
| 46:BW:23:LYS:HG3  | 46:BW:24:ARG:O    | 1.93                     | 0.69              |
| 55:CA:1038:C:H2'  | 55:CA:1039:G:H8   | 1.53                     | 0.69              |
| 55:CA:601:G:H2'   | 55:CA:602:A:H8    | 1.56                     | 0.69              |
| 24:DA:1816:C:O3'  | 24:DA:1817:G:H8   | 1.74                     | 0.69              |
| 27:DD:107:VAL:H   | 27:DD:206:ALA:H   | 1.40                     | 0.69              |
| 33:DJ:44:TYR:HB2  | 40:DQ:63:ARG:CZ   | 2.21                     | 0.69              |
| 21:AA:1144:G:N2   | 21:AA:1146:A:H62  | 1.90                     | 0.69              |
| 24:BA:2292:U:H2'  | 24:BA:2293:G:C8   | 2.26                     | 0.69              |
| 39:BP:50:ARG:HG2  | 39:BP:57:ALA:N    | 2.08                     | 0.69              |
| 44:BU:38:ILE:HG22 | 44:BU:39:ASN:N    | 2.06                     | 0.69              |
| 55:CA:1102:A:H2'  | 55:CA:1103:C:C6   | 2.26                     | 0.69              |
| 55:CA:1234:C:H1'  | 55:CA:1364:U:H6   | 1.57                     | 0.69              |
| 6:CG:65:LEU:HD21  | 6:CG:96:ASN:OD1   | 1.92                     | 0.69              |
| 14:CO:47:LYS:N    | 14:CO:47:LYS:HD2  | 2.07                     | 0.69              |
| 24:DA:1867:G:H2'  | 24:DA:1868:C:C6   | 2.28                     | 0.69              |
| 24:DA:76:C:O2'    | 24:DA:77:G:H5'    | 1.91                     | 0.69              |
| 24:DA:983:A:N6    | 24:DA:984:A:C2    | 2.61                     | 0.69              |
| 34:DK:80:ASP:HB2  | 39:DP:67:GLU:OE1  | 1.91                     | 0.69              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 47:DX:31:ASN:ND2   | 47:DX:31:ASN:H    | 1.89                     | 0.69              |
| 19:AT:34:VAL:O     | 19:AT:38:ILE:HG12 | 1.93                     | 0.69              |
| 24:BA:1936:A:H5''  | 24:BA:1937:A:H5'  | 1.74                     | 0.69              |
| 29:BF:35:LEU:HD12  | 29:BF:88:VAL:HB   | 1.72                     | 0.69              |
| 36:BM:108:VAL:HG13 | 36:BM:109:PRO:CD  | 2.21                     | 0.69              |
| 40:BQ:94:LEU:HD11  | 41:BR:4:VAL:CG1   | 2.22                     | 0.69              |
| 55:CA:1424:U:H2'   | 55:CA:1425:U:O4'  | 1.91                     | 0.69              |
| 55:CA:94:G:O2'     | 55:CA:95:C:H5'    | 1.92                     | 0.69              |
| 55:CA:992:U:O2'    | 55:CA:993:G:OP2   | 2.07                     | 0.69              |
| 1:CB:76:SER:O      | 1:CB:79:VAL:HG12  | 1.91                     | 0.69              |
| 2:CC:25:THR:HG23   | 13:CN:75:LYS:HD2  | 1.73                     | 0.69              |
| 15:CP:3:THR:HB     | 15:CP:66:THR:HB   | 1.73                     | 0.69              |
| 24:DA:1477:A:H2'   | 24:DA:1478:G:O4'  | 1.93                     | 0.69              |
| 34:DK:61:VAL:HG11  | 34:DK:112:PHE:CE2 | 2.28                     | 0.69              |
| 21:AA:1032:G:O2'   | 21:AA:1033:G:H5'  | 1.91                     | 0.69              |
| 21:AA:109:A:H2'    | 21:AA:326:G:N2    | 2.04                     | 0.69              |
| 24:BA:1021:A:H61   | 24:BA:1142:A:H61  | 1.36                     | 0.69              |
| 24:BA:1555:G:C8    | 24:BA:1555:G:H5'  | 2.27                     | 0.69              |
| 31:BH:68:ARG:NH2   | 31:BH:72:ILE:HG21 | 2.07                     | 0.69              |
| 35:BL:78:ARG:HB3   | 35:BL:113:ALA:HB3 | 1.74                     | 0.69              |
| 40:BQ:63:ARG:NH1   | 40:BQ:96:ASP:CA   | 2.46                     | 0.69              |
| 55:CA:373:A:H2'    | 55:CA:374:A:C8    | 2.28                     | 0.69              |
| 7:CH:103:VAL:HG12  | 7:CH:124:ILE:HA   | 1.74                     | 0.69              |
| 24:DA:118:A:C8     | 24:DA:119:A:C8    | 2.80                     | 0.69              |
| 24:DA:1439:A:N7    | 24:DA:1440:U:C6   | 2.60                     | 0.69              |
| 24:DA:1676:A:H2    | 24:DA:1993:U:H5'  | 1.53                     | 0.69              |
| 24:DA:414:C:H5''   | 24:DA:1879:C:O2'  | 1.93                     | 0.69              |
| 24:DA:2320:U:H1'   | 24:DA:2333:A:H62  | 1.57                     | 0.69              |
| 24:DA:95:A:H4'     | 48:DY:38:GLN:O    | 1.93                     | 0.69              |
| 43:DT:67:VAL:HB    | 43:DT:76:ARG:HG3  | 1.75                     | 0.69              |
| 24:BA:1790:C:H2'   | 24:BA:1791:A:C5   | 2.28                     | 0.69              |
| 24:BA:1943:U:O2    | 24:BA:1943:U:O4'  | 2.10                     | 0.69              |
| 24:BA:496:G:C5     | 24:BA:497:A:C8    | 2.80                     | 0.69              |
| 24:BA:848:C:H2'    | 24:BA:849:A:H8    | 1.58                     | 0.69              |
| 55:CA:1449:C:O2'   | 55:CA:1450:U:H5'  | 1.93                     | 0.69              |
| 55:CA:250:A:H1'    | 55:CA:252:U:C4    | 2.28                     | 0.69              |
| 55:CA:672:U:H2'    | 55:CA:673:A:C8    | 2.27                     | 0.69              |
| 24:DA:505:A:O2'    | 24:DA:506:G:H5'   | 1.91                     | 0.69              |
| 24:DA:529:A:C8     | 24:DA:2023:C:N4   | 2.60                     | 0.69              |
| 24:DA:85:G:OP2     | 44:DU:6:ARG:HB2   | 1.92                     | 0.69              |
| 21:AA:1218:C:H2'   | 21:AA:1219:A:H8   | 1.57                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:427:U:C4     | 21:AA:428:G:C6     | 2.81                     | 0.69              |
| 3:AD:31:CYS:O      | 3:AD:32:LYS:HB2    | 1.92                     | 0.69              |
| 24:BA:1385:A:C4    | 24:BA:1386:C:C5    | 2.81                     | 0.69              |
| 24:BA:699:A:H4'    | 24:BA:1634:A:N7    | 2.07                     | 0.69              |
| 33:BJ:65:THR:HG23  | 33:BJ:66:GLY:N     | 2.07                     | 0.69              |
| 24:BA:869:G:H4'    | 36:BM:8:LYS:CE     | 2.21                     | 0.69              |
| 45:BV:80:HIS:CD2   | 45:BV:83:LYS:HB2   | 2.27                     | 0.69              |
| 3:CD:105:GLY:HA3   | 3:CD:158:LEU:HD23  | 1.75                     | 0.69              |
| 8:CI:74:GLN:O      | 8:CI:78:ILE:HG13   | 1.92                     | 0.69              |
| 53:D3:23:HIS:O     | 53:D3:46:LYS:HB2   | 1.93                     | 0.69              |
| 24:DA:2216:G:H2'   | 24:DA:2217:G:C8    | 2.27                     | 0.69              |
| 24:DA:2837:A:H2'   | 24:DA:2838:G:H8    | 1.54                     | 0.69              |
| 24:DA:6:A:H2'      | 24:DA:7:G:H8       | 1.57                     | 0.69              |
| 26:DC:38:LYS:HE2   | 26:DC:55:GLY:H     | 1.56                     | 0.69              |
| 30:DG:86:LEU:HA    | 30:DG:163:TYR:HB3  | 1.75                     | 0.69              |
| 8:AI:8:THR:N       | 8:AI:84:ARG:HH12   | 1.90                     | 0.69              |
| 24:BA:10:A:C2'     | 24:BA:11:C:H5'     | 2.22                     | 0.69              |
| 24:BA:1973:G:H2'   | 24:BA:1974:C:C6    | 2.28                     | 0.69              |
| 24:BA:221:A:H2'    | 24:BA:266:G:N7     | 2.07                     | 0.69              |
| 24:BA:2800:A:C2    | 24:BA:2895:G:H1'   | 2.27                     | 0.69              |
| 28:BE:1:MET:HG3    | 28:BE:14:VAL:HG23  | 1.74                     | 0.69              |
| 35:BL:90:VAL:HG13  | 35:BL:95:LEU:HD21  | 1.75                     | 0.69              |
| 55:CA:630:A:N1     | 59:CA:1859:HOH:O   | 2.26                     | 0.69              |
| 2:CC:109:GLU:HB3   | 2:CC:143:LEU:HD22  | 1.73                     | 0.69              |
| 10:CK:14:GLN:HA    | 10:CK:76:TYR:O     | 1.92                     | 0.69              |
| 10:CK:64:VAL:O     | 10:CK:68:ARG:HB2   | 1.93                     | 0.69              |
| 24:DA:1310:G:H2'   | 24:DA:1311:G:O4'   | 1.93                     | 0.69              |
| 24:DA:823:C:H2'    | 24:DA:824:U:H6     | 1.58                     | 0.69              |
| 26:DC:79:ARG:HD3   | 26:DC:81:GLU:OE1   | 1.93                     | 0.69              |
| 28:DE:79:ARG:HG2   | 28:DE:80:SER:H     | 1.57                     | 0.69              |
| 29:DF:109:ARG:HB2  | 29:DF:109:ARG:NH1  | 2.06                     | 0.69              |
| 43:DT:87:LEU:HD23  | 43:DT:88:LYS:N     | 2.08                     | 0.69              |
| 1:AB:22:TRP:HA     | 1:AB:189:ASN:CA    | 2.23                     | 0.69              |
| 3:AD:22:SER:HA     | 3:AD:26:ALA:HB2    | 1.74                     | 0.69              |
| 5:AF:3:HIS:N       | 5:AF:92:THR:HG23   | 2.02                     | 0.69              |
| 30:BG:102:ILE:HD12 | 30:BG:147:LEU:HD11 | 1.73                     | 0.69              |
| 34:BK:111:LYS:HE2  | 34:BK:111:LYS:N    | 2.06                     | 0.69              |
| 46:BW:26:GLY:O     | 46:BW:27:GLY:O     | 2.11                     | 0.69              |
| 46:BW:30:VAL:O     | 46:BW:30:VAL:HG22  | 1.92                     | 0.69              |
| 47:BX:46:VAL:HG21  | 47:BX:67:LEU:HD11  | 1.74                     | 0.69              |
| 3:CD:58:GLN:O      | 3:CD:62:ARG:HG2    | 1.91                     | 0.69              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:CF:5:GLU:HG3    | 5:CF:63:ASN:OD1    | 1.93                     | 0.69              |
| 14:CO:47:LYS:HD2  | 14:CO:47:LYS:H     | 1.58                     | 0.69              |
| 15:CP:24:SER:HB2  | 55:CA:377:G:H5''   | 1.73                     | 0.69              |
| 24:DA:1190:G:H2'  | 24:DA:1191:G:H8    | 1.57                     | 0.69              |
| 24:DA:1635:A:H2'  | 24:DA:1636:U:H6    | 1.57                     | 0.69              |
| 24:DA:2537:U:H2'  | 24:DA:2538:C:H6    | 1.57                     | 0.69              |
| 56:DB:19:C:H2'    | 56:DB:20:G:C8      | 2.28                     | 0.69              |
| 21:AA:36:C:H2'    | 21:AA:37:U:O4'     | 1.92                     | 0.69              |
| 21:AA:549:C:H2'   | 21:AA:550:G:H8     | 1.57                     | 0.69              |
| 21:AA:575:G:H4'   | 21:AA:576:C:O5'    | 1.93                     | 0.69              |
| 6:AG:113:LYS:HB2  | 6:AG:117:LEU:HD12  | 1.73                     | 0.69              |
| 6:AG:115:MET:HA   | 6:AG:118:ARG:HD3   | 1.73                     | 0.69              |
| 11:AL:43:LYS:NZ   | 11:AL:44:PRO:HD2   | 2.08                     | 0.69              |
| 52:B2:12:ARG:HG2  | 52:B2:13:ASN:ND2   | 2.08                     | 0.69              |
| 53:B3:26:ALA:O    | 53:B3:27:ASN:HB2   | 1.91                     | 0.69              |
| 24:BA:1157:G:H2'  | 24:BA:1158:C:C6    | 2.27                     | 0.69              |
| 24:BA:2801:G:O2'  | 24:BA:2802:G:H5'   | 1.91                     | 0.69              |
| 24:BA:646:U:H3'   | 24:BA:647:G:C5'    | 2.23                     | 0.69              |
| 28:BE:18:THR:HG22 | 28:BE:106:LYS:HE3  | 1.73                     | 0.69              |
| 28:BE:111:GLU:HG2 | 28:BE:114:ARG:NH1  | 2.08                     | 0.69              |
| 28:BE:57:LYS:HG3  | 28:BE:58:LYS:H     | 1.57                     | 0.69              |
| 33:BJ:44:TYR:O    | 33:BJ:45:THR:HB    | 1.92                     | 0.69              |
| 24:BA:1131:G:OP1  | 33:BJ:82:GLY:HA2   | 1.93                     | 0.69              |
| 38:BO:16:ARG:O    | 38:BO:19:GLN:N     | 2.26                     | 0.69              |
| 43:BT:48:GLN:HE21 | 43:BT:48:GLN:HA    | 1.58                     | 0.69              |
| 55:CA:591:U:H2'   | 55:CA:592:G:C8     | 2.28                     | 0.69              |
| 5:CF:9:MET:HE1    | 17:CR:64:LEU:HA    | 1.75                     | 0.69              |
| 9:CJ:42:LEU:HB3   | 9:CJ:43:PRO:HD2    | 1.75                     | 0.69              |
| 24:DA:1021:A:C2   | 24:DA:1023:U:C2    | 2.81                     | 0.69              |
| 24:DA:1080:A:H2'  | 24:DA:1081:U:C6    | 2.28                     | 0.69              |
| 24:DA:2307:G:H1'  | 24:DA:2308:G:C5    | 2.27                     | 0.69              |
| 24:DA:2491:U:H5'' | 24:DA:2570:G:H5''  | 1.75                     | 0.69              |
| 44:DU:47:PRO:HB3  | 44:DU:54:PRO:CG    | 2.22                     | 0.69              |
| 45:DV:77:VAL:HG23 | 45:DV:89:ILE:HG21  | 1.75                     | 0.69              |
| 21:AA:1299:A:N3   | 21:AA:1299:A:H2'   | 2.07                     | 0.68              |
| 21:AA:492:C:H2'   | 21:AA:493:A:C8     | 2.28                     | 0.68              |
| 2:AC:27:GLU:O     | 2:AC:31:ASN:HB2    | 1.93                     | 0.68              |
| 5:AF:29:ILE:HG12  | 5:AF:64:VAL:HG11   | 1.73                     | 0.68              |
| 24:BA:558:U:OP2   | 33:BJ:113:PRO:HG2  | 1.93                     | 0.68              |
| 24:BA:638:G:H2'   | 24:BA:639:U:H6     | 1.58                     | 0.68              |
| 27:BD:104:VAL:O   | 27:BD:177:VAL:HG21 | 1.93                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BD:110:THR:CG2  | 27:BD:171:THR:HG22 | 2.23                     | 0.68              |
| 43:BT:32:LEU:H     | 43:BT:83:ALA:HB3   | 1.58                     | 0.68              |
| 46:BW:37:VAL:CG1   | 46:BW:38:ARG:H     | 1.99                     | 0.68              |
| 55:CA:1018:G:H2'   | 55:CA:1019:A:O4'   | 1.93                     | 0.68              |
| 55:CA:560:A:H4'    | 55:CA:561:U:H5''   | 1.74                     | 0.68              |
| 55:CA:880:C:H2'    | 55:CA:880:C:O2     | 1.94                     | 0.68              |
| 8:CI:24:ASN:HD22   | 8:CI:26:LYS:HD2    | 1.57                     | 0.68              |
| 18:CS:79:TYR:O     | 18:CS:80:ARG:HB2   | 1.93                     | 0.68              |
| 24:DA:1014:A:H2'   | 24:DA:1015:U:H6    | 1.57                     | 0.68              |
| 24:DA:1799:G:H4'   | 24:DA:1800:C:O5'   | 1.91                     | 0.68              |
| 24:DA:2492:U:O2'   | 24:DA:2493:U:H5'   | 1.93                     | 0.68              |
| 56:DB:11:C:H5'     | 46:DW:71:LYS:HD3   | 1.73                     | 0.68              |
| 24:DA:1799:G:H2'   | 26:DC:179:GLU:OE1  | 1.91                     | 0.68              |
| 24:DA:797:G:OP1    | 28:DE:57:LYS:HG2   | 1.94                     | 0.68              |
| 12:AM:69:ARG:HH12  | 21:AA:1330:U:H4'   | 1.57                     | 0.68              |
| 21:AA:1363:A:C5    | 21:AA:1365:G:C6    | 2.81                     | 0.68              |
| 9:AJ:26:VAL:O      | 9:AJ:30:LYS:HG2    | 1.93                     | 0.68              |
| 24:BA:1475:G:O2'   | 24:BA:1476:U:OP2   | 2.10                     | 0.68              |
| 24:BA:2197:U:P     | 3:CD:150:LYS:HG3   | 2.33                     | 0.68              |
| 24:BA:2356:U:H4'   | 46:BW:16:GLU:HG3   | 1.74                     | 0.68              |
| 24:BA:321:U:HO2'   | 24:BA:340:A:HO2'   | 1.41                     | 0.68              |
| 24:BA:632:A:H2'    | 24:BA:633:A:C8     | 2.28                     | 0.68              |
| 24:BA:848:C:H2'    | 24:BA:849:A:C8     | 2.28                     | 0.68              |
| 28:BE:23:PHE:CZ    | 28:BE:28:VAL:HG11  | 2.28                     | 0.68              |
| 37:BN:73:ASN:ND2   | 37:BN:76:VAL:HG11  | 2.09                     | 0.68              |
| 40:BQ:63:ARG:CZ    | 40:BQ:96:ASP:HA    | 2.23                     | 0.68              |
| 12:CM:25:GLY:H     | 55:CA:1329:A:H5''  | 1.57                     | 0.68              |
| 55:CA:631:C:H5''   | 55:CA:632:U:O4'    | 1.92                     | 0.68              |
| 4:CE:110:MET:HG2   | 4:CE:139:THR:HG21  | 1.75                     | 0.68              |
| 5:CF:68:GLN:O      | 5:CF:71:ILE:HG22   | 1.93                     | 0.68              |
| 6:CG:3:ARG:HB3     | 55:CA:932:C:OP1    | 1.93                     | 0.68              |
| 10:CK:74:LYS:HD2   | 10:CK:104:PHE:CE1  | 2.28                     | 0.68              |
| 24:DA:1071:G:N7    | 24:DA:1089:A:C6    | 2.61                     | 0.68              |
| 24:DA:2260:C:O2'   | 24:DA:2261:C:H6    | 1.77                     | 0.68              |
| 24:DA:2657:A:O3'   | 30:DG:159:LYS:NZ   | 2.26                     | 0.68              |
| 29:DF:110:ILE:HD13 | 29:DF:110:ILE:H    | 1.56                     | 0.68              |
| 31:DH:80:ILE:HB    | 31:DH:101:ASP:CB   | 2.23                     | 0.68              |
| 24:DA:2010:G:OP1   | 42:DS:41:LYS:HD3   | 1.93                     | 0.68              |
| 31:DH:27:ARG:NH1   | 47:DX:59:ASP:HA    | 2.08                     | 0.68              |
| 21:AA:86:G:C2      | 21:AA:87:C:N4      | 2.61                     | 0.68              |
| 3:AD:10:LEU:HD21   | 3:AD:62:ARG:HG3    | 1.75                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:AE:32:PHE:HD2   | 4:AE:54:GLU:HA     | 1.58                     | 0.68              |
| 9:AJ:59:LYS:HG2   | 21:AA:972:C:H4'    | 1.75                     | 0.68              |
| 24:BA:1388:G:H2'  | 24:BA:1389:G:H8    | 1.58                     | 0.68              |
| 24:BA:1989:G:C2'  | 24:BA:1990:C:H5'   | 2.23                     | 0.68              |
| 24:BA:88:G:C2     | 24:BA:89:A:C8      | 2.82                     | 0.68              |
| 55:CA:1477:U:H2'  | 55:CA:1478:U:H6    | 1.56                     | 0.68              |
| 9:CJ:80:THR:HG22  | 9:CJ:82:LYS:HZ1    | 1.57                     | 0.68              |
| 24:DA:477:A:H2'   | 24:DA:478:A:H8     | 1.56                     | 0.68              |
| 24:DA:656:G:O2'   | 24:DA:657:U:H5'    | 1.94                     | 0.68              |
| 21:AA:1453:G:H2'  | 21:AA:1453:G:N3    | 2.07                     | 0.68              |
| 52:B2:24:THR:HG23 | 52:B2:27:GLY:H     | 1.59                     | 0.68              |
| 24:BA:1303:G:H2'  | 24:BA:1304:A:H8    | 1.58                     | 0.68              |
| 24:BA:1886:U:H2'  | 24:BA:1887:C:C6    | 2.29                     | 0.68              |
| 24:BA:2032:G:H4'  | 59:BA:3484:HOH:O   | 1.92                     | 0.68              |
| 36:BM:57:VAL:HA   | 36:BM:112:LEU:HD21 | 1.75                     | 0.68              |
| 41:BR:49:ILE:O    | 41:BR:49:ILE:HG13  | 1.92                     | 0.68              |
| 48:BY:18:LEU:O    | 48:BY:22:LEU:HB2   | 1.93                     | 0.68              |
| 55:CA:462:G:O5'   | 55:CA:463:U:OP2    | 2.11                     | 0.68              |
| 13:CN:72:PHE:HA   | 13:CN:79:SER:HA    | 1.76                     | 0.68              |
| 24:DA:1560:G:O2'  | 24:DA:1561:C:H5'   | 1.94                     | 0.68              |
| 24:DA:1641:A:H2'  | 24:DA:1642:G:O4'   | 1.94                     | 0.68              |
| 24:DA:1713:A:H4'  | 24:DA:1714:U:OP1   | 1.93                     | 0.68              |
| 24:DA:247:G:H4'   | 24:DA:386:G:C4     | 2.28                     | 0.68              |
| 24:DA:782:A:H5''  | 24:DA:783:A:OP1    | 1.93                     | 0.68              |
| 36:DM:35:ALA:HB3  | 36:DM:99:GLY:N     | 2.08                     | 0.68              |
| 36:DM:62:LYS:HG2  | 36:DM:64:TRP:CZ2   | 2.29                     | 0.68              |
| 42:DS:4:ILE:HG22  | 42:DS:106:VAL:HG13 | 1.74                     | 0.68              |
| 21:AA:1234:C:H1'  | 21:AA:1364:U:C6    | 2.27                     | 0.68              |
| 21:AA:212:G:O2'   | 21:AA:213:G:C8     | 2.32                     | 0.68              |
| 19:AT:43:LYS:CB   | 19:AT:86:ALA:HB1   | 2.21                     | 0.68              |
| 24:BA:100:U:H4'   | 24:BA:101:A:O5'    | 1.94                     | 0.68              |
| 24:BA:1060:U:O4'  | 24:BA:1062:G:H5''  | 1.94                     | 0.68              |
| 24:BA:1673:G:C2'  | 24:BA:1674:G:H5'   | 2.23                     | 0.68              |
| 24:BA:866:A:O2'   | 24:BA:867:C:H5'    | 1.93                     | 0.68              |
| 26:BC:141:HIS:N   | 26:BC:190:THR:O    | 2.23                     | 0.68              |
| 26:BC:230:PRO:HD2 | 26:BC:246:PRO:HA   | 1.75                     | 0.68              |
| 24:BA:2591:C:OP1  | 26:BC:237:ARG:HG3  | 1.92                     | 0.68              |
| 30:BG:88:LEU:HD11 | 30:BG:95:ALA:HB2   | 1.75                     | 0.68              |
| 34:BK:6:THR:O     | 34:BK:6:THR:HG22   | 1.92                     | 0.68              |
| 55:CA:566:G:H4'   | 55:CA:567:G:OP1    | 1.94                     | 0.68              |
| 4:CE:55:VAL:O     | 4:CE:58:ALA:HB3    | 1.94                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:CF:86:ARG:CZ    | 17:CR:63:TYR:HB3  | 2.23                     | 0.68              |
| 9:CJ:26:VAL:O     | 9:CJ:30:LYS:HB3   | 1.92                     | 0.68              |
| 15:CP:40:ASN:HD21 | 15:CP:42:ILE:HB   | 1.58                     | 0.68              |
| 54:D4:36:ARG:HG2  | 54:D4:37:GLN:H    | 1.59                     | 0.68              |
| 24:DA:128:C:H6    | 24:DA:128:C:H5''  | 1.57                     | 0.68              |
| 24:DA:2096:C:H2'  | 24:DA:2097:A:H8   | 1.58                     | 0.68              |
| 24:DA:2681:C:H4'  | 24:DA:2682:A:O5'  | 1.93                     | 0.68              |
| 24:DA:2851:A:H2'  | 24:DA:2852:G:C8   | 2.29                     | 0.68              |
| 37:DN:2:ARG:HG2   | 37:DN:5:LYS:HD3   | 1.75                     | 0.68              |
| 48:DY:20:ASN:ND2  | 48:DY:50:VAL:HG22 | 2.08                     | 0.68              |
| 21:AA:1382:C:HO2' | 21:AA:1383:C:H6   | 1.39                     | 0.68              |
| 21:AA:390:U:H2'   | 21:AA:391:G:C8    | 2.25                     | 0.68              |
| 23:AW:5:U:H2'     | 23:AW:6:U:C6      | 2.28                     | 0.68              |
| 54:B4:9:LYS:O     | 54:B4:10:LEU:HD23 | 1.94                     | 0.68              |
| 24:BA:1399:C:H2'  | 24:BA:1400:U:H6   | 1.58                     | 0.68              |
| 24:BA:800:A:H4'   | 24:BA:801:G:O5'   | 1.93                     | 0.68              |
| 31:BH:27:ARG:NH1  | 31:BH:38:PRO:HG3  | 2.08                     | 0.68              |
| 35:BL:4:ASN:N     | 35:BL:4:ASN:HD22  | 1.91                     | 0.68              |
| 36:BM:24:THR:O    | 36:BM:34:LYS:HE2  | 1.93                     | 0.68              |
| 39:BP:25:VAL:CG1  | 39:BP:46:VAL:HG23 | 2.24                     | 0.68              |
| 40:BQ:65:ASN:ND2  | 40:BQ:69:ARG:NH2  | 2.41                     | 0.68              |
| 55:CA:209:U:H5''  | 55:CA:210:C:OP2   | 1.93                     | 0.68              |
| 6:CG:118:ARG:HH22 | 55:CA:1239:A:C3'  | 1.99                     | 0.68              |
| 8:CI:79:ARG:HD2   | 8:CI:102:PHE:CD1  | 2.28                     | 0.68              |
| 24:DA:2716:C:H2'  | 24:DA:2717:C:H6   | 1.57                     | 0.68              |
| 24:DA:265:A:H5'   | 24:DA:428:A:N1    | 2.08                     | 0.68              |
| 24:DA:620:G:H4'   | 24:DA:621:A:O5'   | 1.92                     | 0.68              |
| 24:DA:665:U:H2'   | 24:DA:666:A:C8    | 2.28                     | 0.68              |
| 24:DA:741:U:O2'   | 24:DA:742:A:O4'   | 2.09                     | 0.68              |
| 21:AA:1306:A:H61  | 21:AA:1331:G:H1'  | 1.57                     | 0.68              |
| 21:AA:174:A:H2'   | 21:AA:175:C:H6    | 1.58                     | 0.68              |
| 21:AA:765:G:H1    | 21:AA:812:G:HO2'  | 1.36                     | 0.68              |
| 21:AA:885:G:N2    | 21:AA:886:G:C4    | 2.62                     | 0.68              |
| 21:AA:978:A:O2'   | 21:AA:979:C:H5'   | 1.94                     | 0.68              |
| 21:AA:71:A:H61    | 21:AA:99:C:C1'    | 2.07                     | 0.68              |
| 2:AC:166:TRP:N    | 2:AC:166:TRP:HE3  | 1.91                     | 0.68              |
| 52:B2:3:ARG:HG2   | 52:B2:3:ARG:NH2   | 1.91                     | 0.68              |
| 24:BA:1073:A:H3'  | 24:BA:1074:G:H5'' | 1.74                     | 0.68              |
| 28:BE:79:ARG:HG2  | 28:BE:80:SER:N    | 2.06                     | 0.68              |
| 55:CA:503:C:H2'   | 55:CA:504:C:H6    | 1.58                     | 0.68              |
| 1:CB:103:TRP:HA   | 1:CB:106:VAL:HB   | 1.74                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CC:122:GLN:O    | 2:CC:127:VAL:HG13  | 1.94                     | 0.68              |
| 13:CN:40:ARG:HH12 | 18:CS:6:LYS:HB2    | 1.58                     | 0.68              |
| 24:DA:1147:A:H2'  | 24:DA:1148:U:H6    | 1.58                     | 0.68              |
| 24:DA:1386:C:O2'  | 24:DA:1387:A:H8    | 1.76                     | 0.68              |
| 24:DA:2408:U:O2'  | 24:DA:2409:G:C8    | 2.39                     | 0.68              |
| 24:DA:2748:A:H1'  | 30:DG:66:THR:CG2   | 2.20                     | 0.68              |
| 24:DA:442:G:C6    | 24:DA:444:C:N4     | 2.62                     | 0.68              |
| 24:DA:478:A:H5''  | 24:DA:479:A:OP2    | 1.94                     | 0.68              |
| 24:DA:92:U:H2'    | 24:DA:93:G:C8      | 2.27                     | 0.68              |
| 26:DC:122:ALA:HB3 | 26:DC:127:ASN:HD22 | 1.58                     | 0.68              |
| 27:DD:125:TRP:CG  | 27:DD:160:LYS:HB3  | 2.29                     | 0.68              |
| 21:AA:1394:A:H62  | 21:AA:1501:C:H4'   | 1.57                     | 0.68              |
| 21:AA:596:A:N6    | 21:AA:645:G:C6     | 2.61                     | 0.68              |
| 24:BA:14:A:H5''   | 24:BA:15:G:OP2     | 1.93                     | 0.68              |
| 24:BA:2276:G:OP2  | 36:BM:83:GLY:O     | 2.12                     | 0.68              |
| 24:BA:2531:A:H5'  | 30:BG:156:TYR:CZ   | 2.28                     | 0.68              |
| 24:BA:370:G:C6    | 24:BA:424:G:N7     | 2.62                     | 0.68              |
| 27:BD:107:VAL:O   | 27:BD:174:SER:O    | 2.11                     | 0.68              |
| 30:BG:93:TYR:O    | 30:BG:105:SER:O    | 2.11                     | 0.68              |
| 43:BT:50:LEU:H    | 43:BT:50:LEU:CD1   | 2.05                     | 0.68              |
| 55:CA:425:G:H2'   | 55:CA:426:U:C6     | 2.28                     | 0.68              |
| 11:CL:49:ARG:HH22 | 55:CA:522:C:H41    | 1.40                     | 0.68              |
| 15:CP:39:PHE:HD1  | 15:CP:50:THR:HG1   | 1.39                     | 0.68              |
| 24:DA:1207:C:H2'  | 24:DA:1208:C:H6    | 1.59                     | 0.68              |
| 24:DA:1994:C:H2'  | 24:DA:1995:U:H6    | 1.57                     | 0.68              |
| 24:DA:297:G:H5''  | 44:DU:84:PHE:CB    | 2.15                     | 0.68              |
| 45:DV:17:SER:OG   | 45:DV:27:PRO:HG3   | 1.94                     | 0.68              |
| 45:DV:29:ILE:CD1  | 45:DV:31:TYR:CE2   | 2.75                     | 0.68              |
| 21:AA:57:G:C5     | 21:AA:58:C:C4      | 2.82                     | 0.68              |
| 1:AB:159:ALA:HB1  | 1:AB:183:PHE:HE2   | 1.59                     | 0.68              |
| 10:AK:85:VAL:HG11 | 10:AK:92:ARG:HG3   | 1.76                     | 0.68              |
| 11:AL:2:THR:HG22  | 11:AL:4:ASN:H      | 1.59                     | 0.68              |
| 22:AV:34:G:H8     | 22:AV:34:G:OP1     | 1.77                     | 0.68              |
| 24:BA:460:A:H2'   | 24:BA:461:C:H6     | 1.57                     | 0.68              |
| 24:BA:522:A:C6    | 24:BA:523:C:C4     | 2.82                     | 0.68              |
| 24:BA:588:U:H2'   | 24:BA:589:U:C6     | 2.28                     | 0.68              |
| 24:BA:725:G:C6    | 24:BA:726:G:N1     | 2.62                     | 0.68              |
| 44:BU:46:LYS:HG2  | 44:BU:47:PRO:HD2   | 1.76                     | 0.68              |
| 55:CA:1036:A:O2'  | 55:CA:1037:C:H5'   | 1.93                     | 0.68              |
| 55:CA:1442:G:O6   | 55:CA:1461:G:C2    | 2.47                     | 0.68              |
| 9:CJ:51:VAL:HB    | 13:CN:80:ARG:HB2   | 1.76                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:2657:A:O2'  | 24:DA:2658:C:H5'   | 1.94                     | 0.68              |
| 27:DD:106:LYS:O   | 27:DD:107:VAL:HB   | 1.94                     | 0.68              |
| 27:DD:10:GLY:O    | 27:DD:11:MET:HB2   | 1.93                     | 0.68              |
| 28:DE:61:ARG:HD2  | 28:DE:61:ARG:O     | 1.93                     | 0.68              |
| 21:AA:1530:G:O2'  | 21:AA:1531:A:C8    | 2.36                     | 0.68              |
| 21:AA:872:A:C4    | 21:AA:874:G:N7     | 2.62                     | 0.68              |
| 16:AQ:12:VAL:HB   | 16:AQ:21:VAL:HG22  | 1.76                     | 0.68              |
| 24:BA:84:A:H62    | 24:BA:101:A:H2     | 1.42                     | 0.68              |
| 24:BA:1964:G:H4'  | 24:BA:1965:C:OP2   | 1.93                     | 0.68              |
| 24:BA:704:G:O2'   | 24:BA:726:G:N2     | 2.27                     | 0.68              |
| 24:BA:833:A:H2'   | 24:BA:834:G:C8     | 2.28                     | 0.68              |
| 24:BA:976:G:C2    | 24:BA:977:G:N7     | 2.61                     | 0.68              |
| 26:BC:159:THR:O   | 26:BC:194:VAL:HG12 | 1.93                     | 0.68              |
| 28:BE:82:GLY:O    | 28:BE:83:VAL:HB    | 1.93                     | 0.68              |
| 36:BM:1:MET:O     | 36:BM:2:LEU:HB2    | 1.92                     | 0.68              |
| 43:BT:43:ILE:O    | 43:BT:43:ILE:HG13  | 1.94                     | 0.68              |
| 13:CN:2:LYS:HG3   | 55:CA:1048:G:H5''  | 1.74                     | 0.68              |
| 55:CA:1064:G:H4'  | 55:CA:1065:U:O5'   | 1.91                     | 0.68              |
| 55:CA:591:U:H2'   | 55:CA:592:G:H8     | 1.58                     | 0.68              |
| 9:CJ:40:ILE:HG12  | 55:CA:1125:U:C6    | 2.28                     | 0.68              |
| 24:DA:1079:C:C4   | 24:DA:1088:A:H2    | 2.12                     | 0.68              |
| 24:DA:1933:G:N2   | 24:DA:1968:G:H1'   | 2.08                     | 0.68              |
| 24:DA:2311:A:H3'  | 24:DA:2312:U:H6    | 1.59                     | 0.68              |
| 26:DC:77:VAL:HG23 | 26:DC:112:GLY:H    | 1.59                     | 0.68              |
| 30:DG:115:GLN:HG2 | 30:DG:116:LEU:N    | 2.08                     | 0.68              |
| 48:DY:28:LEU:HG   | 48:DY:42:LEU:HD22  | 1.76                     | 0.68              |
| 21:AA:994:A:O2'   | 21:AA:995:C:H5'    | 1.93                     | 0.67              |
| 9:AJ:93:ALA:O     | 9:AJ:96:VAL:HG22   | 1.94                     | 0.67              |
| 24:BA:2813:A:C2   | 24:BA:2887:A:N6    | 2.62                     | 0.67              |
| 30:BG:23:ILE:HD12 | 30:BG:23:ILE:H     | 1.59                     | 0.67              |
| 31:BH:38:PRO:HB2  | 31:BH:40:THR:HG23  | 1.76                     | 0.67              |
| 33:BJ:73:VAL:CG2  | 33:BJ:74:TYR:H     | 1.98                     | 0.67              |
| 6:CG:41:ILE:O     | 6:CG:45:ALA:HB3    | 1.93                     | 0.67              |
| 24:DA:1307:A:H62  | 24:DA:1606:C:H6    | 1.43                     | 0.67              |
| 24:DA:53:A:C2     | 24:DA:179:C:H4'    | 2.28                     | 0.67              |
| 24:DA:478:A:C6    | 24:DA:480:A:C5     | 2.82                     | 0.67              |
| 24:DA:655:A:O2'   | 24:DA:656:G:C8     | 2.44                     | 0.67              |
| 24:DA:74:A:H4'    | 24:DA:75:G:O5'     | 1.93                     | 0.67              |
| 24:DA:789:A:N1    | 59:DA:3322:HOH:O   | 2.26                     | 0.67              |
| 29:DF:65:LEU:HD23 | 29:DF:65:LEU:H     | 1.60                     | 0.67              |
| 30:DG:88:LEU:HD13 | 30:DG:93:TYR:HB3   | 1.75                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:DU:35:VAL:HG12 | 44:DU:36:GLU:H     | 1.60                     | 0.67              |
| 21:AA:185:U:H2'   | 21:AA:186:C:C6     | 2.29                     | 0.67              |
| 21:AA:275:G:O2'   | 21:AA:276:G:H5'    | 1.94                     | 0.67              |
| 21:AA:473:U:H2'   | 21:AA:474:G:C8     | 2.27                     | 0.67              |
| 7:AH:30:LYS:HG2   | 21:AA:590:U:OP1    | 1.94                     | 0.67              |
| 7:AH:7:ALA:HB2    | 7:AH:76:ARG:HG3    | 1.75                     | 0.67              |
| 8:AI:8:THR:HG21   | 8:AI:10:ARG:HH21   | 1.59                     | 0.67              |
| 14:AO:2:LEU:HD22  | 14:AO:34:GLN:HG2   | 1.76                     | 0.67              |
| 24:BA:1676:A:H2   | 24:BA:1993:U:H5'   | 1.59                     | 0.67              |
| 24:BA:949:G:C2'   | 24:BA:950:G:H5'    | 2.25                     | 0.67              |
| 30:BG:104:LEU:HB2 | 30:BG:112:VAL:HG22 | 1.76                     | 0.67              |
| 33:BJ:45:THR:HG23 | 33:BJ:45:THR:O     | 1.95                     | 0.67              |
| 34:BK:21:CYS:HA   | 34:BK:41:ILE:HD12  | 1.76                     | 0.67              |
| 41:BR:39:LEU:N    | 41:BR:39:LEU:HD23  | 2.09                     | 0.67              |
| 46:BW:14:ASP:OD2  | 46:BW:16:GLU:OE1   | 2.11                     | 0.67              |
| 55:CA:1303:C:H3'  | 55:CA:1304:G:C8    | 2.29                     | 0.67              |
| 1:CB:20:ARG:HH21  | 1:CB:38:HIS:CD2    | 2.12                     | 0.67              |
| 2:CC:5:HIS:CE1    | 2:CC:7:ASN:HB3     | 2.28                     | 0.67              |
| 6:CG:30:MET:O     | 6:CG:31:VAL:HB     | 1.94                     | 0.67              |
| 11:CL:18:SER:O    | 11:CL:21:PRO:HD3   | 1.94                     | 0.67              |
| 24:DA:2285:C:C5   | 51:D1:5:ARG:NH2    | 2.62                     | 0.67              |
| 24:DA:1686:C:H2'  | 24:DA:1687:G:O4'   | 1.94                     | 0.67              |
| 24:DA:1713:A:O2'  | 24:DA:1715:G:H5'   | 1.94                     | 0.67              |
| 24:DA:2066:C:H2'  | 24:DA:2067:G:H8    | 1.59                     | 0.67              |
| 24:DA:729:G:O2'   | 24:DA:1775:U:H1'   | 1.92                     | 0.67              |
| 24:DA:973:A:H1'   | 24:DA:1188:U:C5    | 2.29                     | 0.67              |
| 41:DR:21:ARG:HB2  | 41:DR:93:PHE:HD1   | 1.60                     | 0.67              |
| 21:AA:1054:C:OP2  | 21:AA:1197:A:OP2   | 2.12                     | 0.67              |
| 1:AB:143:LEU:HB2  | 1:AB:147:LEU:HD12  | 1.75                     | 0.67              |
| 1:AB:63:LYS:HG2   | 1:AB:224:ARG:NH1   | 2.09                     | 0.67              |
| 1:AB:99:MET:HA    | 1:AB:106:VAL:HG21  | 1.76                     | 0.67              |
| 3:AD:145:ARG:O    | 3:AD:149:LYS:HG3   | 1.94                     | 0.67              |
| 6:AG:125:ASP:OD2  | 6:AG:130:LYS:HG3   | 1.94                     | 0.67              |
| 8:AI:129:ARG:HH21 | 21:AA:966:G:N2     | 1.90                     | 0.67              |
| 13:AN:15:LEU:HD23 | 13:AN:18:LYS:HD2   | 1.76                     | 0.67              |
| 16:AQ:16:MET:HG3  | 16:AQ:20:ILE:HA    | 1.77                     | 0.67              |
| 24:BA:1256:G:H21  | 28:BE:77:ILE:HG13  | 1.59                     | 0.67              |
| 24:BA:2358:A:H61  | 35:BL:54:GLN:NE2   | 1.92                     | 0.67              |
| 24:BA:459:U:H2'   | 24:BA:460:A:C8     | 2.28                     | 0.67              |
| 41:BR:62:GLU:HG3  | 41:BR:62:GLU:O     | 1.92                     | 0.67              |
| 55:CA:787:A:C2    | 55:CA:796:C:N3     | 2.62                     | 0.67              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:CG:46:LEU:HD11   | 6:CG:57:GLU:OE2   | 1.94                     | 0.67              |
| 6:CG:149:ALA:HB2   | 10:CK:55:ARG:HG3  | 1.75                     | 0.67              |
| 24:DA:254:G:N7     | 53:D3:4:LYS:HE2   | 2.09                     | 0.67              |
| 24:DA:1731:G:HO2'  | 24:DA:1732:C:H5'' | 1.57                     | 0.67              |
| 30:DG:112:VAL:HG13 | 30:DG:150:TYR:HE1 | 1.59                     | 0.67              |
| 34:DK:60:ALA:HA    | 34:DK:87:LEU:CD2  | 2.24                     | 0.67              |
| 35:DL:9:ALA:HB3    | 35:DL:12:SER:HB3  | 1.75                     | 0.67              |
| 43:DT:6:ARG:O      | 43:DT:9:LYS:HD2   | 1.93                     | 0.67              |
| 48:DY:17:GLU:HG3   | 48:DY:53:VAL:HG11 | 1.77                     | 0.67              |
| 16:AQ:58:VAL:HG22  | 16:AQ:59:GLU:H    | 1.60                     | 0.67              |
| 18:AS:54:ARG:HG2   | 21:AA:958:A:C6    | 2.30                     | 0.67              |
| 50:B0:43:THR:HG23  | 50:B0:47:TYR:O    | 1.94                     | 0.67              |
| 24:BA:321:U:O2'    | 24:BA:340:A:O2'   | 2.06                     | 0.67              |
| 31:BH:96:THR:O     | 31:BH:97:ARG:HG3  | 1.95                     | 0.67              |
| 34:BK:18:ARG:NH1   | 34:BK:18:ARG:HG3  | 2.06                     | 0.67              |
| 46:BW:39:GLN:HG3   | 46:BW:42:THR:HB   | 1.76                     | 0.67              |
| 55:CA:1305:G:H22   | 55:CA:1331:G:H2'  | 1.60                     | 0.67              |
| 55:CA:181:A:H1'    | 55:CA:182:A:C2    | 2.28                     | 0.67              |
| 55:CA:279:A:H5''   | 55:CA:280:C:H3'   | 1.77                     | 0.67              |
| 55:CA:890:G:HO2'   | 55:CA:891:U:P     | 2.17                     | 0.67              |
| 24:DA:1060:U:H5''  | 24:DA:1061:U:OP1  | 1.94                     | 0.67              |
| 24:DA:1197:G:H5'   | 24:DA:1227:G:O2'  | 1.95                     | 0.67              |
| 24:DA:1210:G:H5''  | 24:DA:1211:C:H3'  | 1.75                     | 0.67              |
| 24:DA:2728:U:O2'   | 24:DA:2729:G:H8   | 1.77                     | 0.67              |
| 24:DA:311:A:O2'    | 24:DA:332:A:H5'   | 1.95                     | 0.67              |
| 24:DA:53:A:O2'     | 24:DA:54:G:H5'    | 1.93                     | 0.67              |
| 24:DA:817:C:O2'    | 24:DA:839:U:H5''  | 1.94                     | 0.67              |
| 28:DE:133:LEU:O    | 28:DE:137:LYS:HB2 | 1.95                     | 0.67              |
| 37:DN:71:ARG:HB2   | 37:DN:71:ARG:HH21 | 1.59                     | 0.67              |
| 21:AA:1005:A:H2'   | 21:AA:1006:G:O4'  | 1.94                     | 0.67              |
| 21:AA:77:A:H8      | 21:AA:77:A:OP2    | 1.78                     | 0.67              |
| 21:AA:994:A:C5     | 21:AA:1216:A:H4'  | 2.29                     | 0.67              |
| 1:AB:89:PHE:CB     | 1:AB:149:GLY:HA2  | 2.25                     | 0.67              |
| 4:AE:83:PRO:CB     | 4:AE:97:PRO:HD3   | 2.24                     | 0.67              |
| 10:AK:85:VAL:HG12  | 10:AK:86:LYS:H    | 1.58                     | 0.67              |
| 24:BA:1557:C:H2'   | 24:BA:1558:C:C6   | 2.29                     | 0.67              |
| 24:BA:2557:G:H2'   | 24:BA:2558:C:H6   | 1.59                     | 0.67              |
| 24:BA:869:G:O2'    | 36:BM:8:LYS:HD3   | 1.94                     | 0.67              |
| 38:BO:24:THR:HG22  | 38:BO:42:PRO:HD3  | 1.77                     | 0.67              |
| 24:BA:2354:C:C4'   | 46:BW:31:LEU:HD22 | 2.24                     | 0.67              |
| 55:CA:559:A:H4'    | 55:CA:560:A:C5'   | 2.25                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:CJ:35:GLN:HG2    | 9:CJ:76:ILE:HG23   | 1.75                     | 0.67              |
| 12:CM:36:ALA:HB2   | 12:CM:55:LEU:HD21  | 1.76                     | 0.67              |
| 20:CU:24:LYS:HG3   | 20:CU:25:ALA:N     | 2.06                     | 0.67              |
| 24:DA:1439:A:N6    | 24:DA:1551:A:C2    | 2.63                     | 0.67              |
| 24:DA:1759:A:H2'   | 24:DA:1760:C:C6    | 2.29                     | 0.67              |
| 24:DA:612:G:C2     | 24:DA:614:A:H1'    | 2.30                     | 0.67              |
| 43:DT:29:THR:HB    | 43:DT:87:LEU:N     | 2.09                     | 0.67              |
| 46:DW:9:THR:HG23   | 46:DW:10:ARG:HG3   | 1.75                     | 0.67              |
| 21:AA:1137:C:H5'   | 21:AA:1138:G:OP1   | 1.93                     | 0.67              |
| 21:AA:721:G:H4'    | 21:AA:722:G:O5'    | 1.93                     | 0.67              |
| 21:AA:765:G:H22    | 21:AA:812:G:HO2'   | 1.41                     | 0.67              |
| 1:AB:163:ILE:O     | 1:AB:185:ILE:HG12  | 1.95                     | 0.67              |
| 12:AM:28:ARG:NH1   | 12:AM:28:ARG:HB3   | 2.09                     | 0.67              |
| 13:AN:70:HIS:CE1   | 21:AA:974:A:H1'    | 2.29                     | 0.67              |
| 24:BA:1783:A:C2    | 24:BA:2587:A:C5    | 2.83                     | 0.67              |
| 24:BA:2822:G:P     | 27:BD:115:GLY:HA3  | 2.34                     | 0.67              |
| 32:BI:33:ASN:HD22  | 32:BI:64:ARG:NH2   | 1.92                     | 0.67              |
| 33:BJ:81:ILE:HG23  | 33:BJ:82:GLY:N     | 2.08                     | 0.67              |
| 55:CA:1508:A:H2'   | 55:CA:1509:C:H6    | 1.58                     | 0.67              |
| 54:D4:7:VAL:HG13   | 54:D4:8:LYS:H      | 1.60                     | 0.67              |
| 24:DA:1590:A:H2'   | 24:DA:1591:A:C8    | 2.30                     | 0.67              |
| 24:DA:2547:A:H1'   | 24:DA:2566:A:N6    | 2.08                     | 0.67              |
| 26:DC:166:ARG:HG3  | 26:DC:166:ARG:O    | 1.95                     | 0.67              |
| 26:DC:75:ALA:HB2   | 26:DC:95:TYR:CD1   | 2.29                     | 0.67              |
| 29:DF:104:THR:HG22 | 29:DF:105:ILE:HG13 | 1.76                     | 0.67              |
| 29:DF:42:ALA:HB2   | 29:DF:49:LEU:HD21  | 1.76                     | 0.67              |
| 34:DK:7:MET:HA     | 34:DK:7:MET:CE     | 2.24                     | 0.67              |
| 43:DT:38:ALA:HB1   | 43:DT:81:LYS:NZ    | 2.10                     | 0.67              |
| 21:AA:769:G:H4'    | 21:AA:1513:A:H4'   | 1.77                     | 0.67              |
| 1:AB:205:ALA:HB3   | 1:AB:208:ALA:HB2   | 1.76                     | 0.67              |
| 24:BA:49:A:H61     | 24:BA:177:G:H2'    | 1.59                     | 0.67              |
| 24:BA:312:G:H2'    | 24:BA:313:G:H8     | 1.60                     | 0.67              |
| 24:BA:825:A:C1'    | 35:BL:54:GLN:HE21  | 2.07                     | 0.67              |
| 26:BC:77:VAL:O     | 26:BC:77:VAL:HG22  | 1.94                     | 0.67              |
| 36:BM:83:GLY:O     | 36:BM:85:GLY:N     | 2.28                     | 0.67              |
| 46:BW:18:LYS:HA    | 46:BW:36:ILE:HG13  | 1.76                     | 0.67              |
| 49:BZ:26:LEU:O     | 49:BZ:37:ARG:NH1   | 2.27                     | 0.67              |
| 55:CA:613:C:H2'    | 55:CA:614:C:C6     | 2.29                     | 0.67              |
| 55:CA:70:U:H4'     | 55:CA:71:A:OP1     | 1.95                     | 0.67              |
| 24:DA:1223:G:N2    | 24:DA:1225:G:H3'   | 2.08                     | 0.67              |
| 24:DA:2400:G:H2'   | 24:DA:2401:U:O4'   | 1.94                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:2408:U:HO2' | 24:DA:2409:G:H8    | 0.75                     | 0.67              |
| 24:DA:855:G:N3    | 46:DW:23:LYS:HE3   | 2.07                     | 0.67              |
| 33:DJ:44:TYR:O    | 33:DJ:45:THR:HB    | 1.93                     | 0.67              |
| 48:DY:1:MET:N     | 48:DY:1:MET:HE2    | 2.10                     | 0.67              |
| 3:AD:101:VAL:HG13 | 3:AD:106:PHE:HB2   | 1.77                     | 0.67              |
| 23:AW:4:U:N3      | 22:AX:37:A:C2      | 2.63                     | 0.67              |
| 54:B4:24:ARG:HG2  | 54:B4:24:ARG:NH2   | 2.10                     | 0.67              |
| 24:BA:1322:A:O3'  | 42:BS:84:ARG:NH1   | 2.27                     | 0.67              |
| 24:BA:2888:C:H2'  | 24:BA:2889:C:H6    | 1.60                     | 0.67              |
| 33:BJ:111:LYS:HD3 | 33:BJ:112:GLY:H    | 1.60                     | 0.67              |
| 33:BJ:21:THR:CG2  | 33:BJ:22:GLY:N     | 2.51                     | 0.67              |
| 33:BJ:56:VAL:HG12 | 33:BJ:57:LEU:H     | 1.58                     | 0.67              |
| 40:BQ:77:LYS:HE2  | 40:BQ:116:LEU:HD23 | 1.77                     | 0.67              |
| 47:BX:76:LYS:HG3  | 47:BX:77:TYR:H     | 1.59                     | 0.67              |
| 1:CB:79:VAL:HG13  | 1:CB:80:LYS:H      | 1.60                     | 0.67              |
| 24:DA:2036:C:O2'  | 24:DA:2037:A:H8    | 1.72                     | 0.67              |
| 24:DA:2592:G:H2'  | 24:DA:2593:U:H6    | 1.60                     | 0.67              |
| 24:DA:417:C:H2'   | 24:DA:418:C:H6     | 1.60                     | 0.67              |
| 24:DA:627:A:O2'   | 24:DA:628:G:O4'    | 2.13                     | 0.67              |
| 21:AA:1505:G:H5'' | 59:AA:1801:HOH:O   | 1.93                     | 0.67              |
| 24:BA:1190:G:H2'  | 24:BA:1191:G:H8    | 1.59                     | 0.67              |
| 24:BA:1361:G:C5   | 24:BA:1371:G:N2    | 2.63                     | 0.67              |
| 24:BA:33:C:H4'    | 24:BA:34:U:OP1     | 1.95                     | 0.67              |
| 24:BA:988:A:OP2   | 49:BZ:11:SER:HB3   | 1.95                     | 0.67              |
| 25:BB:7:G:O2'     | 38:BO:38:GLN:NE2   | 2.28                     | 0.67              |
| 46:BW:28:GLU:HG3  | 46:BW:29:SER:H     | 1.60                     | 0.67              |
| 19:CT:73:ARG:NH1  | 55:CA:261:U:C4     | 2.63                     | 0.67              |
| 55:CA:928:G:O2'   | 55:CA:1533:C:OP1   | 2.12                     | 0.67              |
| 24:DA:375:G:H8    | 24:DA:375:G:H5''   | 1.60                     | 0.67              |
| 24:DA:85:G:O2'    | 24:DA:86:G:C8      | 2.47                     | 0.67              |
| 24:DA:973:A:OP1   | 24:DA:973:A:H8     | 1.78                     | 0.67              |
| 26:DC:9:SER:O     | 26:DC:12:ARG:HB2   | 1.95                     | 0.67              |
| 24:DA:1008:A:H5'' | 33:DJ:37:ARG:HH22  | 1.58                     | 0.67              |
| 45:DV:77:VAL:HG23 | 45:DV:89:ILE:CG2   | 2.25                     | 0.67              |
| 49:DZ:20:LYS:O    | 49:DZ:24:LEU:HD13  | 1.95                     | 0.67              |
| 21:AA:1258:G:O2'  | 21:AA:1259:C:C5'   | 2.41                     | 0.67              |
| 21:AA:355:C:C4    | 21:AA:356:A:N7     | 2.62                     | 0.67              |
| 21:AA:463:U:C4    | 21:AA:464:U:O4     | 2.48                     | 0.67              |
| 8:AI:129:ARG:HH22 | 21:AA:967:C:H1'    | 1.60                     | 0.67              |
| 1:AB:69:VAL:HG21  | 1:AB:160:LEU:HD21  | 1.76                     | 0.67              |
| 3:AD:50:TYR:CE2   | 3:AD:54:LEU:HD12   | 2.29                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:2848:G:O2'  | 24:BA:2867:G:N2    | 2.27                     | 0.67              |
| 24:BA:64:A:H2'    | 24:BA:65:U:H6      | 1.60                     | 0.67              |
| 29:BF:134:GLN:HG3 | 29:BF:140:ILE:HG12 | 1.75                     | 0.67              |
| 41:BR:14:VAL:HG11 | 41:BR:98:ILE:HD12  | 1.76                     | 0.67              |
| 55:CA:1284:C:H2'  | 55:CA:1285:A:C8    | 2.30                     | 0.67              |
| 11:CL:98:ARG:HB2  | 11:CL:116:TYR:HA   | 1.77                     | 0.67              |
| 50:D0:26:SER:O    | 50:D0:27:LEU:HD13  | 1.95                     | 0.67              |
| 21:AA:484:G:OP1   | 21:AA:484:G:H8     | 1.76                     | 0.66              |
| 4:AE:149:PRO:HA   | 4:AE:152:VAL:HG13  | 1.77                     | 0.66              |
| 24:BA:2466:C:OP1  | 54:B4:4:ARG:HB2    | 1.95                     | 0.66              |
| 24:BA:858:G:H21   | 24:BA:2268:A:H2'   | 1.59                     | 0.66              |
| 24:BA:919:U:H6    | 24:BA:919:U:H5''   | 1.59                     | 0.66              |
| 39:BP:50:ARG:HB3  | 39:BP:57:ALA:N     | 2.04                     | 0.66              |
| 55:CA:735:C:HO2'  | 55:CA:736:C:H6     | 1.43                     | 0.66              |
| 6:CG:135:LYS:O    | 6:CG:139:ASP:HB2   | 1.94                     | 0.66              |
| 22:CV:27:G:H8     | 22:CV:27:G:H5''    | 1.60                     | 0.66              |
| 24:DA:2056:G:C2   | 24:DA:2057:G:C8    | 2.83                     | 0.66              |
| 24:DA:2311:A:H4'  | 24:DA:2312:U:OP2   | 1.95                     | 0.66              |
| 24:DA:823:C:H2'   | 24:DA:824:U:C6     | 2.30                     | 0.66              |
| 35:DL:79:LEU:HB3  | 35:DL:114:GLY:H    | 1.59                     | 0.66              |
| 42:DS:88:ARG:HG3  | 42:DS:88:ARG:HH21  | 1.60                     | 0.66              |
| 21:AA:121:U:H5''  | 21:AA:121:U:H6     | 1.60                     | 0.66              |
| 1:AB:67:LEU:HD21  | 1:AB:91:VAL:HG23   | 1.77                     | 0.66              |
| 3:AD:104:MET:SD   | 3:AD:179:GLY:HA3   | 2.35                     | 0.66              |
| 4:AE:85:LYS:HG3   | 4:AE:94:PHE:HB2    | 1.78                     | 0.66              |
| 7:AH:21:LYS:HE2   | 7:AH:21:LYS:HA     | 1.76                     | 0.66              |
| 12:AM:67:ASP:C    | 12:AM:70:ARG:HD2   | 2.13                     | 0.66              |
| 54:B4:36:ARG:HG2  | 54:B4:37:GLN:N     | 2.05                     | 0.66              |
| 24:BA:143:C:H2'   | 24:BA:144:A:C8     | 2.29                     | 0.66              |
| 24:BA:1340:U:H6   | 24:BA:1603:A:H5'   | 1.59                     | 0.66              |
| 24:BA:1695:G:H2'  | 24:BA:1696:G:O4'   | 1.95                     | 0.66              |
| 24:BA:1731:G:C4   | 24:BA:1733:G:N7    | 2.64                     | 0.66              |
| 24:BA:2792:A:O2'  | 24:BA:2793:C:H5'   | 1.95                     | 0.66              |
| 24:BA:509:C:H5''  | 24:BA:509:C:H6     | 1.59                     | 0.66              |
| 26:BC:259:ASN:O   | 26:BC:260:LYS:HB2  | 1.96                     | 0.66              |
| 33:BJ:43:GLU:O    | 33:BJ:44:TYR:C     | 2.33                     | 0.66              |
| 45:BV:40:ILE:HG22 | 45:BV:41:GLU:N     | 2.09                     | 0.66              |
| 46:BW:50:VAL:O    | 46:BW:52:CYS:N     | 2.27                     | 0.66              |
| 55:CA:1070:U:H2'  | 55:CA:1071:C:H6    | 1.60                     | 0.66              |
| 1:CB:128:LEU:HB2  | 1:CB:132:GLU:HG2   | 1.75                     | 0.66              |
| 6:CG:100:MET:HA   | 6:CG:103:ILE:HD12  | 1.77                     | 0.66              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:CG:77:ARG:CZ     | 55:CA:1381:U:H3   | 2.08                     | 0.66              |
| 24:DA:1303:G:H2'   | 24:DA:1304:A:H8   | 1.59                     | 0.66              |
| 24:DA:1810:A:H2'   | 24:DA:1811:G:O4'  | 1.93                     | 0.66              |
| 24:DA:2292:U:H2'   | 24:DA:2293:G:C8   | 2.30                     | 0.66              |
| 24:DA:2631:G:C2'   | 24:DA:2632:A:H5'' | 2.22                     | 0.66              |
| 24:DA:45:G:H5'     | 24:DA:46:G:OP1    | 1.96                     | 0.66              |
| 37:DN:2:ARG:CD     | 37:DN:5:LYS:HB3   | 2.25                     | 0.66              |
| 21:AA:792:A:O2'    | 21:AA:794:A:N7    | 2.20                     | 0.66              |
| 1:AB:107:ARG:HH21  | 1:AB:108:GLN:HE22 | 1.41                     | 0.66              |
| 6:AG:31:VAL:HG22   | 6:AG:32:ASP:OD1   | 1.95                     | 0.66              |
| 12:AM:70:ARG:HG2   | 12:AM:71:GLU:N    | 2.10                     | 0.66              |
| 17:AR:24:ASP:HB3   | 17:AR:27:THR:OG1  | 1.94                     | 0.66              |
| 20:AU:10:PRO:O     | 20:AU:11:PHE:HB3  | 1.95                     | 0.66              |
| 24:BA:2054:A:H2'   | 50:B0:4:GLN:OE1   | 1.95                     | 0.66              |
| 24:BA:1652:A:C2    | 24:BA:2006:C:N3   | 2.63                     | 0.66              |
| 24:BA:2312:U:O2    | 29:BF:38:GLY:HA3  | 1.95                     | 0.66              |
| 24:BA:2417:C:H2'   | 24:BA:2418:A:H8   | 1.60                     | 0.66              |
| 24:BA:197:A:N6     | 24:BA:2430:A:H2'  | 2.07                     | 0.66              |
| 24:BA:2438:U:O2'   | 24:BA:2439:A:H5'' | 1.95                     | 0.66              |
| 24:BA:181:A:H1'    | 24:BA:435:C:H5'   | 1.76                     | 0.66              |
| 26:BC:251:THR:HG22 | 26:BC:252:LYS:N   | 2.07                     | 0.66              |
| 30:BG:11:PRO:O     | 30:BG:14:VAL:HG22 | 1.95                     | 0.66              |
| 48:BY:9:LYS:HA     | 48:BY:9:LYS:HZ1   | 1.58                     | 0.66              |
| 1:CB:208:ALA:O     | 1:CB:211:LEU:HB3  | 1.95                     | 0.66              |
| 1:CB:61:SER:OG     | 1:CB:224:ARG:HA   | 1.95                     | 0.66              |
| 8:CI:96:GLU:HA     | 8:CI:99:LYS:HE2   | 1.75                     | 0.66              |
| 24:DA:123:G:H4'    | 24:DA:1376:C:H5'  | 1.77                     | 0.66              |
| 24:DA:1281:G:C6    | 24:DA:1290:C:N4   | 2.63                     | 0.66              |
| 24:DA:1498:C:O2'   | 24:DA:1499:C:H5'  | 1.95                     | 0.66              |
| 24:DA:1695:G:H8    | 26:DC:7:PRO:O     | 1.78                     | 0.66              |
| 24:DA:234:U:HO2'   | 24:DA:235:U:H6    | 1.41                     | 0.66              |
| 24:DA:479:A:O2'    | 24:DA:480:A:H5''  | 1.95                     | 0.66              |
| 24:DA:480:A:H3'    | 24:DA:481:G:H5''  | 1.76                     | 0.66              |
| 24:DA:27:G:H1'     | 24:DA:513:A:H61   | 1.61                     | 0.66              |
| 30:DG:148:ARG:HB2  | 30:DG:152:ARG:NH2 | 2.09                     | 0.66              |
| 30:DG:164:ALA:O    | 30:DG:165:ASP:HB2 | 1.95                     | 0.66              |
| 35:DL:119:PRO:HB3  | 35:DL:139:GLY:O   | 1.94                     | 0.66              |
| 39:DP:109:ILE:O    | 39:DP:110:LYS:HG3 | 1.95                     | 0.66              |
| 21:AA:1215:G:O2'   | 21:AA:1216:A:H5'  | 1.95                     | 0.66              |
| 4:AE:109:ALA:O     | 4:AE:111:ARG:N    | 2.27                     | 0.66              |
| 10:AK:23:HIS:HB3   | 10:AK:30:ILE:HG13 | 1.78                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:1654:A:H1'  | 27:BD:118:PHE:CD1  | 2.30                     | 0.66              |
| 24:BA:2531:A:OP1  | 30:BG:174:LYS:HG3  | 1.95                     | 0.66              |
| 24:BA:478:A:C6    | 24:BA:480:A:C6     | 2.83                     | 0.66              |
| 31:BH:48:GLU:HA   | 31:BH:51:ARG:CG    | 2.24                     | 0.66              |
| 40:BQ:81:GLY:HA2  | 40:BQ:116:LEU:HD13 | 1.77                     | 0.66              |
| 55:CA:1207:G:H2'  | 55:CA:1208:C:H6    | 1.60                     | 0.66              |
| 55:CA:51:A:H4'    | 55:CA:52:C:OP2     | 1.94                     | 0.66              |
| 4:CE:125:LYS:HG2  | 4:CE:126:ALA:H     | 1.59                     | 0.66              |
| 8:CI:30:ASN:ND2   | 8:CI:66:VAL:H      | 1.93                     | 0.66              |
| 10:CK:20:ALA:HB3  | 10:CK:83:VAL:HG13  | 1.77                     | 0.66              |
| 13:CN:47:LEU:O    | 13:CN:50:LEU:HG    | 1.95                     | 0.66              |
| 24:DA:251:A:H2'   | 24:DA:252:G:O4'    | 1.95                     | 0.66              |
| 33:DJ:73:VAL:HG23 | 33:DJ:74:TYR:H     | 1.59                     | 0.66              |
| 40:DQ:4:LYS:CE    | 40:DQ:7:VAL:H      | 2.08                     | 0.66              |
| 47:DX:29:LEU:HB2  | 47:DX:30:PRO:CD    | 2.26                     | 0.66              |
| 49:DZ:18:LYS:O    | 49:DZ:22:THR:HG23  | 1.95                     | 0.66              |
| 21:AA:1031:C:O2'  | 21:AA:1032:G:H5''  | 1.96                     | 0.66              |
| 8:AI:128:LYS:HD3  | 8:AI:129:ARG:H     | 1.61                     | 0.66              |
| 11:AL:42:LYS:HE2  | 11:AL:43:LYS:HZ1   | 1.60                     | 0.66              |
| 24:BA:1655:A:H4'  | 27:BD:119:ALA:O    | 1.95                     | 0.66              |
| 28:BE:145:ASP:HA  | 28:BE:166:LYS:O    | 1.96                     | 0.66              |
| 55:CA:1033:G:O2'  | 55:CA:1034:G:O4'   | 2.13                     | 0.66              |
| 55:CA:9:G:H2'     | 55:CA:10:A:C8      | 2.29                     | 0.66              |
| 55:CA:1412:C:H2'  | 55:CA:1413:A:C8    | 2.30                     | 0.66              |
| 55:CA:1523:G:H2'  | 55:CA:1524:C:C6    | 2.30                     | 0.66              |
| 55:CA:564:C:H6    | 55:CA:564:C:H5'    | 1.60                     | 0.66              |
| 8:CI:90:ASP:HB3   | 8:CI:93:LEU:HD23   | 1.76                     | 0.66              |
| 8:CI:112:ARG:HH22 | 9:CJ:64:GLN:NE2    | 1.93                     | 0.66              |
| 24:DA:686:U:O4    | 52:D2:12:ARG:HG3   | 1.95                     | 0.66              |
| 24:DA:1666:G:O3'  | 34:DK:6:THR:HA     | 1.96                     | 0.66              |
| 24:DA:1956:U:O2'  | 24:DA:1957:C:C5'   | 2.44                     | 0.66              |
| 24:DA:861:A:O2'   | 24:DA:862:G:H5'    | 1.96                     | 0.66              |
| 24:DA:996:A:H5'   | 40:DQ:91:ARG:NH1   | 2.10                     | 0.66              |
| 26:DC:143:VAL:HB  | 26:DC:153:LEU:HB3  | 1.77                     | 0.66              |
| 26:DC:71:ASP:O    | 26:DC:73:ILE:HG12  | 1.95                     | 0.66              |
| 27:DD:16:THR:HG22 | 27:DD:20:VAL:H     | 1.59                     | 0.66              |
| 30:DG:72:ASN:O    | 30:DG:76:ILE:HG12  | 1.95                     | 0.66              |
| 32:DI:74:PRO:HB2  | 32:DI:77:VAL:HG22  | 1.76                     | 0.66              |
| 21:AA:1038:C:H2'  | 21:AA:1039:G:C8    | 2.31                     | 0.66              |
| 21:AA:1418:A:H8   | 21:AA:1418:A:H3'   | 1.61                     | 0.66              |
| 21:AA:300:A:H1'   | 21:AA:565:U:O2     | 1.96                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AL:49:ARG:NH2   | 21:AA:522:C:H41    | 1.93                     | 0.66              |
| 2:AC:32:LEU:O      | 2:AC:35:ASP:HB3    | 1.96                     | 0.66              |
| 3:AD:106:PHE:HB3   | 3:AD:144:ILE:HD11  | 1.77                     | 0.66              |
| 7:AH:29:SER:HB2    | 7:AH:32:LYS:NZ     | 2.11                     | 0.66              |
| 9:AJ:17:LEU:HD23   | 9:AJ:17:LEU:O      | 1.96                     | 0.66              |
| 50:B0:9:ARG:HH21   | 50:B0:9:ARG:HG3    | 1.59                     | 0.66              |
| 24:BA:1721:G:O2'   | 24:BA:1722:A:H8    | 1.78                     | 0.66              |
| 24:BA:249:C:H5'    | 24:BA:2394:C:O2'   | 1.95                     | 0.66              |
| 26:BC:143:VAL:HG12 | 26:BC:144:GLU:O    | 1.96                     | 0.66              |
| 28:BE:104:ALA:O    | 28:BE:108:ILE:HG22 | 1.94                     | 0.66              |
| 29:BF:107:VAL:CG1  | 29:BF:113:PHE:CZ   | 2.79                     | 0.66              |
| 42:BS:73:LYS:HB3   | 42:BS:106:VAL:HB   | 1.78                     | 0.66              |
| 55:CA:869:G:H4'    | 55:CA:872:A:C8     | 2.31                     | 0.66              |
| 8:CI:87:MET:HG3    | 8:CI:94:ARG:HE     | 1.60                     | 0.66              |
| 16:CQ:25:GLU:HG2   | 16:CQ:40:THR:HG22  | 1.78                     | 0.66              |
| 19:CT:30:PHE:HE2   | 19:CT:52:GLU:HG2   | 1.59                     | 0.66              |
| 24:DA:1084:A:H2'   | 24:DA:1085:A:H5'   | 1.75                     | 0.66              |
| 24:DA:1296:G:N2    | 24:DA:1645:G:C4    | 2.64                     | 0.66              |
| 24:DA:2312:U:OP2   | 29:DF:70:ARG:HD2   | 1.96                     | 0.66              |
| 24:DA:248:G:H5'    | 24:DA:250:G:N7     | 2.10                     | 0.66              |
| 24:DA:2800:A:O2'   | 24:DA:2801:G:H4'   | 1.95                     | 0.66              |
| 24:DA:749:A:H2'    | 24:DA:750:A:H8     | 1.60                     | 0.66              |
| 24:DA:962:G:O2'    | 24:DA:963:U:H5'    | 1.96                     | 0.66              |
| 44:DU:43:LYS:HG2   | 44:DU:45:GLN:HG2   | 1.76                     | 0.66              |
| 49:DZ:30:ARG:NH2   | 49:DZ:33:HIS:HB2   | 2.11                     | 0.66              |
| 1:AB:108:GLN:H     | 1:AB:108:GLN:NE2   | 1.92                     | 0.66              |
| 9:AJ:11:LYS:HB3    | 9:AJ:71:LEU:HD13   | 1.77                     | 0.66              |
| 19:AT:26:MET:HA    | 19:AT:29:THR:OG1   | 1.94                     | 0.66              |
| 27:BD:140:HIS:CE1  | 59:BD:403:HOH:O    | 2.42                     | 0.66              |
| 32:BI:3:LYS:HD2    | 32:BI:4:VAL:HG23   | 1.78                     | 0.66              |
| 42:BS:42:LYS:O     | 42:BS:45:VAL:HG13  | 1.95                     | 0.66              |
| 55:CA:513:C:O2'    | 55:CA:514:C:O4'    | 2.14                     | 0.66              |
| 55:CA:982:U:H4'    | 55:CA:983:A:O5'    | 1.94                     | 0.66              |
| 8:CI:83:THR:OG1    | 8:CI:97:LEU:HD13   | 1.95                     | 0.66              |
| 12:CM:33:LEU:HB3   | 12:CM:38:ILE:HB    | 1.78                     | 0.66              |
| 22:CX:34:G:H2'     | 22:CX:35:A:H8      | 1.58                     | 0.66              |
| 24:DA:1309:G:H4'   | 52:D2:7:PRO:HB2    | 1.78                     | 0.66              |
| 24:DA:1594:U:H2'   | 24:DA:1595:C:C6    | 2.30                     | 0.66              |
| 26:DC:209:ALA:HA   | 26:DC:212:TRP:CE2  | 2.31                     | 0.66              |
| 31:DH:83:LYS:HZ1   | 31:DH:91:PHE:HD2   | 1.42                     | 0.66              |
| 35:DL:100:ILE:O    | 35:DL:101:ILE:HB   | 1.95                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:DP:56:SER:HB2  | 39:DP:75:THR:HG21  | 1.77                     | 0.66              |
| 43:DT:69:ARG:O    | 43:DT:74:ILE:HD12  | 1.95                     | 0.66              |
| 44:DU:83:GLY:O    | 44:DU:93:ARG:HA    | 1.95                     | 0.66              |
| 21:AA:131:A:C2    | 21:AA:132:C:C4     | 2.84                     | 0.66              |
| 21:AA:210:C:H4'   | 21:AA:211:G:C2     | 2.31                     | 0.66              |
| 3:AD:47:LEU:H     | 3:AD:47:LEU:HD23   | 1.61                     | 0.66              |
| 24:BA:1499:C:H2'  | 24:BA:1500:G:H8    | 1.59                     | 0.66              |
| 24:BA:163:C:O2'   | 24:BA:164:C:H5''   | 1.96                     | 0.66              |
| 24:BA:2346:A:H3'  | 24:BA:2347:C:H5''  | 1.78                     | 0.66              |
| 33:BJ:38:GLY:O    | 33:BJ:43:GLU:HB2   | 1.95                     | 0.66              |
| 36:BM:107:GLY:O   | 36:BM:108:VAL:HG23 | 1.94                     | 0.66              |
| 36:BM:54:THR:O    | 36:BM:56:ALA:N     | 2.29                     | 0.66              |
| 41:BR:16:GLU:HA   | 41:BR:98:ILE:CG2   | 2.24                     | 0.66              |
| 44:BU:35:VAL:HB   | 44:BU:38:ILE:HG13  | 1.78                     | 0.66              |
| 55:CA:109:A:H61   | 55:CA:324:G:H1'    | 1.60                     | 0.66              |
| 1:CB:127:LYS:HE3  | 1:CB:132:GLU:HG3   | 1.77                     | 0.66              |
| 3:CD:8:LEU:O      | 3:CD:12:ARG:HB2    | 1.96                     | 0.66              |
| 24:DA:1069:A:H2'  | 24:DA:1072:C:OP2   | 1.94                     | 0.66              |
| 24:DA:2067:G:H4'  | 24:DA:2068:U:OP2   | 1.94                     | 0.66              |
| 24:DA:2838:G:H1'  | 37:DN:45:ARG:NH2   | 2.08                     | 0.66              |
| 29:DF:147:ARG:O   | 29:DF:148:VAL:HG22 | 1.95                     | 0.66              |
| 39:DP:86:LYS:HA   | 39:DP:86:LYS:HZ2   | 1.61                     | 0.66              |
| 41:DR:9:GLY:H     | 41:DR:10:LYS:HD2   | 1.59                     | 0.66              |
| 4:AE:76:ASN:HB3   | 4:AE:81:GLN:HG2    | 1.78                     | 0.66              |
| 7:AH:99:GLY:HA3   | 7:AH:129:ALA:HB2   | 1.77                     | 0.66              |
| 8:AI:29:ILE:HA    | 8:AI:64:ILE:O      | 1.96                     | 0.66              |
| 53:B3:15:LYS:HE2  | 53:B3:19:GLY:HA2   | 1.77                     | 0.66              |
| 24:BA:2725:A:HO2' | 24:BA:2726:A:H2'   | 1.60                     | 0.66              |
| 25:BB:90:C:C6     | 25:BB:90:C:H5''    | 2.31                     | 0.66              |
| 31:BH:1:MET:HG2   | 31:BH:23:ALA:HA    | 1.77                     | 0.66              |
| 39:BP:50:ARG:HD2  | 39:BP:51:ASN:N     | 2.10                     | 0.66              |
| 42:BS:20:VAL:HG11 | 42:BS:44:ALA:HA    | 1.78                     | 0.66              |
| 55:CA:108:G:H5'   | 55:CA:109:A:H5''   | 1.77                     | 0.66              |
| 55:CA:682:G:H2'   | 55:CA:683:G:H8     | 1.61                     | 0.66              |
| 6:CG:115:MET:CE   | 6:CG:119:LEU:HB3   | 2.25                     | 0.66              |
| 24:DA:1060:U:C4'  | 24:DA:1061:U:H5''  | 2.26                     | 0.66              |
| 24:DA:1915:U:H2'  | 24:DA:1916:A:H8    | 1.57                     | 0.66              |
| 24:DA:2590:A:H2'  | 24:DA:2591:C:C6    | 2.31                     | 0.66              |
| 24:DA:2798:U:H5'  | 24:DA:2800:A:C6    | 2.31                     | 0.66              |
| 24:DA:2852:G:H2'  | 24:DA:2853:C:O4'   | 1.95                     | 0.66              |
| 24:DA:628:G:H2'   | 24:DA:629:G:C8     | 2.30                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DD:178:VAL:HG12 | 27:DD:179:ARG:HG3  | 1.76                     | 0.66              |
| 24:DA:995:C:O2     | 33:DJ:3:THR:HG23   | 1.96                     | 0.66              |
| 40:DQ:69:ARG:HB2   | 40:DQ:69:ARG:NH2   | 2.11                     | 0.66              |
| 21:AA:1082:A:C6    | 21:AA:1083:U:C4    | 2.84                     | 0.66              |
| 17:AR:40:PRO:HB2   | 17:AR:42:ARG:HG2   | 1.78                     | 0.66              |
| 24:BA:2388:A:C2'   | 24:BA:2389:G:H5'   | 2.26                     | 0.66              |
| 32:BI:33:ASN:HD22  | 32:BI:64:ARG:HH22  | 1.41                     | 0.66              |
| 35:BL:81:ASP:O     | 35:BL:82:LEU:HB3   | 1.96                     | 0.66              |
| 45:BV:25:LYS:HD3   | 45:BV:43:ASP:HA    | 1.78                     | 0.66              |
| 55:CA:892:A:H2'    | 55:CA:893:C:C6     | 2.31                     | 0.66              |
| 24:DA:1079:C:H41   | 24:DA:1088:A:H5''  | 1.61                     | 0.66              |
| 24:DA:2091:C:OP2   | 24:DA:2092:U:H3'   | 1.96                     | 0.66              |
| 24:DA:2847:U:H2'   | 24:DA:2848:G:H5'   | 1.78                     | 0.66              |
| 24:DA:614:A:O2'    | 24:DA:615:U:H5'    | 1.96                     | 0.66              |
| 24:DA:668:A:H2'    | 24:DA:670:A:N6     | 2.08                     | 0.66              |
| 24:DA:974:G:H1'    | 24:DA:975:A:C8     | 2.31                     | 0.66              |
| 26:DC:82:TYR:O     | 26:DC:84:PRO:HD3   | 1.96                     | 0.66              |
| 28:DE:130:LYS:H    | 28:DE:160:ALA:HB2  | 1.61                     | 0.66              |
| 34:DK:13:ASN:HD21  | 34:DK:97:THR:N     | 1.93                     | 0.66              |
| 34:DK:13:ASN:H     | 34:DK:13:ASN:HD22  | 1.44                     | 0.66              |
| 45:DV:44:HIS:NE2   | 45:DV:85:LYS:HB2   | 2.11                     | 0.66              |
| 21:AA:950:U:H2'    | 21:AA:951:G:H8     | 1.61                     | 0.65              |
| 1:AB:22:TRP:CA     | 1:AB:189:ASN:HA    | 2.24                     | 0.65              |
| 24:BA:103:A:H2'    | 24:BA:104:A:C8     | 2.30                     | 0.65              |
| 24:BA:1071:G:C8    | 24:BA:1089:A:N6    | 2.65                     | 0.65              |
| 24:BA:1206:G:H2'   | 24:BA:1207:C:C6    | 2.30                     | 0.65              |
| 24:BA:2146:C:H4'   | 24:BA:2147:A:O5'   | 1.95                     | 0.65              |
| 26:BC:156:SER:O    | 26:BC:194:VAL:HG11 | 1.96                     | 0.65              |
| 30:BG:83:THR:HA    | 30:BG:84:LYS:NZ    | 2.11                     | 0.65              |
| 30:BG:96:ALA:O     | 30:BG:97:VAL:HB    | 1.96                     | 0.65              |
| 40:BQ:91:ARG:HB3   | 40:BQ:93:ILE:HG22  | 1.76                     | 0.65              |
| 55:CA:120:A:H2'    | 55:CA:121:U:H5''   | 1.78                     | 0.65              |
| 24:DA:1008:A:H4'   | 24:DA:1009:A:OP1   | 1.95                     | 0.65              |
| 24:DA:1063:G:H2'   | 24:DA:1064:C:C6    | 2.31                     | 0.65              |
| 24:DA:1252:G:H5''  | 59:DA:3287:HOH:O   | 1.95                     | 0.65              |
| 24:DA:1437:C:H2'   | 24:DA:1438:U:C6    | 2.32                     | 0.65              |
| 24:DA:1730:C:O2'   | 24:DA:1731:G:H5''  | 1.96                     | 0.65              |
| 24:DA:228:C:H5'    | 24:DA:229:C:C5     | 2.31                     | 0.65              |
| 41:DR:62:GLU:HB3   | 41:DR:97:LYS:HB3   | 1.78                     | 0.65              |
| 43:DT:67:VAL:HG23  | 43:DT:75:GLY:O     | 1.97                     | 0.65              |
| 24:DA:64:A:O2'     | 43:DT:69:ARG:HG2   | 1.96                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:171:A:H2'   | 21:AA:172:A:C8    | 2.31                     | 0.65              |
| 21:AA:792:A:H1'   | 21:AA:794:A:N7    | 2.11                     | 0.65              |
| 4:AE:59:ILE:O     | 4:AE:62:ALA:HB3   | 1.96                     | 0.65              |
| 7:AH:88:LYS:HG3   | 7:AH:89:ASP:H     | 1.61                     | 0.65              |
| 24:BA:1616:A:H4'  | 24:BA:1617:C:OP2  | 1.96                     | 0.65              |
| 24:BA:1957:C:H5'' | 24:BA:1958:C:OP2  | 1.96                     | 0.65              |
| 24:BA:1997:C:OP2  | 27:BD:129:THR:OG1 | 2.13                     | 0.65              |
| 24:BA:2599:G:N7   | 26:BC:234:GLY:HA2 | 2.11                     | 0.65              |
| 24:BA:2793:C:H2'  | 24:BA:2794:C:C6   | 2.30                     | 0.65              |
| 25:BB:29:A:H2'    | 25:BB:30:C:C6     | 2.31                     | 0.65              |
| 25:BB:64:G:H2'    | 25:BB:65:U:C6     | 2.32                     | 0.65              |
| 27:BD:114:LYS:HE3 | 27:BD:114:LYS:N   | 2.12                     | 0.65              |
| 24:BA:675:A:H4'   | 28:BE:62:GLN:NE2  | 2.11                     | 0.65              |
| 32:BI:126:ARG:HA  | 32:BI:129:GLU:HB2 | 1.79                     | 0.65              |
| 33:BJ:16:TYR:HA   | 33:BJ:138:GLN:O   | 1.95                     | 0.65              |
| 34:BK:28:SER:O    | 34:BK:29:HIS:HB2  | 1.95                     | 0.65              |
| 40:BQ:82:LEU:CD2  | 40:BQ:112:ALA:HB2 | 2.26                     | 0.65              |
| 55:CA:52:C:C4     | 55:CA:360:G:N2    | 2.64                     | 0.65              |
| 55:CA:721:G:H4'   | 55:CA:722:G:C5'   | 2.25                     | 0.65              |
| 8:CI:125:GLN:NE2  | 55:CA:1232:U:H5'' | 2.12                     | 0.65              |
| 9:CJ:37:ARG:HB3   | 9:CJ:74:VAL:O     | 1.96                     | 0.65              |
| 9:CJ:9:ARG:HH21   | 9:CJ:71:LEU:CD2   | 2.08                     | 0.65              |
| 12:CM:2:ARG:HD2   | 12:CM:8:ILE:HG12  | 1.76                     | 0.65              |
| 24:DA:1236:G:O2'  | 24:DA:1237:A:H8   | 1.79                     | 0.65              |
| 24:DA:2037:A:O2'  | 24:DA:2038:G:O4'  | 2.13                     | 0.65              |
| 24:DA:2860:A:H8   | 24:DA:2860:A:O5'  | 1.79                     | 0.65              |
| 24:DA:677:A:O2'   | 24:DA:2071:A:H5'  | 1.97                     | 0.65              |
| 24:DA:752:A:O2'   | 24:DA:753:A:P     | 2.54                     | 0.65              |
| 56:DB:98:G:H1     | 45:DV:14:LYS:HB2  | 1.60                     | 0.65              |
| 12:AM:101:THR:OG1 | 21:AA:1225:A:H5'' | 1.96                     | 0.65              |
| 1:AB:143:LEU:HD12 | 1:AB:147:LEU:HD12 | 1.77                     | 0.65              |
| 4:AE:37:VAL:HG11  | 4:AE:113:VAL:HA   | 1.77                     | 0.65              |
| 4:AE:155:LYS:HB3  | 7:AH:64:TYR:C     | 2.16                     | 0.65              |
| 24:BA:1566:A:O2'  | 24:BA:1567:G:H5'  | 1.97                     | 0.65              |
| 24:BA:1625:C:H5'' | 24:BA:1626:A:OP2  | 1.96                     | 0.65              |
| 24:BA:709:U:H2'   | 24:BA:710:U:H6    | 1.56                     | 0.65              |
| 33:BJ:43:GLU:O    | 33:BJ:45:THR:N    | 2.29                     | 0.65              |
| 37:BN:37:THR:HA   | 37:BN:110:MET:SD  | 2.36                     | 0.65              |
| 40:BQ:63:ARG:HH12 | 40:BQ:96:ASP:CB   | 2.08                     | 0.65              |
| 24:BA:994:C:O2    | 41:BR:10:LYS:NZ   | 2.29                     | 0.65              |
| 55:CA:1051:C:O2'  | 55:CA:1052:U:C6   | 2.48                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:CA:1319:A:C6   | 55:CA:1323:G:C4    | 2.85                     | 0.65              |
| 55:CA:818:G:O2'   | 55:CA:819:A:H5''   | 1.96                     | 0.65              |
| 3:CD:171:GLU:HG2  | 3:CD:180:THR:HB    | 1.76                     | 0.65              |
| 4:CE:148:SER:O    | 4:CE:152:VAL:HG23  | 1.95                     | 0.65              |
| 4:CE:14:LEU:HG    | 4:CE:15:ILE:N      | 2.10                     | 0.65              |
| 5:CF:70:VAL:O     | 5:CF:73:GLU:HB2    | 1.96                     | 0.65              |
| 7:CH:88:LYS:HG3   | 7:CH:89:ASP:OD1    | 1.96                     | 0.65              |
| 12:CM:69:ARG:HA   | 12:CM:72:ILE:HG22  | 1.78                     | 0.65              |
| 24:DA:1270:C:N4   | 24:DA:1648:U:O4    | 2.29                     | 0.65              |
| 55:CA:1494:G:H4'  | 24:DA:1913:A:N7    | 2.12                     | 0.65              |
| 24:DA:1935:G:H1'  | 24:DA:1964:G:C2    | 2.31                     | 0.65              |
| 24:DA:2264:C:C2   | 24:DA:2277:G:N2    | 2.63                     | 0.65              |
| 24:DA:2751:G:O2'  | 24:DA:2752:C:H5'   | 1.96                     | 0.65              |
| 24:DA:27:G:H1'    | 24:DA:513:A:N6     | 2.11                     | 0.65              |
| 24:DA:445:C:H2'   | 24:DA:446:G:C8     | 2.31                     | 0.65              |
| 24:DA:533:G:H2'   | 24:DA:534:U:C6     | 2.31                     | 0.65              |
| 24:DA:975:A:H2'   | 24:DA:976:G:H8     | 1.62                     | 0.65              |
| 27:DD:117:GLY:HA2 | 27:DD:164:GLN:OE1  | 1.96                     | 0.65              |
| 27:DD:38:LYS:HB3  | 27:DD:38:LYS:HZ3   | 1.60                     | 0.65              |
| 21:AA:1003:G:N2   | 21:AA:1005:A:H5'   | 2.11                     | 0.65              |
| 21:AA:339:C:N3    | 21:AA:351:G:O6     | 2.29                     | 0.65              |
| 22:AX:30:G:C4     | 22:AX:31:A:C8      | 2.85                     | 0.65              |
| 24:BA:1139:G:O2'  | 24:BA:1140:C:H5'   | 1.96                     | 0.65              |
| 24:BA:1253:A:C3'  | 24:BA:1254:A:H5'   | 2.27                     | 0.65              |
| 24:BA:532:A:C8    | 24:BA:2021:C:C6    | 2.85                     | 0.65              |
| 24:BA:763:G:N7    | 24:BA:765:C:C5     | 2.65                     | 0.65              |
| 26:BC:106:PRO:HA  | 26:BC:141:HIS:CE1  | 2.30                     | 0.65              |
| 26:BC:245:THR:OG1 | 26:BC:249:VAL:HB   | 1.96                     | 0.65              |
| 28:BE:110:SER:O   | 28:BE:113:VAL:HG12 | 1.96                     | 0.65              |
| 33:BJ:25:LEU:HD22 | 33:BJ:25:LEU:C     | 2.16                     | 0.65              |
| 39:BP:33:GLU:CB   | 39:BP:38:ARG:HH11  | 2.09                     | 0.65              |
| 40:BQ:4:LYS:NZ    | 40:BQ:7:VAL:HG13   | 2.12                     | 0.65              |
| 55:CA:390:U:O2'   | 55:CA:391:G:H5'    | 1.97                     | 0.65              |
| 55:CA:865:A:C2    | 55:CA:918:A:H4'    | 2.31                     | 0.65              |
| 2:CC:110:LEU:HD11 | 2:CC:203:LYS:NZ    | 2.11                     | 0.65              |
| 2:CC:120:THR:O    | 2:CC:120:THR:HG22  | 1.97                     | 0.65              |
| 24:DA:1062:G:OP1  | 24:DA:1070:A:H4'   | 1.97                     | 0.65              |
| 24:DA:13:A:O2'    | 24:DA:15:G:N7      | 2.29                     | 0.65              |
| 24:DA:140:C:H5'   | 24:DA:141:G:H21    | 1.61                     | 0.65              |
| 24:DA:1496:A:H2'  | 24:DA:1498:C:N4    | 2.12                     | 0.65              |
| 24:DA:1832:C:N4   | 24:DA:1833:C:C4    | 2.64                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:2308:G:O6    | 24:DA:2311:A:C6    | 2.49                     | 0.65              |
| 24:DA:704:G:H1'    | 24:DA:727:A:N6     | 2.12                     | 0.65              |
| 24:DA:75:G:H4'     | 48:DY:48:ARG:NH2   | 2.12                     | 0.65              |
| 24:DA:852:U:H2'    | 24:DA:853:C:C6     | 2.30                     | 0.65              |
| 35:DL:142:ILE:HG22 | 35:DL:144:GLU:H    | 1.61                     | 0.65              |
| 44:DU:14:THR:HB    | 44:DU:68:ASN:HB3   | 1.78                     | 0.65              |
| 44:DU:82:VAL:H     | 44:DU:96:LYS:HZ2   | 1.44                     | 0.65              |
| 48:DY:19:LEU:HA    | 48:DY:22:LEU:HB2   | 1.77                     | 0.65              |
| 21:AA:1084:G:OP1   | 21:AA:1086:U:H5''  | 1.97                     | 0.65              |
| 21:AA:338:A:N1     | 21:AA:351:G:C6     | 2.65                     | 0.65              |
| 21:AA:582:C:C2     | 21:AA:583:A:C8     | 2.85                     | 0.65              |
| 3:AD:117:VAL:HA    | 3:AD:122:ILE:HD11  | 1.79                     | 0.65              |
| 4:AE:13:LYS:HG3    | 4:AE:112:ALA:HB1   | 1.79                     | 0.65              |
| 4:AE:90:GLY:O      | 4:AE:129:SER:HB3   | 1.97                     | 0.65              |
| 7:AH:87:ARG:HG3    | 7:AH:90:GLU:OE2    | 1.96                     | 0.65              |
| 8:AI:3:ASN:CG      | 8:AI:4:GLN:H       | 2.00                     | 0.65              |
| 10:AK:85:VAL:O     | 10:AK:112:VAL:HG22 | 1.96                     | 0.65              |
| 12:AM:109:LYS:NZ   | 21:AA:1227:A:H5'   | 2.11                     | 0.65              |
| 16:AQ:76:ARG:HG2   | 16:AQ:77:VAL:N     | 2.12                     | 0.65              |
| 24:BA:2210:U:H4'   | 24:BA:2211:A:H5'   | 1.78                     | 0.65              |
| 24:BA:2868:A:H2'   | 24:BA:2869:G:H8    | 1.56                     | 0.65              |
| 24:BA:491:G:C2     | 24:BA:492:A:H1'    | 2.31                     | 0.65              |
| 24:BA:860:U:C5'    | 24:BA:860:U:H6     | 2.08                     | 0.65              |
| 26:BC:109:LEU:HD23 | 26:BC:110:LYS:N    | 2.12                     | 0.65              |
| 42:BS:63:GLY:O     | 42:BS:64:ALA:HB3   | 1.96                     | 0.65              |
| 46:BW:9:THR:HG23   | 46:BW:10:ARG:CD    | 2.24                     | 0.65              |
| 55:CA:1228:C:O2'   | 55:CA:1229:A:H5'   | 1.95                     | 0.65              |
| 55:CA:632:U:H3'    | 55:CA:633:G:H5'    | 1.78                     | 0.65              |
| 55:CA:662:U:H2'    | 55:CA:663:A:C8     | 2.32                     | 0.65              |
| 24:DA:1050:A:O2'   | 24:DA:1051:G:H5'   | 1.96                     | 0.65              |
| 24:DA:2184:A:H2'   | 24:DA:2185:U:C6    | 2.31                     | 0.65              |
| 24:DA:2210:U:H4'   | 24:DA:2211:A:O5'   | 1.97                     | 0.65              |
| 24:DA:417:C:H2'    | 24:DA:418:C:C6     | 2.32                     | 0.65              |
| 24:DA:634:C:H2'    | 24:DA:635:C:C6     | 2.31                     | 0.65              |
| 21:AA:130:A:O2'    | 21:AA:263:A:O2'    | 2.13                     | 0.65              |
| 21:AA:306:A:H2'    | 21:AA:307:C:H6     | 1.61                     | 0.65              |
| 21:AA:653:U:O2'    | 21:AA:654:G:H5'    | 1.96                     | 0.65              |
| 21:AA:984:C:O2'    | 21:AA:985:C:C6     | 2.44                     | 0.65              |
| 6:AG:26:VAL:HG12   | 6:AG:42:VAL:HG21   | 1.78                     | 0.65              |
| 16:AQ:11:VAL:HB    | 16:AQ:55:GLY:H     | 1.60                     | 0.65              |
| 37:BN:24:MET:HG2   | 37:BN:44:LEU:CD2   | 2.26                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:BW:29:SER:HA   | 46:BW:63:ASP:HB3   | 1.77                     | 0.65              |
| 55:CA:109:A:N6    | 55:CA:324:G:H1'    | 2.12                     | 0.65              |
| 1:CB:212:TYR:O    | 1:CB:216:VAL:HG23  | 1.96                     | 0.65              |
| 4:CE:55:VAL:N     | 4:CE:56:PRO:HD2    | 2.11                     | 0.65              |
| 24:DA:1079:C:N4   | 24:DA:1088:A:N3    | 2.45                     | 0.65              |
| 24:DA:1558:C:H1'  | 24:DA:1560:G:N7    | 2.12                     | 0.65              |
| 24:DA:454:A:H4'   | 24:DA:455:C:OP2    | 1.95                     | 0.65              |
| 24:DA:459:U:O2'   | 24:DA:460:A:H5'    | 1.96                     | 0.65              |
| 24:DA:53:A:H2'    | 24:DA:54:G:O4'     | 1.97                     | 0.65              |
| 24:DA:740:C:H5'   | 24:DA:1784:A:C3'   | 2.19                     | 0.65              |
| 56:DB:46:A:H2'    | 56:DB:47:C:H6      | 1.62                     | 0.65              |
| 31:DH:84:ALA:H    | 31:DH:148:ALA:HA   | 1.61                     | 0.65              |
| 33:DJ:75:TYR:CD1  | 33:DJ:84:ILE:HD11  | 2.32                     | 0.65              |
| 34:DK:39:ILE:HD11 | 34:DK:62:VAL:HG23  | 1.79                     | 0.65              |
| 21:AA:9:G:C6      | 21:AA:26:A:N6      | 2.65                     | 0.65              |
| 12:AM:39:ALA:HB3  | 12:AM:42:VAL:HG13  | 1.78                     | 0.65              |
| 16:AQ:58:VAL:HG22 | 16:AQ:59:GLU:N     | 2.12                     | 0.65              |
| 24:BA:1027:A:N3   | 24:BA:1027:A:H2'   | 2.11                     | 0.65              |
| 40:BQ:48:ASP:O    | 40:BQ:51:GLN:N     | 2.30                     | 0.65              |
| 55:CA:1101:A:H4'  | 55:CA:1102:A:O5'   | 1.96                     | 0.65              |
| 55:CA:570:G:H2'   | 55:CA:571:U:C6     | 2.32                     | 0.65              |
| 1:CB:25:LYS:HD2   | 1:CB:25:LYS:H      | 1.61                     | 0.65              |
| 11:CL:65:TYR:HD1  | 11:CL:66:ILE:N     | 1.94                     | 0.65              |
| 15:CP:68:SER:HB3  | 15:CP:71:VAL:HG12  | 1.79                     | 0.65              |
| 5:CF:86:ARG:NH1   | 17:CR:63:TYR:HB3   | 2.11                     | 0.65              |
| 24:DA:1069:A:N6   | 24:DA:1073:A:H5''  | 2.12                     | 0.65              |
| 24:DA:1078:U:H4'  | 24:DA:1079:C:O5'   | 1.97                     | 0.65              |
| 24:DA:121:G:C2    | 24:DA:131:A:C5     | 2.85                     | 0.65              |
| 24:DA:1334:G:O2'  | 24:DA:1335:C:H5'   | 1.96                     | 0.65              |
| 24:DA:2459:A:O2'  | 24:DA:2460:U:H5'   | 1.96                     | 0.65              |
| 24:DA:2585:U:O2'  | 24:DA:2586:U:H5'   | 1.97                     | 0.65              |
| 24:DA:734:A:C4    | 24:DA:735:A:C8     | 2.84                     | 0.65              |
| 21:AA:1239:A:H1'  | 21:AA:1241:G:C4    | 2.32                     | 0.65              |
| 21:AA:1384:C:H2'  | 21:AA:1385:G:H8    | 1.61                     | 0.65              |
| 21:AA:1417:G:N2   | 21:AA:1482:G:H2'   | 2.11                     | 0.65              |
| 2:AC:119:ILE:HG21 | 2:AC:197:VAL:HG11  | 1.77                     | 0.65              |
| 3:AD:103:ARG:O    | 3:AD:167:PRO:HG2   | 1.96                     | 0.65              |
| 54:B4:9:LYS:C     | 54:B4:10:LEU:HD23  | 2.17                     | 0.65              |
| 24:BA:479:A:O2'   | 24:BA:481:G:H5'    | 1.96                     | 0.65              |
| 25:BB:78:A:H2'    | 25:BB:79:G:O4'     | 1.96                     | 0.65              |
| 34:BK:112:PHE:O   | 34:BK:115:ILE:HG22 | 1.97                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BM:96:ILE:C    | 36:BM:96:ILE:HD12 | 2.17                     | 0.65              |
| 39:BP:56:SER:O    | 39:BP:75:THR:HG23 | 1.96                     | 0.65              |
| 55:CA:1504:G:H4'  | 55:CA:1505:G:H5'  | 1.77                     | 0.65              |
| 1:CB:79:VAL:HG11  | 1:CB:92:ASN:HB3   | 1.78                     | 0.65              |
| 4:CE:38:VAL:HG12  | 4:CE:39:GLY:N     | 2.10                     | 0.65              |
| 54:D4:36:ARG:HG2  | 54:D4:37:GLN:N    | 2.11                     | 0.65              |
| 24:DA:1298:C:H2'  | 24:DA:1299:G:O4'  | 1.97                     | 0.65              |
| 24:DA:471:A:H5''  | 28:DE:79:ARG:HH12 | 1.61                     | 0.65              |
| 26:DC:2:VAL:O     | 26:DC:3:VAL:HB    | 1.97                     | 0.65              |
| 40:DQ:10:ARG:HA   | 40:DQ:13:HIS:HB2  | 1.79                     | 0.65              |
| 21:AA:1076:U:H2'  | 21:AA:1077:G:C8   | 2.31                     | 0.65              |
| 21:AA:1125:U:O2'  | 21:AA:1126:U:O5'  | 2.13                     | 0.65              |
| 24:BA:2021:C:P    | 50:B0:8:THR:HG21  | 2.36                     | 0.65              |
| 24:BA:1373:A:H2'  | 24:BA:1374:G:O4'  | 1.96                     | 0.65              |
| 24:BA:1427:A:H4'  | 24:BA:1428:C:O5'  | 1.96                     | 0.65              |
| 24:BA:1842:G:H2'  | 24:BA:1843:C:C6   | 2.32                     | 0.65              |
| 24:BA:229:C:H2'   | 24:BA:230:G:O4'   | 1.97                     | 0.65              |
| 24:BA:2483:C:H2'  | 24:BA:2484:G:O4'  | 1.95                     | 0.65              |
| 24:BA:436:C:HO2'  | 24:BA:437:U:H6    | 1.45                     | 0.65              |
| 24:BA:540:C:O2'   | 24:BA:541:A:H5'   | 1.97                     | 0.65              |
| 39:BP:37:LYS:HD3  | 39:BP:37:LYS:N    | 2.11                     | 0.65              |
| 40:BQ:68:ALA:HB1  | 40:BQ:73:ILE:HG23 | 1.77                     | 0.65              |
| 40:BQ:91:ARG:HD3  | 41:BR:11:GLN:CG   | 2.26                     | 0.65              |
| 43:BT:38:ALA:HB1  | 43:BT:43:ILE:HG22 | 1.79                     | 0.65              |
| 24:BA:2364:C:H4'  | 46:BW:55:ASP:OD1  | 1.97                     | 0.65              |
| 55:CA:25:C:H2'    | 55:CA:26:A:C8     | 2.32                     | 0.65              |
| 7:CH:39:LEU:HB2   | 7:CH:45:ILE:HD11  | 1.78                     | 0.65              |
| 18:CS:52:ASN:HD21 | 18:CS:55:GLN:H    | 1.44                     | 0.65              |
| 22:CX:34:G:H2'    | 22:CX:35:A:C8     | 2.32                     | 0.65              |
| 24:DA:1328:A:H2'  | 24:DA:1330:C:C5   | 2.31                     | 0.65              |
| 24:DA:1386:C:O2'  | 24:DA:1387:A:C8   | 2.50                     | 0.65              |
| 24:DA:1555:G:N2   | 24:DA:1556:C:C2   | 2.65                     | 0.65              |
| 24:DA:1608:A:C8   | 24:DA:1611:C:N4   | 2.65                     | 0.65              |
| 24:DA:1734:G:HO2' | 24:DA:1735:A:H8   | 1.43                     | 0.65              |
| 24:DA:2895:G:O2'  | 24:DA:2896:C:H6   | 1.79                     | 0.65              |
| 56:DB:115:A:H2'   | 56:DB:116:G:C8    | 2.32                     | 0.65              |
| 27:DD:29:VAL:HB   | 27:DD:98:VAL:CG1  | 2.26                     | 0.65              |
| 33:DJ:20:ALA:HA   | 33:DJ:23:LYS:HG3  | 1.79                     | 0.65              |
| 33:DJ:30:THR:HG23 | 33:DJ:31:GLU:N    | 2.12                     | 0.65              |
| 40:DQ:24:TYR:O    | 40:DQ:27:ARG:HB3  | 1.97                     | 0.65              |
| 21:AA:1225:A:N3   | 21:AA:1225:A:H2'  | 2.11                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:1299:A:O2'   | 21:AA:1300:G:H4'   | 1.97                     | 0.65              |
| 8:AI:122:ARG:CZ    | 21:AA:1343:G:H1'   | 2.27                     | 0.65              |
| 21:AA:17:U:H2'     | 21:AA:18:C:C6      | 2.32                     | 0.65              |
| 21:AA:451:A:H1'    | 21:AA:452:A:N7     | 2.12                     | 0.65              |
| 4:AE:81:GLN:HG2    | 4:AE:149:PRO:CG    | 2.17                     | 0.65              |
| 8:AI:129:ARG:NH2   | 21:AA:966:G:N2     | 2.41                     | 0.65              |
| 54:B4:9:LYS:H      | 54:B4:9:LYS:CD     | 2.10                     | 0.65              |
| 24:BA:1422:G:C4    | 24:BA:1423:G:C8    | 2.85                     | 0.65              |
| 24:BA:2629:U:O2'   | 24:BA:2630:G:OP2   | 2.15                     | 0.65              |
| 24:BA:553:G:H2'    | 24:BA:554:U:O4'    | 1.96                     | 0.65              |
| 24:BA:653:U:OP1    | 24:BA:653:U:H4'    | 1.96                     | 0.65              |
| 34:BK:19:VAL:HG22  | 34:BK:41:ILE:HG13  | 1.78                     | 0.65              |
| 2:CC:198:LYS:HE2   | 55:CA:1058:G:OP1   | 1.97                     | 0.65              |
| 55:CA:1311:A:H2'   | 55:CA:1312:G:O4'   | 1.97                     | 0.65              |
| 55:CA:765:G:C5     | 55:CA:812:G:C6     | 2.85                     | 0.65              |
| 55:CA:93:U:H2'     | 55:CA:95:C:H5      | 1.62                     | 0.65              |
| 7:CH:104:SER:O     | 7:CH:122:GLY:HA3   | 1.97                     | 0.65              |
| 20:CU:15:LEU:HD12  | 20:CU:15:LEU:O     | 1.97                     | 0.65              |
| 24:DA:515:A:H2     | 24:DA:1260:A:N3    | 1.95                     | 0.65              |
| 24:DA:1277:G:O2'   | 24:DA:1278:C:O4'   | 2.14                     | 0.65              |
| 24:DA:1312:U:HO2'  | 24:DA:1314:C:N4    | 1.95                     | 0.65              |
| 24:DA:1400:U:H2'   | 24:DA:1401:G:O4'   | 1.96                     | 0.65              |
| 24:DA:1421:G:H8    | 24:DA:1421:G:OP2   | 1.80                     | 0.65              |
| 24:DA:1683:U:O2'   | 24:DA:1684:G:H8    | 1.80                     | 0.65              |
| 24:DA:1787:A:C2    | 24:DA:1788:C:C4    | 2.85                     | 0.65              |
| 24:DA:2260:C:O2'   | 24:DA:2261:C:C6    | 2.50                     | 0.65              |
| 24:DA:2061:G:C8    | 24:DA:2501:C:H4'   | 2.32                     | 0.65              |
| 24:DA:2742:G:OP1   | 54:D4:36:ARG:HD3   | 1.97                     | 0.65              |
| 24:DA:303:G:O2'    | 24:DA:304:U:O4'    | 2.12                     | 0.65              |
| 24:DA:810:U:O4     | 35:DL:30:THR:HG22  | 1.97                     | 0.65              |
| 28:DE:105:LEU:HD12 | 28:DE:200:LEU:HD11 | 1.79                     | 0.65              |
| 34:DK:54:LYS:H     | 34:DK:54:LYS:HD2   | 1.61                     | 0.65              |
| 38:DO:17:LYS:HE3   | 38:DO:17:LYS:O     | 1.97                     | 0.65              |
| 21:AA:1295:U:H2'   | 21:AA:1296:C:H6    | 1.61                     | 0.64              |
| 4:AE:17:VAL:HG23   | 4:AE:33:THR:O      | 1.97                     | 0.64              |
| 16:AQ:11:VAL:HG12  | 16:AQ:12:VAL:N     | 2.12                     | 0.64              |
| 24:BA:1125:G:C6    | 24:BA:1126:A:N6    | 2.65                     | 0.64              |
| 24:BA:1496:A:H2'   | 24:BA:1498:C:N4    | 2.12                     | 0.64              |
| 24:BA:169:G:H2'    | 24:BA:170:U:H6     | 1.61                     | 0.64              |
| 24:BA:2020:A:C2    | 24:BA:2022:U:O4'   | 2.50                     | 0.64              |
| 24:BA:2543:G:H2'   | 24:BA:2544:G:C8    | 2.32                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:9:G:C6       | 24:BA:2629:U:C6    | 2.85                     | 0.64              |
| 24:BA:2741:A:H2'   | 24:BA:2742:G:O4'   | 1.95                     | 0.64              |
| 24:BA:541:A:C2     | 24:BA:553:G:C2     | 2.85                     | 0.64              |
| 24:BA:842:U:O4     | 59:BA:3593:HOH:O   | 2.10                     | 0.64              |
| 35:BL:14:LYS:HG3   | 35:BL:15:ALA:N     | 2.12                     | 0.64              |
| 15:CP:78:VAL:O     | 15:CP:80:LYS:HG3   | 1.97                     | 0.64              |
| 24:DA:18:U:H2'     | 24:DA:19:A:O4'     | 1.97                     | 0.64              |
| 24:DA:243:U:O2'    | 24:DA:244:A:H5'    | 1.98                     | 0.64              |
| 24:DA:752:A:O2'    | 24:DA:753:A:OP2    | 2.15                     | 0.64              |
| 27:DD:30:GLU:HG2   | 27:DD:185:ASN:ND2  | 2.12                     | 0.64              |
| 35:DL:47:ARG:HG2   | 35:DL:47:ARG:NH2   | 2.11                     | 0.64              |
| 36:DM:108:VAL:HG21 | 36:DM:112:LEU:HB3  | 1.78                     | 0.64              |
| 39:DP:5:LYS:HE2    | 39:DP:9:GLN:NE2    | 2.12                     | 0.64              |
| 40:DQ:4:LYS:HE3    | 40:DQ:7:VAL:HG13   | 1.77                     | 0.64              |
| 48:DY:39:GLN:O     | 48:DY:42:LEU:HB2   | 1.97                     | 0.64              |
| 21:AA:1124:G:H3'   | 21:AA:1145:A:N6    | 2.11                     | 0.64              |
| 21:AA:41:G:H2'     | 21:AA:42:G:C8      | 2.32                     | 0.64              |
| 2:AC:6:PRO:O       | 2:AC:10:ARG:HG2    | 1.97                     | 0.64              |
| 24:BA:1965:C:H2'   | 24:BA:1966:A:C8    | 2.32                     | 0.64              |
| 24:BA:2799:A:O2'   | 24:BA:2800:A:H4'   | 1.97                     | 0.64              |
| 24:BA:960:A:H2'    | 24:BA:962:G:H5'    | 1.79                     | 0.64              |
| 27:BD:101:PHE:CE2  | 27:BD:203:VAL:HG22 | 2.31                     | 0.64              |
| 33:BJ:88:THR:CG2   | 33:BJ:90:GLU:HG3   | 2.27                     | 0.64              |
| 41:BR:14:VAL:HG11  | 41:BR:98:ILE:CD1   | 2.28                     | 0.64              |
| 55:CA:1504:G:C3'   | 55:CA:1505:G:H5'   | 2.27                     | 0.64              |
| 2:CC:59:PRO:HG2    | 2:CC:62:SER:HB3    | 1.79                     | 0.64              |
| 7:CH:9:MET:SD      | 7:CH:32:LYS:HG3    | 2.36                     | 0.64              |
| 24:DA:2190:G:H3'   | 24:DA:2191:A:O4'   | 1.97                     | 0.64              |
| 24:DA:2226:C:H2'   | 24:DA:2227:A:C8    | 2.32                     | 0.64              |
| 24:DA:2519:U:C6    | 24:DA:2542:A:N6    | 2.64                     | 0.64              |
| 24:DA:2788:C:O2    | 24:DA:2809:A:H2    | 1.80                     | 0.64              |
| 24:DA:2895:G:O2'   | 24:DA:2896:C:C6    | 2.50                     | 0.64              |
| 24:DA:75:G:HO2'    | 24:DA:76:C:H6      | 1.42                     | 0.64              |
| 56:DB:74:U:H2'     | 56:DB:75:G:O4'     | 1.97                     | 0.64              |
| 26:DC:224:MET:SD   | 26:DC:229:HIS:HB2  | 2.37                     | 0.64              |
| 24:DA:1695:G:H8    | 26:DC:7:PRO:HB2    | 1.59                     | 0.64              |
| 21:AA:1394:A:HO2'  | 21:AA:1395:C:P     | 2.19                     | 0.64              |
| 3:AD:166:LYS:NZ    | 3:AD:166:LYS:HB3   | 2.11                     | 0.64              |
| 11:AL:78:VAL:O     | 11:AL:102:ASP:HB2  | 1.97                     | 0.64              |
| 19:AT:24:ARG:HG2   | 19:AT:28:ARG:NH1   | 2.12                     | 0.64              |
| 19:AT:80:ALA:O     | 19:AT:84:LYS:HB2   | 1.97                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:1095:A:H2'   | 24:BA:1096:A:C8    | 2.32                     | 0.64              |
| 24:BA:1339:G:N2    | 24:BA:1603:A:H1'   | 2.12                     | 0.64              |
| 24:BA:1408:G:H2'   | 24:BA:1409:U:H6    | 1.61                     | 0.64              |
| 24:BA:1779:U:H5    | 24:BA:1784:A:N7    | 1.95                     | 0.64              |
| 24:BA:1794:A:H2'   | 24:BA:1795:C:C6    | 2.30                     | 0.64              |
| 24:BA:1796:U:H2'   | 24:BA:1797:G:C8    | 2.32                     | 0.64              |
| 24:BA:1805:A:C5    | 24:BA:1806:C:H5    | 2.16                     | 0.64              |
| 25:BB:57:A:C2      | 25:BB:58:A:C4      | 2.85                     | 0.64              |
| 31:BH:82:SER:O     | 31:BH:83:LYS:HB2   | 1.97                     | 0.64              |
| 37:BN:55:ALA:HB1   | 37:BN:80:PHE:N     | 2.13                     | 0.64              |
| 39:BP:24:THR:HG22  | 39:BP:87:ARG:H     | 1.61                     | 0.64              |
| 41:BR:49:ILE:CB    | 41:BR:51:VAL:O     | 2.45                     | 0.64              |
| 24:BA:1187:G:H5''  | 41:BR:83:TYR:CE2   | 2.32                     | 0.64              |
| 43:BT:39:THR:O     | 43:BT:39:THR:HG22  | 1.97                     | 0.64              |
| 55:CA:33:A:H2'     | 55:CA:34:C:C6      | 2.31                     | 0.64              |
| 2:CC:139:ASN:HB3   | 2:CC:142:ARG:NH2   | 2.11                     | 0.64              |
| 11:CL:29:LYS:O     | 11:CL:80:LEU:HD12  | 1.97                     | 0.64              |
| 24:DA:1275:A:H2'   | 24:DA:1275:A:N3    | 2.13                     | 0.64              |
| 24:DA:1782:U:O2'   | 24:DA:1783:A:H5'   | 1.97                     | 0.64              |
| 24:DA:2707:U:H2'   | 24:DA:2708:G:C8    | 2.32                     | 0.64              |
| 24:DA:741:U:H2'    | 24:DA:742:A:H8     | 1.61                     | 0.64              |
| 56:DB:24:G:H1'     | 56:DB:27:C:N4      | 2.12                     | 0.64              |
| 44:DU:58:VAL:HG12  | 44:DU:60:LYS:H     | 1.61                     | 0.64              |
| 1:AB:212:TYR:HA    | 1:AB:215:ALA:HB3   | 1.78                     | 0.64              |
| 1:AB:40:ILE:HD13   | 1:AB:201:GLY:CA    | 2.26                     | 0.64              |
| 5:AF:38:ARG:HG3    | 5:AF:39:LEU:N      | 2.11                     | 0.64              |
| 12:AM:106:ARG:HH11 | 12:AM:106:ARG:HA   | 1.63                     | 0.64              |
| 14:AO:21:THR:HG21  | 21:AA:658:C:H1'    | 1.79                     | 0.64              |
| 19:AT:20:ASN:O     | 19:AT:24:ARG:HB2   | 1.97                     | 0.64              |
| 24:BA:1059:G:H1'   | 32:BI:127:SER:HB2  | 1.77                     | 0.64              |
| 24:BA:1266:G:OP2   | 50:B0:16:ARG:NE    | 2.28                     | 0.64              |
| 24:BA:2484:G:OP1   | 36:BM:44:ARG:HD3   | 1.98                     | 0.64              |
| 24:BA:493:G:H2'    | 24:BA:494:G:O4'    | 1.98                     | 0.64              |
| 26:BC:12:ARG:HG2   | 26:BC:12:ARG:HH11  | 1.61                     | 0.64              |
| 24:BA:2747:G:HO2'  | 30:BG:66:THR:HG22  | 1.60                     | 0.64              |
| 30:BG:85:LYS:HG2   | 30:BG:131:VAL:HG12 | 1.80                     | 0.64              |
| 46:BW:28:GLU:CG    | 46:BW:29:SER:H     | 2.11                     | 0.64              |
| 55:CA:1381:U:O2'   | 55:CA:1382:C:H5'   | 1.96                     | 0.64              |
| 55:CA:275:G:O2'    | 55:CA:276:G:H5'    | 1.98                     | 0.64              |
| 55:CA:695:A:H61    | 55:CA:797:C:H1'    | 1.62                     | 0.64              |
| 3:CD:18:LEU:HB2    | 3:CD:20:LEU:HG     | 1.78                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:CI:18:VAL:HG11  | 8:CI:82:ILE:HA    | 1.80                     | 0.64              |
| 9:CJ:44:THR:HG22  | 9:CJ:45:ARG:H     | 1.61                     | 0.64              |
| 24:DA:1601:G:H2'  | 24:DA:1602:U:O4'  | 1.96                     | 0.64              |
| 24:DA:1835:G:N2   | 24:DA:1836:C:C2   | 2.65                     | 0.64              |
| 24:DA:2543:G:O6   | 24:DA:2765:A:C5   | 2.50                     | 0.64              |
| 24:DA:390:U:O2'   | 24:DA:391:A:C8    | 2.50                     | 0.64              |
| 24:DA:223:A:H2    | 24:DA:407:G:N3    | 1.95                     | 0.64              |
| 24:DA:764:A:N1    | 24:DA:1789:A:O2'  | 2.31                     | 0.64              |
| 56:DB:12:C:H4'    | 56:DB:13:G:OP1    | 1.95                     | 0.64              |
| 21:AA:236:A:H2'   | 21:AA:237:G:H8    | 1.63                     | 0.64              |
| 21:AA:532:A:H2    | 21:AA:1206:G:H21  | 1.46                     | 0.64              |
| 1:AB:183:PHE:CD2  | 1:AB:183:PHE:N    | 2.65                     | 0.64              |
| 3:AD:195:ASN:N    | 3:AD:195:ASN:HD22 | 1.96                     | 0.64              |
| 24:BA:1436:G:N2   | 24:BA:1557:C:C2   | 2.65                     | 0.64              |
| 24:BA:2195:U:H2'  | 24:BA:2196:C:H6   | 1.60                     | 0.64              |
| 24:BA:494:G:H21   | 42:BS:57:ASN:HD21 | 1.44                     | 0.64              |
| 24:BA:672:C:C2    | 24:BA:809:G:N2    | 2.65                     | 0.64              |
| 26:BC:229:HIS:CD2 | 26:BC:246:PRO:HB3 | 2.32                     | 0.64              |
| 28:BE:146:VAL:HA  | 28:BE:185:LYS:O   | 1.96                     | 0.64              |
| 35:BL:93:ASN:ND2  | 35:BL:94:THR:N    | 2.45                     | 0.64              |
| 36:BM:78:LEU:C    | 36:BM:80:VAL:H    | 2.01                     | 0.64              |
| 41:BR:28:ALA:O    | 41:BR:63:VAL:HG21 | 1.98                     | 0.64              |
| 19:CT:22:SER:HB2  | 55:CA:1458:G:H4'  | 1.78                     | 0.64              |
| 55:CA:93:U:C2     | 55:CA:95:C:N4     | 2.65                     | 0.64              |
| 22:CV:39:U:H2'    | 22:CV:40:C:C6     | 2.33                     | 0.64              |
| 24:DA:465:G:H4'   | 52:D2:16:HIS:HD2  | 1.62                     | 0.64              |
| 24:DA:1078:U:H4'  | 24:DA:1079:C:C5'  | 2.28                     | 0.64              |
| 24:DA:572:A:OP1   | 59:DA:3603:HOH:O  | 2.15                     | 0.64              |
| 26:DC:128:THR:CG2 | 26:DC:188:ARG:HB3 | 2.28                     | 0.64              |
| 4:AE:55:VAL:O     | 4:AE:58:ALA:HB3   | 1.98                     | 0.64              |
| 5:AF:11:HIS:HD2   | 5:AF:12:PRO:HD2   | 1.62                     | 0.64              |
| 5:AF:2:ARG:HB3    | 5:AF:92:THR:OG1   | 1.98                     | 0.64              |
| 8:AI:40:ARG:HA    | 8:AI:44:ARG:HB3   | 1.80                     | 0.64              |
| 8:AI:62:LEU:HD12  | 8:AI:64:ILE:HD11  | 1.79                     | 0.64              |
| 17:AR:63:TYR:CE1  | 21:AA:734:G:N2    | 2.62                     | 0.64              |
| 24:BA:2094:A:H2'  | 24:BA:2095:A:H8   | 1.60                     | 0.64              |
| 24:BA:401:A:H2'   | 24:BA:402:A:C8    | 2.33                     | 0.64              |
| 26:BC:43:ASN:HB3  | 26:BC:45:ASN:H    | 1.63                     | 0.64              |
| 24:BA:1131:G:C8   | 33:BJ:77:HIS:CE1  | 2.86                     | 0.64              |
| 42:BS:13:SER:O    | 42:BS:14:ALA:HB2  | 1.98                     | 0.64              |
| 55:CA:1356:G:H2'  | 55:CA:1357:A:H8   | 1.59                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CC:133:MET:HB2  | 2:CC:150:VAL:HG21 | 1.79                     | 0.64              |
| 2:CC:171:ARG:HB3  | 55:CA:1106:G:H5'' | 1.79                     | 0.64              |
| 3:CD:96:ARG:HE    | 3:CD:133:SER:HA   | 1.61                     | 0.64              |
| 4:CE:147:ASN:HD21 | 7:CH:72:GLU:HG3   | 1.61                     | 0.64              |
| 9:CJ:54:SER:HB2   | 55:CA:1060:U:H4'  | 1.80                     | 0.64              |
| 12:CM:2:ARG:HD3   | 12:CM:2:ARG:H     | 1.59                     | 0.64              |
| 7:CH:85:TYR:CE1   | 16:CQ:36:PHE:HE2  | 2.15                     | 0.64              |
| 24:DA:1598:A:H2'  | 24:DA:1599:U:C6   | 2.32                     | 0.64              |
| 24:DA:233:A:O2'   | 24:DA:234:U:H6    | 1.81                     | 0.64              |
| 24:DA:2716:C:O2'  | 24:DA:2717:C:H5'  | 1.97                     | 0.64              |
| 24:DA:1:G:H2'     | 24:DA:2:G:C8      | 2.31                     | 0.64              |
| 29:DF:107:VAL:C   | 29:DF:109:ARG:N   | 2.51                     | 0.64              |
| 31:DH:84:ALA:HA   | 31:DH:89:LYS:O    | 1.96                     | 0.64              |
| 46:DW:49:ASN:ND2  | 46:DW:81:ILE:HG23 | 2.13                     | 0.64              |
| 21:AA:1086:U:O2'  | 21:AA:1087:G:H5'  | 1.98                     | 0.64              |
| 50:B0:10:SER:O    | 50:B0:14:MET:HG3  | 1.97                     | 0.64              |
| 24:BA:250:G:H2'   | 24:BA:251:A:C8    | 2.33                     | 0.64              |
| 24:BA:373:U:OP2   | 24:BA:400:G:N1    | 2.28                     | 0.64              |
| 24:BA:898:C:H2'   | 24:BA:899:A:O4'   | 1.98                     | 0.64              |
| 24:BA:919:U:H6    | 24:BA:919:U:C5'   | 2.11                     | 0.64              |
| 30:BG:73:SER:HA   | 30:BG:76:ILE:CG2  | 2.27                     | 0.64              |
| 32:BI:71:LYS:HG2  | 32:BI:72:THR:H    | 1.62                     | 0.64              |
| 35:BL:7:SER:HB2   | 35:BL:8:PRO:HD2   | 1.80                     | 0.64              |
| 40:BQ:4:LYS:HG3   | 40:BQ:5:ARG:N     | 2.13                     | 0.64              |
| 55:CA:652:U:O2'   | 55:CA:653:U:H6    | 1.81                     | 0.64              |
| 24:DA:1138:G:H2'  | 24:DA:1139:G:O4'  | 1.98                     | 0.64              |
| 24:DA:1141:U:H5'' | 24:DA:1142:A:OP1  | 1.98                     | 0.64              |
| 24:DA:1465:G:H2'  | 24:DA:1466:U:O4'  | 1.98                     | 0.64              |
| 24:DA:1499:C:O2'  | 24:DA:1500:G:H5'  | 1.98                     | 0.64              |
| 24:DA:2093:G:N2   | 24:DA:2094:A:C4   | 2.66                     | 0.64              |
| 24:DA:2148:G:O2'  | 24:DA:2149:U:C6   | 2.51                     | 0.64              |
| 24:DA:2235:G:H2'  | 24:DA:2236:U:H6   | 1.61                     | 0.64              |
| 24:DA:2259:U:C4   | 24:DA:2427:C:N4   | 2.65                     | 0.64              |
| 24:DA:2756:U:H3   | 24:DA:2758:A:H62  | 1.44                     | 0.64              |
| 24:DA:2850:A:O2'  | 24:DA:2851:A:H5'  | 1.98                     | 0.64              |
| 26:DC:181:ARG:HG3 | 26:DC:265:PHE:O   | 1.98                     | 0.64              |
| 27:DD:4:LEU:HD23  | 27:DD:101:PHE:CE1 | 2.33                     | 0.64              |
| 24:DA:2269:G:O3'  | 46:DW:18:LYS:HE2  | 1.98                     | 0.64              |
| 21:AA:1394:A:N6   | 21:AA:1501:C:H4'  | 2.13                     | 0.64              |
| 17:AR:38:ILE:O    | 21:AA:719:C:O2'   | 2.16                     | 0.64              |
| 4:AE:11:GLN:CG    | 4:AE:116:VAL:HA   | 2.28                     | 0.64              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:AE:79:THR:CB    | 4:AE:121:ASN:HD21  | 2.10                     | 0.64              |
| 6:AG:147:ASN:H    | 6:AG:147:ASN:ND2   | 1.96                     | 0.64              |
| 16:AQ:46:HIS:HB2  | 16:AQ:66:LEU:HD12  | 1.79                     | 0.64              |
| 54:B4:10:LEU:HD12 | 54:B4:33:HIS:CD2   | 2.32                     | 0.64              |
| 24:BA:1057:A:C8   | 24:BA:1086:A:C8    | 2.85                     | 0.64              |
| 24:BA:143:C:H2'   | 24:BA:144:A:H8     | 1.62                     | 0.64              |
| 24:BA:1874:C:H2'  | 24:BA:1875:G:O4'   | 1.98                     | 0.64              |
| 24:BA:276:U:O2'   | 24:BA:278:A:N7     | 2.31                     | 0.64              |
| 24:BA:63:A:C2     | 24:BA:64:A:C8      | 2.86                     | 0.64              |
| 26:BC:16:VAL:HB   | 26:BC:203:VAL:HB   | 1.78                     | 0.64              |
| 35:BL:79:LEU:HB2  | 35:BL:114:GLY:O    | 1.98                     | 0.64              |
| 36:BM:55:ARG:HG3  | 36:BM:55:ARG:O     | 1.98                     | 0.64              |
| 46:BW:72:GLY:C    | 46:BW:74:LYS:H     | 2.01                     | 0.64              |
| 55:CA:1434:A:H2'  | 55:CA:1435:G:O4'   | 1.98                     | 0.64              |
| 6:CG:2:ARG:HD3    | 55:CA:932:C:H5''   | 1.79                     | 0.64              |
| 4:CE:104:ILE:O    | 4:CE:104:ILE:HG23  | 1.98                     | 0.64              |
| 24:DA:2537:U:H2'  | 24:DA:2538:C:C6    | 2.33                     | 0.64              |
| 24:DA:73:A:O5'    | 24:DA:73:A:H8      | 1.81                     | 0.64              |
| 24:DA:865:C:H5''  | 24:DA:866:A:OP1    | 1.97                     | 0.64              |
| 27:DD:107:VAL:CG1 | 27:DD:109:VAL:HG23 | 2.27                     | 0.64              |
| 30:DG:10:VAL:HB   | 30:DG:14:VAL:HG21  | 1.78                     | 0.64              |
| 34:DK:104:THR:O   | 34:DK:107:LEU:HD22 | 1.97                     | 0.64              |
| 44:DU:26:ASN:OD1  | 44:DU:34:ILE:HD12  | 1.98                     | 0.64              |
| 46:DW:18:LYS:H    | 46:DW:36:ILE:HG12  | 1.62                     | 0.64              |
| 18:AS:77:ARG:HH22 | 21:AA:1322:C:P     | 2.21                     | 0.64              |
| 21:AA:1360:A:H2'  | 21:AA:1361:G:H8    | 1.63                     | 0.64              |
| 21:AA:1500:A:OP1  | 21:AA:1508:A:OP1   | 2.16                     | 0.64              |
| 3:AD:53:GLN:NE2   | 3:AD:201:GLU:HG2   | 2.13                     | 0.64              |
| 4:AE:75:LEU:HD21  | 4:AE:119:VAL:HG13  | 1.80                     | 0.64              |
| 8:AI:122:ARG:NH1  | 21:AA:1343:G:H1'   | 2.13                     | 0.64              |
| 24:BA:1387:A:H2'  | 24:BA:1388:G:H8    | 1.62                     | 0.64              |
| 24:BA:1553:A:N7   | 24:BA:1555:G:C6    | 2.66                     | 0.64              |
| 26:BC:180:MET:HG3 | 26:BC:268:ARG:HH11 | 1.60                     | 0.64              |
| 27:BD:121:THR:O   | 27:BD:122:VAL:HG23 | 1.97                     | 0.64              |
| 32:BI:48:ILE:HG13 | 32:BI:49:GLU:H     | 1.62                     | 0.64              |
| 42:BS:88:ARG:NE   | 42:BS:94:ASP:OD1   | 2.30                     | 0.64              |
| 24:BA:2269:G:H4'  | 46:BW:18:LYS:HE2   | 1.78                     | 0.64              |
| 55:CA:1050:G:O2'  | 55:CA:1051:C:C6    | 2.48                     | 0.64              |
| 55:CA:1163:A:C2   | 55:CA:1174:G:C2    | 2.86                     | 0.64              |
| 55:CA:1533:C:H2'  | 55:CA:1534:A:H5''  | 1.78                     | 0.64              |
| 55:CA:239:U:OP1   | 55:CA:239:U:H4'    | 1.97                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:815:A:OP2   | 55:CA:816:A:C8    | 2.51                     | 0.64              |
| 55:CA:977:A:C8    | 55:CA:1223:C:N3   | 2.65                     | 0.64              |
| 8:CI:51:LEU:HB2   | 8:CI:56:MET:SD    | 2.38                     | 0.64              |
| 18:CS:49:ALA:HB1  | 18:CS:56:HIS:HB3  | 1.80                     | 0.64              |
| 24:DA:1056:G:H1'  | 24:DA:1103:A:N1   | 2.13                     | 0.64              |
| 24:DA:1439:A:N1   | 24:DA:1552:A:C4   | 2.65                     | 0.64              |
| 24:DA:1645:G:H5'' | 24:DA:1646:C:H5'  | 1.78                     | 0.64              |
| 24:DA:2384:U:H5'' | 24:DA:2386:A:OP1  | 1.98                     | 0.64              |
| 24:DA:300:A:OP2   | 44:DU:96:LYS:HD3  | 1.97                     | 0.64              |
| 24:DA:411:G:H4'   | 24:DA:412:A:OP1   | 1.97                     | 0.64              |
| 24:DA:607:U:H5    | 24:DA:619:G:C4    | 2.16                     | 0.64              |
| 21:AA:1173:U:H2'  | 21:AA:1174:G:C8   | 2.33                     | 0.64              |
| 21:AA:1361:G:C2'  | 21:AA:1362:A:H5'  | 2.27                     | 0.64              |
| 1:AB:71:THR:O     | 1:AB:72:LYS:HG2   | 1.98                     | 0.64              |
| 16:AQ:12:VAL:HG13 | 16:AQ:16:MET:HE1  | 1.80                     | 0.64              |
| 24:BA:1181:U:O2'  | 24:BA:1182:G:C8   | 2.48                     | 0.64              |
| 24:BA:216:A:H2'   | 24:BA:217:A:C8    | 2.32                     | 0.64              |
| 24:BA:2297:A:N1   | 24:BA:2321:U:C5   | 2.63                     | 0.64              |
| 24:BA:592:A:O2'   | 53:B3:2:LYS:HA    | 1.98                     | 0.64              |
| 24:BA:77:G:C5     | 24:BA:78:U:C5     | 2.86                     | 0.64              |
| 25:BB:116:G:H4'   | 38:BO:54:VAL:O    | 1.99                     | 0.64              |
| 29:BF:40:GLY:CA   | 29:BF:84:ILE:HD11 | 2.28                     | 0.64              |
| 35:BL:85:VAL:HG21 | 35:BL:94:THR:HG23 | 1.80                     | 0.64              |
| 41:BR:51:VAL:HB   | 41:BR:52:PRO:CD   | 2.28                     | 0.64              |
| 49:BZ:6:ILE:O     | 49:BZ:34:THR:HA   | 1.97                     | 0.64              |
| 55:CA:1184:G:H3'  | 55:CA:1184:G:OP1  | 1.97                     | 0.64              |
| 55:CA:6:G:N3      | 55:CA:6:G:C2'     | 2.59                     | 0.64              |
| 55:CA:765:G:C8    | 55:CA:812:G:C2    | 2.86                     | 0.64              |
| 55:CA:960:U:H5'   | 55:CA:961:U:H5''  | 1.78                     | 0.64              |
| 8:CI:27:ILE:HD13  | 8:CI:62:LEU:HG    | 1.78                     | 0.64              |
| 17:CR:32:ILE:HA   | 17:CR:39:VAL:HG23 | 1.80                     | 0.64              |
| 24:DA:2350:C:H5   | 53:D3:41:ARG:NH1  | 1.95                     | 0.64              |
| 24:DA:1213:A:HO2' | 24:DA:1214:A:H8   | 1.45                     | 0.64              |
| 24:DA:1654:A:HO2' | 24:DA:1655:A:H8   | 0.76                     | 0.64              |
| 24:DA:2623:G:O2'  | 24:DA:2624:G:H5'  | 1.98                     | 0.64              |
| 24:DA:319:G:H2'   | 24:DA:320:A:O4'   | 1.98                     | 0.64              |
| 28:DE:111:GLU:HA  | 28:DE:114:ARG:HE  | 1.61                     | 0.64              |
| 45:DV:55:GLU:O    | 45:DV:57:TYR:N    | 2.31                     | 0.64              |
| 21:AA:94:G:H5''   | 21:AA:95:C:C5     | 2.33                     | 0.63              |
| 4:AE:11:GLN:HG3   | 4:AE:116:VAL:HG12 | 1.80                     | 0.63              |
| 7:AH:82:LEU:HD12  | 11:AL:3:VAL:HG11  | 1.78                     | 0.63              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:B1:12:SER:HB2   | 51:B1:48:TYR:CZ   | 2.33                     | 0.63              |
| 24:BA:1508:A:O2'   | 24:BA:1509:A:O4'  | 2.17                     | 0.63              |
| 24:BA:475:C:O2'    | 24:BA:476:G:H5'   | 1.97                     | 0.63              |
| 24:BA:522:A:C5     | 24:BA:523:C:C5    | 2.86                     | 0.63              |
| 24:BA:533:G:H2'    | 24:BA:534:U:C6    | 2.34                     | 0.63              |
| 30:BG:66:THR:O     | 30:BG:70:LEU:HG   | 1.97                     | 0.63              |
| 38:BO:74:VAL:O     | 38:BO:78:VAL:HG22 | 1.97                     | 0.63              |
| 39:BP:72:VAL:O     | 39:BP:72:VAL:HG23 | 1.97                     | 0.63              |
| 55:CA:1283:U:O2'   | 55:CA:1284:C:C5'  | 2.45                     | 0.63              |
| 55:CA:1455:G:H2'   | 55:CA:1456:A:H8   | 1.61                     | 0.63              |
| 55:CA:189:A:H3'    | 55:CA:190:A:C8    | 2.33                     | 0.63              |
| 24:DA:1074:G:H2'   | 24:DA:1075:C:C6   | 2.34                     | 0.63              |
| 24:DA:1328:A:H2'   | 24:DA:1330:C:C4   | 2.33                     | 0.63              |
| 24:DA:13:A:H5''    | 24:DA:14:A:OP1    | 1.97                     | 0.63              |
| 24:DA:1560:G:C2'   | 24:DA:1561:C:H5'  | 2.28                     | 0.63              |
| 24:DA:225:C:O2'    | 24:DA:226:A:O4'   | 2.16                     | 0.63              |
| 24:DA:2712:C:C2    | 24:DA:2715:C:OP1  | 2.50                     | 0.63              |
| 24:DA:2902:C:O2'   | 24:DA:2903:U:C5'  | 2.46                     | 0.63              |
| 24:DA:724:U:H2'    | 24:DA:725:G:O4'   | 1.97                     | 0.63              |
| 27:DD:159:LYS:HE2  | 27:DD:160:LYS:H   | 1.63                     | 0.63              |
| 44:DU:26:ASN:O     | 44:DU:34:ILE:HB   | 1.98                     | 0.63              |
| 21:AA:1192:C:H2'   | 21:AA:1193:G:O4'  | 1.98                     | 0.63              |
| 21:AA:1444:U:H1'   | 21:AA:1459:G:N2   | 2.13                     | 0.63              |
| 21:AA:236:A:H2'    | 21:AA:237:G:C8    | 2.34                     | 0.63              |
| 10:AK:45:THR:OG1   | 10:AK:48:GLY:HA3  | 1.97                     | 0.63              |
| 11:AL:50:LYS:HD2   | 11:AL:50:LYS:N    | 2.13                     | 0.63              |
| 16:AQ:44:HIS:HE1   | 21:AA:276:G:O3'   | 1.82                     | 0.63              |
| 24:BA:1075:C:H2'   | 24:BA:1076:C:C6   | 2.33                     | 0.63              |
| 24:BA:1372:U:O2'   | 24:BA:1373:A:H5'  | 1.98                     | 0.63              |
| 24:BA:2407:A:H2'   | 24:BA:2408:U:H6   | 1.62                     | 0.63              |
| 24:BA:2742:G:O2'   | 24:BA:2743:U:H5'  | 1.97                     | 0.63              |
| 27:BD:191:GLY:O    | 27:BD:192:ALA:HB3 | 1.98                     | 0.63              |
| 31:BH:130:VAL:HG23 | 31:BH:131:SER:H   | 1.63                     | 0.63              |
| 37:BN:8:ARG:HB3    | 37:BN:10:LEU:HD22 | 1.79                     | 0.63              |
| 55:CA:1320:C:H2'   | 55:CA:1321:U:O4'  | 1.99                     | 0.63              |
| 1:CB:133:ALA:HA    | 1:CB:137:THR:HG21 | 1.79                     | 0.63              |
| 1:CB:59:ILE:HA     | 1:CB:62:ARG:HD3   | 1.79                     | 0.63              |
| 13:CN:52:ARG:CZ    | 13:CN:52:ARG:HA   | 2.26                     | 0.63              |
| 24:DA:1799:G:H8    | 26:DC:179:GLU:OE1 | 1.82                     | 0.63              |
| 24:DA:2882:A:H4'   | 37:DN:97:ILE:HG12 | 1.80                     | 0.63              |
| 24:DA:64:A:H2'     | 24:DA:65:U:C6     | 2.34                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:DB:40:U:O2'     | 56:DB:45:A:N6      | 2.31                     | 0.63              |
| 59:AN:204:HOH:O    | 21:AA:1359:C:H5''  | 1.98                     | 0.63              |
| 21:AA:423:G:HO2'   | 21:AA:424:G:C4'    | 2.11                     | 0.63              |
| 24:BA:570:G:H2'    | 24:BA:2030:A:N7    | 2.13                     | 0.63              |
| 24:BA:233:A:N6     | 24:BA:428:A:H61    | 1.96                     | 0.63              |
| 26:BC:108:GLY:O    | 26:BC:109:LEU:HD22 | 1.98                     | 0.63              |
| 55:CA:1003:G:N2    | 55:CA:1005:A:H5''  | 2.14                     | 0.63              |
| 55:CA:1324:A:H2'   | 55:CA:1325:C:C6    | 2.34                     | 0.63              |
| 55:CA:205:A:C6     | 55:CA:206:C:N4     | 2.66                     | 0.63              |
| 55:CA:320:A:H2'    | 55:CA:321:A:C8     | 2.33                     | 0.63              |
| 55:CA:558:G:H2'    | 55:CA:559:A:H2     | 1.64                     | 0.63              |
| 14:CO:77:TYR:OH    | 14:CO:87:ARG:HD3   | 1.97                     | 0.63              |
| 24:DA:272:A:O2'    | 24:DA:273:G:H8     | 1.80                     | 0.63              |
| 24:DA:556:A:C8     | 24:DA:556:A:OP2    | 2.52                     | 0.63              |
| 24:DA:607:U:H5     | 24:DA:619:G:C5     | 2.16                     | 0.63              |
| 24:DA:674:G:O2'    | 28:DE:69:ARG:HG2   | 1.98                     | 0.63              |
| 24:DA:866:A:O2'    | 24:DA:867:C:H6     | 1.82                     | 0.63              |
| 37:DN:90:ARG:NH2   | 37:DN:116:VAL:HG11 | 2.14                     | 0.63              |
| 41:DR:27:ILE:HG22  | 41:DR:28:ALA:N     | 2.13                     | 0.63              |
| 41:DR:87:GLN:HG2   | 41:DR:88:GLY:N     | 2.13                     | 0.63              |
| 21:AA:1238:A:H5'   | 21:AA:1336:C:N4    | 2.07                     | 0.63              |
| 21:AA:466:A:H5'    | 21:AA:467:U:OP2    | 1.99                     | 0.63              |
| 4:AE:19:ARG:HB2    | 4:AE:32:PHE:CE1    | 2.34                     | 0.63              |
| 6:AG:86:VAL:HG13   | 6:AG:87:PRO:HD2    | 1.80                     | 0.63              |
| 7:AH:29:SER:HB3    | 7:AH:32:LYS:CG     | 2.27                     | 0.63              |
| 4:AE:83:PRO:HG2    | 7:AH:95:MET:HG2    | 1.80                     | 0.63              |
| 24:BA:1059:G:C6    | 24:BA:1060:U:N3    | 2.65                     | 0.63              |
| 24:BA:1517:G:C2    | 24:BA:1518:C:C2    | 2.86                     | 0.63              |
| 24:BA:822:G:C5     | 24:BA:836:G:N2     | 2.67                     | 0.63              |
| 24:BA:2680:U:OP2   | 27:BD:114:LYS:HE2  | 1.98                     | 0.63              |
| 28:BE:196:VAL:HG13 | 28:BE:200:LEU:HD23 | 1.81                     | 0.63              |
| 47:BX:2:ARG:HD2    | 47:BX:29:LEU:HD12  | 1.80                     | 0.63              |
| 47:BX:31:ASN:O     | 47:BX:51:SER:HA    | 1.99                     | 0.63              |
| 55:CA:1064:G:O2'   | 55:CA:1190:G:N2    | 2.31                     | 0.63              |
| 55:CA:1432:G:H1'   | 55:CA:1468:A:H61   | 1.61                     | 0.63              |
| 5:CF:11:HIS:HD2    | 5:CF:13:ASP:H      | 1.46                     | 0.63              |
| 6:CG:149:ALA:CB    | 10:CK:55:ARG:HG3   | 2.29                     | 0.63              |
| 24:DA:1180:U:H2'   | 24:DA:1181:U:O4'   | 1.98                     | 0.63              |
| 24:DA:1854:A:H61   | 24:DA:1888:G:H1'   | 1.63                     | 0.63              |
| 24:DA:2345:G:H4'   | 24:DA:2346:A:O5'   | 1.96                     | 0.63              |
| 24:DA:2592:G:C5    | 24:DA:2593:U:C5    | 2.86                     | 0.63              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 56:DB:46:A:H2'     | 56:DB:47:C:C6     | 2.33                     | 0.63              |
| 26:DC:17:LYS:HD3   | 26:DC:18:VAL:N    | 2.14                     | 0.63              |
| 27:DD:114:LYS:HB2  | 27:DD:116:LYS:HE3 | 1.81                     | 0.63              |
| 27:DD:34:VAL:CG1   | 27:DD:48:ILE:HD11 | 2.27                     | 0.63              |
| 31:DH:50:ARG:HA    | 31:DH:53:GLU:HB3  | 1.81                     | 0.63              |
| 34:DK:87:LEU:HD12  | 34:DK:92:GLU:HA   | 1.80                     | 0.63              |
| 44:DU:3:LYS:HG2    | 44:DU:84:PHE:HZ   | 1.63                     | 0.63              |
| 45:DV:75:GLN:HB2   | 45:DV:90:ASP:O    | 1.99                     | 0.63              |
| 21:AA:1129:C:H1'   | 21:AA:1130:A:N7   | 2.14                     | 0.63              |
| 21:AA:1261:A:H61   | 21:AA:1274:A:H2'  | 1.62                     | 0.63              |
| 2:AC:42:LEU:HD21   | 2:AC:67:ILE:HD11  | 1.79                     | 0.63              |
| 3:AD:55:ARG:NH1    | 3:AD:58:GLN:HB3   | 2.13                     | 0.63              |
| 24:BA:528:A:H2     | 24:BA:2043:C:H5'  | 1.64                     | 0.63              |
| 24:BA:2383:G:H2'   | 24:BA:2384:U:H6   | 1.64                     | 0.63              |
| 33:BJ:124:VAL:HG23 | 33:BJ:125:TYR:H   | 1.63                     | 0.63              |
| 35:BL:109:LYS:HG2  | 35:BL:126:ARG:HB3 | 1.79                     | 0.63              |
| 39:BP:50:ARG:CD    | 39:BP:51:ASN:N    | 2.61                     | 0.63              |
| 55:CA:1327:C:C4    | 55:CA:1328:C:N4   | 2.66                     | 0.63              |
| 55:CA:393:A:H2'    | 55:CA:394:G:H8    | 1.63                     | 0.63              |
| 55:CA:908:A:H2'    | 55:CA:909:A:H8    | 1.62                     | 0.63              |
| 1:CB:17:HIS:HA     | 1:CB:37:VAL:HG21  | 1.80                     | 0.63              |
| 12:CM:57:ASP:O     | 12:CM:61:LYS:HG3  | 1.98                     | 0.63              |
| 19:CT:26:MET:HE3   | 19:CT:30:PHE:HD1  | 1.63                     | 0.63              |
| 20:CU:16:ARG:NE    | 20:CU:16:ARG:HA   | 2.12                     | 0.63              |
| 24:DA:1345:C:O2'   | 24:DA:1346:G:H5'  | 1.99                     | 0.63              |
| 24:DA:142:A:H2'    | 24:DA:143:C:C5    | 2.33                     | 0.63              |
| 24:DA:2010:G:C6    | 24:DA:2011:U:C4   | 2.87                     | 0.63              |
| 24:DA:2262:U:H4'   | 24:DA:2328:A:C2   | 2.34                     | 0.63              |
| 24:DA:339:U:H2'    | 24:DA:340:A:C8    | 2.34                     | 0.63              |
| 24:DA:741:U:H2'    | 24:DA:742:A:C8    | 2.34                     | 0.63              |
| 24:DA:776:G:C8     | 24:DA:793:A:C4    | 2.86                     | 0.63              |
| 24:DA:786:C:H4'    | 24:DA:1780:A:N7   | 2.13                     | 0.63              |
| 24:DA:7:G:H4'      | 33:DJ:15:TRP:CH2  | 2.34                     | 0.63              |
| 24:DA:833:A:H2'    | 24:DA:834:G:H8    | 1.59                     | 0.63              |
| 24:DA:983:A:C6     | 24:DA:984:A:C2    | 2.87                     | 0.63              |
| 27:DD:124:ARG:NH1  | 27:DD:125:TRP:CZ2 | 2.67                     | 0.63              |
| 21:AA:206:C:H2'    | 21:AA:207:C:O4'   | 1.98                     | 0.63              |
| 4:AE:90:GLY:C      | 4:AE:129:SER:HB3  | 2.19                     | 0.63              |
| 4:AE:33:THR:HB     | 4:AE:49:TYR:HE1   | 1.63                     | 0.63              |
| 8:AI:110:VAL:HG21  | 21:AA:1370:G:O5'  | 1.98                     | 0.63              |
| 13:AN:29:ILE:HG23  | 13:AN:34:ASN:CG   | 2.19                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:1062:G:C8   | 24:BA:1088:A:C8   | 2.87                     | 0.63              |
| 24:BA:2020:A:H5'  | 50:B0:8:THR:HG22  | 1.80                     | 0.63              |
| 24:BA:221:A:H4'   | 24:BA:222:A:O5'   | 1.98                     | 0.63              |
| 24:BA:748:G:O5'   | 42:BS:89:ALA:HB2  | 1.99                     | 0.63              |
| 25:BB:9:G:OP1     | 38:BO:15:ARG:HD2  | 1.98                     | 0.63              |
| 27:BD:151:THR:HB  | 27:BD:152:PRO:HD3 | 1.80                     | 0.63              |
| 48:BY:47:ARG:HG3  | 48:BY:47:ARG:HH21 | 1.64                     | 0.63              |
| 55:CA:1306:A:H61  | 55:CA:1331:G:H1'  | 1.64                     | 0.63              |
| 55:CA:300:A:H1'   | 55:CA:565:U:O2    | 1.98                     | 0.63              |
| 3:CD:35:GLN:HG3   | 3:CD:36:ALA:H     | 1.64                     | 0.63              |
| 4:CE:80:LEU:HB3   | 4:CE:97:PRO:HB3   | 1.80                     | 0.63              |
| 10:CK:30:ILE:HG23 | 10:CK:45:THR:HG22 | 1.81                     | 0.63              |
| 13:CN:19:TYR:CD2  | 13:CN:51:PRO:HG3  | 2.33                     | 0.63              |
| 24:DA:103:A:H2'   | 24:DA:104:A:C8    | 2.34                     | 0.63              |
| 24:DA:105:C:H2'   | 24:DA:106:C:C6    | 2.34                     | 0.63              |
| 24:DA:1386:C:HO2' | 24:DA:1387:A:H8   | 1.44                     | 0.63              |
| 24:DA:2572:A:O2'  | 24:DA:2573:C:OP2  | 2.15                     | 0.63              |
| 24:DA:476:G:O2'   | 24:DA:477:A:H3'   | 1.99                     | 0.63              |
| 30:DG:85:LYS:O    | 30:DG:86:LEU:HG   | 1.98                     | 0.63              |
| 24:DA:2726:A:O2'  | 34:DK:67:LYS:NZ   | 2.31                     | 0.63              |
| 38:DO:13:ARG:O    | 38:DO:17:LYS:HB2  | 1.99                     | 0.63              |
| 42:DS:24:ILE:HG21 | 42:DS:36:LEU:HD21 | 1.81                     | 0.63              |
| 45:DV:29:ILE:CD1  | 45:DV:31:TYR:HE2  | 2.11                     | 0.63              |
| 21:AA:1054:C:C4   | 22:AX:34:G:H1'    | 2.34                     | 0.63              |
| 8:AI:113:LYS:HE2  | 8:AI:118:ARG:O    | 1.99                     | 0.63              |
| 12:AM:94:LEU:HD22 | 12:AM:95:PRO:HD2  | 1.80                     | 0.63              |
| 24:BA:1204:A:H1'  | 24:BA:1206:G:C5   | 2.33                     | 0.63              |
| 24:BA:2691:C:O2'  | 24:BA:2692:G:H5'  | 1.99                     | 0.63              |
| 24:BA:2728:U:O2'  | 24:BA:2729:G:C8   | 2.52                     | 0.63              |
| 24:BA:614:A:O2'   | 24:BA:615:U:OP2   | 2.13                     | 0.63              |
| 24:BA:652:U:H5''  | 24:BA:653:U:O5'   | 1.98                     | 0.63              |
| 27:BD:70:LYS:O    | 27:BD:71:ALA:HB3  | 1.98                     | 0.63              |
| 32:BI:53:PRO:O    | 32:BI:74:PRO:HD2  | 1.98                     | 0.63              |
| 33:BJ:111:LYS:HD3 | 33:BJ:112:GLY:N   | 2.13                     | 0.63              |
| 45:BV:44:HIS:HE1  | 45:BV:86:LEU:H    | 1.47                     | 0.63              |
| 55:CA:1127:G:O2'  | 55:CA:1128:C:H5'  | 1.98                     | 0.63              |
| 55:CA:1264:U:H2'  | 55:CA:1265:C:C6   | 2.33                     | 0.63              |
| 55:CA:1300:G:O2'  | 55:CA:1303:C:N4   | 2.31                     | 0.63              |
| 55:CA:371:A:O2'   | 55:CA:372:C:H5'   | 1.99                     | 0.63              |
| 55:CA:397:A:N6    | 55:CA:548:G:C5    | 2.66                     | 0.63              |
| 3:CD:2:ARG:HE     | 3:CD:114:ARG:HD2  | 1.64                     | 0.63              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:CL:19:ASN:N     | 11:CL:19:ASN:HD22 | 1.95                     | 0.63              |
| 15:CP:36:VAL:O     | 15:CP:36:VAL:HG13 | 1.99                     | 0.63              |
| 37:DN:98:LEU:HD21  | 50:D0:53:VAL:HG11 | 1.80                     | 0.63              |
| 24:DA:2053:G:N2    | 24:DA:2054:A:C4   | 2.66                     | 0.63              |
| 24:DA:2448:A:H3'   | 24:DA:2449:U:H6   | 1.63                     | 0.63              |
| 24:DA:918:A:C6     | 24:DA:919:U:H1'   | 2.33                     | 0.63              |
| 28:DE:126:VAL:HG22 | 28:DE:127:GLU:OE2 | 1.98                     | 0.63              |
| 30:DG:106:LEU:HB2  | 30:DG:108:PHE:HE1 | 1.63                     | 0.63              |
| 36:DM:19:GLY:N     | 36:DM:38:ARG:HH21 | 1.92                     | 0.63              |
| 41:DR:70:GLU:CD    | 41:DR:70:GLU:H    | 2.02                     | 0.63              |
| 21:AA:76:G:H2'     | 21:AA:76:G:N3     | 2.14                     | 0.63              |
| 1:AB:51:GLU:O      | 1:AB:54:ALA:HB3   | 1.98                     | 0.63              |
| 12:AM:44:ILE:N     | 12:AM:44:ILE:HD12 | 2.13                     | 0.63              |
| 51:B1:8:ILE:HG22   | 51:B1:9:LYS:N     | 2.14                     | 0.63              |
| 24:BA:1247:A:C4    | 24:BA:1249:U:C5   | 2.87                     | 0.63              |
| 24:BA:2156:G:H2'   | 24:BA:2157:G:N2   | 2.13                     | 0.63              |
| 24:BA:945:A:C4     | 24:BA:2448:A:C2   | 2.86                     | 0.63              |
| 24:BA:320:A:O2'    | 24:BA:322:A:H8    | 1.82                     | 0.63              |
| 24:BA:455:C:H42    | 24:BA:473:G:H5'   | 1.62                     | 0.63              |
| 24:BA:84:A:N1      | 24:BA:103:A:C5    | 2.67                     | 0.63              |
| 30:BG:123:GLU:CD   | 30:BG:124:CYS:H   | 2.02                     | 0.63              |
| 37:BN:106:ASP:C    | 37:BN:106:ASP:OD1 | 2.37                     | 0.63              |
| 40:BQ:13:HIS:HD2   | 40:BQ:31:TYR:CD1  | 2.17                     | 0.63              |
| 40:BQ:86:SER:O     | 40:BQ:88:GLU:N    | 2.31                     | 0.63              |
| 42:BS:2:GLU:O      | 42:BS:107:VAL:O   | 2.16                     | 0.63              |
| 46:BW:14:ASP:O     | 46:BW:15:SER:HB2  | 1.97                     | 0.63              |
| 55:CA:1106:G:H2'   | 55:CA:1107:C:H6   | 1.62                     | 0.63              |
| 55:CA:1490:U:O2'   | 55:CA:1491:G:H5'  | 1.99                     | 0.63              |
| 9:CJ:57:VAL:HG23   | 55:CA:972:C:O2'   | 1.97                     | 0.63              |
| 1:CB:113:LEU:HD13  | 1:CB:143:LEU:HB3  | 1.81                     | 0.63              |
| 3:CD:205:LYS:HD3   | 55:CA:8:A:C6      | 2.34                     | 0.63              |
| 3:CD:29:THR:C      | 3:CD:30:LYS:HD3   | 2.19                     | 0.63              |
| 11:CL:109:ARG:NH2  | 11:CL:116:TYR:CE2 | 2.67                     | 0.63              |
| 53:D3:18:LYS:HD2   | 53:D3:19:GLY:H    | 1.64                     | 0.63              |
| 24:DA:1079:C:C4    | 24:DA:1088:A:C2   | 2.87                     | 0.63              |
| 24:DA:121:G:H2'    | 24:DA:122:G:C8    | 2.34                     | 0.63              |
| 24:DA:1695:G:H2'   | 24:DA:1695:G:N3   | 2.14                     | 0.63              |
| 24:DA:1748:C:H2'   | 24:DA:1749:A:H8   | 1.63                     | 0.63              |
| 24:DA:217:A:O2'    | 24:DA:218:A:H5'   | 1.99                     | 0.63              |
| 26:DC:183:VAL:HG13 | 26:DC:185:ALA:H   | 1.64                     | 0.63              |
| 36:DM:34:LYS:HB2   | 36:DM:131:VAL:CG2 | 2.29                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:DW:39:GLN:HG2  | 46:DW:42:THR:HB   | 1.79                     | 0.63              |
| 47:DX:63:ILE:CD1  | 47:DX:64:ASP:H    | 2.11                     | 0.63              |
| 49:DZ:7:THR:O     | 49:DZ:54:VAL:HA   | 1.99                     | 0.63              |
| 21:AA:1226:C:H4'  | 21:AA:1227:A:OP1  | 1.98                     | 0.63              |
| 21:AA:1405:G:O2'  | 21:AA:1519:A:H5'  | 1.99                     | 0.63              |
| 1:AB:107:ARG:HE   | 1:AB:108:GLN:HE22 | 1.44                     | 0.63              |
| 2:AC:180:ASP:O    | 2:AC:181:ILE:HD13 | 1.99                     | 0.63              |
| 6:AG:69:ARG:HG3   | 6:AG:95:ARG:HG2   | 1.81                     | 0.63              |
| 23:AW:5:U:H2'     | 23:AW:6:U:C5      | 2.34                     | 0.63              |
| 24:BA:1747:U:H2'  | 24:BA:1748:C:C6   | 2.34                     | 0.63              |
| 24:BA:2853:C:O2'  | 24:BA:2854:G:H5'  | 1.99                     | 0.63              |
| 24:BA:923:G:H4'   | 46:BW:25:PHE:CZ   | 2.33                     | 0.63              |
| 46:BW:23:LYS:HD2  | 46:BW:24:ARG:N    | 2.13                     | 0.63              |
| 47:BX:67:LEU:HD13 | 47:BX:77:TYR:CE1  | 2.34                     | 0.63              |
| 55:CA:1050:G:HO2' | 55:CA:1051:C:H6   | 1.36                     | 0.63              |
| 55:CA:67:C:O2'    | 55:CA:68:G:C8     | 2.51                     | 0.63              |
| 55:CA:865:A:H2    | 55:CA:918:A:H4'   | 1.63                     | 0.63              |
| 9:CJ:8:ILE:HG22   | 9:CJ:100:ILE:HG12 | 1.80                     | 0.63              |
| 2:CC:5:HIS:ND1    | 13:CN:88:MET:HB3  | 2.14                     | 0.63              |
| 24:DA:1439:A:N7   | 24:DA:1440:U:N1   | 2.47                     | 0.63              |
| 24:DA:1809:A:C2   | 24:DA:1810:A:C4   | 2.87                     | 0.63              |
| 24:DA:476:G:H4'   | 24:DA:502:A:N1    | 2.14                     | 0.63              |
| 24:DA:600:G:H5''  | 28:DE:27:LEU:HD22 | 1.80                     | 0.63              |
| 24:DA:812:C:O2'   | 24:DA:813:U:H5'   | 1.98                     | 0.63              |
| 56:DB:11:C:C5     | 56:DB:12:C:C5     | 2.86                     | 0.63              |
| 37:DN:45:ARG:HG2  | 37:DN:95:THR:HG21 | 1.81                     | 0.63              |
| 37:DN:98:LEU:O    | 37:DN:112:TYR:HB2 | 1.99                     | 0.63              |
| 49:DZ:16:LEU:CD2  | 49:DZ:16:LEU:H    | 2.12                     | 0.63              |
| 21:AA:664:G:H2'   | 21:AA:666:G:OP1   | 1.98                     | 0.62              |
| 21:AA:781:A:H5'   | 21:AA:782:A:OP2   | 1.98                     | 0.62              |
| 2:AC:78:LYS:NZ    | 2:AC:78:LYS:HB3   | 2.13                     | 0.62              |
| 53:B3:53:ASP:HA   | 53:B3:56:LEU:HD23 | 1.81                     | 0.62              |
| 24:BA:2185:U:H2'  | 24:BA:2186:G:C8   | 2.34                     | 0.62              |
| 24:BA:2408:U:O2'  | 24:BA:2409:G:H5'  | 1.99                     | 0.62              |
| 24:BA:2532:G:N7   | 24:BA:2533:U:C5   | 2.66                     | 0.62              |
| 24:BA:373:U:O2'   | 24:BA:374:A:H5'   | 1.99                     | 0.62              |
| 24:BA:620:G:H4'   | 24:BA:621:A:O5'   | 1.99                     | 0.62              |
| 24:BA:783:A:H4'   | 24:BA:1779:U:O2   | 1.98                     | 0.62              |
| 55:CA:121:U:OP1   | 55:CA:121:U:H3'   | 1.99                     | 0.62              |
| 55:CA:1530:G:O2'  | 55:CA:1531:A:H8   | 1.82                     | 0.62              |
| 1:CB:34:ARG:HD3   | 1:CB:35:ASN:HB2   | 1.79                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:CH:28:SER:HA    | 7:CH:58:LEU:HD12  | 1.81                     | 0.62              |
| 9:CJ:17:LEU:HD21  | 9:CJ:95:GLY:HA3   | 1.79                     | 0.62              |
| 12:CM:28:ARG:HA   | 12:CM:31:ALA:HB3  | 1.79                     | 0.62              |
| 24:DA:1061:U:O2'  | 24:DA:1062:G:H5'' | 1.99                     | 0.62              |
| 24:DA:1470:A:OP2  | 24:DA:1470:A:H8   | 1.81                     | 0.62              |
| 24:DA:1439:A:H1'  | 24:DA:1553:A:N6   | 2.14                     | 0.62              |
| 24:DA:2258:C:H2'  | 24:DA:2426:A:H4'  | 1.81                     | 0.62              |
| 24:DA:329:G:OP1   | 24:DA:329:G:H3'   | 1.99                     | 0.62              |
| 24:DA:468:G:H4'   | 28:DE:57:LYS:HG2  | 1.80                     | 0.62              |
| 24:DA:75:G:O2'    | 24:DA:76:C:H6     | 1.82                     | 0.62              |
| 29:DF:46:LYS:HD3  | 29:DF:46:LYS:O    | 1.98                     | 0.62              |
| 34:DK:25:LEU:HD23 | 34:DK:25:LEU:H    | 1.64                     | 0.62              |
| 41:DR:4:VAL:HG22  | 41:DR:40:MET:HB3  | 1.82                     | 0.62              |
| 42:DS:20:VAL:HG23 | 42:DS:23:LEU:HD12 | 1.81                     | 0.62              |
| 48:DY:18:LEU:O    | 48:DY:18:LEU:HD13 | 1.98                     | 0.62              |
| 21:AA:1432:G:H1'  | 21:AA:1468:A:H61  | 1.62                     | 0.62              |
| 21:AA:446:G:H2'   | 21:AA:447:G:O4'   | 2.00                     | 0.62              |
| 5:AF:11:HIS:CE1   | 5:AF:13:ASP:HB2   | 2.34                     | 0.62              |
| 5:AF:91:ARG:HG3   | 5:AF:92:THR:N     | 2.13                     | 0.62              |
| 11:AL:43:LYS:HZ2  | 11:AL:44:PRO:HD2  | 1.63                     | 0.62              |
| 16:AQ:79:GLU:C    | 16:AQ:80:LYS:HD3  | 2.19                     | 0.62              |
| 24:BA:1020:A:H4'  | 24:BA:1021:A:O5'  | 1.98                     | 0.62              |
| 24:BA:1721:G:O2'  | 24:BA:1722:A:C8   | 2.50                     | 0.62              |
| 24:BA:58:G:N2     | 24:BA:70:G:C4     | 2.67                     | 0.62              |
| 24:BA:855:G:H21   | 46:BW:23:LYS:CG   | 2.06                     | 0.62              |
| 29:BF:121:PHE:HD1 | 29:BF:126:ASN:O   | 1.82                     | 0.62              |
| 31:BH:76:GLU:HG2  | 31:BH:106:ALA:HB2 | 1.79                     | 0.62              |
| 39:BP:37:LYS:HD3  | 39:BP:37:LYS:H    | 1.63                     | 0.62              |
| 47:BX:5:GLN:HE21  | 47:BX:49:ARG:H    | 1.45                     | 0.62              |
| 55:CA:1264:U:H2'  | 55:CA:1265:C:H6   | 1.65                     | 0.62              |
| 55:CA:1239:A:N6   | 55:CA:1299:A:H62  | 1.97                     | 0.62              |
| 55:CA:463:U:H2'   | 55:CA:464:U:C6    | 2.34                     | 0.62              |
| 55:CA:654:G:C2'   | 55:CA:655:A:H8    | 2.11                     | 0.62              |
| 54:D4:7:VAL:HG13  | 54:D4:8:LYS:N     | 2.14                     | 0.62              |
| 24:DA:1352:U:C5   | 24:DA:1377:G:C6   | 2.87                     | 0.62              |
| 24:DA:140:C:H5'   | 24:DA:141:G:N2    | 2.13                     | 0.62              |
| 24:DA:2748:A:C4   | 24:DA:2757:A:N6   | 2.67                     | 0.62              |
| 24:DA:33:C:H2'    | 24:DA:446:G:H22   | 1.64                     | 0.62              |
| 28:DE:61:ARG:HE   | 28:DE:65:THR:HB   | 1.64                     | 0.62              |
| 32:DI:104:GLN:HA  | 32:DI:107:GLU:CB  | 2.29                     | 0.62              |
| 43:DT:13:ALA:O    | 43:DT:32:LEU:HB2  | 1.99                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 43:DT:15:HIS:CE1   | 43:DT:80:TRP:CH2  | 2.87                     | 0.62              |
| 21:AA:1376:U:H2'   | 21:AA:1377:A:C8   | 2.32                     | 0.62              |
| 21:AA:497:G:O2'    | 21:AA:498:A:C8    | 2.46                     | 0.62              |
| 1:AB:89:PHE:CE1    | 1:AB:153:MET:HG3  | 2.33                     | 0.62              |
| 24:BA:1166:G:C2    | 24:BA:1184:U:O2   | 2.53                     | 0.62              |
| 24:BA:1287:A:H5'   | 37:BN:103:ARG:HD2 | 1.80                     | 0.62              |
| 24:BA:1576:U:H2'   | 24:BA:1577:C:H6   | 1.64                     | 0.62              |
| 24:BA:2673:G:N3    | 24:BA:2674:G:C8   | 2.67                     | 0.62              |
| 24:BA:83:A:OP1     | 44:BU:91:LYS:HE3  | 1.99                     | 0.62              |
| 26:BC:80:LEU:CD1   | 26:BC:109:LEU:HG  | 2.29                     | 0.62              |
| 28:BE:150:THR:HG21 | 28:BE:153:LEU:HA  | 1.80                     | 0.62              |
| 40:BQ:91:ARG:NE    | 41:BR:11:GLN:H    | 1.97                     | 0.62              |
| 55:CA:1071:C:H2'   | 55:CA:1072:G:C8   | 2.34                     | 0.62              |
| 55:CA:115:G:H5'    | 55:CA:116:A:OP1   | 1.99                     | 0.62              |
| 55:CA:1283:U:O2'   | 55:CA:1284:C:H5'  | 1.98                     | 0.62              |
| 55:CA:1453:G:H2'   | 55:CA:1453:G:N3   | 2.15                     | 0.62              |
| 55:CA:1513:A:H2'   | 55:CA:1514:G:C8   | 2.35                     | 0.62              |
| 55:CA:642:A:O2'    | 55:CA:643:C:C6    | 2.50                     | 0.62              |
| 55:CA:82:G:C5      | 55:CA:89:U:C5     | 2.87                     | 0.62              |
| 6:CG:77:ARG:CZ     | 55:CA:1381:U:N3   | 2.62                     | 0.62              |
| 13:CN:79:SER:O     | 13:CN:83:VAL:HG23 | 2.00                     | 0.62              |
| 17:CR:25:ILE:HB    | 17:CR:67:LEU:HD21 | 1.81                     | 0.62              |
| 24:DA:1213:A:O2'   | 24:DA:1214:A:H5'  | 1.99                     | 0.62              |
| 24:DA:1895:C:C2    | 24:DA:1896:G:C8   | 2.87                     | 0.62              |
| 24:DA:1980:G:C5    | 24:DA:1982:U:O4   | 2.53                     | 0.62              |
| 24:DA:538:A:H5''   | 33:DJ:7:LYS:HZ3   | 1.63                     | 0.62              |
| 24:DA:7:G:H4'      | 33:DJ:15:TRP:CZ2  | 2.33                     | 0.62              |
| 24:DA:843:G:H2'    | 24:DA:844:A:H8    | 1.64                     | 0.62              |
| 56:DB:19:C:H2'     | 56:DB:20:G:H8     | 1.63                     | 0.62              |
| 33:DJ:35:ARG:HG2   | 33:DJ:40:HIS:CD2  | 2.34                     | 0.62              |
| 24:DA:832:U:OP1    | 35:DL:39:LYS:N    | 2.33                     | 0.62              |
| 37:DN:114:GLU:HG3  | 37:DN:118:ARG:HD3 | 1.81                     | 0.62              |
| 45:DV:63:ILE:O     | 45:DV:70:ILE:HD11 | 1.99                     | 0.62              |
| 46:DW:39:GLN:O     | 46:DW:56:HIS:HB3  | 2.00                     | 0.62              |
| 21:AA:1008:U:H2'   | 21:AA:1009:U:C6   | 2.34                     | 0.62              |
| 21:AA:1464:U:H2'   | 21:AA:1465:A:H8   | 1.64                     | 0.62              |
| 21:AA:33:A:O2'     | 21:AA:34:C:H5'    | 1.99                     | 0.62              |
| 2:AC:142:ARG:HB3   | 2:AC:143:LEU:HD13 | 1.81                     | 0.62              |
| 4:AE:57:ALA:HB1    | 4:AE:61:LYS:HE3   | 1.79                     | 0.62              |
| 8:AI:20:ILE:HG23   | 8:AI:60:LEU:HD12  | 1.81                     | 0.62              |
| 14:AO:57:ARG:HB3   | 14:AO:57:ARG:NH1  | 2.14                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:AQ:11:VAL:HG12 | 16:AQ:12:VAL:H    | 1.64                     | 0.62              |
| 24:BA:1070:A:C2   | 24:BA:1097:U:H4'  | 2.34                     | 0.62              |
| 24:BA:2675:A:O2'  | 24:BA:2676:C:H5'  | 1.98                     | 0.62              |
| 24:BA:747:U:C2    | 24:BA:2613:U:O4   | 2.52                     | 0.62              |
| 24:BA:876:C:H2'   | 24:BA:877:A:O4'   | 1.99                     | 0.62              |
| 24:BA:954:G:C4    | 24:BA:955:U:C6    | 2.87                     | 0.62              |
| 25:BB:15:A:H1'    | 25:BB:109:A:N7    | 2.14                     | 0.62              |
| 26:BC:109:LEU:CD2 | 26:BC:110:LYS:H   | 2.11                     | 0.62              |
| 26:BC:251:THR:CG2 | 26:BC:252:LYS:H   | 2.07                     | 0.62              |
| 27:BD:149:ASN:CG  | 27:BD:150:GLN:H   | 2.03                     | 0.62              |
| 46:BW:67:LYS:HB3  | 46:BW:80:SER:H    | 1.64                     | 0.62              |
| 55:CA:991:U:C4    | 55:CA:1212:U:H4'  | 2.35                     | 0.62              |
| 55:CA:1293:C:H2'  | 55:CA:1294:G:C8   | 2.34                     | 0.62              |
| 55:CA:687:A:C2    | 55:CA:704:A:C6    | 2.87                     | 0.62              |
| 1:CB:125:PHE:HD1  | 1:CB:137:THR:HG22 | 1.64                     | 0.62              |
| 3:CD:25:ARG:NH1   | 3:CD:30:LYS:HG2   | 2.14                     | 0.62              |
| 4:CE:93:VAL:HG12  | 4:CE:126:ALA:CB   | 2.30                     | 0.62              |
| 6:CG:70:PRO:O     | 6:CG:95:ARG:HD2   | 1.99                     | 0.62              |
| 7:CH:26:MET:O     | 7:CH:57:GLU:HG3   | 1.99                     | 0.62              |
| 9:CJ:45:ARG:HH21  | 55:CA:1279:G:H5'' | 1.62                     | 0.62              |
| 14:CO:25:GLU:HG2  | 14:CO:80:LEU:HD12 | 1.80                     | 0.62              |
| 24:DA:1082:U:N3   | 24:DA:1086:A:C5   | 2.67                     | 0.62              |
| 24:DA:1381:G:H2'  | 24:DA:1382:G:H5'' | 1.81                     | 0.62              |
| 24:DA:1722:A:N6   | 24:DA:1738:G:H1'  | 2.14                     | 0.62              |
| 24:DA:1830:C:H2'  | 24:DA:1831:G:H8   | 1.64                     | 0.62              |
| 24:DA:2287:A:C5   | 24:DA:2289:G:C8   | 2.87                     | 0.62              |
| 24:DA:2500:U:H5'' | 24:DA:2501:C:OP2  | 1.98                     | 0.62              |
| 24:DA:2734:A:N6   | 24:DA:2770:G:H1'  | 2.14                     | 0.62              |
| 24:DA:849:A:H2'   | 24:DA:850:U:H6    | 1.64                     | 0.62              |
| 26:DC:28:PRO:HB3  | 26:DC:62:ARG:HH22 | 1.65                     | 0.62              |
| 41:DR:48:LYS:H    | 41:DR:48:LYS:HD2  | 1.63                     | 0.62              |
| 21:AA:1043:G:H2'  | 21:AA:1044:A:H8   | 1.64                     | 0.62              |
| 21:AA:1468:A:H2'  | 21:AA:1469:C:H5'' | 1.81                     | 0.62              |
| 21:AA:1517:G:H1'  | 24:BA:1919:A:O3'  | 2.00                     | 0.62              |
| 21:AA:374:A:H5''  | 21:AA:452:A:N1    | 2.15                     | 0.62              |
| 21:AA:747:A:H5'   | 21:AA:748:G:OP2   | 1.99                     | 0.62              |
| 4:AE:15:ILE:HD13  | 4:AE:35:LEU:HG    | 1.81                     | 0.62              |
| 8:AI:34:LEU:HD11  | 8:AI:47:VAL:HG21  | 1.82                     | 0.62              |
| 9:AJ:50:THR:HG22  | 9:AJ:64:GLN:HG2   | 1.81                     | 0.62              |
| 24:BA:1026:G:H2'  | 24:BA:1027:A:H8   | 1.61                     | 0.62              |
| 24:BA:1136:G:N2   | 24:BA:1137:G:C4   | 2.68                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:2094:A:H2'  | 24:BA:2095:A:C8   | 2.35                     | 0.62              |
| 24:BA:9:G:C6      | 24:BA:2629:U:C5   | 2.87                     | 0.62              |
| 24:BA:2896:C:H2'  | 24:BA:2897:U:C6   | 2.35                     | 0.62              |
| 24:BA:391:A:C6    | 24:BA:411:G:C2    | 2.87                     | 0.62              |
| 24:BA:690:G:H2'   | 24:BA:691:C:O4'   | 2.00                     | 0.62              |
| 27:BD:99:GLU:CG   | 27:BD:100:LEU:H   | 2.12                     | 0.62              |
| 31:BH:18:GLN:HE21 | 31:BH:18:GLN:HA   | 1.64                     | 0.62              |
| 32:BI:7:TYR:HA    | 32:BI:58:ILE:HB   | 1.81                     | 0.62              |
| 38:BO:31:THR:HG23 | 38:BO:33:ARG:H    | 1.65                     | 0.62              |
| 34:BK:76:VAL:HB   | 39:BP:72:VAL:HG22 | 1.80                     | 0.62              |
| 43:BT:27:SER:O    | 43:BT:28:ASN:OD1  | 2.18                     | 0.62              |
| 53:D3:15:LYS:NZ   | 53:D3:19:GLY:HA2  | 2.15                     | 0.62              |
| 24:DA:1157:G:H2'  | 24:DA:1158:C:C6   | 2.34                     | 0.62              |
| 24:DA:1333:G:O2'  | 24:DA:1334:G:H8   | 1.81                     | 0.62              |
| 24:DA:1639:C:C2'  | 24:DA:1640:A:H5'' | 2.28                     | 0.62              |
| 24:DA:2867:G:N3   | 24:DA:2867:G:C2'  | 2.61                     | 0.62              |
| 24:DA:364:C:O2'   | 24:DA:365:U:O4'   | 2.13                     | 0.62              |
| 29:DF:134:GLN:NE2 | 29:DF:136:ILE:H   | 1.97                     | 0.62              |
| 32:DI:76:ALA:HB2  | 32:DI:131:THR:HB  | 1.80                     | 0.62              |
| 40:DQ:60:TRP:O    | 40:DQ:64:ILE:HG12 | 1.99                     | 0.62              |
| 41:DR:4:VAL:HG23  | 41:DR:39:LEU:HG   | 1.82                     | 0.62              |
| 24:DA:2262:U:H5'' | 46:DW:38:ARG:NH2  | 2.14                     | 0.62              |
| 21:AA:1160:G:O2'  | 21:AA:1161:C:C5'  | 2.48                     | 0.62              |
| 21:AA:246:A:C4    | 21:AA:282:A:N6    | 2.68                     | 0.62              |
| 1:AB:17:HIS:CD2   | 1:AB:202:ASN:HD21 | 2.17                     | 0.62              |
| 1:AB:94:ARG:HG2   | 21:AA:1100:C:OP1  | 1.99                     | 0.62              |
| 1:AB:95:TRP:CZ2   | 1:AB:99:MET:HG2   | 2.35                     | 0.62              |
| 4:AE:19:ARG:HB2   | 4:AE:32:PHE:CD1   | 2.35                     | 0.62              |
| 5:AF:49:TYR:CE2   | 5:AF:51:ILE:HB    | 2.35                     | 0.62              |
| 24:BA:1082:U:N3   | 24:BA:1086:A:C6   | 2.67                     | 0.62              |
| 24:BA:528:A:H8    | 24:BA:528:A:H3'   | 1.65                     | 0.62              |
| 31:BH:21:VAL:HG21 | 31:BH:25:TYR:HD2  | 1.65                     | 0.62              |
| 49:BZ:5:LYS:H     | 49:BZ:5:LYS:HD2   | 1.64                     | 0.62              |
| 55:CA:1235:U:H2'  | 55:CA:1236:A:H8   | 1.65                     | 0.62              |
| 55:CA:373:A:H2'   | 55:CA:374:A:H8    | 1.64                     | 0.62              |
| 3:CD:109:THR:HG21 | 55:CA:408:A:OP1   | 1.99                     | 0.62              |
| 55:CA:510:A:N3    | 55:CA:543:U:H1'   | 2.14                     | 0.62              |
| 24:DA:1744:A:H3'  | 24:DA:1745:A:H8   | 1.64                     | 0.62              |
| 24:DA:2052:A:O2'  | 24:DA:2053:G:H5'  | 1.99                     | 0.62              |
| 24:DA:2344:U:O2'  | 24:DA:2345:G:H5'' | 1.99                     | 0.62              |
| 24:DA:2695:U:H2'  | 24:DA:2696:U:C6   | 2.34                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:271:G:O2'   | 24:DA:272:A:C5'   | 2.43                     | 0.62              |
| 24:DA:2788:C:O2'  | 24:DA:2809:A:N3   | 2.26                     | 0.62              |
| 24:DA:41:C:H2'    | 24:DA:42:A:C8     | 2.35                     | 0.62              |
| 24:DA:834:G:H1'   | 24:DA:2358:A:N3   | 2.15                     | 0.62              |
| 28:DE:108:ILE:O   | 28:DE:112:LEU:HB2 | 1.99                     | 0.62              |
| 29:DF:48:LEU:HD23 | 29:DF:48:LEU:H    | 1.64                     | 0.62              |
| 43:DT:29:THR:H    | 43:DT:87:LEU:CB   | 2.13                     | 0.62              |
| 46:DW:13:ARG:HG3  | 46:DW:14:ASP:N    | 2.08                     | 0.62              |
| 21:AA:266:G:O2'   | 21:AA:267:C:P     | 2.57                     | 0.62              |
| 21:AA:375:U:C4    | 21:AA:376:G:N7    | 2.68                     | 0.62              |
| 2:AC:184:ASN:HD22 | 2:AC:185:THR:N    | 1.96                     | 0.62              |
| 2:AC:24:ASN:ND2   | 2:AC:25:THR:H     | 1.96                     | 0.62              |
| 11:AL:42:LYS:HB3  | 11:AL:43:LYS:HZ1  | 1.65                     | 0.62              |
| 24:BA:1973:G:C5   | 24:BA:1974:C:C5   | 2.88                     | 0.62              |
| 24:BA:2383:G:C4   | 24:BA:2384:U:C5   | 2.88                     | 0.62              |
| 35:BL:110:VAL:O   | 35:BL:111:ILE:HB  | 1.99                     | 0.62              |
| 38:BO:105:ALA:O   | 38:BO:106:LEU:HB3 | 2.00                     | 0.62              |
| 18:CS:33:TRP:HB2  | 55:CA:1014:A:C2   | 2.35                     | 0.62              |
| 55:CA:1533:C:C2'  | 55:CA:1534:A:H5'' | 2.29                     | 0.62              |
| 55:CA:358:U:H2'   | 55:CA:359:G:H8    | 1.64                     | 0.62              |
| 6:CG:124:SER:O    | 6:CG:128:GLU:HG2  | 1.99                     | 0.62              |
| 9:CJ:84:VAL:HG23  | 9:CJ:85:ASP:N     | 2.11                     | 0.62              |
| 35:DL:62:PRO:O    | 53:D3:12:ARG:HB3  | 1.99                     | 0.62              |
| 24:DA:1965:C:H2'  | 24:DA:1966:A:C8   | 2.35                     | 0.62              |
| 28:DE:88:ARG:HB3  | 28:DE:89:PRO:HD2  | 1.82                     | 0.62              |
| 32:DI:106:GLN:HA  | 32:DI:109:ALA:HB3 | 1.81                     | 0.62              |
| 49:DZ:23:LEU:HD12 | 49:DZ:28:LEU:HD21 | 1.80                     | 0.62              |
| 8:AI:17:ARG:HH22  | 21:AA:1129:C:C5'  | 2.12                     | 0.62              |
| 21:AA:1348:U:HO2' | 21:AA:1349:A:H8   | 1.46                     | 0.62              |
| 21:AA:1394:A:O2'  | 21:AA:1395:C:OP1  | 2.18                     | 0.62              |
| 21:AA:49:U:O4     | 21:AA:365:U:H5    | 1.82                     | 0.62              |
| 21:AA:595:A:H1'   | 21:AA:596:A:N7    | 2.15                     | 0.62              |
| 1:AB:75:ALA:O     | 1:AB:79:VAL:HG23  | 1.99                     | 0.62              |
| 7:AH:88:LYS:O     | 7:AH:91:LEU:HB2   | 2.00                     | 0.62              |
| 9:AJ:19:ASP:HA    | 9:AJ:22:THR:HB    | 1.82                     | 0.62              |
| 11:AL:2:THR:HB    | 11:AL:5:GLN:HG3   | 1.81                     | 0.62              |
| 11:AL:43:LYS:CD   | 11:AL:43:LYS:H    | 2.08                     | 0.62              |
| 24:BA:1021:A:N6   | 24:BA:1142:A:H61  | 1.98                     | 0.62              |
| 24:BA:1082:U:N3   | 24:BA:1086:A:C5   | 2.68                     | 0.62              |
| 24:BA:1717:A:H2'  | 24:BA:1718:G:O4'  | 1.98                     | 0.62              |
| 24:BA:216:A:H2'   | 24:BA:217:A:H8    | 1.64                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:1782:U:H1'   | 24:BA:2609:U:O4'   | 1.99                     | 0.62              |
| 25:BB:54:G:H2'     | 25:BB:55:U:H6      | 1.64                     | 0.62              |
| 26:BC:259:ASN:C    | 26:BC:261:ARG:H    | 2.03                     | 0.62              |
| 30:BG:29:ASN:CG    | 30:BG:30:GLY:N     | 2.51                     | 0.62              |
| 34:BK:71:ARG:HG3   | 34:BK:106:GLU:OE2  | 1.99                     | 0.62              |
| 35:BL:87:GLY:O     | 35:BL:89:VAL:N     | 2.31                     | 0.62              |
| 36:BM:45:GLN:O     | 36:BM:46:ILE:C     | 2.37                     | 0.62              |
| 46:BW:72:GLY:N     | 46:BW:73:PRO:HD2   | 2.14                     | 0.62              |
| 49:BZ:15:ARG:HG3   | 49:BZ:15:ARG:HH11  | 1.64                     | 0.62              |
| 55:CA:64:G:H4'     | 55:CA:65:A:H5''    | 1.81                     | 0.62              |
| 3:CD:90:LEU:HD11   | 3:CD:194:ILE:HD11  | 1.82                     | 0.62              |
| 53:D3:41:ARG:CG    | 53:D3:41:ARG:HH21  | 2.13                     | 0.62              |
| 24:DA:1103:A:H8    | 24:DA:1103:A:O5'   | 1.82                     | 0.62              |
| 24:DA:1338:G:H4'   | 43:DT:18:GLU:OE2   | 1.99                     | 0.62              |
| 24:DA:1397:U:H5''  | 24:DA:1398:C:H5    | 1.65                     | 0.62              |
| 24:DA:1440:U:C2    | 24:DA:1441:G:C8    | 2.88                     | 0.62              |
| 24:DA:16:C:H2'     | 24:DA:17:G:C8      | 2.32                     | 0.62              |
| 24:DA:1906:G:C2    | 24:DA:1925:C:O2    | 2.53                     | 0.62              |
| 24:DA:2547:A:H1'   | 24:DA:2566:A:C6    | 2.34                     | 0.62              |
| 24:DA:2721:A:H2'   | 24:DA:2722:G:O4'   | 1.99                     | 0.62              |
| 24:DA:437:U:O2'    | 24:DA:438:G:O4'    | 2.15                     | 0.62              |
| 24:DA:629:G:H4'    | 24:DA:650:C:O2     | 1.99                     | 0.62              |
| 26:DC:28:PRO:HG3   | 26:DC:62:ARG:NH1   | 2.15                     | 0.62              |
| 28:DE:126:VAL:HG11 | 28:DE:134:LEU:HD22 | 1.81                     | 0.62              |
| 33:DJ:111:LYS:HB2  | 33:DJ:115:GLY:N    | 2.15                     | 0.62              |
| 21:AA:1003:G:H21   | 21:AA:1005:A:H5'   | 1.64                     | 0.62              |
| 21:AA:1087:G:N2    | 21:AA:1088:G:C4    | 2.67                     | 0.62              |
| 21:AA:5:U:O2'      | 21:AA:6:G:OP2      | 2.18                     | 0.62              |
| 21:AA:90:C:O2'     | 21:AA:91:U:C6      | 2.50                     | 0.62              |
| 1:AB:158:ASP:C     | 1:AB:180:ILE:HG23  | 2.19                     | 0.62              |
| 9:AJ:84:VAL:O      | 9:AJ:88:MET:HG2    | 2.00                     | 0.62              |
| 24:BA:1054:A:H2'   | 24:BA:1055:G:C8    | 2.35                     | 0.62              |
| 24:BA:1060:U:C4'   | 24:BA:1061:U:H5'   | 2.29                     | 0.62              |
| 24:BA:1456:G:C5    | 24:BA:1457:U:C5    | 2.88                     | 0.62              |
| 24:BA:1499:C:O2'   | 24:BA:1500:G:H5'   | 1.98                     | 0.62              |
| 24:BA:2103:C:H2'   | 24:BA:2104:C:H5'   | 1.82                     | 0.62              |
| 24:BA:2239:G:O2'   | 24:BA:2240:U:H5'   | 2.00                     | 0.62              |
| 24:BA:231:A:C6     | 24:BA:232:G:C2     | 2.88                     | 0.62              |
| 24:BA:572:A:OP1    | 24:BA:573:U:H5     | 1.83                     | 0.62              |
| 29:BF:34:THR:HG23  | 29:BF:89:THR:HG23  | 1.81                     | 0.62              |
| 33:BJ:88:THR:HG22  | 33:BJ:91:GLU:CG    | 2.30                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:542:G:O2'   | 55:CA:543:U:H5'   | 2.00                     | 0.62              |
| 55:CA:765:G:C5    | 55:CA:812:G:C5    | 2.88                     | 0.62              |
| 7:CH:102:VAL:HG22 | 7:CH:126:CYS:SG   | 2.40                     | 0.62              |
| 9:CJ:59:LYS:HG2   | 55:CA:972:C:H4'   | 1.82                     | 0.62              |
| 10:CK:15:VAL:HG13 | 10:CK:36:ARG:HH12 | 1.65                     | 0.62              |
| 19:CT:67:HIS:HB3  | 19:CT:68:LYS:HD2  | 1.81                     | 0.62              |
| 24:DA:2421:G:N7   | 53:D3:30:HIS:CD2  | 2.66                     | 0.62              |
| 24:DA:1073:A:H3'  | 24:DA:1074:G:C8   | 2.35                     | 0.62              |
| 24:DA:1213:A:H62  | 24:DA:1236:G:H1'  | 1.63                     | 0.62              |
| 24:DA:1655:A:H2'  | 24:DA:1656:C:C6   | 2.33                     | 0.62              |
| 24:DA:2638:G:O2'  | 24:DA:2639:A:C8   | 2.53                     | 0.62              |
| 24:DA:2686:G:C2   | 24:DA:2687:U:C2   | 2.87                     | 0.62              |
| 24:DA:753:A:C2    | 24:DA:754:U:N3    | 2.68                     | 0.62              |
| 24:DA:84:A:C5     | 24:DA:103:A:N6    | 2.68                     | 0.62              |
| 26:DC:171:VAL:N   | 26:DC:185:ALA:HB2 | 2.14                     | 0.62              |
| 24:DA:1567:G:H3'  | 26:DC:84:PRO:HG3  | 1.81                     | 0.62              |
| 27:DD:5:VAL:H     | 27:DD:32:ASN:ND2  | 1.97                     | 0.62              |
| 27:DD:68:PHE:HB3  | 27:DD:73:VAL:HA   | 1.81                     | 0.62              |
| 42:DS:28:LYS:HA   | 42:DS:70:LYS:HA   | 1.82                     | 0.62              |
| 21:AA:104:G:N2    | 21:AA:105:G:C4    | 2.68                     | 0.62              |
| 21:AA:1064:G:H1'  | 21:AA:1066:C:C5   | 2.34                     | 0.62              |
| 21:AA:1074:G:H2'  | 21:AA:1075:U:O4'  | 1.99                     | 0.62              |
| 21:AA:1137:C:H4'  | 21:AA:1138:G:H5'' | 1.81                     | 0.62              |
| 21:AA:1305:G:H22  | 21:AA:1331:G:H2'  | 1.63                     | 0.62              |
| 21:AA:1411:C:C2'  | 21:AA:1412:C:H5'  | 2.30                     | 0.62              |
| 21:AA:519:C:H2'   | 21:AA:520:A:H8    | 1.63                     | 0.62              |
| 7:AH:87:ARG:O     | 7:AH:121:GLY:HA3  | 2.00                     | 0.62              |
| 9:AJ:11:LYS:HE2   | 9:AJ:71:LEU:HD11  | 1.80                     | 0.62              |
| 10:AK:28:ASN:CG   | 10:AK:46:ALA:HB3  | 2.20                     | 0.62              |
| 6:AG:149:ALA:HB2  | 10:AK:60:PHE:HD2  | 1.64                     | 0.62              |
| 16:AQ:12:VAL:CB   | 16:AQ:21:VAL:HG22 | 2.30                     | 0.62              |
| 18:AS:17:LYS:HA   | 18:AS:20:LYS:HZ2  | 1.65                     | 0.62              |
| 22:AX:30:G:N3     | 22:AX:31:A:C8     | 2.67                     | 0.62              |
| 24:BA:1919:A:H2'  | 24:BA:1919:A:N3   | 2.14                     | 0.62              |
| 24:BA:1931:U:O2'  | 24:BA:1932:A:H5'  | 2.00                     | 0.62              |
| 24:BA:1977:A:H2'  | 24:BA:1978:A:O4'  | 1.99                     | 0.62              |
| 24:BA:2267:A:H3'  | 24:BA:2268:A:H5'' | 1.81                     | 0.62              |
| 24:BA:2728:U:O2'  | 24:BA:2729:G:H8   | 1.83                     | 0.62              |
| 24:BA:2794:C:C2   | 24:BA:2803:G:N2   | 2.68                     | 0.62              |
| 24:BA:704:G:H2'   | 24:BA:726:G:H22   | 1.64                     | 0.62              |
| 25:BB:56:G:H4'    | 25:BB:57:A:O5'    | 1.99                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BB:70:C:H2'     | 25:BB:71:C:H6      | 1.65                     | 0.62              |
| 30:BG:155:PRO:O    | 30:BG:170:THR:HA   | 2.00                     | 0.62              |
| 37:BN:73:ASN:HD22  | 37:BN:76:VAL:CG1   | 2.13                     | 0.62              |
| 39:BP:19:PHE:O     | 39:BP:20:ARG:HB3   | 1.99                     | 0.62              |
| 43:BT:32:LEU:N     | 43:BT:32:LEU:HD23  | 2.15                     | 0.62              |
| 43:BT:52:GLU:HG3   | 43:BT:52:GLU:O     | 2.00                     | 0.62              |
| 55:CA:61:G:O6      | 55:CA:107:G:C6     | 2.53                     | 0.62              |
| 8:CI:70:GLY:C      | 8:CI:71:ILE:HD12   | 2.20                     | 0.62              |
| 24:DA:1567:G:H1'   | 24:DA:1568:G:C6    | 2.35                     | 0.62              |
| 24:DA:708:G:N2     | 24:DA:724:U:H1'    | 2.15                     | 0.62              |
| 24:DA:832:U:P      | 35:DL:38:GLN:H     | 2.22                     | 0.62              |
| 28:DE:130:LYS:CB   | 28:DE:133:LEU:HB3  | 2.29                     | 0.62              |
| 28:DE:5:LEU:HA     | 28:DE:120:VAL:HG13 | 1.82                     | 0.62              |
| 30:DG:103:ASN:HD22 | 30:DG:111:PRO:HB2  | 1.64                     | 0.62              |
| 24:DA:2515:C:OP1   | 33:DJ:81:ILE:HG22  | 2.00                     | 0.62              |
| 36:DM:49:ALA:HB2   | 36:DM:123:LYS:HB2  | 1.82                     | 0.62              |
| 48:DY:2:LYS:HD2    | 48:DY:4:LYS:HE3    | 1.82                     | 0.62              |
| 21:AA:738:C:H2'    | 21:AA:739:C:H6     | 1.65                     | 0.61              |
| 21:AA:89:U:O2'     | 21:AA:90:C:C5'     | 2.48                     | 0.61              |
| 24:BA:10:A:H2'     | 24:BA:11:C:H5'     | 1.80                     | 0.61              |
| 24:BA:1734:G:H2'   | 24:BA:1735:A:H8    | 1.65                     | 0.61              |
| 24:BA:2209:G:C6    | 24:BA:2210:U:C4    | 2.87                     | 0.61              |
| 24:BA:2352:A:N1    | 46:BW:30:VAL:HG11  | 2.15                     | 0.61              |
| 24:BA:2521:C:C2    | 24:BA:2545:G:N2    | 2.68                     | 0.61              |
| 24:BA:2716:C:O2'   | 24:BA:2717:C:H5'   | 2.00                     | 0.61              |
| 25:BB:51:G:H21     | 25:BB:53:A:H62     | 1.47                     | 0.61              |
| 27:BD:12:THR:CG2   | 27:BD:13:ARG:N     | 2.63                     | 0.61              |
| 32:BI:105:LEU:HA   | 32:BI:108:ILE:HB   | 1.82                     | 0.61              |
| 33:BJ:88:THR:HG22  | 33:BJ:91:GLU:HB2   | 1.82                     | 0.61              |
| 24:BA:1996:C:H5    | 34:BK:32:TYR:HH    | 1.48                     | 0.61              |
| 44:BU:73:ASN:HD22  | 44:BU:76:THR:H     | 1.48                     | 0.61              |
| 55:CA:1067:A:H1'   | 55:CA:1068:G:C8    | 2.35                     | 0.61              |
| 55:CA:1440:U:OP2   | 55:CA:1440:U:H6    | 1.82                     | 0.61              |
| 55:CA:404:G:H2'    | 55:CA:405:U:C6     | 2.33                     | 0.61              |
| 14:CO:42:PHE:CZ    | 14:CO:52:ARG:HA    | 2.35                     | 0.61              |
| 19:CT:26:MET:HE3   | 19:CT:30:PHE:CD1   | 2.34                     | 0.61              |
| 24:DA:1033:U:H4'   | 24:DA:1034:G:OP1   | 1.98                     | 0.61              |
| 24:DA:1625:C:H5''  | 24:DA:1626:A:OP2   | 2.00                     | 0.61              |
| 24:DA:2211:A:OP2   | 24:DA:2211:A:H4'   | 2.00                     | 0.61              |
| 24:DA:2468:A:O2'   | 24:DA:2469:A:C8    | 2.53                     | 0.61              |
| 24:DA:2638:G:O2'   | 24:DA:2639:A:H8    | 1.83                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:2766:A:N3   | 24:DA:2766:A:H2'   | 2.13                     | 0.61              |
| 24:DA:45:G:H5'    | 24:DA:46:G:H5'     | 1.81                     | 0.61              |
| 24:DA:500:G:N2    | 24:DA:503:A:C8     | 2.68                     | 0.61              |
| 24:DA:686:U:H2'   | 24:DA:788:A:C2     | 2.35                     | 0.61              |
| 24:DA:866:A:O2'   | 24:DA:867:C:C6     | 2.53                     | 0.61              |
| 56:DB:116:G:H2'   | 56:DB:117:G:H8     | 1.65                     | 0.61              |
| 36:DM:50:ARG:O    | 36:DM:53:MET:HB3   | 1.99                     | 0.61              |
| 43:DT:48:GLN:HA   | 43:DT:48:GLN:HE21  | 1.65                     | 0.61              |
| 44:DU:10:VAL:HG12 | 44:DU:71:ILE:HA    | 1.82                     | 0.61              |
| 45:DV:6:ALA:HB3   | 45:DV:65:VAL:HB    | 1.81                     | 0.61              |
| 47:DX:32:LEU:HD13 | 47:DX:50:VAL:O     | 2.00                     | 0.61              |
| 21:AA:1378:C:C5   | 21:AA:1379:G:C8    | 2.88                     | 0.61              |
| 21:AA:68:G:C6     | 21:AA:69:G:H1'     | 2.35                     | 0.61              |
| 21:AA:827:U:O4    | 21:AA:870:U:H1'    | 1.99                     | 0.61              |
| 7:AH:106:SER:O    | 21:AA:641:U:H4'    | 1.99                     | 0.61              |
| 51:B1:39:ASP:OD1  | 51:B1:42:VAL:HB    | 1.99                     | 0.61              |
| 24:BA:1442:U:H2'  | 24:BA:1443:U:C6    | 2.35                     | 0.61              |
| 24:BA:572:A:C2    | 24:BA:2033:A:C2    | 2.88                     | 0.61              |
| 24:BA:2183:A:H2'  | 24:BA:2184:A:C8    | 2.36                     | 0.61              |
| 24:BA:2305:U:C4   | 24:BA:2306:C:N3    | 2.69                     | 0.61              |
| 24:BA:2879:A:H4'  | 24:BA:2880:C:OP1   | 2.00                     | 0.61              |
| 24:BA:790:U:HO2'  | 24:BA:791:C:C5'    | 2.13                     | 0.61              |
| 26:BC:52:HIS:CE1  | 26:BC:218:THR:HG23 | 2.35                     | 0.61              |
| 24:BA:2313:C:H5'' | 29:BF:87:LYS:HD3   | 1.82                     | 0.61              |
| 33:BJ:18:VAL:HG22 | 33:BJ:140:LEU:CD1  | 2.30                     | 0.61              |
| 37:BN:70:THR:HB   | 37:BN:75:ILE:HD11  | 1.82                     | 0.61              |
| 46:BW:24:ARG:HB2  | 46:BW:65:LYS:HD3   | 1.81                     | 0.61              |
| 55:CA:219:U:H2'   | 55:CA:220:G:H8     | 1.64                     | 0.61              |
| 55:CA:717:U:C4    | 55:CA:734:G:N7     | 2.68                     | 0.61              |
| 55:CA:858:G:O6    | 59:CA:1824:HOH:O   | 2.16                     | 0.61              |
| 55:CA:913:A:H1'   | 55:CA:914:A:O4'    | 2.00                     | 0.61              |
| 3:CD:30:LYS:HD3   | 3:CD:30:LYS:N      | 2.15                     | 0.61              |
| 5:CF:45:ARG:HG2   | 5:CF:46:GLN:H      | 1.66                     | 0.61              |
| 24:DA:1346:G:H2'  | 24:DA:1347:A:H8    | 1.65                     | 0.61              |
| 24:DA:1355:G:N2   | 24:DA:1377:G:H1'   | 2.15                     | 0.61              |
| 24:DA:1923:U:H2'  | 24:DA:1924:C:H6    | 1.64                     | 0.61              |
| 24:DA:1944:U:O4'  | 24:DA:1955:U:H1'   | 2.00                     | 0.61              |
| 24:DA:2093:G:C6   | 24:DA:2225:A:C8    | 2.88                     | 0.61              |
| 24:DA:2303:G:H2'  | 24:DA:2304:G:C8    | 2.33                     | 0.61              |
| 24:DA:2340:A:H2'  | 24:DA:2341:G:C8    | 2.36                     | 0.61              |
| 24:DA:2543:G:O4'  | 24:DA:2766:A:H5''  | 2.00                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:2544:G:H5'  | 24:DA:2645:G:C8   | 2.35                     | 0.61              |
| 24:DA:2728:U:O2'  | 24:DA:2729:G:C8   | 2.50                     | 0.61              |
| 24:DA:323:C:OP1   | 24:DA:324:A:H8    | 1.83                     | 0.61              |
| 24:DA:85:G:O2'    | 24:DA:86:G:H8     | 1.80                     | 0.61              |
| 26:DC:175:LEU:O   | 26:DC:178:GLY:N   | 2.31                     | 0.61              |
| 37:DN:12:ARG:HG3  | 37:DN:13:ASN:H    | 1.64                     | 0.61              |
| 41:DR:80:ARG:HA   | 41:DR:80:ARG:HE   | 1.64                     | 0.61              |
| 46:DW:67:LYS:HB3  | 46:DW:80:SER:HB2  | 1.82                     | 0.61              |
| 49:DZ:30:ARG:HH21 | 49:DZ:33:HIS:HB2  | 1.63                     | 0.61              |
| 21:AA:1203:C:H2'  | 21:AA:1204:A:H8   | 1.65                     | 0.61              |
| 21:AA:1228:C:O2'  | 21:AA:1229:A:C8   | 2.52                     | 0.61              |
| 21:AA:174:A:H2'   | 21:AA:175:C:C6    | 2.34                     | 0.61              |
| 21:AA:806:C:H2'   | 21:AA:807:A:C8    | 2.34                     | 0.61              |
| 21:AA:82:G:O2'    | 21:AA:83:C:H4'    | 2.00                     | 0.61              |
| 1:AB:160:LEU:O    | 1:AB:183:PHE:HD2  | 1.84                     | 0.61              |
| 2:AC:139:ASN:HA   | 2:AC:142:ARG:HB2  | 1.81                     | 0.61              |
| 4:AE:32:PHE:HD2   | 4:AE:54:GLU:CA    | 2.12                     | 0.61              |
| 13:AN:62:ARG:HB3  | 13:AN:67:GLY:HA2  | 1.82                     | 0.61              |
| 15:AP:52:LEU:O    | 15:AP:54:LEU:HD12 | 2.00                     | 0.61              |
| 24:BA:1649:G:O6   | 24:BA:2009:A:N6   | 2.33                     | 0.61              |
| 24:BA:2791:G:H2'  | 24:BA:2792:A:H8   | 1.65                     | 0.61              |
| 24:BA:2796:U:C4   | 24:BA:2798:U:C4   | 2.89                     | 0.61              |
| 24:BA:322:A:C2    | 24:BA:340:A:C6    | 2.88                     | 0.61              |
| 24:BA:541:A:N1    | 24:BA:553:G:C6    | 2.69                     | 0.61              |
| 24:BA:746:U:HO2'  | 24:BA:747:U:P     | 2.23                     | 0.61              |
| 24:BA:799:G:N1    | 24:BA:800:A:N6    | 2.48                     | 0.61              |
| 24:BA:923:G:H5'   | 46:BW:25:PHE:CZ   | 2.35                     | 0.61              |
| 46:BW:77:LYS:O    | 46:BW:78:PHE:HB2  | 1.99                     | 0.61              |
| 49:BZ:3:THR:C     | 49:BZ:4:ILE:HG22  | 2.20                     | 0.61              |
| 55:CA:1095:U:H2'  | 55:CA:1096:C:H6   | 1.62                     | 0.61              |
| 55:CA:656:G:N2    | 55:CA:751:U:C2    | 2.67                     | 0.61              |
| 4:CE:93:VAL:HG12  | 4:CE:126:ALA:HB1  | 1.81                     | 0.61              |
| 4:CE:131:ASN:C    | 4:CE:131:ASN:HD22 | 2.03                     | 0.61              |
| 8:CI:97:LEU:HA    | 8:CI:100:ALA:HB3  | 1.82                     | 0.61              |
| 15:CP:52:LEU:O    | 15:CP:53:ASP:HB2  | 2.00                     | 0.61              |
| 24:DA:1346:G:H2'  | 24:DA:1347:A:C8   | 2.36                     | 0.61              |
| 24:DA:1554:U:H5'' | 24:DA:1555:G:OP2  | 2.00                     | 0.61              |
| 24:DA:1716:U:HO2' | 24:DA:1717:A:H8   | 0.70                     | 0.61              |
| 24:DA:1992:G:H22  | 24:DA:1996:C:H2'  | 1.66                     | 0.61              |
| 24:DA:2468:A:O2'  | 24:DA:2469:A:H8   | 1.83                     | 0.61              |
| 24:DA:2629:U:H5'' | 24:DA:2630:G:OP1  | 2.00                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:422:A:H2'   | 24:DA:423:A:C8     | 2.35                     | 0.61              |
| 24:DA:444:C:O2'   | 24:DA:445:C:H5'    | 1.99                     | 0.61              |
| 27:DD:16:THR:HG22 | 27:DD:20:VAL:N     | 2.15                     | 0.61              |
| 29:DF:169:LEU:HB3 | 29:DF:174:PHE:HB2  | 1.82                     | 0.61              |
| 33:DJ:73:VAL:HB   | 33:DJ:75:TYR:CE2   | 2.35                     | 0.61              |
| 21:AA:1076:U:C2   | 21:AA:1077:G:C8    | 2.89                     | 0.61              |
| 21:AA:31:G:H21    | 21:AA:46:G:H5''    | 1.64                     | 0.61              |
| 21:AA:954:G:C6    | 21:AA:955:U:N3     | 2.68                     | 0.61              |
| 51:B1:24:LYS:HE2  | 51:B1:52:LYS:HB2   | 1.82                     | 0.61              |
| 24:BA:1131:G:C4   | 33:BJ:77:HIS:ND1   | 2.68                     | 0.61              |
| 24:BA:1179:G:C2   | 24:BA:1180:U:O2'   | 2.53                     | 0.61              |
| 24:BA:1815:A:H1'  | 24:BA:1817:G:C8    | 2.35                     | 0.61              |
| 24:BA:2492:U:H2'  | 24:BA:2493:U:C6    | 2.35                     | 0.61              |
| 24:BA:271:G:HO2'  | 24:BA:272:A:H8     | 1.49                     | 0.61              |
| 24:BA:794:A:H2'   | 24:BA:795:C:H6     | 1.66                     | 0.61              |
| 24:BA:2680:U:H5'  | 27:BD:194:PRO:HA   | 1.82                     | 0.61              |
| 31:BH:62:LEU:HD12 | 31:BH:63:ALA:N     | 2.15                     | 0.61              |
| 33:BJ:88:THR:HG22 | 33:BJ:91:GLU:CB    | 2.31                     | 0.61              |
| 55:CA:1129:C:O2'  | 55:CA:1130:A:C8    | 2.53                     | 0.61              |
| 55:CA:60:A:H4'    | 55:CA:61:G:O5'     | 1.99                     | 0.61              |
| 55:CA:722:G:N3    | 55:CA:722:G:H2'    | 2.15                     | 0.61              |
| 55:CA:801:U:O2'   | 55:CA:802:A:H5'    | 2.01                     | 0.61              |
| 2:CC:149:LYS:HG3  | 2:CC:168:ARG:HB2   | 1.82                     | 0.61              |
| 12:CM:2:ARG:HA    | 12:CM:7:ASN:O      | 1.99                     | 0.61              |
| 13:CN:6:LYS:O     | 13:CN:10:VAL:HG23  | 2.00                     | 0.61              |
| 20:CU:28:LEU:HD23 | 20:CU:29:ALA:N     | 2.16                     | 0.61              |
| 24:DA:1177:G:H2'  | 24:DA:1178:C:C6    | 2.36                     | 0.61              |
| 24:DA:1570:A:C6   | 24:DA:1571:A:C6    | 2.89                     | 0.61              |
| 24:DA:2092:U:H4'  | 24:DA:2093:G:C5'   | 2.18                     | 0.61              |
| 24:DA:2240:U:O2'  | 24:DA:2241:A:O4'   | 2.18                     | 0.61              |
| 24:DA:2310:C:H42  | 29:DF:76:PHE:HZ    | 1.47                     | 0.61              |
| 24:DA:565:C:H2'   | 24:DA:566:U:O4'    | 2.00                     | 0.61              |
| 24:DA:637:A:OP2   | 35:DL:112:LEU:HD22 | 2.01                     | 0.61              |
| 27:DD:45:TYR:HE2  | 27:DD:47:ALA:HB3   | 1.65                     | 0.61              |
| 31:DH:68:ARG:CD   | 31:DH:71:LYS:HD3   | 2.30                     | 0.61              |
| 33:DJ:45:THR:HG21 | 33:DJ:50:THR:HG23  | 1.82                     | 0.61              |
| 35:DL:110:VAL:HB  | 35:DL:127:VAL:HA   | 1.83                     | 0.61              |
| 41:DR:21:ARG:HB2  | 41:DR:93:PHE:CD1   | 2.35                     | 0.61              |
| 21:AA:1055:A:N6   | 21:AA:1206:G:C6    | 2.68                     | 0.61              |
| 21:AA:845:A:H3'   | 21:AA:846:G:O4'    | 2.00                     | 0.61              |
| 21:AA:964:A:OP1   | 59:AA:1829:HOH:O   | 2.16                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AN:20:PHE:C     | 13:AN:22:LYS:N     | 2.54                     | 0.61              |
| 16:AQ:44:HIS:O     | 16:AQ:70:LYS:HA    | 2.00                     | 0.61              |
| 21:AA:1230:C:C5'   | 22:AV:30:G:H5''    | 2.30                     | 0.61              |
| 24:BA:669:G:H3'    | 24:BA:670:A:C8     | 2.35                     | 0.61              |
| 24:BA:852:U:H2'    | 24:BA:853:C:C6     | 2.35                     | 0.61              |
| 27:BD:114:LYS:HZ2  | 27:BD:116:LYS:HE2  | 1.65                     | 0.61              |
| 32:BI:10:LEU:HD13  | 32:BI:27:LEU:HA    | 1.83                     | 0.61              |
| 37:BN:38:LEU:HD12  | 37:BN:38:LEU:C     | 2.21                     | 0.61              |
| 37:BN:73:ASN:HA    | 37:BN:76:VAL:CG1   | 2.26                     | 0.61              |
| 42:BS:14:ALA:O     | 42:BS:18:ARG:HG3   | 2.00                     | 0.61              |
| 3:CD:195:ASN:HB3   | 3:CD:197:HIS:NE2   | 2.15                     | 0.61              |
| 11:CL:91:GLY:O     | 11:CL:93:ARG:HG3   | 1.99                     | 0.61              |
| 12:CM:106:ARG:HH21 | 12:CM:112:ARG:CZ   | 2.13                     | 0.61              |
| 24:DA:686:U:C4     | 52:D2:12:ARG:HG3   | 2.35                     | 0.61              |
| 24:DA:942:G:O2'    | 24:DA:1189:A:H1'   | 2.01                     | 0.61              |
| 24:DA:1698:A:H1'   | 24:DA:1700:A:OP2   | 2.00                     | 0.61              |
| 24:DA:2284:A:H1'   | 24:DA:2325:G:N2    | 2.15                     | 0.61              |
| 24:DA:2297:A:N6    | 24:DA:2319:G:O2'   | 2.33                     | 0.61              |
| 24:DA:2544:G:H2'   | 24:DA:2545:G:C8    | 2.35                     | 0.61              |
| 24:DA:292:U:H2'    | 24:DA:293:U:C6     | 2.36                     | 0.61              |
| 24:DA:279:A:H61    | 24:DA:361:G:H1'    | 1.65                     | 0.61              |
| 24:DA:444:C:O2'    | 24:DA:445:C:H6     | 1.75                     | 0.61              |
| 24:DA:927:A:H2'    | 24:DA:928:A:C8     | 2.35                     | 0.61              |
| 56:DB:86:G:HO2'    | 56:DB:87:U:H6      | 1.49                     | 0.61              |
| 28:DE:110:SER:O    | 28:DE:113:VAL:HG12 | 1.99                     | 0.61              |
| 33:DJ:5:THR:HA     | 33:DJ:44:TYR:CD2   | 2.35                     | 0.61              |
| 3:AD:43:ARG:C      | 3:AD:45:PRO:HD3    | 2.21                     | 0.61              |
| 8:AI:19:PHE:O      | 8:AI:62:LEU:HA     | 2.00                     | 0.61              |
| 9:AJ:14:ASP:CB     | 9:AJ:17:LEU:HB3    | 2.30                     | 0.61              |
| 24:BA:1061:U:H3'   | 24:BA:1062:G:H5''  | 1.83                     | 0.61              |
| 24:BA:1670:C:O2    | 24:BA:1670:C:H2'   | 2.00                     | 0.61              |
| 24:BA:1980:G:O2'   | 24:BA:1982:U:OP2   | 2.14                     | 0.61              |
| 24:BA:215:G:H4'    | 24:BA:216:A:H4'    | 1.83                     | 0.61              |
| 24:BA:2308:G:O2'   | 24:BA:2310:C:H5    | 1.74                     | 0.61              |
| 26:BC:230:PRO:CD   | 26:BC:246:PRO:HA   | 2.30                     | 0.61              |
| 26:BC:29:PHE:CE2   | 26:BC:31:PRO:HG2   | 2.35                     | 0.61              |
| 39:BP:3:ILE:HD13   | 39:BP:3:ILE:C      | 2.20                     | 0.61              |
| 55:CA:1233:G:H2'   | 55:CA:1234:C:C6    | 2.35                     | 0.61              |
| 55:CA:568:G:N2     | 55:CA:883:C:C2     | 2.68                     | 0.61              |
| 18:CS:50:VAL:HG11  | 18:CS:70:LEU:HB3   | 1.82                     | 0.61              |
| 22:CV:39:U:H2'     | 22:CV:40:C:H6      | 1.66                     | 0.61              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:DA:1395:A:H4'   | 24:DA:1397:U:C5   | 2.35                     | 0.61              |
| 24:DA:1438:U:H5'   | 24:DA:1517:G:OP1  | 2.01                     | 0.61              |
| 24:DA:1914:C:H2'   | 24:DA:1915:U:C6   | 2.36                     | 0.61              |
| 24:DA:1956:U:O2'   | 24:DA:1957:C:H5'  | 2.01                     | 0.61              |
| 24:DA:2064:C:O2'   | 24:DA:2065:C:O4'  | 2.15                     | 0.61              |
| 24:DA:2733:A:H2'   | 24:DA:2734:A:O4'  | 2.00                     | 0.61              |
| 24:DA:329:G:H4'    | 24:DA:330:A:OP1   | 2.00                     | 0.61              |
| 24:DA:33:C:O2      | 24:DA:447:A:N6    | 2.34                     | 0.61              |
| 24:DA:537:G:N2     | 24:DA:557:C:N4    | 2.48                     | 0.61              |
| 24:DA:77:G:O2'     | 24:DA:78:U:O4'    | 2.06                     | 0.61              |
| 24:DA:972:A:N1     | 24:DA:973:A:N6    | 2.48                     | 0.61              |
| 24:DA:1789:A:OP1   | 26:DC:219:VAL:HA  | 2.01                     | 0.61              |
| 35:DL:117:THR:HG22 | 35:DL:118:THR:H   | 1.66                     | 0.61              |
| 35:DL:141:LYS:HD2  | 35:DL:142:ILE:N   | 2.14                     | 0.61              |
| 35:DL:17:LYS:HZ3   | 35:DL:19:LEU:HD22 | 1.66                     | 0.61              |
| 49:DZ:40:THR:H     | 49:DZ:43:ILE:HD11 | 1.65                     | 0.61              |
| 21:AA:1382:C:O2'   | 21:AA:1383:C:H6   | 1.83                     | 0.61              |
| 20:AU:48:LYS:HG2   | 21:AA:723:U:H5''  | 1.82                     | 0.61              |
| 22:AX:27:G:H5''    | 22:AX:27:G:C8     | 2.32                     | 0.61              |
| 24:BA:1730:C:C2'   | 24:BA:1731:G:H5'' | 2.31                     | 0.61              |
| 24:BA:2388:A:C3'   | 24:BA:2389:G:H5'  | 2.29                     | 0.61              |
| 24:BA:272:A:O2'    | 24:BA:273:G:O4'   | 2.15                     | 0.61              |
| 24:BA:27:G:H1'     | 24:BA:513:A:N6    | 2.14                     | 0.61              |
| 24:BA:598:U:H2'    | 24:BA:599:A:H8    | 1.65                     | 0.61              |
| 24:BA:687:C:O2'    | 24:BA:1780:A:N1   | 2.33                     | 0.61              |
| 25:BB:20:G:C2      | 25:BB:64:G:C2     | 2.89                     | 0.61              |
| 25:BB:40:U:HO2'    | 25:BB:43:C:H5     | 1.44                     | 0.61              |
| 28:BE:146:VAL:HG23 | 28:BE:167:VAL:CG2 | 2.29                     | 0.61              |
| 28:BE:58:LYS:HG3   | 28:BE:71:GLY:HA2  | 1.82                     | 0.61              |
| 29:BF:134:GLN:H    | 29:BF:134:GLN:NE2 | 1.99                     | 0.61              |
| 30:BG:52:GLY:O     | 30:BG:53:PRO:O    | 2.19                     | 0.61              |
| 35:BL:65:GLY:O     | 35:BL:66:PHE:HB3  | 2.00                     | 0.61              |
| 36:BM:56:ALA:H     | 36:BM:58:LYS:H    | 1.47                     | 0.61              |
| 55:CA:1053:G:O6    | 55:CA:1199:U:H2'  | 2.00                     | 0.61              |
| 55:CA:384:G:H2'    | 55:CA:385:C:C6    | 2.35                     | 0.61              |
| 1:CB:163:ILE:CG2   | 1:CB:203:ASP:HA   | 2.31                     | 0.61              |
| 4:CE:13:LYS:HA     | 4:CE:13:LYS:HE2   | 1.81                     | 0.61              |
| 24:DA:1287:A:O2'   | 24:DA:1288:G:C5'  | 2.48                     | 0.61              |
| 24:DA:1341:G:O2'   | 24:DA:1398:C:H5'' | 2.01                     | 0.61              |
| 24:DA:2439:A:H1'   | 24:DA:2586:U:O3'  | 2.01                     | 0.61              |
| 24:DA:397:U:OP1    | 47:DX:30:PRO:CA   | 2.48                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:412:A:N7     | 24:DA:2412:A:H1'   | 2.15                     | 0.61              |
| 28:DE:119:ILE:HG13 | 28:DE:119:ILE:O    | 1.99                     | 0.61              |
| 31:DH:49:ALA:O     | 31:DH:53:GLU:N     | 2.34                     | 0.61              |
| 31:DH:57:LYS:HD2   | 31:DH:57:LYS:O     | 2.00                     | 0.61              |
| 4:AE:53:ARG:HH21   | 21:AA:1071:C:H5''  | 1.66                     | 0.61              |
| 6:AG:52:ARG:HH22   | 6:AG:121:ASN:HA    | 1.66                     | 0.61              |
| 7:AH:24:VAL:HG23   | 7:AH:62:LEU:HD21   | 1.83                     | 0.61              |
| 9:AJ:45:ARG:HB2    | 9:AJ:69:THR:HB     | 1.82                     | 0.61              |
| 13:AN:63:CYS:HB2   | 13:AN:79:SER:OG    | 2.00                     | 0.61              |
| 19:AT:81:GLN:HA    | 19:AT:84:LYS:HB2   | 1.82                     | 0.61              |
| 20:AU:19:LYS:C     | 20:AU:21:SER:H     | 2.04                     | 0.61              |
| 24:BA:1027:A:N1    | 24:BA:1126:A:C4    | 2.69                     | 0.61              |
| 24:BA:2291:U:H2'   | 24:BA:2292:U:C5    | 2.36                     | 0.61              |
| 24:BA:228:C:H4'    | 24:BA:229:C:H5''   | 1.83                     | 0.61              |
| 24:BA:460:A:H2'    | 24:BA:461:C:C6     | 2.36                     | 0.61              |
| 24:BA:1059:G:O2'   | 32:BI:128:ILE:HD13 | 2.01                     | 0.61              |
| 32:BI:89:SER:OG    | 32:BI:135:MET:HA   | 1.99                     | 0.61              |
| 38:BO:11:ALA:HB2   | 38:BO:96:GLY:N     | 2.14                     | 0.61              |
| 45:BV:21:ARG:HA    | 45:BV:25:LYS:O     | 2.00                     | 0.61              |
| 2:CC:191:THR:O     | 55:CA:1206:G:H4'   | 2.01                     | 0.61              |
| 6:CG:29:LEU:HG     | 55:CA:1240:U:C4    | 2.36                     | 0.61              |
| 55:CA:575:G:C6     | 55:CA:821:G:N7     | 2.69                     | 0.61              |
| 9:CJ:52:LEU:HD21   | 9:CJ:59:LYS:HA     | 1.83                     | 0.61              |
| 54:D4:3:VAL:O      | 54:D4:4:ARG:HB2    | 2.01                     | 0.61              |
| 24:DA:1586:A:H2'   | 24:DA:1587:G:H8    | 1.66                     | 0.61              |
| 24:DA:1311:G:N2    | 24:DA:1603:A:H62   | 1.87                     | 0.61              |
| 24:DA:2239:G:O2'   | 24:DA:2240:U:H6    | 1.83                     | 0.61              |
| 24:DA:391:A:H2'    | 24:DA:392:U:H6     | 1.66                     | 0.61              |
| 24:DA:962:G:H2'    | 24:DA:963:U:C6     | 2.36                     | 0.61              |
| 29:DF:39:VAL:HG22  | 29:DF:49:LEU:HG    | 1.83                     | 0.61              |
| 30:DG:167:VAL:HG23 | 30:DG:168:VAL:H    | 1.64                     | 0.61              |
| 39:DP:102:ARG:HD2  | 39:DP:106:ALA:O    | 1.99                     | 0.61              |
| 40:DQ:60:TRP:O     | 40:DQ:63:ARG:HG2   | 2.00                     | 0.61              |
| 46:DW:33:GLY:O     | 46:DW:34:SER:CB    | 2.48                     | 0.61              |
| 47:DX:6:VAL:HG22   | 47:DX:7:THR:HG23   | 1.82                     | 0.61              |
| 21:AA:33:A:H2'     | 21:AA:34:C:C6      | 2.35                     | 0.61              |
| 21:AA:428:G:C2     | 21:AA:430:A:N6     | 2.69                     | 0.61              |
| 21:AA:439:U:H2'    | 21:AA:440:C:H5'    | 1.81                     | 0.61              |
| 2:AC:46:LEU:HB3    | 2:AC:49:ALA:HB3    | 1.83                     | 0.61              |
| 7:AH:106:SER:HB3   | 21:AA:640:A:N3     | 2.16                     | 0.61              |
| 24:BA:1084:A:H2'   | 24:BA:1085:A:H8    | 1.66                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:1885:A:H2'   | 24:BA:1886:U:C6    | 2.36                     | 0.61              |
| 24:BA:2287:A:N7    | 24:BA:2289:G:C8    | 2.69                     | 0.61              |
| 29:BF:13:LYS:HD2   | 29:BF:13:LYS:C     | 2.20                     | 0.61              |
| 33:BJ:103:ILE:HG13 | 33:BJ:104:ALA:N    | 2.16                     | 0.61              |
| 33:BJ:88:THR:CG2   | 33:BJ:91:GLU:H     | 2.14                     | 0.61              |
| 40:BQ:18:LYS:O     | 40:BQ:21:LYS:HG3   | 2.00                     | 0.61              |
| 55:CA:1071:C:H2'   | 55:CA:1072:G:H8    | 1.66                     | 0.61              |
| 55:CA:1215:G:C2    | 55:CA:1216:A:C8    | 2.88                     | 0.61              |
| 16:CQ:70:LYS:HD3   | 55:CA:254:G:H5''   | 1.82                     | 0.61              |
| 55:CA:413:G:N2     | 55:CA:428:G:O2'    | 2.34                     | 0.61              |
| 55:CA:664:G:H2'    | 55:CA:666:G:OP1    | 2.01                     | 0.61              |
| 1:CB:30:ILE:HG21   | 1:CB:38:HIS:ND1    | 2.16                     | 0.61              |
| 13:CN:20:PHE:HE1   | 13:CN:54:SER:HB2   | 1.65                     | 0.61              |
| 24:DA:1430:G:O2'   | 24:DA:1431:A:H5'   | 2.01                     | 0.61              |
| 24:DA:1441:G:C6    | 24:DA:1442:U:C4    | 2.89                     | 0.61              |
| 24:DA:1734:G:O2'   | 24:DA:1735:A:H8    | 1.82                     | 0.61              |
| 24:DA:1809:A:C2'   | 24:DA:1810:A:C8    | 2.84                     | 0.61              |
| 24:DA:2021:C:H5''  | 24:DA:2022:U:OP2   | 2.01                     | 0.61              |
| 24:DA:2267:A:N6    | 24:DA:2271:G:O6    | 2.34                     | 0.61              |
| 24:DA:2333:A:C2    | 24:DA:2335:A:N6    | 2.69                     | 0.61              |
| 24:DA:2695:U:H2'   | 24:DA:2696:U:H6    | 1.65                     | 0.61              |
| 24:DA:2836:U:O2'   | 24:DA:2837:A:H5''  | 2.00                     | 0.61              |
| 24:DA:323:C:H3'    | 24:DA:323:C:OP2    | 2.01                     | 0.61              |
| 24:DA:70:G:O2'     | 24:DA:71:A:H5'     | 2.01                     | 0.61              |
| 24:DA:76:C:O2'     | 24:DA:77:G:C5'     | 2.49                     | 0.61              |
| 24:DA:851:C:H2'    | 24:DA:852:U:C6     | 2.35                     | 0.61              |
| 24:DA:861:A:H2'    | 24:DA:862:G:C8     | 2.36                     | 0.61              |
| 24:DA:923:G:H1'    | 46:DW:23:LYS:HZ1   | 1.62                     | 0.61              |
| 24:DA:945:A:H5'    | 24:DA:946:C:OP2    | 2.01                     | 0.61              |
| 27:DD:141:ARG:HB3  | 27:DD:141:ARG:NH1  | 2.16                     | 0.61              |
| 28:DE:105:LEU:HD23 | 28:DE:177:PRO:HG3  | 1.82                     | 0.61              |
| 28:DE:45:ALA:O     | 28:DE:46:GLN:HB2   | 2.00                     | 0.61              |
| 36:DM:38:ARG:O     | 36:DM:126:ILE:HG21 | 2.00                     | 0.61              |
| 36:DM:133:LYS:O    | 36:DM:134:THR:HB   | 2.00                     | 0.61              |
| 37:DN:33:ILE:HA    | 37:DN:114:GLU:HB2  | 1.83                     | 0.61              |
| 21:AA:198:G:O2'    | 21:AA:199:A:C8     | 2.40                     | 0.61              |
| 2:AC:46:LEU:HD21   | 2:AC:86:LEU:HD11   | 1.83                     | 0.61              |
| 3:AD:63:ILE:HG23   | 3:AD:64:TYR:CD1    | 2.35                     | 0.61              |
| 7:AH:45:ILE:HD12   | 7:AH:60:LEU:HD22   | 1.82                     | 0.61              |
| 15:AP:18:GLN:NE2   | 15:AP:35:ARG:HD2   | 2.16                     | 0.61              |
| 24:BA:2250:G:O5'   | 24:BA:2250:G:H8    | 1.84                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:860:U:C1'    | 24:BA:2268:A:H5'   | 2.31                     | 0.61              |
| 24:BA:327:G:O2'    | 24:BA:328:U:H5'    | 2.01                     | 0.61              |
| 24:BA:919:U:H6     | 24:BA:919:U:C4'    | 2.14                     | 0.61              |
| 24:BA:946:C:O2'    | 24:BA:947:A:H5'    | 2.00                     | 0.61              |
| 26:BC:94:LEU:HD12  | 26:BC:95:TYR:N     | 2.16                     | 0.61              |
| 28:BE:157:LEU:HG   | 28:BE:169:VAL:HG11 | 1.82                     | 0.61              |
| 34:BK:121:GLU:HG2  | 34:BK:122:VAL:HG23 | 1.82                     | 0.61              |
| 36:BM:101:VAL:HG13 | 36:BM:101:VAL:O    | 2.01                     | 0.61              |
| 55:CA:1077:G:C6    | 55:CA:1081:A:N6    | 2.69                     | 0.61              |
| 55:CA:205:A:C5     | 55:CA:206:C:N4     | 2.69                     | 0.61              |
| 55:CA:654:G:C2'    | 55:CA:655:A:C8     | 2.84                     | 0.61              |
| 55:CA:990:C:H2'    | 55:CA:991:U:O4'    | 2.01                     | 0.61              |
| 15:CP:66:THR:HG22  | 15:CP:67:ILE:N     | 2.16                     | 0.61              |
| 50:D0:30:ASP:OD1   | 50:D0:47:TYR:HB3   | 2.01                     | 0.61              |
| 24:DA:1014:A:C5    | 24:DA:1015:U:C5    | 2.89                     | 0.61              |
| 24:DA:1635:A:H2'   | 24:DA:1636:U:C6    | 2.36                     | 0.61              |
| 24:DA:214:G:H1'    | 24:DA:217:A:H5'    | 1.83                     | 0.61              |
| 24:DA:2611:C:O2'   | 24:DA:2612:C:O4'   | 2.18                     | 0.61              |
| 24:DA:2643:G:C5    | 24:DA:2644:G:N7    | 2.68                     | 0.61              |
| 24:DA:503:A:H5''   | 24:DA:504:A:O5'    | 2.01                     | 0.61              |
| 24:DA:867:C:HO2'   | 24:DA:868:U:H6     | 1.47                     | 0.61              |
| 30:DG:93:TYR:N     | 30:DG:93:TYR:CD2   | 2.67                     | 0.61              |
| 32:DI:109:ALA:HB1  | 32:DI:125:THR:HA   | 1.83                     | 0.61              |
| 33:DJ:94:ALA:O     | 33:DJ:95:ARG:HB3   | 2.01                     | 0.61              |
| 36:DM:41:LEU:C     | 36:DM:93:VAL:HG23  | 2.22                     | 0.61              |
| 45:DV:16:ALA:HA    | 45:DV:19:ARG:CZ    | 2.31                     | 0.61              |
| 21:AA:1091:U:H1'   | 21:AA:1095:U:O2    | 2.00                     | 0.60              |
| 4:AE:83:PRO:HB3    | 4:AE:96:GLN:HA     | 1.83                     | 0.60              |
| 6:AG:71:THR:O      | 6:AG:90:VAL:HG12   | 2.01                     | 0.60              |
| 19:AT:60:GLN:O     | 19:AT:66:ILE:HG22  | 2.00                     | 0.60              |
| 53:B3:30:HIS:O     | 53:B3:31:ILE:C     | 2.39                     | 0.60              |
| 24:BA:1429:G:C4    | 24:BA:1568:G:C2    | 2.88                     | 0.60              |
| 24:BA:1747:U:H2'   | 24:BA:1748:C:H6    | 1.66                     | 0.60              |
| 24:BA:2424:C:HO2'  | 24:BA:2429:G:H4'   | 1.65                     | 0.60              |
| 59:BA:3293:HOH:O   | 28:BE:98:LYS:HE2   | 2.00                     | 0.60              |
| 36:BM:132:THR:HG22 | 36:BM:133:LYS:N    | 2.16                     | 0.60              |
| 37:BN:55:ALA:HA    | 37:BN:80:PHE:CE1   | 2.35                     | 0.60              |
| 42:BS:73:LYS:CE    | 42:BS:74:ILE:H     | 2.12                     | 0.60              |
| 47:BX:3:VAL:HG22   | 47:BX:10:ARG:HB3   | 1.83                     | 0.60              |
| 55:CA:1036:A:C2'   | 55:CA:1037:C:H5'   | 2.31                     | 0.60              |
| 55:CA:1169:A:H2'   | 55:CA:1170:A:C8    | 2.36                     | 0.60              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 55:CA:1182:G:C3'   | 55:CA:1183:U:H5'  | 2.31                     | 0.60              |
| 55:CA:1242:G:N2    | 55:CA:1243:C:H1'  | 2.16                     | 0.60              |
| 55:CA:1514:G:H2'   | 55:CA:1515:G:H8   | 1.64                     | 0.60              |
| 55:CA:166:U:H2'    | 55:CA:167:A:H5'   | 1.83                     | 0.60              |
| 55:CA:765:G:C4     | 55:CA:812:G:C6    | 2.89                     | 0.60              |
| 1:CB:107:ARG:HA    | 1:CB:110:ILE:HG13 | 1.82                     | 0.60              |
| 8:CI:33:SER:H      | 8:CI:36:GLN:HG3   | 1.65                     | 0.60              |
| 13:CN:73:LEU:HD12  | 13:CN:83:VAL:HG21 | 1.83                     | 0.60              |
| 18:CS:54:ARG:HG2   | 18:CS:55:GLN:N    | 2.13                     | 0.60              |
| 24:DA:1830:C:H5'   | 26:DC:14:HIS:CE1  | 2.36                     | 0.60              |
| 24:DA:2093:G:C5    | 24:DA:2225:A:C5   | 2.89                     | 0.60              |
| 24:DA:2417:C:H2'   | 24:DA:2418:A:H8   | 1.66                     | 0.60              |
| 31:DH:61:VAL:HG13  | 31:DH:62:LEU:HG   | 1.83                     | 0.60              |
| 34:DK:13:ASN:N     | 34:DK:13:ASN:HD22 | 1.97                     | 0.60              |
| 37:DN:63:ARG:O     | 37:DN:67:PHE:HB2  | 2.01                     | 0.60              |
| 43:DT:58:VAL:HG23  | 43:DT:85:VAL:HA   | 1.83                     | 0.60              |
| 21:AA:888:G:H4'    | 21:AA:1488:G:O2'  | 2.00                     | 0.60              |
| 24:BA:1343:G:H2'   | 24:BA:1344:U:H6   | 1.65                     | 0.60              |
| 24:BA:2291:U:H2'   | 24:BA:2292:U:C6   | 2.36                     | 0.60              |
| 24:BA:2850:A:H2'   | 24:BA:2851:A:C8   | 2.36                     | 0.60              |
| 24:BA:796:C:H2'    | 24:BA:797:G:C8    | 2.31                     | 0.60              |
| 24:BA:826:U:O2'    | 35:BL:53:GLY:CA   | 2.47                     | 0.60              |
| 24:BA:854:C:O2     | 24:BA:924:G:C2    | 2.54                     | 0.60              |
| 29:BF:110:ILE:HG22 | 29:BF:110:ILE:O   | 1.99                     | 0.60              |
| 30:BG:132:LEU:HD23 | 30:BG:132:LEU:N   | 2.16                     | 0.60              |
| 24:BA:1064:C:H4'   | 32:BI:90:GLY:N    | 2.15                     | 0.60              |
| 24:BA:1190:G:OP1   | 35:BL:32:GLY:HA2  | 2.01                     | 0.60              |
| 35:BL:62:PRO:HG2   | 53:B3:24:LYS:HB3  | 1.82                     | 0.60              |
| 47:BX:52:ALA:O     | 47:BX:53:LYS:CB   | 2.48                     | 0.60              |
| 55:CA:588:G:C5     | 55:CA:589:U:C4    | 2.89                     | 0.60              |
| 55:CA:969:A:O2'    | 55:CA:970:C:H5'   | 2.02                     | 0.60              |
| 1:CB:58:LYS:HE2    | 1:CB:62:ARG:HD2   | 1.82                     | 0.60              |
| 4:CE:94:PHE:O      | 4:CE:124:ALA:HB1  | 2.00                     | 0.60              |
| 4:CE:24:VAL:HG23   | 4:CE:26:GLY:H     | 1.66                     | 0.60              |
| 18:CS:20:LYS:NZ    | 18:CS:27:LYS:HD3  | 2.16                     | 0.60              |
| 24:DA:1056:G:H1'   | 24:DA:1103:A:H61  | 1.64                     | 0.60              |
| 24:DA:1238:G:O2'   | 24:DA:1239:G:H5'  | 2.02                     | 0.60              |
| 24:DA:1360:G:H2'   | 24:DA:1361:G:H5'  | 1.83                     | 0.60              |
| 24:DA:1784:A:C4'   | 24:DA:1785:A:O5'  | 2.44                     | 0.60              |
| 24:DA:2489:U:H2'   | 24:DA:2490:G:O4'  | 2.01                     | 0.60              |
| 24:DA:2531:A:C4    | 24:DA:2532:G:C8   | 2.89                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:2571:U:C4   | 24:DA:2574:G:C8   | 2.89                     | 0.60              |
| 24:DA:2714:G:H2'  | 24:DA:2715:C:H6   | 1.65                     | 0.60              |
| 24:DA:477:A:H2'   | 24:DA:478:A:C8    | 2.35                     | 0.60              |
| 24:DA:522:A:H2'   | 24:DA:523:C:H6    | 1.66                     | 0.60              |
| 24:DA:671:C:O2'   | 24:DA:672:C:C6    | 2.54                     | 0.60              |
| 56:DB:65:U:H3'    | 56:DB:108:A:H62   | 1.64                     | 0.60              |
| 29:DF:74:ALA:HB3  | 29:DF:78:ILE:CD1  | 2.31                     | 0.60              |
| 34:DK:13:ASN:H    | 34:DK:13:ASN:ND2  | 1.99                     | 0.60              |
| 34:DK:76:VAL:HB   | 39:DP:72:VAL:HG22 | 1.82                     | 0.60              |
| 36:DM:25:ASP:OD2  | 45:DV:79:ARG:HD2  | 2.00                     | 0.60              |
| 24:DA:2336:A:N7   | 46:DW:40:ARG:NH2  | 2.49                     | 0.60              |
| 48:DY:28:LEU:HD11 | 48:DY:43:LEU:HD13 | 1.81                     | 0.60              |
| 20:AU:38:GLU:HB2  | 21:AA:1526:G:P    | 2.40                     | 0.60              |
| 21:AA:201:G:H5''  | 21:AA:202:G:OP2   | 2.01                     | 0.60              |
| 21:AA:270:A:H2'   | 21:AA:271:C:C6    | 2.37                     | 0.60              |
| 10:AK:125:LYS:O   | 10:AK:126:ARG:HB2 | 2.00                     | 0.60              |
| 13:AN:40:ARG:HH12 | 13:AN:44:VAL:CG2  | 2.13                     | 0.60              |
| 10:AK:124:LYS:O   | 20:AU:33:ARG:NE   | 2.34                     | 0.60              |
| 50:B0:9:ARG:CG    | 50:B0:9:ARG:HH21  | 2.14                     | 0.60              |
| 24:BA:1064:C:O3'  | 32:BI:90:GLY:HA2  | 2.02                     | 0.60              |
| 24:BA:1364:G:OP2  | 47:BX:1:SER:N     | 2.26                     | 0.60              |
| 24:BA:2279:G:N7   | 46:BW:10:ARG:NH2  | 2.48                     | 0.60              |
| 24:BA:27:G:N2     | 24:BA:512:G:O2'   | 2.34                     | 0.60              |
| 24:BA:509:C:H5''  | 24:BA:509:C:C6    | 2.35                     | 0.60              |
| 33:BJ:58:ASN:HD21 | 33:BJ:128:ASN:HB2 | 1.66                     | 0.60              |
| 33:BJ:64:VAL:O    | 33:BJ:65:THR:HB   | 2.00                     | 0.60              |
| 37:BN:23:ASN:ND2  | 37:BN:23:ASN:N    | 2.50                     | 0.60              |
| 48:BY:39:GLN:HB2  | 48:BY:41:HIS:HD2  | 1.64                     | 0.60              |
| 55:CA:1226:C:O2'  | 55:CA:1227:A:H5'  | 2.00                     | 0.60              |
| 55:CA:198:G:C2'   | 55:CA:199:A:H8    | 2.14                     | 0.60              |
| 55:CA:247:G:C6    | 55:CA:278:G:C2    | 2.88                     | 0.60              |
| 55:CA:801:U:H2'   | 55:CA:802:A:H8    | 1.66                     | 0.60              |
| 1:CB:212:TYR:HA   | 1:CB:215:ALA:HB3  | 1.82                     | 0.60              |
| 6:CG:110:ARG:HG2  | 6:CG:112:ASP:OD1  | 2.02                     | 0.60              |
| 11:CL:113:ARG:HB3 | 11:CL:118:VAL:HB  | 1.84                     | 0.60              |
| 11:CL:2:THR:HB    | 11:CL:5:GLN:H     | 1.65                     | 0.60              |
| 12:CM:28:ARG:HD2  | 12:CM:28:ARG:O    | 2.01                     | 0.60              |
| 12:CM:2:ARG:HD2   | 12:CM:8:ILE:HG23  | 1.82                     | 0.60              |
| 24:DA:1051:G:H2'  | 24:DA:1052:C:C6   | 2.36                     | 0.60              |
| 24:DA:127:A:H5''  | 24:DA:128:C:C6    | 2.36                     | 0.60              |
| 24:DA:2259:U:C2   | 24:DA:2260:C:C5   | 2.89                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:279:A:N6    | 24:DA:361:G:H1'   | 2.16                     | 0.60              |
| 26:DC:144:GLU:HG3 | 26:DC:151:GLY:N   | 2.16                     | 0.60              |
| 28:DE:24:ASN:HB3  | 28:DE:27:LEU:HB3  | 1.82                     | 0.60              |
| 28:DE:47:LYS:CB   | 28:DE:51:GLU:HB2  | 2.30                     | 0.60              |
| 35:DL:92:LEU:CD2  | 35:DL:124:GLY:HA3 | 2.31                     | 0.60              |
| 21:AA:251:G:C6    | 21:AA:266:G:O6    | 2.54                     | 0.60              |
| 21:AA:790:A:C6    | 21:AA:791:G:C6    | 2.89                     | 0.60              |
| 4:AE:123:LEU:O    | 4:AE:124:ALA:HB2  | 2.01                     | 0.60              |
| 7:AH:1:SER:HB2    | 21:AA:877:G:H21   | 1.67                     | 0.60              |
| 54:B4:36:ARG:CG   | 54:B4:37:GLN:H    | 1.99                     | 0.60              |
| 24:BA:1122:G:N3   | 24:BA:1122:G:H2'  | 2.16                     | 0.60              |
| 24:BA:1779:U:C5   | 24:BA:1784:A:N7   | 2.69                     | 0.60              |
| 24:BA:2725:A:O2'  | 24:BA:2726:A:O5'  | 2.16                     | 0.60              |
| 24:BA:448:U:H4'   | 24:BA:449:A:OP2   | 2.01                     | 0.60              |
| 24:BA:616:A:H2'   | 24:BA:617:G:C8    | 2.37                     | 0.60              |
| 28:BE:37:ALA:C    | 28:BE:39:ALA:H    | 2.05                     | 0.60              |
| 29:BF:43:ILE:HG22 | 29:BF:82:TYR:CE1  | 2.37                     | 0.60              |
| 34:BK:118:LEU:O   | 34:BK:119:ALA:O   | 2.19                     | 0.60              |
| 34:BK:11:ALA:O    | 34:BK:99:ILE:HA   | 2.02                     | 0.60              |
| 37:BN:73:ASN:O    | 37:BN:76:VAL:HG12 | 2.02                     | 0.60              |
| 40:BQ:57:ARG:NH2  | 40:BQ:92:LYS:HD2  | 2.17                     | 0.60              |
| 40:BQ:93:ILE:HG23 | 40:BQ:94:LEU:N    | 2.16                     | 0.60              |
| 46:BW:23:LYS:HE3  | 46:BW:24:ARG:HG3  | 1.82                     | 0.60              |
| 55:CA:1256:A:C4   | 55:CA:1278:G:C6   | 2.90                     | 0.60              |
| 55:CA:1316:G:N2   | 55:CA:1318:A:H3'  | 2.17                     | 0.60              |
| 55:CA:106:C:O2    | 55:CA:379:C:H4'   | 2.01                     | 0.60              |
| 55:CA:509:A:C2    | 55:CA:510:A:C2    | 2.89                     | 0.60              |
| 8:CI:27:ILE:HA    | 8:CI:62:LEU:HB2   | 1.82                     | 0.60              |
| 24:DA:1080:A:O2'  | 24:DA:1081:U:O4'  | 2.16                     | 0.60              |
| 24:DA:1282:U:H2'  | 24:DA:1283:G:O4'  | 2.01                     | 0.60              |
| 24:DA:1773:A:N7   | 24:DA:1829:A:H1'  | 2.15                     | 0.60              |
| 24:DA:2019:A:H4'  | 40:DQ:33:VAL:HG21 | 1.83                     | 0.60              |
| 24:DA:2235:G:H2'  | 24:DA:2236:U:C6   | 2.35                     | 0.60              |
| 24:DA:2746:U:H1'  | 30:DG:138:GLN:NE2 | 2.08                     | 0.60              |
| 24:DA:33:C:H2'    | 24:DA:446:G:N2    | 2.17                     | 0.60              |
| 24:DA:82:U:H2'    | 24:DA:83:A:O4'    | 2.01                     | 0.60              |
| 37:DN:99:LYS:O    | 50:D0:41:HIS:HB2  | 2.01                     | 0.60              |
| 38:DO:8:ILE:H     | 38:DO:8:ILE:HD12  | 1.65                     | 0.60              |
| 44:DU:3:LYS:HG2   | 44:DU:84:PHE:CZ   | 2.36                     | 0.60              |
| 46:DW:8:SER:O     | 46:DW:9:THR:HB    | 2.02                     | 0.60              |
| 21:AA:1050:G:O2'  | 21:AA:1051:C:H5'  | 2.01                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:1054:C:C5   | 22:AX:34:G:C1'    | 2.83                     | 0.60              |
| 21:AA:1443:C:H2'  | 21:AA:1444:U:O4'  | 2.01                     | 0.60              |
| 21:AA:197:A:O2'   | 21:AA:198:G:C8    | 2.54                     | 0.60              |
| 21:AA:543:U:C2'   | 21:AA:544:G:H5'   | 2.32                     | 0.60              |
| 21:AA:575:G:C6    | 21:AA:821:G:C8    | 2.90                     | 0.60              |
| 21:AA:724:G:O2'   | 21:AA:725:G:H5'   | 2.01                     | 0.60              |
| 21:AA:792:A:C4    | 21:AA:794:A:N6    | 2.70                     | 0.60              |
| 21:AA:914:A:H2'   | 21:AA:915:A:H8    | 1.66                     | 0.60              |
| 21:AA:977:A:H3'   | 21:AA:1362:A:H62  | 1.67                     | 0.60              |
| 1:AB:41:ASN:HD22  | 1:AB:42:LEU:H     | 1.48                     | 0.60              |
| 7:AH:74:ILE:HD12  | 7:AH:127:TYR:O    | 2.02                     | 0.60              |
| 19:AT:68:LYS:HB2  | 19:AT:68:LYS:NZ   | 2.16                     | 0.60              |
| 24:BA:1038:G:O2'  | 24:BA:1039:A:H5'  | 2.02                     | 0.60              |
| 24:BA:1105:U:H2'  | 24:BA:1106:G:H8   | 1.66                     | 0.60              |
| 24:BA:1022:G:N2   | 24:BA:1142:A:C2   | 2.62                     | 0.60              |
| 24:BA:1271:G:OP2  | 59:BA:3391:HOH:O  | 2.16                     | 0.60              |
| 24:BA:13:A:H4'    | 24:BA:14:A:OP1    | 2.01                     | 0.60              |
| 24:BA:200:U:O2'   | 24:BA:201:C:H5'   | 2.00                     | 0.60              |
| 24:BA:363:G:H2'   | 24:BA:364:C:H6    | 1.65                     | 0.60              |
| 24:BA:528:A:C8    | 24:BA:528:A:C3'   | 2.83                     | 0.60              |
| 24:BA:604:G:O6    | 24:BA:625:G:C6    | 2.54                     | 0.60              |
| 24:BA:812:C:H4'   | 40:BQ:12:ARG:HH22 | 1.66                     | 0.60              |
| 24:BA:92:U:H6     | 24:BA:92:U:H5''   | 1.66                     | 0.60              |
| 27:BD:118:PHE:HD2 | 27:BD:119:ALA:N   | 1.99                     | 0.60              |
| 28:BE:154:ASP:OD2 | 28:BE:157:LEU:HB3 | 2.02                     | 0.60              |
| 31:BH:31:VAL:O    | 31:BH:32:PRO:C    | 2.37                     | 0.60              |
| 46:BW:30:VAL:HG23 | 46:BW:60:ALA:O    | 2.02                     | 0.60              |
| 55:CA:1410:A:H5'' | 55:CA:1411:C:OP1  | 2.02                     | 0.60              |
| 55:CA:1423:G:H2'  | 55:CA:1424:U:H6   | 1.65                     | 0.60              |
| 55:CA:57:G:H2'    | 55:CA:58:C:C6     | 2.36                     | 0.60              |
| 10:CK:51:PHE:HE2  | 10:CK:64:VAL:HG21 | 1.65                     | 0.60              |
| 10:CK:74:LYS:HA   | 10:CK:78:ILE:HD11 | 1.83                     | 0.60              |
| 15:CP:56:ARG:O    | 15:CP:59:HIS:HB3  | 2.01                     | 0.60              |
| 24:DA:1303:G:H2'  | 24:DA:1304:A:C8   | 2.35                     | 0.60              |
| 24:DA:170:U:H2'   | 24:DA:171:U:H6    | 1.66                     | 0.60              |
| 24:DA:571:U:C2    | 24:DA:2030:A:C5   | 2.89                     | 0.60              |
| 24:DA:2624:G:H1'  | 50:D0:18:HIS:HE1  | 1.66                     | 0.60              |
| 56:DB:38:C:C4'    | 38:DO:100:HIS:NE2 | 2.63                     | 0.60              |
| 29:DF:160:LYS:HD3 | 29:DF:161:SER:N   | 2.17                     | 0.60              |
| 34:DK:19:VAL:HG12 | 34:DK:41:ILE:HG12 | 1.83                     | 0.60              |
| 46:DW:22:VAL:O    | 46:DW:23:LYS:HG3  | 2.02                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:1055:A:N6    | 21:AA:1206:G:C5    | 2.69                     | 0.60              |
| 21:AA:11:G:C5      | 21:AA:12:U:C5      | 2.90                     | 0.60              |
| 21:AA:1343:G:H2'   | 21:AA:1344:C:C6    | 2.36                     | 0.60              |
| 21:AA:182:A:C2     | 21:AA:184:G:C8     | 2.90                     | 0.60              |
| 21:AA:414:A:C2'    | 21:AA:415:A:H5'    | 2.31                     | 0.60              |
| 24:BA:1372:U:C2'   | 24:BA:1373:A:H5'   | 2.31                     | 0.60              |
| 24:BA:1854:A:N6    | 24:BA:1888:G:H1'   | 2.17                     | 0.60              |
| 24:BA:2762:C:N4    | 24:BA:2763:G:C6    | 2.70                     | 0.60              |
| 26:BC:236:GLY:O    | 26:BC:237:ARG:HB2  | 2.02                     | 0.60              |
| 28:BE:47:LYS:HB3   | 28:BE:51:GLU:HG3   | 1.82                     | 0.60              |
| 29:BF:131:VAL:HG22 | 29:BF:151:LEU:H    | 1.66                     | 0.60              |
| 30:BG:33:THR:CA    | 30:BG:34:ARG:HH11  | 2.14                     | 0.60              |
| 59:BA:3787:HOH:O   | 33:BJ:39:LYS:HE3   | 2.00                     | 0.60              |
| 44:BU:43:LYS:O     | 44:BU:57:ILE:HA    | 2.01                     | 0.60              |
| 46:BW:47:GLY:N     | 46:BW:80:SER:HB3   | 2.15                     | 0.60              |
| 55:CA:1135:U:H5'   | 55:CA:1136:C:OP2   | 2.01                     | 0.60              |
| 55:CA:1308:U:O2    | 55:CA:1330:U:C2    | 2.54                     | 0.60              |
| 16:CQ:67:SER:HA    | 55:CA:265:G:H4'    | 1.83                     | 0.60              |
| 55:CA:463:U:H2'    | 55:CA:464:U:C5     | 2.37                     | 0.60              |
| 55:CA:920:U:O2'    | 55:CA:921:U:H5'    | 2.02                     | 0.60              |
| 3:CD:31:CYS:O      | 3:CD:32:LYS:HB2    | 2.00                     | 0.60              |
| 6:CG:132:THR:O     | 6:CG:133:ALA:HB2   | 2.02                     | 0.60              |
| 12:CM:22:TYR:O     | 12:CM:65:GLU:HG2   | 2.01                     | 0.60              |
| 12:CM:80:MET:SD    | 12:CM:91:ARG:HB3   | 2.42                     | 0.60              |
| 15:CP:75:ILE:HA    | 15:CP:78:VAL:HG23  | 1.83                     | 0.60              |
| 20:CU:13:VAL:HG22  | 20:CU:15:LEU:HD23  | 1.83                     | 0.60              |
| 24:DA:222:A:N6     | 24:DA:232:G:H1'    | 2.16                     | 0.60              |
| 24:DA:757:G:H2'    | 24:DA:758:C:H5'    | 1.83                     | 0.60              |
| 24:DA:959:A:H2'    | 24:DA:960:A:H8     | 1.65                     | 0.60              |
| 29:DF:91:ARG:NH2   | 29:DF:91:ARG:HB3   | 2.16                     | 0.60              |
| 39:DP:86:LYS:HA    | 39:DP:86:LYS:NZ    | 2.17                     | 0.60              |
| 40:DQ:71:ASN:HD21  | 40:DQ:106:THR:HG23 | 1.67                     | 0.60              |
| 42:DS:71:VAL:O     | 42:DS:71:VAL:HG13  | 2.01                     | 0.60              |
| 21:AA:1194:U:H2'   | 21:AA:1195:C:C6    | 2.36                     | 0.60              |
| 18:AS:5:LYS:HA     | 21:AA:1313:U:OP2   | 2.02                     | 0.60              |
| 21:AA:587:G:N1     | 21:AA:755:G:C6     | 2.69                     | 0.60              |
| 21:AA:570:G:H1'    | 21:AA:820:U:C4     | 2.36                     | 0.60              |
| 21:AA:866:C:C4     | 21:AA:867:G:H1'    | 2.37                     | 0.60              |
| 21:AA:895:G:C4     | 21:AA:896:C:C5     | 2.89                     | 0.60              |
| 21:AA:95:C:H2'     | 21:AA:96:U:C6      | 2.36                     | 0.60              |
| 24:BA:1195:G:N2    | 24:BA:1196:C:C2    | 2.69                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:161:A:H3'   | 24:BA:162:U:H5''   | 1.83                     | 0.60              |
| 24:BA:2259:U:H2'  | 24:BA:2260:C:H6    | 1.66                     | 0.60              |
| 24:BA:2493:U:H2'  | 24:BA:2494:G:O4'   | 2.01                     | 0.60              |
| 24:BA:2832:U:O2   | 24:BA:2834:G:N1    | 2.34                     | 0.60              |
| 25:BB:76:G:O5'    | 25:BB:76:G:H8      | 1.83                     | 0.60              |
| 40:BQ:68:ALA:O    | 40:BQ:71:ASN:N     | 2.34                     | 0.60              |
| 47:BX:33:HIS:O    | 47:BX:34:SER:O     | 2.19                     | 0.60              |
| 55:CA:1228:C:O2'  | 55:CA:1229:A:H8    | 1.84                     | 0.60              |
| 55:CA:140:U:H2'   | 55:CA:141:G:O4'    | 2.02                     | 0.60              |
| 19:CT:35:TYR:OH   | 55:CA:259:G:H5'    | 2.01                     | 0.60              |
| 55:CA:714:G:H2'   | 55:CA:715:A:C8     | 2.37                     | 0.60              |
| 3:CD:59:LYS:O     | 3:CD:63:ILE:HG13   | 2.02                     | 0.60              |
| 10:CK:44:ALA:HB3  | 10:CK:69:CYS:HB2   | 1.83                     | 0.60              |
| 12:CM:69:ARG:HD2  | 12:CM:69:ARG:N     | 2.17                     | 0.60              |
| 22:CX:33:U:H5'    | 22:CX:34:G:OP2     | 2.02                     | 0.60              |
| 24:DA:1055:G:N3   | 24:DA:1055:G:H2'   | 2.16                     | 0.60              |
| 24:DA:1071:G:N7   | 24:DA:1089:A:C5    | 2.70                     | 0.60              |
| 24:DA:1196:C:H1'  | 24:DA:1226:A:C4    | 2.37                     | 0.60              |
| 24:DA:2674:G:H2'  | 24:DA:2675:A:C8    | 2.34                     | 0.60              |
| 24:DA:417:C:H2'   | 24:DA:418:C:O4'    | 2.01                     | 0.60              |
| 29:DF:103:ILE:HA  | 29:DF:107:VAL:HG21 | 1.84                     | 0.60              |
| 33:DJ:74:TYR:OH   | 33:DJ:100:VAL:HG13 | 2.01                     | 0.60              |
| 24:DA:627:A:H5''  | 35:DL:78:ARG:HH12  | 1.66                     | 0.60              |
| 21:AA:1034:G:H2'  | 21:AA:1035:A:C8    | 2.37                     | 0.60              |
| 21:AA:1082:A:C2   | 21:AA:1083:U:C2    | 2.90                     | 0.60              |
| 21:AA:15:G:C8     | 21:AA:1396:A:C2    | 2.89                     | 0.60              |
| 21:AA:274:A:O2'   | 21:AA:275:G:H8     | 1.84                     | 0.60              |
| 21:AA:324:G:O6    | 59:AA:1847:HOH:O   | 2.16                     | 0.60              |
| 4:AE:112:ALA:O    | 4:AE:116:VAL:HG13  | 2.01                     | 0.60              |
| 4:AE:84:VAL:HG23  | 4:AE:145:ASN:HD21  | 1.66                     | 0.60              |
| 5:AF:3:HIS:H      | 5:AF:92:THR:CG2    | 2.08                     | 0.60              |
| 24:BA:1079:C:C4   | 24:BA:1088:A:H2    | 2.18                     | 0.60              |
| 24:BA:1097:U:H3'  | 24:BA:1098:A:H4'   | 1.84                     | 0.60              |
| 24:BA:1115:G:HO2' | 24:BA:1116:G:P     | 2.25                     | 0.60              |
| 24:BA:1315:C:C2   | 24:BA:1338:G:N2    | 2.69                     | 0.60              |
| 24:BA:2063:C:C4   | 24:BA:2064:C:C5    | 2.89                     | 0.60              |
| 24:BA:2287:A:C8   | 24:BA:2289:G:C8    | 2.90                     | 0.60              |
| 24:BA:2353:G:O2'  | 46:BW:31:LEU:HD23  | 2.01                     | 0.60              |
| 24:BA:2404:U:O2   | 24:BA:2414:G:C2    | 2.54                     | 0.60              |
| 30:BG:85:LYS:HA   | 30:BG:130:ILE:O    | 2.01                     | 0.60              |
| 34:BK:64:ARG:NH1  | 34:BK:101:GLY:HA3  | 2.17                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BL:85:VAL:CG2  | 35:BL:94:THR:HG23  | 2.32                     | 0.60              |
| 38:BO:75:GLY:HA2  | 38:BO:106:LEU:HD12 | 1.83                     | 0.60              |
| 46:BW:24:ARG:O    | 46:BW:25:PHE:HB2   | 2.01                     | 0.60              |
| 55:CA:1167:A:N7   | 55:CA:1169:A:N6    | 2.49                     | 0.60              |
| 55:CA:120:A:H3'   | 55:CA:121:U:C5'    | 2.31                     | 0.60              |
| 55:CA:415:A:H3'   | 55:CA:416:G:H8     | 1.67                     | 0.60              |
| 55:CA:607:A:H2'   | 55:CA:608:A:C8     | 2.36                     | 0.60              |
| 55:CA:891:U:O2'   | 55:CA:892:A:H5'    | 2.01                     | 0.60              |
| 12:CM:69:ARG:NH2  | 55:CA:1330:U:H5'   | 2.17                     | 0.60              |
| 51:D1:5:ARG:HD2   | 51:D1:25:ASN:HB2   | 1.82                     | 0.60              |
| 24:DA:1008:A:OP1  | 24:DA:1008:A:H8    | 1.84                     | 0.60              |
| 24:DA:1078:U:H4'  | 24:DA:1079:C:H5''  | 1.83                     | 0.60              |
| 24:DA:1455:G:H2'  | 24:DA:1456:G:C8    | 2.36                     | 0.60              |
| 24:DA:1555:G:O2'  | 24:DA:1556:C:H5'   | 2.01                     | 0.60              |
| 24:DA:1738:G:O2'  | 24:DA:1739:A:H8    | 1.85                     | 0.60              |
| 24:DA:1738:G:O2'  | 24:DA:1739:A:C8    | 2.55                     | 0.60              |
| 24:DA:23:G:H2'    | 24:DA:24:G:H8      | 1.67                     | 0.60              |
| 26:DC:166:ARG:CB  | 26:DC:171:VAL:HG22 | 2.31                     | 0.60              |
| 30:DG:15:ASP:HB3  | 30:DG:26:LYS:H     | 1.67                     | 0.60              |
| 31:DH:93:SER:HB3  | 31:DH:121:VAL:HG21 | 1.83                     | 0.60              |
| 34:DK:41:ILE:HG22 | 34:DK:58:LEU:O     | 2.01                     | 0.60              |
| 38:DO:26:LEU:HD23 | 38:DO:92:PHE:CE1   | 2.37                     | 0.60              |
| 45:DV:14:LYS:HG3  | 45:DV:18:ARG:HD2   | 1.84                     | 0.60              |
| 21:AA:1256:A:H1'  | 21:AA:1258:G:C5    | 2.37                     | 0.60              |
| 21:AA:335:C:H2'   | 21:AA:336:A:C8     | 2.37                     | 0.60              |
| 10:AK:86:LYS:HE3  | 21:AA:707:U:OP1    | 2.02                     | 0.60              |
| 21:AA:830:G:H2'   | 21:AA:831:A:H8     | 1.67                     | 0.60              |
| 1:AB:108:GLN:HE21 | 1:AB:108:GLN:N     | 1.94                     | 0.60              |
| 8:AI:123:ARG:HB3  | 21:AA:1343:G:O3'   | 2.01                     | 0.60              |
| 24:BA:1287:A:OP2  | 37:BN:103:ARG:HG3  | 2.02                     | 0.60              |
| 24:BA:2134:A:N6   | 24:BA:2157:G:C5    | 2.70                     | 0.60              |
| 24:BA:547:A:C8    | 24:BA:548:G:N3     | 2.70                     | 0.60              |
| 24:BA:789:A:OP1   | 24:BA:790:U:H5     | 1.85                     | 0.60              |
| 24:BA:880:G:H8    | 24:BA:880:G:O5'    | 1.83                     | 0.60              |
| 29:BF:161:SER:OG  | 29:BF:164:GLU:HG3  | 2.01                     | 0.60              |
| 24:BA:2352:A:C2   | 46:BW:30:VAL:HG11  | 2.37                     | 0.60              |
| 55:CA:1091:U:H2'  | 55:CA:1093:A:OP2   | 2.01                     | 0.60              |
| 55:CA:1518:A:H2'  | 55:CA:1519:A:C8    | 2.37                     | 0.60              |
| 55:CA:21:G:H2'    | 55:CA:22:G:C8      | 2.37                     | 0.60              |
| 55:CA:425:G:O2'   | 55:CA:426:U:O4'    | 2.19                     | 0.60              |
| 55:CA:686:U:O4    | 55:CA:703:G:H1'    | 2.02                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:CC:26:LYS:HA   | 2:CC:26:LYS:HE3   | 1.82                     | 0.60              |
| 10:CK:74:LYS:HG3 | 10:CK:78:ILE:HG12 | 1.82                     | 0.60              |
| 24:DA:1213:A:H2' | 24:DA:1214:A:C8   | 2.37                     | 0.60              |
| 24:DA:1245:G:H4' | 28:DE:33:VAL:CG1  | 2.31                     | 0.60              |
| 24:DA:1440:U:H2' | 24:DA:1441:G:H8   | 1.67                     | 0.60              |
| 24:DA:1706:C:H5' | 24:DA:1707:G:OP2  | 2.01                     | 0.60              |
| 24:DA:1967:C:H6  | 24:DA:1967:C:H5'' | 1.66                     | 0.60              |
| 24:DA:860:U:C4   | 24:DA:2268:A:C4   | 2.90                     | 0.60              |
| 24:DA:312:G:H2'  | 24:DA:313:G:H8    | 1.65                     | 0.60              |
| 24:DA:673:C:C2'  | 24:DA:674:G:H5'   | 2.31                     | 0.60              |
| 24:DA:923:G:H1'  | 46:DW:23:LYS:HZ2  | 1.64                     | 0.60              |
| 24:DA:1993:U:H4' | 27:DD:133:THR:CG2 | 2.31                     | 0.60              |
| 29:DF:47:LYS:HA  | 29:DF:50:ASP:HB3  | 1.84                     | 0.60              |
| 34:DK:101:GLY:O  | 34:DK:120:PRO:HB3 | 2.00                     | 0.60              |
| 39:DP:62:LYS:O   | 39:DP:63:ILE:HB   | 2.01                     | 0.60              |
| 47:DX:30:PRO:HG2 | 47:DX:32:LEU:CD2  | 2.32                     | 0.60              |
| 47:DX:1:SER:O    | 47:DX:3:VAL:N     | 2.35                     | 0.60              |
| 21:AA:1252:A:H2' | 21:AA:1253:G:O4'  | 2.02                     | 0.60              |
| 21:AA:397:A:N7   | 21:AA:547:A:O2'   | 2.35                     | 0.60              |
| 2:AC:141:MET:HG3 | 2:AC:169:GLU:OE2  | 2.02                     | 0.60              |
| 3:AD:54:LEU:O    | 3:AD:54:LEU:HD23  | 2.01                     | 0.60              |
| 24:BA:1060:U:H6  | 24:BA:1060:U:OP1  | 1.84                     | 0.60              |
| 24:BA:1429:G:N3  | 24:BA:1568:G:C2   | 2.70                     | 0.60              |
| 24:BA:1515:A:H2' | 24:BA:1516:G:O4'  | 2.02                     | 0.60              |
| 24:BA:2026:U:H2' | 24:BA:2027:G:O4'  | 2.02                     | 0.60              |
| 24:BA:2331:G:N2  | 24:BA:2385:C:C2   | 2.70                     | 0.60              |
| 24:BA:2358:A:N6  | 35:BL:54:GLN:HE22 | 1.98                     | 0.60              |
| 24:BA:2691:C:O3' | 24:BA:2871:U:H4'  | 2.02                     | 0.60              |
| 24:BA:639:U:H2'  | 24:BA:640:C:H6    | 1.59                     | 0.60              |
| 24:BA:997:G:O2'  | 24:BA:998:C:H5'   | 2.01                     | 0.60              |
| 26:BC:66:PHE:HB3 | 26:BC:150:GLY:O   | 2.02                     | 0.60              |
| 24:BA:1224:U:H4' | 41:BR:88:GLY:O    | 2.02                     | 0.60              |
| 55:CA:1423:G:O2' | 55:CA:1424:U:H5'  | 2.01                     | 0.60              |
| 55:CA:1477:U:H2' | 55:CA:1478:U:C6   | 2.35                     | 0.60              |
| 55:CA:431:A:H2'  | 55:CA:431:A:N3    | 2.16                     | 0.60              |
| 7:CH:76:ARG:HD3  | 7:CH:77:VAL:N     | 2.17                     | 0.60              |
| 19:CT:23:ARG:HB3 | 19:CT:60:GLN:NE2  | 2.14                     | 0.60              |
| 24:DA:1126:A:H4' | 24:DA:1127:A:O5'  | 2.02                     | 0.60              |
| 24:DA:1311:G:H1' | 24:DA:1313:U:O4   | 2.02                     | 0.60              |
| 24:DA:1417:C:H4' | 24:DA:1587:G:H21  | 1.66                     | 0.60              |
| 24:DA:2770:G:O5' | 24:DA:2770:G:H8   | 1.84                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:324:A:N6    | 24:DA:339:U:H5'    | 2.17                     | 0.60              |
| 24:DA:682:G:H2'   | 24:DA:683:U:H6     | 1.67                     | 0.60              |
| 26:DC:131:MET:HA  | 26:DC:134:ILE:HG12 | 1.84                     | 0.60              |
| 37:DN:8:ARG:HG2   | 37:DN:10:LEU:HD22  | 1.84                     | 0.60              |
| 45:DV:31:TYR:O    | 45:DV:31:TYR:CD1   | 2.54                     | 0.60              |
| 21:AA:930:C:H2'   | 21:AA:931:C:O4'    | 2.02                     | 0.59              |
| 1:AB:182:VAL:HG12 | 1:AB:183:PHE:N     | 2.17                     | 0.59              |
| 2:AC:13:ILE:HG12  | 2:AC:14:VAL:HG22   | 1.83                     | 0.59              |
| 9:AJ:6:ILE:HD11   | 9:AJ:79:PRO:HA     | 1.84                     | 0.59              |
| 11:AL:43:LYS:HZ2  | 11:AL:43:LYS:N     | 2.00                     | 0.59              |
| 11:AL:42:LYS:HD2  | 11:AL:90:PRO:HG3   | 1.83                     | 0.59              |
| 54:B4:7:VAL:HG23  | 54:B4:8:LYS:H      | 1.67                     | 0.59              |
| 24:BA:1408:G:C2   | 24:BA:1595:C:O2    | 2.55                     | 0.59              |
| 24:BA:1681:G:O2'  | 24:BA:1762:A:C2'   | 2.50                     | 0.59              |
| 24:BA:2410:G:C2   | 24:BA:2411:A:H1'   | 2.37                     | 0.59              |
| 24:BA:434:U:H4'   | 24:BA:435:C:OP1    | 2.01                     | 0.59              |
| 26:BC:85:ASN:OD1  | 26:BC:85:ASN:N     | 2.35                     | 0.59              |
| 27:BD:101:PHE:HE2 | 27:BD:203:VAL:CG2  | 2.15                     | 0.59              |
| 43:BT:38:ALA:HB1  | 43:BT:43:ILE:CG2   | 2.32                     | 0.59              |
| 24:BA:923:G:N3    | 46:BW:23:LYS:HE2   | 2.17                     | 0.59              |
| 55:CA:1239:A:N6   | 55:CA:1299:A:N6    | 2.49                     | 0.59              |
| 16:CQ:64:ARG:HD3  | 55:CA:130:A:H8     | 1.67                     | 0.59              |
| 55:CA:211:G:C2'   | 55:CA:211:G:N3     | 2.56                     | 0.59              |
| 55:CA:576:C:H2'   | 55:CA:578:C:OP2    | 2.02                     | 0.59              |
| 55:CA:92:U:H2'    | 55:CA:93:U:C6      | 2.36                     | 0.59              |
| 3:CD:167:PRO:HB3  | 3:CD:169:TRP:CH2   | 2.37                     | 0.59              |
| 3:CD:197:HIS:O    | 3:CD:200:VAL:HB    | 2.02                     | 0.59              |
| 11:CL:72:ASN:HD21 | 11:CL:104:SER:H    | 1.48                     | 0.59              |
| 20:CU:36:PHE:HD1  | 20:CU:40:PRO:HB3   | 1.66                     | 0.59              |
| 24:DA:1181:U:H2'  | 24:DA:1182:G:C8    | 2.37                     | 0.59              |
| 24:DA:1439:A:C2   | 24:DA:1552:A:C4    | 2.89                     | 0.59              |
| 24:DA:167:A:C2    | 24:DA:168:G:H1'    | 2.37                     | 0.59              |
| 24:DA:1867:G:H2'  | 24:DA:1868:C:H6    | 1.66                     | 0.59              |
| 24:DA:2096:C:H2'  | 24:DA:2097:A:C8    | 2.37                     | 0.59              |
| 24:DA:2714:G:H2'  | 24:DA:2715:C:C6    | 2.37                     | 0.59              |
| 24:DA:279:A:N6    | 24:DA:361:G:O2'    | 2.35                     | 0.59              |
| 24:DA:335:C:O2'   | 24:DA:336:C:H5'    | 2.01                     | 0.59              |
| 24:DA:49:A:N6     | 24:DA:177:G:C5     | 2.70                     | 0.59              |
| 24:DA:782:A:C8    | 24:DA:782:A:OP1    | 2.46                     | 0.59              |
| 24:DA:876:C:H3'   | 24:DA:877:A:H8     | 1.66                     | 0.59              |
| 24:DA:975:A:H2'   | 24:DA:976:G:C8     | 2.36                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:DA:1789:A:H5''  | 26:DC:218:THR:O   | 2.01                     | 0.59              |
| 30:DG:95:ALA:HB3   | 30:DG:127:GLN:HA  | 1.83                     | 0.59              |
| 21:AA:1269:A:H2    | 21:AA:1312:G:N3   | 1.99                     | 0.59              |
| 21:AA:15:G:N7      | 21:AA:1396:A:C2   | 2.70                     | 0.59              |
| 21:AA:1464:U:H2'   | 21:AA:1465:A:C8   | 2.37                     | 0.59              |
| 21:AA:214:C:H2'    | 21:AA:215:C:C6    | 2.38                     | 0.59              |
| 4:AE:154:ALA:HB3   | 7:AH:65:PHE:CD1   | 2.38                     | 0.59              |
| 24:BA:1027:A:N1    | 24:BA:1126:A:N3   | 2.50                     | 0.59              |
| 24:BA:1083:U:O2    | 24:BA:1086:A:N6   | 2.36                     | 0.59              |
| 24:BA:1286:A:H4'   | 24:BA:1287:A:OP1  | 2.02                     | 0.59              |
| 24:BA:14:A:N6      | 24:BA:15:G:C2     | 2.69                     | 0.59              |
| 24:BA:1683:U:H2'   | 24:BA:1684:G:C8   | 2.37                     | 0.59              |
| 24:BA:1936:A:H2    | 24:BA:1943:U:O4   | 1.85                     | 0.59              |
| 24:BA:411:G:H5''   | 24:BA:412:A:OP1   | 2.02                     | 0.59              |
| 24:BA:558:U:P      | 33:BJ:113:PRO:HG2 | 2.42                     | 0.59              |
| 28:BE:97:ASN:HB2   | 28:BE:100:MET:HG3 | 1.84                     | 0.59              |
| 29:BF:68:LYS:N     | 29:BF:68:LYS:HD2  | 2.17                     | 0.59              |
| 36:BM:35:ALA:O     | 36:BM:36:VAL:CB   | 2.45                     | 0.59              |
| 55:CA:1084:G:C5    | 55:CA:1085:U:C4   | 2.90                     | 0.59              |
| 55:CA:1213:A:C8    | 55:CA:1215:G:C5   | 2.90                     | 0.59              |
| 55:CA:1415:G:C2    | 55:CA:1486:G:C4   | 2.90                     | 0.59              |
| 55:CA:1461:G:H2'   | 55:CA:1462:C:C6   | 2.37                     | 0.59              |
| 55:CA:170:U:O2'    | 55:CA:171:A:H5'   | 2.01                     | 0.59              |
| 55:CA:223:A:H2'    | 55:CA:224:U:C6    | 2.35                     | 0.59              |
| 55:CA:983:A:C2'    | 55:CA:984:C:H5'   | 2.31                     | 0.59              |
| 4:CE:95:MET:HE1    | 4:CE:143:LEU:HD11 | 1.84                     | 0.59              |
| 10:CK:19:VAL:HB    | 10:CK:34:THR:O    | 2.01                     | 0.59              |
| 12:CM:88:LEU:O     | 12:CM:92:ARG:HB2  | 2.01                     | 0.59              |
| 20:CU:24:LYS:CG    | 20:CU:25:ALA:N    | 2.64                     | 0.59              |
| 24:DA:1815:A:H4'   | 24:DA:1816:C:OP1  | 2.01                     | 0.59              |
| 24:DA:1844:C:C2    | 24:DA:1845:G:C8   | 2.90                     | 0.59              |
| 55:CA:1409:C:H4'   | 24:DA:1915:U:O4   | 2.02                     | 0.59              |
| 24:DA:2092:U:C4'   | 24:DA:2093:G:H5'' | 2.17                     | 0.59              |
| 24:DA:375:G:H5''   | 24:DA:375:G:C8    | 2.36                     | 0.59              |
| 24:DA:985:C:N4     | 24:DA:986:C:H41   | 2.01                     | 0.59              |
| 26:DC:173:LEU:HD22 | 26:DC:181:ARG:O   | 2.00                     | 0.59              |
| 33:DJ:37:ARG:HG3   | 33:DJ:118:MET:SD  | 2.41                     | 0.59              |
| 34:DK:1:MET:HA     | 34:DK:33:ALA:O    | 2.02                     | 0.59              |
| 38:DO:24:THR:HG22  | 38:DO:41:ALA:HA   | 1.85                     | 0.59              |
| 40:DQ:34:ALA:O     | 40:DQ:38:VAL:HG23 | 2.02                     | 0.59              |
| 42:DS:66:ILE:HA    | 42:DS:69:LEU:HD13 | 1.83                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 44:DU:81:ARG:HD2   | 44:DU:81:ARG:N    | 2.17                     | 0.59              |
| 46:DW:31:LEU:C     | 46:DW:33:GLY:H    | 2.05                     | 0.59              |
| 21:AA:11:G:C6      | 21:AA:12:U:C4     | 2.90                     | 0.59              |
| 21:AA:1055:A:C6    | 21:AA:1206:G:C5   | 2.90                     | 0.59              |
| 21:AA:308:C:H2'    | 21:AA:309:A:H8    | 1.67                     | 0.59              |
| 21:AA:511:C:N3     | 21:AA:512:U:C4    | 2.70                     | 0.59              |
| 21:AA:722:G:H2'    | 21:AA:722:G:N3    | 2.16                     | 0.59              |
| 4:AE:155:LYS:HD2   | 4:AE:156:ARG:CG   | 2.31                     | 0.59              |
| 5:AF:11:HIS:CD2    | 5:AF:12:PRO:HD2   | 2.37                     | 0.59              |
| 24:BA:1738:G:O2'   | 24:BA:1739:A:H8   | 1.85                     | 0.59              |
| 24:BA:529:A:H2'    | 24:BA:2023:C:H41  | 1.67                     | 0.59              |
| 24:BA:2217:G:H2'   | 24:BA:2218:G:H8   | 1.66                     | 0.59              |
| 24:BA:2286:G:H4'   | 24:BA:2287:A:O4'  | 2.01                     | 0.59              |
| 24:BA:2812:G:H5'   | 24:BA:2813:A:OP2  | 2.02                     | 0.59              |
| 24:BA:2888:C:H2'   | 24:BA:2889:C:C6   | 2.36                     | 0.59              |
| 24:BA:289:G:H2'    | 24:BA:290:U:O4'   | 2.01                     | 0.59              |
| 24:BA:418:C:H2'    | 24:BA:419:U:O4'   | 2.02                     | 0.59              |
| 27:BD:118:PHE:HD2  | 27:BD:119:ALA:H   | 1.50                     | 0.59              |
| 37:BN:114:GLU:HB2  | 37:BN:118:ARG:HD3 | 1.83                     | 0.59              |
| 39:BP:50:ARG:CB    | 39:BP:57:ALA:N    | 2.56                     | 0.59              |
| 55:CA:481:G:H1'    | 55:CA:482:A:N7    | 2.18                     | 0.59              |
| 3:CD:87:GLU:OE2    | 3:CD:187:ARG:HB2  | 2.02                     | 0.59              |
| 4:CE:22:LYS:HB3    | 4:CE:29:ILE:HG21  | 1.84                     | 0.59              |
| 6:CG:12:LEU:HD22   | 6:CG:13:PRO:O     | 2.01                     | 0.59              |
| 9:CJ:90:LEU:HD23   | 9:CJ:92:LEU:HD11  | 1.85                     | 0.59              |
| 18:CS:28:LYS:HB3   | 18:CS:29:PRO:HD2  | 1.84                     | 0.59              |
| 24:DA:1290:C:O2'   | 24:DA:1291:C:H6   | 1.84                     | 0.59              |
| 24:DA:770:G:H1'    | 24:DA:1379:U:C4   | 2.37                     | 0.59              |
| 24:DA:1343:G:C5    | 24:DA:1597:A:N6   | 2.70                     | 0.59              |
| 24:DA:1700:A:C2'   | 24:DA:1701:A:H5'  | 2.32                     | 0.59              |
| 24:DA:2015:A:C6    | 50:D0:2:VAL:HG11  | 2.37                     | 0.59              |
| 24:DA:746:U:H5'    | 24:DA:748:G:O4'   | 2.02                     | 0.59              |
| 56:DB:75:G:H1      | 56:DB:102:G:N2    | 1.99                     | 0.59              |
| 29:DF:136:ILE:HG22 | 29:DF:142:TYR:CG  | 2.38                     | 0.59              |
| 29:DF:33:ILE:HB    | 29:DF:90:LEU:HB2  | 1.84                     | 0.59              |
| 30:DG:18:ILE:HD12  | 30:DG:42:VAL:HG13 | 1.83                     | 0.59              |
| 21:AA:280:C:H3'    | 21:AA:281:G:H5'   | 1.84                     | 0.59              |
| 1:AB:103:TRP:CZ2   | 1:AB:154:GLY:HA2  | 2.37                     | 0.59              |
| 1:AB:168:GLU:HB3   | 1:AB:171:ALA:HB3  | 1.82                     | 0.59              |
| 2:AC:27:GLU:CD     | 2:AC:27:GLU:H     | 2.04                     | 0.59              |
| 3:AD:125:ASN:OD1   | 3:AD:140:ASP:HA   | 2.02                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AD:98:ASP:CB     | 3:AD:114:ARG:HG2   | 2.31                     | 0.59              |
| 18:AS:62:THR:HG22  | 18:AS:63:ASP:N     | 2.16                     | 0.59              |
| 22:AV:39:U:H2'     | 22:AV:40:C:H6      | 1.66                     | 0.59              |
| 24:BA:2485:G:N2    | 24:BA:2486:C:C2    | 2.70                     | 0.59              |
| 24:BA:2502:G:H5'   | 24:BA:2503:A:C5'   | 2.33                     | 0.59              |
| 24:BA:26:G:C2      | 24:BA:27:G:N2      | 2.71                     | 0.59              |
| 24:BA:447:A:C2     | 24:BA:454:A:C8     | 2.89                     | 0.59              |
| 26:BC:20:ASN:HB3   | 26:BC:23:LEU:HD23  | 1.85                     | 0.59              |
| 27:BD:186:LEU:HD11 | 39:BP:3:ILE:CD1    | 2.32                     | 0.59              |
| 30:BG:168:VAL:O    | 30:BG:170:THR:HG23 | 2.02                     | 0.59              |
| 24:BA:811:U:C4     | 35:BL:21:ARG:CZ    | 2.85                     | 0.59              |
| 37:BN:65:LEU:HD11  | 37:BN:69:ARG:NH2   | 2.17                     | 0.59              |
| 55:CA:1077:G:N1    | 55:CA:1081:A:C6    | 2.71                     | 0.59              |
| 55:CA:1087:G:O2'   | 55:CA:1088:G:H5'   | 2.03                     | 0.59              |
| 12:CM:102:LYS:CA   | 55:CA:1226:C:H5    | 2.08                     | 0.59              |
| 1:CB:187:ASP:HB2   | 1:CB:202:ASN:O     | 2.02                     | 0.59              |
| 2:CC:9:ILE:HG23    | 2:CC:10:ARG:N      | 2.18                     | 0.59              |
| 11:CL:24:GLU:O     | 11:CL:25:ALA:HB3   | 2.02                     | 0.59              |
| 53:D3:18:LYS:CD    | 53:D3:19:GLY:H     | 2.15                     | 0.59              |
| 24:DA:1206:G:C2    | 24:DA:1207:C:C2    | 2.91                     | 0.59              |
| 24:DA:1209:U:O3'   | 24:DA:1212:G:H5'   | 2.03                     | 0.59              |
| 24:DA:1210:G:H1'   | 24:DA:1212:G:C2    | 2.37                     | 0.59              |
| 24:DA:2143:C:H5'   | 24:DA:2144:G:OP2   | 2.01                     | 0.59              |
| 24:DA:2425:A:H5'   | 24:DA:2427:C:H5'   | 1.83                     | 0.59              |
| 24:DA:873:C:H4'    | 36:DM:64:TRP:CD1   | 2.38                     | 0.59              |
| 56:DB:60:C:H2'     | 56:DB:61:G:C8      | 2.36                     | 0.59              |
| 34:DK:108:ARG:HA   | 34:DK:116:ILE:HD13 | 1.84                     | 0.59              |
| 36:DM:136:MET:OXT  | 36:DM:136:MET:CG   | 2.45                     | 0.59              |
| 39:DP:91:VAL:HG11  | 39:DP:96:LEU:HD11  | 1.84                     | 0.59              |
| 49:DZ:6:ILE:O      | 49:DZ:34:THR:HA    | 2.03                     | 0.59              |
| 21:AA:1088:G:C6    | 21:AA:1089:G:N7    | 2.71                     | 0.59              |
| 21:AA:1502:A:O2'   | 21:AA:1503:A:P     | 2.61                     | 0.59              |
| 21:AA:223:A:H2'    | 21:AA:224:U:H6     | 1.68                     | 0.59              |
| 1:AB:110:ILE:HD11  | 1:AB:147:LEU:HD13  | 1.82                     | 0.59              |
| 3:AD:130:ASN:HB3   | 21:AA:619:U:H3     | 1.67                     | 0.59              |
| 4:AE:136:VAL:O     | 4:AE:136:VAL:HG22  | 2.02                     | 0.59              |
| 4:AE:152:VAL:HB    | 4:AE:155:LYS:HZ2   | 1.68                     | 0.59              |
| 5:AF:16:GLU:HG2    | 3:CD:191:SER:CB    | 2.24                     | 0.59              |
| 6:AG:9:ARG:NH1     | 21:AA:1346:A:C4    | 2.70                     | 0.59              |
| 7:AH:77:VAL:HG23   | 7:AH:126:CYS:HA    | 1.84                     | 0.59              |
| 10:AK:28:ASN:HD21  | 10:AK:47:GLY:N     | 1.93                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:AK:49:SER:HA   | 10:AK:68:ARG:NH2  | 2.17                     | 0.59              |
| 50:B0:42:ILE:HG22 | 50:B0:43:THR:O    | 2.02                     | 0.59              |
| 35:BL:59:ARG:HA   | 53:B3:12:ARG:NH2  | 2.17                     | 0.59              |
| 24:BA:1555:G:H5'  | 24:BA:1555:G:H8   | 1.65                     | 0.59              |
| 24:BA:2657:A:O2'  | 24:BA:2658:C:H5'  | 2.02                     | 0.59              |
| 24:BA:322:A:H1'   | 24:BA:339:U:O2    | 2.03                     | 0.59              |
| 24:BA:53:A:H2'    | 24:BA:54:G:O4'    | 2.02                     | 0.59              |
| 32:BI:120:ASP:HB3 | 32:BI:123:ALA:HB3 | 1.83                     | 0.59              |
| 33:BJ:13:ARG:O    | 33:BJ:14:ASP:HB2  | 2.02                     | 0.59              |
| 33:BJ:43:GLU:O    | 33:BJ:45:THR:HG22 | 2.00                     | 0.59              |
| 33:BJ:4:PHE:O     | 33:BJ:44:TYR:CE1  | 2.56                     | 0.59              |
| 36:BM:41:LEU:HA   | 36:BM:45:GLN:OE1  | 2.03                     | 0.59              |
| 55:CA:1336:C:H1'  | 55:CA:1337:G:C6   | 2.38                     | 0.59              |
| 55:CA:1446:A:H2'  | 55:CA:1447:A:C5'  | 2.32                     | 0.59              |
| 55:CA:164:G:H2'   | 55:CA:165:G:H5'   | 1.83                     | 0.59              |
| 55:CA:374:A:H5''  | 55:CA:452:A:C6    | 2.37                     | 0.59              |
| 55:CA:395:C:H2'   | 55:CA:396:C:C6    | 2.37                     | 0.59              |
| 2:CC:56:ILE:HG23  | 2:CC:65:VAL:HG22  | 1.85                     | 0.59              |
| 11:CL:86:VAL:HG11 | 11:CL:89:LEU:HD23 | 1.83                     | 0.59              |
| 14:CO:83:ARG:O    | 14:CO:83:ARG:HG2  | 2.02                     | 0.59              |
| 51:D1:5:ARG:NH2   | 51:D1:23:THR:HB   | 2.18                     | 0.59              |
| 24:DA:1074:G:OP2  | 24:DA:1074:G:C8   | 2.56                     | 0.59              |
| 24:DA:1437:C:H2'  | 24:DA:1438:U:H6   | 1.67                     | 0.59              |
| 24:DA:616:A:O2'   | 24:DA:617:G:H5'   | 2.02                     | 0.59              |
| 24:DA:777:G:HO2'  | 24:DA:778:G:H8    | 1.50                     | 0.59              |
| 32:DI:16:MET:SD   | 32:DI:19:PRO:HG2  | 2.42                     | 0.59              |
| 34:DK:87:LEU:N    | 34:DK:87:LEU:HD23 | 2.17                     | 0.59              |
| 21:AA:1143:G:O2'  | 21:AA:1144:G:H5'  | 2.01                     | 0.59              |
| 13:AN:81:ILE:HG21 | 21:AA:1202:U:N3   | 2.18                     | 0.59              |
| 21:AA:512:U:H2'   | 21:AA:513:C:C6    | 2.37                     | 0.59              |
| 21:AA:21:G:H1'    | 21:AA:915:A:H61   | 1.67                     | 0.59              |
| 1:AB:142:LYS:NZ   | 21:AA:1098:C:P    | 2.76                     | 0.59              |
| 1:AB:184:ALA:HB3  | 1:AB:195:VAL:HG22 | 1.83                     | 0.59              |
| 2:AC:91:ALA:C     | 2:AC:93:ILE:H     | 2.05                     | 0.59              |
| 4:AE:142:GLY:O    | 4:AE:143:LEU:HD23 | 2.02                     | 0.59              |
| 6:AG:110:ARG:NH1  | 6:AG:122:GLU:HG2  | 2.17                     | 0.59              |
| 24:BA:1084:A:H2'  | 24:BA:1085:A:C8   | 2.38                     | 0.59              |
| 24:BA:1234:U:H2'  | 24:BA:1235:G:O4'  | 2.03                     | 0.59              |
| 24:BA:1334:G:O2'  | 24:BA:1335:C:H5'  | 2.02                     | 0.59              |
| 24:BA:2556:C:H2'  | 24:BA:2557:G:H5'  | 1.84                     | 0.59              |
| 27:BD:191:GLY:O   | 27:BD:192:ALA:CB  | 2.50                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BL:28:GLY:O    | 35:BL:29:LYS:HB3   | 2.00                     | 0.59              |
| 40:BQ:63:ARG:CZ   | 40:BQ:95:ALA:O     | 2.51                     | 0.59              |
| 40:BQ:96:ASP:C    | 40:BQ:98:ALA:N     | 2.54                     | 0.59              |
| 24:BA:571:U:O3'   | 41:BR:80:ARG:NH2   | 2.36                     | 0.59              |
| 42:BS:38:TYR:HD2  | 50:B0:38:LEU:HD21  | 1.67                     | 0.59              |
| 55:CA:1068:G:O2'  | 55:CA:1069:C:H5'   | 2.03                     | 0.59              |
| 55:CA:1119:C:H2'  | 55:CA:1120:C:C6    | 2.33                     | 0.59              |
| 55:CA:1172:C:O2'  | 55:CA:1173:U:H5'   | 2.01                     | 0.59              |
| 55:CA:1206:G:H2'  | 55:CA:1207:G:O4'   | 2.02                     | 0.59              |
| 55:CA:149:A:H1'   | 55:CA:1446:A:H2    | 1.66                     | 0.59              |
| 55:CA:198:G:H2'   | 55:CA:199:A:C8     | 2.36                     | 0.59              |
| 55:CA:199:A:O2'   | 55:CA:200:G:O4'    | 2.21                     | 0.59              |
| 55:CA:242:G:N2    | 55:CA:285:C:C2     | 2.71                     | 0.59              |
| 55:CA:302:G:C4    | 55:CA:303:A:C8     | 2.91                     | 0.59              |
| 55:CA:704:A:H2'   | 55:CA:705:G:C8     | 2.33                     | 0.59              |
| 1:CB:185:ILE:HD12 | 1:CB:202:ASN:N     | 2.18                     | 0.59              |
| 1:CB:49:PHE:HB3   | 1:CB:199:ILE:CG2   | 2.32                     | 0.59              |
| 13:CN:20:PHE:HA   | 13:CN:24:ALA:HB2   | 1.85                     | 0.59              |
| 14:CO:63:ARG:HH22 | 24:DA:715:A:C5'    | 2.07                     | 0.59              |
| 16:CQ:17:GLU:HB2  | 55:CA:255:G:O4'    | 2.02                     | 0.59              |
| 20:CU:40:PRO:HA   | 20:CU:43:GLU:CB    | 2.32                     | 0.59              |
| 24:DA:1439:A:N1   | 24:DA:1552:A:C8    | 2.71                     | 0.59              |
| 24:DA:1313:U:C6   | 24:DA:1610:A:H8    | 2.19                     | 0.59              |
| 24:DA:1645:G:OP1  | 24:DA:1646:C:H5'   | 2.03                     | 0.59              |
| 24:DA:1683:U:O2'  | 24:DA:1684:G:C8    | 2.53                     | 0.59              |
| 24:DA:1716:U:O2'  | 24:DA:1717:A:H5'   | 2.01                     | 0.59              |
| 24:DA:1768:C:O2'  | 24:DA:1958:C:H4'   | 2.02                     | 0.59              |
| 24:DA:2093:G:N7   | 24:DA:2225:A:C4    | 2.70                     | 0.59              |
| 24:DA:2142:A:C3'  | 24:DA:2143:C:H4'   | 2.31                     | 0.59              |
| 24:DA:633:A:H8    | 24:DA:633:A:O5'    | 1.86                     | 0.59              |
| 26:DC:158:GLY:H   | 26:DC:194:VAL:HG13 | 1.68                     | 0.59              |
| 27:DD:36:GLN:HE21 | 27:DD:38:LYS:HZ1   | 1.50                     | 0.59              |
| 30:DG:8:VAL:HA    | 30:DG:68:ARG:HH21  | 1.67                     | 0.59              |
| 38:DO:30:ARG:HG2  | 38:DO:31:THR:N     | 2.17                     | 0.59              |
| 41:DR:33:VAL:HG23 | 41:DR:61:ALA:HB3   | 1.83                     | 0.59              |
| 44:DU:44:HIS:HD2  | 44:DU:57:ILE:HG21  | 1.66                     | 0.59              |
| 44:DU:81:ARG:HB2  | 44:DU:96:LYS:HD2   | 1.84                     | 0.59              |
| 44:DU:81:ARG:HD2  | 44:DU:81:ARG:H     | 1.66                     | 0.59              |
| 56:DB:73:A:N6     | 45:DV:31:TYR:CE2   | 2.71                     | 0.59              |
| 24:DA:1808:A:N6   | 47:DX:27:ARG:HD2   | 2.18                     | 0.59              |
| 21:AA:1142:G:H2'  | 21:AA:1143:G:O4'   | 2.02                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 21:AA:512:U:C2     | 21:AA:513:C:C5    | 2.90                     | 0.59              |
| 21:AA:721:G:H4'    | 21:AA:722:G:C5'   | 2.33                     | 0.59              |
| 1:AB:138:ARG:HA    | 1:AB:141:GLU:OE2  | 2.02                     | 0.59              |
| 7:AH:31:LEU:HD22   | 21:AA:643:C:H5''  | 1.85                     | 0.59              |
| 17:AR:64:LEU:HB2   | 17:AR:66:LEU:HG   | 1.83                     | 0.59              |
| 24:BA:1079:C:C4    | 24:BA:1080:A:N7   | 2.70                     | 0.59              |
| 24:BA:1513:U:O2'   | 24:BA:1514:G:H5'  | 2.02                     | 0.59              |
| 24:BA:1676:A:C2    | 24:BA:1993:U:H5'  | 2.37                     | 0.59              |
| 24:BA:2400:G:C5    | 24:BA:2401:U:C5   | 2.91                     | 0.59              |
| 24:BA:288:U:H2'    | 24:BA:289:G:H8    | 1.68                     | 0.59              |
| 24:BA:609:A:H2'    | 24:BA:610:C:O4'   | 2.02                     | 0.59              |
| 24:BA:2052:A:OP1   | 27:BD:145:SER:HA  | 2.03                     | 0.59              |
| 27:BD:47:ALA:HB1   | 27:BD:82:PHE:O    | 2.03                     | 0.59              |
| 36:BM:1:MET:O      | 36:BM:2:LEU:CB    | 2.49                     | 0.59              |
| 48:BY:42:LEU:O     | 48:BY:45:GLN:O    | 2.20                     | 0.59              |
| 55:CA:1249:C:H2'   | 55:CA:1250:A:H5'' | 1.85                     | 0.59              |
| 55:CA:1443:C:H2'   | 55:CA:1444:U:O4'  | 2.01                     | 0.59              |
| 55:CA:147:G:H2'    | 55:CA:148:G:H8    | 1.65                     | 0.59              |
| 55:CA:534:U:O2'    | 55:CA:535:A:H5'   | 2.02                     | 0.59              |
| 24:DA:1337:G:OP2   | 24:DA:1337:G:H8   | 1.86                     | 0.59              |
| 24:DA:1341:G:O2'   | 24:DA:1398:C:C5'  | 2.50                     | 0.59              |
| 24:DA:1521:G:C6    | 24:DA:1522:A:N6   | 2.71                     | 0.59              |
| 24:DA:1945:G:H2'   | 24:DA:1946:U:C6   | 2.37                     | 0.59              |
| 24:DA:2092:U:H5    | 24:DA:2226:C:OP2  | 1.84                     | 0.59              |
| 24:DA:387:U:H4'    | 24:DA:388:G:O5'   | 2.02                     | 0.59              |
| 24:DA:851:C:O4'    | 49:DZ:46:MET:HG2  | 2.02                     | 0.59              |
| 28:DE:131:THR:HG22 | 28:DE:161:ALA:H   | 1.67                     | 0.59              |
| 30:DG:162:ARG:HB2  | 30:DG:166:GLU:HB3 | 1.84                     | 0.59              |
| 34:DK:2:ILE:HG22   | 34:DK:3:GLN:N     | 2.17                     | 0.59              |
| 35:DL:127:VAL:HG13 | 35:DL:132:ARG:HB2 | 1.85                     | 0.59              |
| 38:DO:79:ALA:HB1   | 38:DO:114:GLY:HA3 | 1.84                     | 0.59              |
| 45:DV:29:ILE:HG22  | 45:DV:39:ALA:HA   | 1.83                     | 0.59              |
| 47:DX:53:LYS:HA    | 47:DX:56:ARG:CB   | 2.23                     | 0.59              |
| 21:AA:1180:A:H5''  | 21:AA:1181:G:OP2  | 2.02                     | 0.59              |
| 21:AA:1395:C:OP2   | 21:AA:1395:C:H3'  | 2.02                     | 0.59              |
| 3:AD:196:GLU:C     | 3:AD:198:LEU:H    | 2.04                     | 0.59              |
| 4:AE:93:VAL:HG11   | 4:AE:139:THR:HG23 | 1.85                     | 0.59              |
| 5:AF:54:LEU:HD22   | 5:AF:55:HIS:H     | 1.67                     | 0.59              |
| 8:AI:113:LYS:HG3   | 8:AI:119:LYS:HA   | 1.83                     | 0.59              |
| 11:AL:110:LYS:HB2  | 21:AA:538:G:H5''  | 1.85                     | 0.59              |
| 11:AL:89:LEU:HB2   | 11:AL:92:VAL:CG2  | 2.32                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:AV:27:G:H5''    | 22:AV:27:G:C8     | 2.37                     | 0.59              |
| 51:B1:10:LEU:O     | 51:B1:19:PHE:HB2  | 2.03                     | 0.59              |
| 24:BA:1343:G:O2'   | 24:BA:1344:U:H5'  | 2.03                     | 0.59              |
| 24:BA:1539:U:O2'   | 24:BA:1540:G:O4'  | 2.20                     | 0.59              |
| 24:BA:2259:U:H2'   | 24:BA:2260:C:C6   | 2.38                     | 0.59              |
| 24:BA:2307:G:C2    | 24:BA:2311:A:N7   | 2.71                     | 0.59              |
| 24:BA:2726:A:O2'   | 24:BA:2727:A:H5'  | 2.02                     | 0.59              |
| 24:BA:2795:C:C2    | 24:BA:2802:G:N2   | 2.71                     | 0.59              |
| 24:BA:822:G:C6     | 24:BA:836:G:C2    | 2.91                     | 0.59              |
| 24:BA:949:G:H2'    | 24:BA:950:G:H5'   | 1.84                     | 0.59              |
| 31:BH:68:ARG:HH21  | 31:BH:69:ALA:HA   | 1.68                     | 0.59              |
| 38:BO:35:ILE:O     | 38:BO:53:THR:HG23 | 2.03                     | 0.59              |
| 42:BS:12:SER:OG    | 42:BS:13:SER:N    | 2.35                     | 0.59              |
| 46:BW:23:LYS:HD2   | 46:BW:24:ARG:H    | 1.66                     | 0.59              |
| 46:BW:39:GLN:HG3   | 46:BW:42:THR:N    | 2.18                     | 0.59              |
| 3:CD:147:LYS:HD3   | 3:CD:148:ALA:N    | 2.18                     | 0.59              |
| 7:CH:94:VAL:HB     | 7:CH:99:GLY:O     | 2.02                     | 0.59              |
| 53:D3:32:LEU:HA    | 53:D3:35:LYS:HG3  | 1.84                     | 0.59              |
| 24:DA:176:A:H3'    | 24:DA:177:G:N2    | 2.17                     | 0.59              |
| 24:DA:2460:U:O2'   | 24:DA:2461:A:O4'  | 2.12                     | 0.59              |
| 24:DA:249:C:H4'    | 24:DA:250:G:O5'   | 2.03                     | 0.59              |
| 24:DA:2577:A:H2    | 50:D0:1:ALA:N     | 2.00                     | 0.59              |
| 24:DA:2692:G:H2'   | 24:DA:2693:G:C8   | 2.38                     | 0.59              |
| 24:DA:2836:U:C2    | 24:DA:2837:A:N7   | 2.71                     | 0.59              |
| 56:DB:46:A:OP1     | 38:DO:3:LYS:HD2   | 2.02                     | 0.59              |
| 26:DC:8:THR:O      | 26:DC:9:SER:CB    | 2.50                     | 0.59              |
| 28:DE:149:ILE:HG23 | 28:DE:188:MET:CA  | 2.32                     | 0.59              |
| 33:DJ:45:THR:C     | 33:DJ:47:HIS:N    | 2.56                     | 0.59              |
| 36:DM:8:LYS:HA     | 36:DM:8:LYS:HE3   | 1.84                     | 0.59              |
| 39:DP:5:LYS:HE2    | 39:DP:9:GLN:HE22  | 1.67                     | 0.59              |
| 43:DT:28:ASN:HB2   | 43:DT:87:LEU:HB3  | 1.83                     | 0.59              |
| 21:AA:1103:C:O2'   | 21:AA:1104:G:O5'  | 2.21                     | 0.59              |
| 8:AI:105:ARG:HH21  | 21:AA:1117:A:H5'' | 1.67                     | 0.59              |
| 21:AA:602:A:H2'    | 21:AA:603:U:C6    | 2.37                     | 0.59              |
| 21:AA:842:U:H3'    | 21:AA:843:U:C5'   | 2.32                     | 0.59              |
| 2:AC:110:LEU:HD21  | 2:AC:143:LEU:HD23 | 1.85                     | 0.59              |
| 4:AE:156:ARG:HA    | 7:AH:63:LYS:HE2   | 1.84                     | 0.59              |
| 22:AV:35:A:C2      | 22:AV:36:A:C8     | 2.91                     | 0.59              |
| 24:BA:1050:A:C2    | 24:BA:2751:G:C5   | 2.90                     | 0.59              |
| 24:BA:1555:G:C6    | 24:BA:1556:C:N4   | 2.71                     | 0.59              |
| 24:BA:1585:C:O5'   | 24:BA:1585:C:H6   | 1.86                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:2312:U:H2'  | 24:BA:2313:C:H5'  | 1.85                     | 0.59              |
| 24:BA:995:C:O2'   | 24:BA:996:A:P     | 2.60                     | 0.59              |
| 25:BB:40:U:O2'    | 25:BB:43:C:H5     | 1.86                     | 0.59              |
| 33:BJ:11:VAL:HG11 | 33:BJ:50:THR:HA   | 1.84                     | 0.59              |
| 36:BM:8:LYS:HD2   | 36:BM:8:LYS:N     | 2.18                     | 0.59              |
| 43:BT:73:ARG:CZ   | 43:BT:73:ARG:HB3  | 2.33                     | 0.59              |
| 46:BW:43:LYS:HG3  | 46:BW:79:ILE:HD11 | 1.82                     | 0.59              |
| 55:CA:1116:U:O2'  | 55:CA:1117:A:H5'  | 2.03                     | 0.59              |
| 55:CA:13:U:HO2'   | 55:CA:14:U:P      | 2.24                     | 0.59              |
| 55:CA:397:A:N7    | 55:CA:547:A:O2'   | 2.36                     | 0.59              |
| 55:CA:425:G:H2'   | 55:CA:426:U:H6    | 1.68                     | 0.59              |
| 55:CA:432:A:H2'   | 55:CA:433:G:O4'   | 2.02                     | 0.59              |
| 55:CA:436:C:C2    | 55:CA:437:U:C5    | 2.90                     | 0.59              |
| 55:CA:519:C:C2'   | 55:CA:520:A:C8    | 2.84                     | 0.59              |
| 55:CA:564:C:O2'   | 55:CA:565:U:H5'   | 2.03                     | 0.59              |
| 55:CA:817:C:H1'   | 55:CA:819:A:H5'   | 1.84                     | 0.59              |
| 3:CD:57:LYS:HE2   | 3:CD:58:GLN:OE1   | 2.03                     | 0.59              |
| 4:CE:96:GLN:OE1   | 4:CE:123:LEU:HD12 | 2.03                     | 0.59              |
| 12:CM:97:ARG:CZ   | 55:CA:1308:U:C5   | 2.85                     | 0.59              |
| 22:CV:40:C:H2'    | 22:CV:41:C:C6     | 2.38                     | 0.59              |
| 24:DA:1001:A:C8   | 24:DA:1002:G:C8   | 2.90                     | 0.59              |
| 24:DA:1746:A:H2'  | 24:DA:1747:U:C6   | 2.38                     | 0.59              |
| 24:DA:2324:U:H5'  | 24:DA:2325:G:C5'  | 2.26                     | 0.59              |
| 24:DA:2415:G:C2   | 24:DA:2416:C:C2   | 2.91                     | 0.59              |
| 24:DA:2493:U:C2'  | 24:DA:2494:G:H5'' | 2.32                     | 0.59              |
| 31:DH:27:ARG:HH21 | 31:DH:27:ARG:HB2  | 1.67                     | 0.59              |
| 34:DK:18:ARG:HB2  | 34:DK:45:GLU:HB2  | 1.84                     | 0.59              |
| 44:DU:35:VAL:HB   | 44:DU:38:ILE:HD13 | 1.85                     | 0.59              |
| 21:AA:1021:A:C2'  | 21:AA:1022:A:H5'' | 2.32                     | 0.59              |
| 21:AA:1251:A:H2'  | 21:AA:1252:A:C8   | 2.38                     | 0.59              |
| 21:AA:1360:A:H2'  | 21:AA:1361:G:C8   | 2.38                     | 0.59              |
| 21:AA:1415:G:O2'  | 21:AA:1416:G:H5'  | 2.03                     | 0.59              |
| 21:AA:228:A:H2'   | 21:AA:229:U:H6    | 1.68                     | 0.59              |
| 21:AA:654:G:O2'   | 21:AA:655:A:H5'   | 2.03                     | 0.59              |
| 21:AA:996:A:H2'   | 21:AA:997:U:H6    | 1.68                     | 0.59              |
| 1:AB:94:ARG:HG2   | 21:AA:1100:C:P    | 2.43                     | 0.59              |
| 4:AE:113:VAL:HG11 | 4:AE:136:VAL:HG23 | 1.84                     | 0.59              |
| 7:AH:85:TYR:CD2   | 7:AH:123:GLU:HB2  | 2.37                     | 0.59              |
| 11:AL:2:THR:HB    | 11:AL:5:GLN:CG    | 2.33                     | 0.59              |
| 24:BA:1343:G:C4   | 24:BA:1344:U:C5   | 2.90                     | 0.59              |
| 24:BA:1361:G:C4   | 24:BA:1371:G:N2   | 2.71                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:858:G:N2    | 24:BA:2268:A:H2'  | 2.18                     | 0.59              |
| 24:BA:2683:C:O2   | 34:BK:70:ARG:NH2  | 2.33                     | 0.59              |
| 24:BA:2790:U:H4'  | 24:BA:2791:G:OP1  | 2.00                     | 0.59              |
| 24:BA:2834:G:H2'  | 24:BA:2879:A:N6   | 2.18                     | 0.59              |
| 24:BA:554:U:C4    | 24:BA:555:G:C6    | 2.90                     | 0.59              |
| 27:BD:118:PHE:O   | 27:BD:120:GLY:N   | 2.36                     | 0.59              |
| 30:BG:72:ASN:O    | 30:BG:76:ILE:HG22 | 2.03                     | 0.59              |
| 30:BG:86:LEU:HB3  | 30:BG:162:ARG:O   | 2.03                     | 0.59              |
| 36:BM:42:THR:OG1  | 36:BM:45:GLN:HG3  | 2.03                     | 0.59              |
| 37:BN:23:ASN:H    | 37:BN:23:ASN:ND2  | 1.99                     | 0.59              |
| 39:BP:80:VAL:HG12 | 39:BP:81:ASP:N    | 2.17                     | 0.59              |
| 40:BQ:6:GLY:HA2   | 40:BQ:9:ALA:CB    | 2.31                     | 0.59              |
| 40:BQ:63:ARG:HH22 | 40:BQ:96:ASP:CB   | 2.15                     | 0.59              |
| 46:BW:35:ILE:O    | 46:BW:37:VAL:N    | 2.36                     | 0.59              |
| 55:CA:1157:A:H1'  | 55:CA:1181:G:C2   | 2.37                     | 0.59              |
| 55:CA:1194:U:H2'  | 55:CA:1195:C:H6   | 1.66                     | 0.59              |
| 1:CB:20:ARG:HG3   | 55:CA:831:A:OP1   | 2.02                     | 0.59              |
| 55:CA:880:C:H2'   | 55:CA:881:G:H5'   | 1.85                     | 0.59              |
| 55:CA:938:A:N6    | 55:CA:939:G:C6    | 2.71                     | 0.59              |
| 5:CF:8:PHE:HE2    | 5:CF:62:MET:CE    | 2.15                     | 0.59              |
| 6:CG:116:ALA:O    | 6:CG:120:ALA:HB3  | 2.03                     | 0.59              |
| 24:DA:1079:C:H41  | 24:DA:1088:A:C5'  | 2.15                     | 0.59              |
| 24:DA:2485:G:O2'  | 24:DA:2486:C:H5'  | 2.03                     | 0.59              |
| 24:DA:2660:A:H2   | 24:DA:2661:G:C8   | 2.21                     | 0.59              |
| 24:DA:300:A:H1'   | 24:DA:333:G:H21   | 1.68                     | 0.59              |
| 24:DA:46:G:N2     | 24:DA:47:C:C2     | 2.71                     | 0.59              |
| 24:DA:810:U:O2'   | 24:DA:811:U:H5    | 1.86                     | 0.59              |
| 56:DB:24:G:H1'    | 56:DB:27:C:H42    | 1.68                     | 0.59              |
| 33:DJ:45:THR:C    | 33:DJ:47:HIS:H    | 2.06                     | 0.59              |
| 33:DJ:59:ALA:O    | 33:DJ:62:VAL:HG12 | 2.03                     | 0.59              |
| 37:DN:33:ILE:HG23 | 37:DN:114:GLU:HB2 | 1.83                     | 0.59              |
| 38:DO:23:ALA:HB1  | 38:DO:90:VAL:HG12 | 1.85                     | 0.59              |
| 21:AA:1342:C:H2'  | 21:AA:1343:G:C8   | 2.38                     | 0.58              |
| 15:AP:1:MET:HB2   | 21:AA:135:C:C2    | 2.38                     | 0.58              |
| 21:AA:1418:A:H3'  | 21:AA:1418:A:C8   | 2.37                     | 0.58              |
| 21:AA:267:C:O2'   | 21:AA:268:U:H5'   | 2.02                     | 0.58              |
| 21:AA:922:G:H2'   | 21:AA:923:A:H8    | 1.68                     | 0.58              |
| 3:AD:90:LEU:O     | 3:AD:93:LEU:HB2   | 2.03                     | 0.58              |
| 24:BA:222:A:C6    | 24:BA:224:U:O2    | 2.56                     | 0.58              |
| 24:BA:2297:A:N7   | 24:BA:2320:U:N3   | 2.51                     | 0.58              |
| 24:BA:2352:A:N1   | 46:BW:30:VAL:HG21 | 2.18                     | 0.58              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:BA:2650:U:H2'   | 24:BA:2651:C:C6   | 2.38                     | 0.58              |
| 24:BA:2714:G:P     | 59:BA:3555:HOH:O  | 2.61                     | 0.58              |
| 24:BA:580:U:H2'    | 24:BA:581:C:H6    | 1.68                     | 0.58              |
| 24:BA:914:G:H8     | 24:BA:914:G:H5''  | 1.67                     | 0.58              |
| 24:BA:946:C:H2'    | 24:BA:947:A:H8    | 1.68                     | 0.58              |
| 27:BD:190:LYS:HG3  | 27:BD:190:LYS:O   | 2.03                     | 0.58              |
| 27:BD:45:TYR:HD1   | 27:BD:45:TYR:H    | 1.50                     | 0.58              |
| 28:BE:131:THR:HG22 | 28:BE:160:ALA:HA  | 1.84                     | 0.58              |
| 24:BA:1140:C:OP1   | 33:BJ:25:LEU:O    | 2.21                     | 0.58              |
| 24:BA:2393:U:H5'   | 35:BL:60:ARG:O    | 2.03                     | 0.58              |
| 55:CA:599:C:H2'    | 55:CA:600:A:C8    | 2.37                     | 0.58              |
| 55:CA:82:G:C2      | 55:CA:83:C:O2'    | 2.55                     | 0.58              |
| 55:CA:977:A:O2'    | 55:CA:1223:C:N4   | 2.29                     | 0.58              |
| 1:CB:114:LYS:HA    | 1:CB:117:GLU:CG   | 2.28                     | 0.58              |
| 1:CB:79:VAL:HG13   | 1:CB:80:LYS:N     | 2.17                     | 0.58              |
| 1:CB:81:ASP:CG     | 1:CB:82:ALA:H     | 2.04                     | 0.58              |
| 4:CE:36:THR:O      | 4:CE:47:PHE:HB2   | 2.03                     | 0.58              |
| 11:CL:6:LEU:HA     | 11:CL:9:LYS:O     | 2.04                     | 0.58              |
| 24:DA:1056:G:H1'   | 24:DA:1103:A:N6   | 2.18                     | 0.58              |
| 24:DA:2327:A:H2'   | 24:DA:2328:A:C8   | 2.38                     | 0.58              |
| 24:DA:2508:G:C2    | 24:DA:2582:G:C6   | 2.91                     | 0.58              |
| 24:DA:2626:C:O2'   | 24:DA:2627:G:H5'  | 2.02                     | 0.58              |
| 24:DA:1998:A:O3'   | 24:DA:2724:U:H4'  | 2.03                     | 0.58              |
| 24:DA:990:A:O2'    | 24:DA:991:C:H5''  | 2.03                     | 0.58              |
| 27:DD:79:LEU:HD22  | 27:DD:79:LEU:N    | 2.18                     | 0.58              |
| 43:DT:43:ILE:CG2   | 43:DT:58:VAL:HG11 | 2.32                     | 0.58              |
| 21:AA:1084:G:C6    | 21:AA:1085:U:O4   | 2.56                     | 0.58              |
| 21:AA:1201:A:H5'   | 21:AA:1203:C:OP2  | 2.03                     | 0.58              |
| 21:AA:336:A:O2'    | 21:AA:1469:C:H1'  | 2.04                     | 0.58              |
| 21:AA:937:A:C5     | 21:AA:938:A:N7    | 2.71                     | 0.58              |
| 6:AG:144:ALA:C     | 6:AG:146:ALA:N    | 2.54                     | 0.58              |
| 6:AG:149:ALA:HB1   | 10:AK:58:THR:OG1  | 2.03                     | 0.58              |
| 15:AP:28:ARG:HH11  | 15:AP:29:ASN:HD21 | 1.50                     | 0.58              |
| 18:AS:76:THR:HG21  | 21:AA:1221:G:H4'  | 1.84                     | 0.58              |
| 21:AA:1340:A:H4'   | 22:AV:31:A:O2'    | 2.03                     | 0.58              |
| 50:B0:9:ARG:HB3    | 50:B0:9:ARG:CZ    | 2.33                     | 0.58              |
| 24:BA:1106:G:C2    | 24:BA:1107:G:C8   | 2.91                     | 0.58              |
| 24:BA:1269:A:O5'   | 24:BA:1269:A:H8   | 1.86                     | 0.58              |
| 24:BA:1289:C:H2'   | 24:BA:1290:C:C6   | 2.38                     | 0.58              |
| 24:BA:1553:A:C8    | 24:BA:1555:G:C6   | 2.91                     | 0.58              |
| 24:BA:387:U:C4'    | 24:BA:388:G:H5''  | 2.31                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:918:A:C6    | 24:BA:919:U:H1'   | 2.38                     | 0.58              |
| 26:BC:255:LYS:C   | 26:BC:257:ARG:H   | 2.07                     | 0.58              |
| 36:BM:64:TRP:CZ3  | 36:BM:106:ASP:HB2 | 2.39                     | 0.58              |
| 36:BM:72:PRO:O    | 36:BM:91:TYR:O    | 2.21                     | 0.58              |
| 37:BN:73:ASN:CA   | 37:BN:76:VAL:HG12 | 2.31                     | 0.58              |
| 38:BO:111:ARG:O   | 38:BO:113:ALA:N   | 2.36                     | 0.58              |
| 39:BP:19:PHE:O    | 39:BP:20:ARG:CB   | 2.50                     | 0.58              |
| 45:BV:61:LEU:O    | 45:BV:71:LYS:HA   | 2.03                     | 0.58              |
| 55:CA:1051:C:O2'  | 55:CA:1052:U:O5'  | 2.21                     | 0.58              |
| 55:CA:1134:G:C5   | 55:CA:1135:U:H1'  | 2.38                     | 0.58              |
| 55:CA:1265:C:H2'  | 55:CA:1266:G:H5'  | 1.85                     | 0.58              |
| 55:CA:283:U:H2'   | 55:CA:284:C:H6    | 1.66                     | 0.58              |
| 55:CA:563:A:N3    | 55:CA:563:A:C2'   | 2.66                     | 0.58              |
| 9:CJ:57:VAL:HG22  | 9:CJ:58:ASN:N     | 2.16                     | 0.58              |
| 24:DA:1136:G:O2'  | 24:DA:1137:G:H8   | 1.86                     | 0.58              |
| 24:DA:1258:U:H2'  | 24:DA:1259:G:H8   | 1.66                     | 0.58              |
| 24:DA:2623:G:N2   | 50:D0:18:HIS:CE1  | 2.71                     | 0.58              |
| 24:DA:2869:G:H2'  | 24:DA:2870:C:O4'  | 2.03                     | 0.58              |
| 24:DA:3:U:H2'     | 24:DA:4:U:C6      | 2.38                     | 0.58              |
| 24:DA:478:A:N6    | 24:DA:480:A:C6    | 2.71                     | 0.58              |
| 24:DA:674:G:H5''  | 28:DE:71:GLY:H    | 1.68                     | 0.58              |
| 24:DA:729:G:C2'   | 24:DA:729:G:N3    | 2.66                     | 0.58              |
| 27:DD:21:SER:O    | 27:DD:23:PRO:HD3  | 2.03                     | 0.58              |
| 29:DF:11:VAL:HG12 | 29:DF:12:VAL:N    | 2.18                     | 0.58              |
| 31:DH:24:GLY:O    | 31:DH:26:ALA:O    | 2.22                     | 0.58              |
| 24:DA:2816:G:O3'  | 37:DN:99:LYS:HE3  | 2.03                     | 0.58              |
| 56:DB:83:G:OP1    | 49:DZ:16:LEU:HD21 | 2.03                     | 0.58              |
| 21:AA:1238:A:C5'  | 21:AA:1336:C:H41  | 2.09                     | 0.58              |
| 21:AA:1533:C:C3'  | 21:AA:1534:A:H5'' | 2.34                     | 0.58              |
| 21:AA:957:U:O2    | 21:AA:959:A:C8    | 2.56                     | 0.58              |
| 21:AA:957:U:O2    | 21:AA:959:A:H8    | 1.87                     | 0.58              |
| 1:AB:19:THR:HG23  | 1:AB:20:ARG:H     | 1.68                     | 0.58              |
| 3:AD:36:ALA:HA    | 3:AD:41:GLY:HA3   | 1.84                     | 0.58              |
| 11:AL:74:GLN:HG3  | 11:AL:75:GLU:HG2  | 1.84                     | 0.58              |
| 24:BA:1059:G:C8   | 24:BA:1060:U:H2'  | 2.38                     | 0.58              |
| 24:BA:1422:G:N3   | 24:BA:1423:G:C8   | 2.71                     | 0.58              |
| 24:BA:1914:C:O2'  | 24:BA:1915:U:H5'  | 2.04                     | 0.58              |
| 24:BA:387:U:H4'   | 24:BA:388:G:C5'   | 2.33                     | 0.58              |
| 24:BA:449:A:H4'   | 40:BQ:2:ARG:NH1   | 2.18                     | 0.58              |
| 24:BA:63:A:O2'    | 24:BA:64:A:H5'    | 2.02                     | 0.58              |
| 24:BA:786:C:C2'   | 24:BA:787:C:H5'   | 2.33                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:914:G:C8     | 24:BA:914:G:H5''   | 2.38                     | 0.58              |
| 27:BD:9:VAL:HG22   | 27:BD:10:GLY:H     | 1.67                     | 0.58              |
| 27:BD:118:PHE:CD2  | 27:BD:119:ALA:N    | 2.71                     | 0.58              |
| 33:BJ:42:ALA:O     | 33:BJ:43:GLU:C     | 2.40                     | 0.58              |
| 34:BK:34:GLY:O     | 34:BK:35:VAL:C     | 2.41                     | 0.58              |
| 45:BV:80:HIS:CD2   | 45:BV:82:TYR:H     | 2.21                     | 0.58              |
| 55:CA:1125:U:C2    | 55:CA:1127:G:N7    | 2.71                     | 0.58              |
| 55:CA:264:C:H2'    | 55:CA:265:G:O4'    | 2.04                     | 0.58              |
| 55:CA:369:G:C6     | 55:CA:393:A:N1     | 2.71                     | 0.58              |
| 55:CA:459:A:H2'    | 55:CA:460:A:C8     | 2.38                     | 0.58              |
| 3:CD:88:ASN:O      | 3:CD:92:LEU:HG     | 2.03                     | 0.58              |
| 5:CF:57:ALA:O      | 5:CF:59:TYR:HD1    | 1.87                     | 0.58              |
| 8:CI:24:ASN:HB2    | 8:CI:26:LYS:HZ2    | 1.68                     | 0.58              |
| 12:CM:92:ARG:HA    | 12:CM:92:ARG:NE    | 2.18                     | 0.58              |
| 24:DA:2643:G:C4    | 24:DA:2644:G:C8    | 2.91                     | 0.58              |
| 24:DA:2686:G:C5    | 24:DA:2687:U:C4    | 2.92                     | 0.58              |
| 24:DA:2774:C:N4    | 24:DA:2775:G:C6    | 2.71                     | 0.58              |
| 24:DA:2823:A:H2'   | 24:DA:2824:C:H5'   | 1.86                     | 0.58              |
| 24:DA:374:A:O2'    | 24:DA:375:G:O4'    | 2.17                     | 0.58              |
| 24:DA:380:G:C2     | 24:DA:395:U:O2     | 2.55                     | 0.58              |
| 24:DA:474:G:H4'    | 24:DA:475:C:OP1    | 2.02                     | 0.58              |
| 24:DA:704:G:H1'    | 24:DA:727:A:H61    | 1.67                     | 0.58              |
| 24:DA:704:G:H2'    | 24:DA:726:G:N2     | 2.18                     | 0.58              |
| 27:DD:149:ASN:O    | 27:DD:151:THR:N    | 2.36                     | 0.58              |
| 29:DF:64:PRO:HA    | 29:DF:88:VAL:CG2   | 2.33                     | 0.58              |
| 31:DH:125:THR:HG22 | 31:DH:146:VAL:HG11 | 1.85                     | 0.58              |
| 31:DH:93:SER:CB    | 31:DH:121:VAL:HG21 | 2.34                     | 0.58              |
| 41:DR:87:GLN:HG2   | 41:DR:88:GLY:H     | 1.66                     | 0.58              |
| 21:AA:251:G:H4'    | 21:AA:252:U:O5'    | 2.03                     | 0.58              |
| 21:AA:557:G:H2'    | 21:AA:558:G:O4'    | 2.03                     | 0.58              |
| 21:AA:765:G:C6     | 21:AA:812:G:C4     | 2.91                     | 0.58              |
| 21:AA:94:G:C4'     | 21:AA:95:C:H5''    | 2.32                     | 0.58              |
| 1:AB:46:VAL:HG13   | 1:AB:49:PHE:CZ     | 2.39                     | 0.58              |
| 5:AF:99:ALA:O      | 5:AF:100:SER:HB2   | 2.03                     | 0.58              |
| 11:AL:20:VAL:N     | 11:AL:21:PRO:HD3   | 2.18                     | 0.58              |
| 14:AO:52:ARG:HG3   | 14:AO:55:LEU:HD23  | 1.85                     | 0.58              |
| 17:AR:63:TYR:HE1   | 21:AA:734:G:N2     | 1.94                     | 0.58              |
| 24:BA:684:G:OP1    | 52:B2:16:HIS:CD2   | 2.57                     | 0.58              |
| 53:B3:21:PHE:O     | 53:B3:22:LYS:O     | 2.21                     | 0.58              |
| 24:BA:1333:G:N3    | 24:BA:1334:G:C8    | 2.71                     | 0.58              |
| 24:BA:1385:A:H1'   | 24:BA:1386:C:C6    | 2.38                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:1388:G:H2'  | 24:BA:1389:G:C8    | 2.39                     | 0.58              |
| 24:BA:2052:A:N6   | 24:BA:2618:G:C2    | 2.72                     | 0.58              |
| 24:BA:256:A:O2'   | 24:BA:257:C:H5'    | 2.04                     | 0.58              |
| 24:BA:2665:A:C2   | 24:BA:2666:C:C6    | 2.92                     | 0.58              |
| 24:BA:2850:A:C2   | 24:BA:2851:A:C4    | 2.90                     | 0.58              |
| 24:BA:522:A:C6    | 24:BA:523:C:N4     | 2.72                     | 0.58              |
| 24:BA:858:G:N3    | 24:BA:2268:A:H2'   | 2.18                     | 0.58              |
| 24:BA:976:G:C2    | 24:BA:977:G:C8     | 2.91                     | 0.58              |
| 27:BD:46:ARG:HG3  | 27:BD:84:LEU:HB2   | 1.86                     | 0.58              |
| 27:BD:89:GLU:HG3  | 27:BD:94:GLN:OE1   | 2.03                     | 0.58              |
| 32:BI:86:LYS:HD2  | 32:BI:86:LYS:H     | 1.67                     | 0.58              |
| 33:BJ:38:GLY:C    | 33:BJ:40:HIS:H     | 2.06                     | 0.58              |
| 42:BS:69:LEU:HG   | 42:BS:107:VAL:HG13 | 1.85                     | 0.58              |
| 55:CA:131:A:C2    | 55:CA:132:C:N3     | 2.72                     | 0.58              |
| 6:CG:77:ARG:NH1   | 55:CA:1381:U:C4    | 2.71                     | 0.58              |
| 55:CA:1417:G:N2   | 55:CA:1484:C:C4    | 2.72                     | 0.58              |
| 55:CA:517:G:H5'   | 55:CA:519:C:C2     | 2.39                     | 0.58              |
| 55:CA:794:A:H2'   | 55:CA:795:C:C6     | 2.38                     | 0.58              |
| 55:CA:953:G:H2'   | 55:CA:954:G:O4'    | 2.04                     | 0.58              |
| 6:CG:116:ALA:C    | 6:CG:120:ALA:HB3   | 2.24                     | 0.58              |
| 8:CI:33:SER:OG    | 8:CI:36:GLN:HG2    | 2.03                     | 0.58              |
| 12:CM:82:LEU:CD2  | 18:CS:60:PHE:HB3   | 2.33                     | 0.58              |
| 13:CN:50:LEU:HB2  | 13:CN:51:PRO:HD3   | 1.84                     | 0.58              |
| 24:DA:1021:A:O2'  | 24:DA:1022:G:H4'   | 2.03                     | 0.58              |
| 24:DA:1049:C:O2'  | 24:DA:1050:A:H5'   | 2.04                     | 0.58              |
| 24:DA:1075:C:O2'  | 24:DA:1076:C:C5'   | 2.51                     | 0.58              |
| 24:DA:240:C:H3'   | 24:DA:241:A:H5''   | 1.86                     | 0.58              |
| 24:DA:2660:A:H2   | 24:DA:2661:G:C5    | 2.21                     | 0.58              |
| 24:DA:720:U:H2'   | 24:DA:721:A:C8     | 2.37                     | 0.58              |
| 24:DA:79:C:H2'    | 24:DA:80:G:O4'     | 2.04                     | 0.58              |
| 24:DA:832:U:O2'   | 24:DA:833:A:O4'    | 2.19                     | 0.58              |
| 24:DA:878:A:H4'   | 24:DA:898:C:N4     | 2.19                     | 0.58              |
| 24:DA:7:G:H2'     | 24:DA:8:C:O4'      | 2.02                     | 0.58              |
| 26:DC:131:MET:HG2 | 26:DC:134:ILE:HD11 | 1.84                     | 0.58              |
| 26:DC:62:ARG:NH2  | 26:DC:62:ARG:HG2   | 2.18                     | 0.58              |
| 28:DE:136:GLN:HA  | 28:DE:139:LYS:HG2  | 1.85                     | 0.58              |
| 30:DG:163:TYR:N   | 30:DG:163:TYR:HD2  | 2.02                     | 0.58              |
| 31:DH:78:VAL:HB   | 31:DH:144:VAL:HA   | 1.85                     | 0.58              |
| 34:DK:71:ARG:CB   | 34:DK:72:PRO:HD3   | 2.22                     | 0.58              |
| 38:DO:62:LEU:HD11 | 38:DO:65:THR:N     | 2.18                     | 0.58              |
| 43:DT:29:THR:N    | 43:DT:87:LEU:HB2   | 2.16                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:AH:50:VAL:O     | 7:AH:50:VAL:HG13  | 2.04                     | 0.58              |
| 10:AK:20:ALA:HB3  | 10:AK:83:VAL:HA   | 1.84                     | 0.58              |
| 19:AT:24:ARG:O    | 19:AT:28:ARG:HG2  | 2.03                     | 0.58              |
| 24:BA:1027:A:N1   | 24:BA:1126:A:H1'  | 2.17                     | 0.58              |
| 24:BA:1257:C:O2'  | 28:BE:79:ARG:N    | 2.36                     | 0.58              |
| 24:BA:1340:U:C6   | 24:BA:1603:A:H5'  | 2.38                     | 0.58              |
| 24:BA:181:A:H2'   | 24:BA:182:A:H8    | 1.67                     | 0.58              |
| 24:BA:2585:U:O2'  | 24:BA:2586:U:H5'  | 2.04                     | 0.58              |
| 25:BB:42:C:O2'    | 25:BB:43:C:H5'    | 2.03                     | 0.58              |
| 55:CA:1245:C:H2'  | 55:CA:1246:A:H8   | 1.68                     | 0.58              |
| 55:CA:1406:U:H1'  | 55:CA:1518:A:H4'  | 1.85                     | 0.58              |
| 55:CA:31:G:C5     | 55:CA:306:A:H1'   | 2.39                     | 0.58              |
| 55:CA:382:A:O2'   | 55:CA:383:A:H5'   | 2.03                     | 0.58              |
| 2:CC:181:ILE:HG12 | 2:CC:202:PHE:HB2  | 1.85                     | 0.58              |
| 2:CC:180:ASP:OD2  | 2:CC:203:LYS:HB2  | 2.04                     | 0.58              |
| 6:CG:63:VAL:O     | 6:CG:67:ASN:HB2   | 2.03                     | 0.58              |
| 11:CL:42:LYS:HG2  | 11:CL:43:LYS:H    | 1.68                     | 0.58              |
| 24:DA:1073:A:H3'  | 24:DA:1074:G:H8   | 1.69                     | 0.58              |
| 24:DA:2315:G:C2   | 24:DA:2316:G:C4   | 2.91                     | 0.58              |
| 24:DA:2446:G:C2   | 24:DA:2501:C:C5   | 2.92                     | 0.58              |
| 24:DA:2687:U:C4   | 24:DA:2688:G:C6   | 2.90                     | 0.58              |
| 24:DA:2756:U:H1'  | 24:DA:2757:A:H5'' | 1.85                     | 0.58              |
| 24:DA:277:G:H2'   | 24:DA:361:G:C6    | 2.39                     | 0.58              |
| 26:DC:147:PRO:HA  | 26:DC:187:CYS:HB3 | 1.85                     | 0.58              |
| 30:DG:70:LEU:O    | 30:DG:74:MET:HB2  | 2.03                     | 0.58              |
| 31:DH:41:LYS:H    | 31:DH:44:ILE:HG23 | 1.68                     | 0.58              |
| 21:AA:1065:U:H5'' | 21:AA:1190:G:H21  | 1.69                     | 0.58              |
| 21:AA:1251:A:H2'  | 21:AA:1252:A:H8   | 1.68                     | 0.58              |
| 21:AA:1338:G:C2   | 21:AA:1339:A:C4   | 2.91                     | 0.58              |
| 21:AA:1463:U:C2   | 21:AA:1464:U:C5   | 2.92                     | 0.58              |
| 21:AA:833:G:N2    | 21:AA:854:U:H1'   | 2.19                     | 0.58              |
| 1:AB:140:LEU:O    | 1:AB:144:GLU:HG2  | 2.03                     | 0.58              |
| 6:AG:34:LYS:HD3   | 6:AG:37:THR:HG21  | 1.86                     | 0.58              |
| 7:AH:74:ILE:CD1   | 7:AH:128:VAL:HG22 | 2.33                     | 0.58              |
| 20:AU:39:LYS:N    | 20:AU:40:PRO:HD2  | 2.19                     | 0.58              |
| 24:BA:1127:A:O2'  | 24:BA:1128:G:H5'  | 2.02                     | 0.58              |
| 24:BA:2021:C:OP1  | 50:B0:8:THR:HG21  | 2.03                     | 0.58              |
| 24:BA:2047:C:C2'  | 24:BA:2048:G:H5'  | 2.33                     | 0.58              |
| 24:BA:494:G:N2    | 42:BS:57:ASN:HD21 | 2.00                     | 0.58              |
| 24:BA:522:A:N6    | 24:BA:523:C:N4    | 2.51                     | 0.58              |
| 24:BA:638:G:C5    | 24:BA:651:G:N2    | 2.72                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:856:G:N2    | 24:BA:857:G:C2    | 2.71                     | 0.58              |
| 24:BA:2682:A:C8   | 27:BD:11:MET:HG3  | 2.38                     | 0.58              |
| 28:BE:148:ILE:HA  | 28:BE:187:VAL:HB  | 1.85                     | 0.58              |
| 41:BR:47:VAL:O    | 41:BR:47:VAL:HG12 | 2.03                     | 0.58              |
| 46:BW:9:THR:OG1   | 46:BW:10:ARG:N    | 2.35                     | 0.58              |
| 55:CA:512:U:HO2'  | 55:CA:513:C:H6    | 1.51                     | 0.58              |
| 55:CA:539:A:H2'   | 55:CA:540:G:C8    | 2.38                     | 0.58              |
| 55:CA:672:U:H2'   | 55:CA:673:A:H8    | 1.68                     | 0.58              |
| 55:CA:721:G:H4'   | 55:CA:722:G:H5''  | 1.86                     | 0.58              |
| 1:CB:89:PHE:HB3   | 1:CB:149:GLY:O    | 2.03                     | 0.58              |
| 3:CD:127:ARG:CZ   | 3:CD:127:ARG:HB2  | 2.31                     | 0.58              |
| 3:CD:190:LEU:O    | 3:CD:190:LEU:HD23 | 2.03                     | 0.58              |
| 4:CE:45:VAL:HB    | 4:CE:117:ALA:HB2  | 1.86                     | 0.58              |
| 5:CF:35:LYS:HE2   | 5:CF:37:HIS:HE1   | 1.68                     | 0.58              |
| 24:DA:1055:G:H2'  | 24:DA:1056:G:H5'  | 1.85                     | 0.58              |
| 24:DA:1087:G:C5   | 24:DA:1089:A:C2   | 2.92                     | 0.58              |
| 24:DA:1289:C:O2'  | 24:DA:1290:C:H6   | 1.86                     | 0.58              |
| 24:DA:1552:A:H2   | 24:DA:1553:A:C8   | 2.21                     | 0.58              |
| 24:DA:1826:G:C6   | 24:DA:1827:U:C4   | 2.90                     | 0.58              |
| 24:DA:2300:C:H2'  | 24:DA:2301:C:C6   | 2.39                     | 0.58              |
| 24:DA:2788:C:H2'  | 24:DA:2789:C:C6   | 2.39                     | 0.58              |
| 24:DA:583:G:C6    | 24:DA:584:C:C4    | 2.92                     | 0.58              |
| 24:DA:848:C:H2'   | 24:DA:849:A:C8    | 2.38                     | 0.58              |
| 34:DK:63:VAL:HG21 | 34:DK:85:VAL:HG23 | 1.85                     | 0.58              |
| 21:AA:1022:A:H2'  | 21:AA:1023:U:O4'  | 2.04                     | 0.58              |
| 21:AA:116:A:H2'   | 21:AA:117:G:C8    | 2.38                     | 0.58              |
| 21:AA:1338:G:H2'  | 21:AA:1339:A:H8   | 1.68                     | 0.58              |
| 21:AA:814:A:C8    | 21:AA:816:A:C8    | 2.91                     | 0.58              |
| 1:AB:24:PRO:HG2   | 21:AA:829:G:O2'   | 2.04                     | 0.58              |
| 2:AC:178:ARG:HD3  | 21:AA:1112:C:H1'  | 1.86                     | 0.58              |
| 7:AH:86:LYS:HD3   | 7:AH:124:ILE:HD11 | 1.84                     | 0.58              |
| 8:AI:21:LYS:NZ    | 8:AI:23:GLY:HA3   | 2.18                     | 0.58              |
| 8:AI:7:GLY:HA3    | 8:AI:85:ALA:HB2   | 1.84                     | 0.58              |
| 19:AT:25:SER:HB3  | 21:AA:1458:G:H5'' | 1.86                     | 0.58              |
| 23:AW:4:U:O2'     | 23:AW:5:U:H5'     | 2.03                     | 0.58              |
| 24:BA:1587:G:H8   | 24:BA:1587:G:OP2  | 1.87                     | 0.58              |
| 24:BA:1660:G:H2'  | 24:BA:1661:G:H8   | 1.69                     | 0.58              |
| 24:BA:1700:A:H2'  | 24:BA:1701:A:O4'  | 2.03                     | 0.58              |
| 24:BA:2581:G:C8   | 24:BA:2610:C:N4   | 2.71                     | 0.58              |
| 24:BA:2627:G:H2'  | 24:BA:2628:C:H6   | 1.67                     | 0.58              |
| 24:BA:2783:U:H2'  | 24:BA:2784:U:C6   | 2.37                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:704:G:C2'   | 24:BA:726:G:H22    | 2.17                     | 0.58              |
| 24:BA:860:U:H2'   | 24:BA:861:A:H8     | 1.69                     | 0.58              |
| 27:BD:140:HIS:CE1 | 59:BD:402:HOH:O    | 2.53                     | 0.58              |
| 30:BG:162:ARG:NH1 | 30:BG:168:VAL:HG21 | 2.18                     | 0.58              |
| 32:BI:58:ILE:O    | 32:BI:60:VAL:HG23  | 2.03                     | 0.58              |
| 55:CA:1242:G:C2'  | 55:CA:1243:C:O5'   | 2.52                     | 0.58              |
| 6:CG:108:ARG:CZ   | 55:CA:1240:U:C6    | 2.87                     | 0.58              |
| 6:CG:45:ALA:HB1   | 6:CG:120:ALA:CB    | 2.22                     | 0.58              |
| 7:CH:65:PHE:CD2   | 7:CH:66:GLN:HG2    | 2.38                     | 0.58              |
| 51:D1:34:GLU:HG3  | 51:D1:49:LYS:HB2   | 1.85                     | 0.58              |
| 24:DA:1090:A:H2'  | 24:DA:1091:G:H5''  | 1.85                     | 0.58              |
| 24:DA:1476:U:O2'  | 24:DA:1477:A:P     | 2.61                     | 0.58              |
| 24:DA:2084:C:H2'  | 24:DA:2085:U:H6    | 1.67                     | 0.58              |
| 24:DA:2253:G:C6   | 24:DA:2254:C:C4    | 2.92                     | 0.58              |
| 24:DA:2077:A:C8   | 24:DA:2435:A:C4    | 2.91                     | 0.58              |
| 24:DA:2653:U:C4   | 24:DA:2654:A:C6    | 2.92                     | 0.58              |
| 24:DA:345:A:O2'   | 24:DA:346:A:C2     | 2.53                     | 0.58              |
| 24:DA:371:A:H61   | 24:DA:401:A:H3'    | 1.68                     | 0.58              |
| 29:DF:109:ARG:NH1 | 29:DF:135:ILE:CG2  | 2.66                     | 0.58              |
| 30:DG:8:VAL:HB    | 30:DG:49:LEU:HB3   | 1.86                     | 0.58              |
| 24:DA:2748:A:C1'  | 30:DG:66:THR:HG22  | 2.27                     | 0.58              |
| 33:DJ:111:LYS:HB2 | 33:DJ:115:GLY:H    | 1.69                     | 0.58              |
| 34:DK:1:MET:HB2   | 34:DK:32:TYR:HB3   | 1.85                     | 0.58              |
| 21:AA:1062:U:H2'  | 21:AA:1063:C:C5    | 2.37                     | 0.58              |
| 21:AA:1518:A:H2'  | 21:AA:1519:A:C8    | 2.38                     | 0.58              |
| 21:AA:33:A:H2'    | 21:AA:34:C:H6      | 1.69                     | 0.58              |
| 21:AA:794:A:O2'   | 21:AA:795:C:H5'    | 2.03                     | 0.58              |
| 1:AB:209:VAL:HB   | 1:AB:213:LEU:HB2   | 1.85                     | 0.58              |
| 4:AE:41:GLY:HA2   | 4:AE:116:VAL:O     | 2.03                     | 0.58              |
| 8:AI:50:PRO:HG3   | 8:AI:82:ILE:HD12   | 1.85                     | 0.58              |
| 13:AN:81:ILE:O    | 13:AN:85:GLU:HG2   | 2.03                     | 0.58              |
| 17:AR:37:LYS:HB3  | 21:AA:719:C:H1'    | 1.85                     | 0.58              |
| 54:B4:25:VAL:HG11 | 54:B4:35:GLN:HE21  | 1.68                     | 0.58              |
| 24:BA:1416:G:O2'  | 24:BA:1417:C:O5'   | 2.22                     | 0.58              |
| 29:BF:165:GLY:O   | 29:BF:168:LEU:HB3  | 2.04                     | 0.58              |
| 36:BM:35:ALA:O    | 36:BM:128:THR:HA   | 2.04                     | 0.58              |
| 43:BT:43:ILE:O    | 43:BT:47:VAL:HG23  | 2.04                     | 0.58              |
| 55:CA:1502:A:O2'  | 55:CA:1503:A:P     | 2.62                     | 0.58              |
| 55:CA:936:C:H2'   | 55:CA:937:A:C8     | 2.39                     | 0.58              |
| 1:CB:139:GLU:HG3  | 1:CB:140:LEU:N     | 2.19                     | 0.58              |
| 4:CE:76:ASN:HB2   | 4:CE:81:GLN:HE22   | 1.68                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:CE:94:PHE:CZ    | 4:CE:95:MET:O     | 2.57                     | 0.58              |
| 10:CK:21:HIS:HD2  | 10:CK:34:THR:HG21 | 1.68                     | 0.58              |
| 24:DA:1113:U:O2'  | 24:DA:1114:C:C6   | 2.50                     | 0.58              |
| 24:DA:1443:U:H2'  | 24:DA:1444:G:H8   | 1.68                     | 0.58              |
| 24:DA:1965:C:C5'  | 24:DA:1966:A:H5'' | 2.34                     | 0.58              |
| 24:DA:2335:A:H2'  | 24:DA:2337:G:N7   | 2.19                     | 0.58              |
| 24:DA:555:G:H8    | 24:DA:555:G:OP2   | 1.85                     | 0.58              |
| 24:DA:54:G:C6     | 24:DA:55:G:N7     | 2.72                     | 0.58              |
| 24:DA:576:U:H2'   | 24:DA:577:G:H8    | 1.67                     | 0.58              |
| 24:DA:646:U:H2'   | 24:DA:647:G:O4'   | 2.04                     | 0.58              |
| 28:DE:60:TRP:CZ2  | 28:DE:71:GLY:HA2  | 2.39                     | 0.58              |
| 30:DG:163:TYR:N   | 30:DG:163:TYR:CD2 | 2.72                     | 0.58              |
| 34:DK:40:LYS:NZ   | 34:DK:89:ASN:HD21 | 2.02                     | 0.58              |
| 37:DN:56:LYS:HA   | 37:DN:84:GLY:HA2  | 1.86                     | 0.58              |
| 24:DA:508:A:H62   | 42:DS:9:HIS:CE1   | 2.22                     | 0.58              |
| 44:DU:45:GLN:HE21 | 44:DU:45:GLN:HA   | 1.67                     | 0.58              |
| 45:DV:79:ARG:CZ   | 45:DV:79:ARG:HB3  | 2.34                     | 0.58              |
| 46:DW:19:ARG:HA   | 46:DW:34:SER:HA   | 1.86                     | 0.58              |
| 21:AA:1341:U:O2'  | 21:AA:1342:C:H5'  | 2.04                     | 0.58              |
| 21:AA:1349:A:C6   | 21:AA:1374:A:C8   | 2.92                     | 0.58              |
| 21:AA:228:A:H2'   | 21:AA:229:U:O4'   | 2.04                     | 0.58              |
| 21:AA:978:A:OP2   | 21:AA:1362:A:N6   | 2.37                     | 0.58              |
| 3:AD:173:ASP:CG   | 3:AD:174:ALA:N    | 2.56                     | 0.58              |
| 16:AQ:58:VAL:HG23 | 16:AQ:76:ARG:O    | 2.04                     | 0.58              |
| 24:BA:1060:U:O4'  | 24:BA:1062:G:C5'  | 2.52                     | 0.58              |
| 24:BA:1447:C:H1'  | 24:BA:1545:A:H1'  | 1.84                     | 0.58              |
| 24:BA:1680:U:H2'  | 24:BA:1681:G:O4'  | 2.03                     | 0.58              |
| 24:BA:2075:U:H2'  | 24:BA:2238:G:H22  | 1.68                     | 0.58              |
| 24:BA:548:G:H5''  | 24:BA:549:G:H5'   | 1.86                     | 0.58              |
| 24:BA:655:A:O2'   | 24:BA:656:G:C8    | 2.57                     | 0.58              |
| 24:BA:666:A:O2'   | 24:BA:667:U:H5'   | 2.02                     | 0.58              |
| 24:BA:745:G:C2'   | 24:BA:746:U:H5'   | 2.32                     | 0.58              |
| 27:BD:14:ILE:O    | 27:BD:14:ILE:HG13 | 2.03                     | 0.58              |
| 30:BG:26:LYS:HB3  | 30:BG:32:LEU:HG   | 1.86                     | 0.58              |
| 31:BH:68:ARG:NH2  | 31:BH:69:ALA:HA   | 2.18                     | 0.58              |
| 39:BP:50:ARG:HD3  | 39:BP:51:ASN:H    | 1.68                     | 0.58              |
| 36:BM:36:VAL:HG22 | 45:BV:82:TYR:CD1  | 2.37                     | 0.58              |
| 55:CA:996:A:N1    | 55:CA:1046:A:H5'  | 2.18                     | 0.58              |
| 9:CJ:62:ARG:NH1   | 55:CA:1366:C:O3'  | 2.36                     | 0.58              |
| 55:CA:500:G:H2'   | 55:CA:501:C:C6    | 2.39                     | 0.58              |
| 55:CA:727:G:N2    | 55:CA:731:G:C4    | 2.71                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CB:44:LYS:O     | 1:CB:48:MET:HG3    | 2.04                     | 0.58              |
| 5:CF:67:PRO:O     | 5:CF:70:VAL:HG22   | 2.03                     | 0.58              |
| 5:CF:92:THR:O     | 5:CF:93:LYS:HG2    | 2.03                     | 0.58              |
| 9:CJ:59:LYS:HB2   | 9:CJ:62:ARG:NH2    | 2.19                     | 0.58              |
| 9:CJ:80:THR:HG22  | 9:CJ:82:LYS:NZ     | 2.17                     | 0.58              |
| 12:CM:32:ILE:HG13 | 12:CM:59:VAL:HB    | 1.84                     | 0.58              |
| 13:CN:60:ARG:HG2  | 13:CN:61:ASN:H     | 1.69                     | 0.58              |
| 17:CR:22:TYR:HE1  | 17:CR:64:LEU:HD12  | 1.69                     | 0.58              |
| 24:DA:1008:A:N6   | 24:DA:1136:G:C6    | 2.71                     | 0.58              |
| 24:DA:1213:A:H2'  | 24:DA:1214:A:H8    | 1.67                     | 0.58              |
| 24:DA:1413:A:H2'  | 24:DA:1414:C:C6    | 2.39                     | 0.58              |
| 24:DA:1552:A:C2'  | 24:DA:1552:A:N3    | 2.59                     | 0.58              |
| 24:DA:1668:A:H5'  | 24:DA:1669:A:C5    | 2.38                     | 0.58              |
| 24:DA:2554:U:H2'  | 24:DA:2555:U:C6    | 2.38                     | 0.58              |
| 24:DA:2567:G:O2'  | 24:DA:2568:U:H5'   | 2.03                     | 0.58              |
| 24:DA:2716:C:H2'  | 24:DA:2717:C:C6    | 2.39                     | 0.58              |
| 24:DA:391:A:H2'   | 24:DA:392:U:C6     | 2.39                     | 0.58              |
| 24:DA:804:A:H2'   | 24:DA:806:C:C4     | 2.39                     | 0.58              |
| 56:DB:12:C:H5''   | 56:DB:15:A:N6      | 2.19                     | 0.58              |
| 27:DD:137:SER:C   | 27:DD:138:LEU:HD22 | 2.24                     | 0.58              |
| 42:DS:31:GLN:O    | 42:DS:35:ILE:HG12  | 2.04                     | 0.58              |
| 21:AA:1365:G:H2'  | 21:AA:1366:C:C6    | 2.39                     | 0.58              |
| 11:AL:82:ARG:N    | 11:AL:95:HIS:O     | 2.37                     | 0.58              |
| 13:AN:48:GLN:HE21 | 13:AN:48:GLN:HA    | 1.69                     | 0.58              |
| 54:B4:9:LYS:H     | 54:B4:9:LYS:CE     | 2.16                     | 0.58              |
| 24:BA:2023:C:O2'  | 24:BA:2024:G:C5'   | 2.50                     | 0.58              |
| 24:BA:464:U:H2'   | 24:BA:465:G:O4'    | 2.03                     | 0.58              |
| 24:BA:2683:C:H4'  | 27:BD:13:ARG:NH2   | 2.19                     | 0.58              |
| 27:BD:47:ALA:HA   | 27:BD:84:LEU:HG    | 1.84                     | 0.58              |
| 30:BG:84:LYS:HD2  | 30:BG:133:LYS:HG2  | 1.86                     | 0.58              |
| 31:BH:97:ARG:HH12 | 55:CA:368:U:P      | 2.27                     | 0.58              |
| 40:BQ:71:ASN:OD1  | 40:BQ:106:THR:HG23 | 2.04                     | 0.58              |
| 40:BQ:8:ILE:HG13  | 40:BQ:9:ALA:N      | 2.18                     | 0.58              |
| 44:BU:53:GLN:N    | 44:BU:54:PRO:CD    | 2.67                     | 0.58              |
| 46:BW:72:GLY:C    | 46:BW:74:LYS:N     | 2.54                     | 0.58              |
| 55:CA:129:A:O2'   | 55:CA:130:A:C8     | 2.56                     | 0.58              |
| 55:CA:68:G:H1'    | 55:CA:151:A:H61    | 1.68                     | 0.58              |
| 55:CA:875:U:O2'   | 55:CA:876:C:O5'    | 2.21                     | 0.58              |
| 3:CD:90:LEU:HD11  | 3:CD:194:ILE:CD1   | 2.34                     | 0.58              |
| 6:CG:114:SER:O    | 6:CG:118:ARG:HG3   | 2.03                     | 0.58              |
| 7:CH:7:ALA:O      | 7:CH:11:THR:HG23   | 2.02                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:CI:40:ARG:HG3   | 8:CI:44:ARG:NH1   | 2.18                     | 0.58              |
| 12:CM:86:ARG:HD3  | 12:CM:96:VAL:HG21 | 1.84                     | 0.58              |
| 19:CT:70:LYS:HA   | 19:CT:73:ARG:HE   | 1.68                     | 0.58              |
| 24:DA:123:G:N2    | 24:DA:124:G:H1'   | 2.18                     | 0.58              |
| 24:DA:1326:U:O2'  | 24:DA:1327:A:H8   | 1.76                     | 0.58              |
| 24:DA:1327:A:O2'  | 24:DA:1328:A:O4'  | 2.11                     | 0.58              |
| 24:DA:1331:G:C4   | 24:DA:1333:G:N7   | 2.72                     | 0.58              |
| 24:DA:170:U:H2'   | 24:DA:171:U:C6    | 2.38                     | 0.58              |
| 24:DA:2210:U:H4'  | 24:DA:2211:A:C5'  | 2.34                     | 0.58              |
| 24:DA:2554:U:H2'  | 24:DA:2555:U:H6   | 1.69                     | 0.58              |
| 56:DB:13:G:N2     | 56:DB:69:G:H21    | 2.01                     | 0.58              |
| 56:DB:66:A:H4'    | 56:DB:67:G:C8     | 2.39                     | 0.58              |
| 26:DC:127:ASN:O   | 26:DC:190:THR:HA  | 2.04                     | 0.58              |
| 27:DD:208:LYS:O   | 27:DD:209:ALA:CB  | 2.52                     | 0.58              |
| 28:DE:150:THR:O   | 28:DE:192:ALA:HB2 | 2.04                     | 0.58              |
| 34:DK:17:ARG:CG   | 34:DK:18:ARG:H    | 2.17                     | 0.58              |
| 40:DQ:89:ILE:HG22 | 40:DQ:91:ARG:H    | 1.68                     | 0.58              |
| 40:DQ:101:ASP:HB2 | 41:DR:2:TYR:OH    | 2.04                     | 0.58              |
| 44:DU:3:LYS:HD3   | 44:DU:82:VAL:HG21 | 1.85                     | 0.58              |
| 21:AA:1348:U:O2'  | 21:AA:1349:A:H8   | 1.86                     | 0.57              |
| 21:AA:71:A:C5     | 21:AA:100:G:C5    | 2.92                     | 0.57              |
| 21:AA:874:G:C6    | 21:AA:875:U:C4    | 2.92                     | 0.57              |
| 1:AB:161:PHE:HA   | 1:AB:183:PHE:O    | 2.04                     | 0.57              |
| 2:AC:149:LYS:HG3  | 2:AC:200:TRP:HB2  | 1.85                     | 0.57              |
| 3:AD:98:ASP:HB3   | 3:AD:114:ARG:HG2  | 1.85                     | 0.57              |
| 24:BA:176:A:N7    | 24:BA:177:G:C6    | 2.72                     | 0.57              |
| 24:BA:2020:A:O2'  | 24:BA:2021:C:H3'  | 2.03                     | 0.57              |
| 24:BA:2079:U:O3'  | 47:BX:20:ALA:HB2  | 2.04                     | 0.57              |
| 24:BA:2552:U:O2   | 24:BA:2554:U:H5'  | 2.04                     | 0.57              |
| 24:BA:505:A:O2'   | 24:BA:506:G:H5'   | 2.04                     | 0.57              |
| 24:BA:60:G:N3     | 24:BA:74:A:C2     | 2.72                     | 0.57              |
| 27:BD:91:THR:O    | 27:BD:93:GLY:N    | 2.35                     | 0.57              |
| 29:BF:30:VAL:CG1  | 29:BF:96:TRP:CH2  | 2.87                     | 0.57              |
| 33:BJ:101:ILE:O   | 33:BJ:105:VAL:CG1 | 2.51                     | 0.57              |
| 39:BP:30:TRP:CH2  | 39:BP:39:LEU:HD11 | 2.39                     | 0.57              |
| 55:CA:1513:A:H2'  | 55:CA:1514:G:H8   | 1.68                     | 0.57              |
| 55:CA:557:G:C6    | 55:CA:558:G:N1    | 2.72                     | 0.57              |
| 3:CD:125:ASN:N    | 3:CD:141:VAL:O    | 2.35                     | 0.57              |
| 8:CI:44:ARG:HA    | 8:CI:46:VAL:HG22  | 1.86                     | 0.57              |
| 12:CM:1:ALA:H3    | 12:CM:2:ARG:CD    | 2.17                     | 0.57              |
| 16:CQ:4:ILE:HG22  | 16:CQ:5:ARG:N     | 2.18                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:D3:3:ILE:HG21   | 53:D3:62:PRO:HG2   | 1.86                     | 0.57              |
| 24:DA:1068:G:H2'   | 24:DA:1069:A:C8    | 2.38                     | 0.57              |
| 24:DA:1623:G:C2    | 24:DA:1624:U:C6    | 2.91                     | 0.57              |
| 24:DA:1950:G:N1    | 24:DA:1954:G:C8    | 2.72                     | 0.57              |
| 24:DA:2212:A:C8    | 24:DA:2214:C:N4    | 2.72                     | 0.57              |
| 24:DA:2812:G:C2    | 24:DA:2813:A:C4    | 2.92                     | 0.57              |
| 24:DA:397:U:O2'    | 24:DA:398:C:O4'    | 2.12                     | 0.57              |
| 24:DA:75:G:O2'     | 24:DA:76:C:C6      | 2.56                     | 0.57              |
| 24:DA:975:A:C4     | 24:DA:990:A:N7     | 2.72                     | 0.57              |
| 56:DB:57:A:H2'     | 56:DB:58:A:C8      | 2.39                     | 0.57              |
| 27:DD:118:PHE:CD1  | 27:DD:119:ALA:N    | 2.72                     | 0.57              |
| 27:DD:53:GLY:HA3   | 27:DD:77:ARG:HG3   | 1.86                     | 0.57              |
| 28:DE:153:LEU:HB2  | 28:DE:171:ASP:HB3  | 1.86                     | 0.57              |
| 29:DF:101:ARG:HH11 | 29:DF:138:PRO:HB3  | 1.69                     | 0.57              |
| 29:DF:35:LEU:HA    | 29:DF:152:ASP:O    | 2.03                     | 0.57              |
| 21:AA:178:C:H2'    | 21:AA:179:A:H8     | 1.69                     | 0.57              |
| 11:AL:49:ARG:HH21  | 21:AA:522:C:H41    | 1.51                     | 0.57              |
| 21:AA:774:G:C6     | 21:AA:775:G:C5     | 2.93                     | 0.57              |
| 1:AB:14:HIS:O      | 1:AB:14:HIS:CG     | 2.56                     | 0.57              |
| 1:AB:24:PRO:HB3    | 21:AA:829:G:O3'    | 2.03                     | 0.57              |
| 3:AD:29:THR:O      | 3:AD:30:LYS:HE2    | 2.04                     | 0.57              |
| 8:AI:112:ARG:HH22  | 9:AJ:64:GLN:HE22   | 1.52                     | 0.57              |
| 24:BA:811:U:H1'    | 24:BA:1251:C:C6    | 2.39                     | 0.57              |
| 24:BA:1387:A:H2'   | 24:BA:1388:G:C8    | 2.39                     | 0.57              |
| 24:BA:2294:G:H5''  | 38:BO:10:ARG:HD3   | 1.85                     | 0.57              |
| 24:BA:2467:C:O2    | 36:BM:123:LYS:HE2  | 2.04                     | 0.57              |
| 24:BA:747:U:C4     | 24:BA:2613:U:C4    | 2.92                     | 0.57              |
| 24:BA:928:A:H2'    | 24:BA:929:U:O4'    | 2.03                     | 0.57              |
| 27:BD:53:GLY:HA3   | 27:BD:77:ARG:HB2   | 1.86                     | 0.57              |
| 28:BE:48:THR:HG22  | 28:BE:86:ALA:HB3   | 1.85                     | 0.57              |
| 31:BH:76:GLU:HB3   | 31:BH:103:VAL:HG12 | 1.85                     | 0.57              |
| 35:BL:55:MET:HA    | 35:BL:55:MET:CE    | 2.34                     | 0.57              |
| 39:BP:26:GLU:HG3   | 39:BP:43:GLU:HB2   | 1.86                     | 0.57              |
| 33:BJ:44:TYR:HA    | 40:BQ:59:LEU:HD21  | 1.86                     | 0.57              |
| 41:BR:25:LEU:H     | 41:BR:94:THR:CG2   | 2.17                     | 0.57              |
| 41:BR:6:GLN:HE21   | 41:BR:9:GLY:HA2    | 1.69                     | 0.57              |
| 42:BS:74:ILE:HD13  | 42:BS:105:VAL:HG22 | 1.86                     | 0.57              |
| 42:BS:25:ARG:NE    | 42:BS:73:LYS:NZ    | 2.52                     | 0.57              |
| 43:BT:67:VAL:HG12  | 43:BT:76:ARG:HG3   | 1.85                     | 0.57              |
| 24:BA:856:G:H1'    | 46:BW:23:LYS:HB3   | 1.86                     | 0.57              |
| 55:CA:1077:G:N2    | 55:CA:1080:A:OP2   | 2.37                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:1145:A:O2'  | 55:CA:1146:A:C8   | 2.56                     | 0.57              |
| 55:CA:1160:G:HO2' | 55:CA:1161:C:H6   | 1.49                     | 0.57              |
| 55:CA:1179:A:H2'  | 55:CA:1180:A:O4'  | 2.03                     | 0.57              |
| 55:CA:1285:A:H4'  | 55:CA:1286:U:OP1  | 2.03                     | 0.57              |
| 55:CA:1441:A:H2'  | 55:CA:1442:G:H8   | 1.69                     | 0.57              |
| 55:CA:1530:G:O2'  | 55:CA:1531:A:C8   | 2.56                     | 0.57              |
| 55:CA:452:A:O2'   | 55:CA:453:G:O4'   | 2.20                     | 0.57              |
| 55:CA:548:G:H2'   | 55:CA:549:C:C6    | 2.39                     | 0.57              |
| 1:CB:99:MET:HA    | 1:CB:106:VAL:HG21 | 1.85                     | 0.57              |
| 2:CC:129:PHE:CE2  | 2:CC:156:LEU:HD13 | 2.39                     | 0.57              |
| 5:CF:86:ARG:HD2   | 55:CA:673:A:H4'   | 1.86                     | 0.57              |
| 6:CG:61:PHE:O     | 6:CG:63:VAL:N     | 2.37                     | 0.57              |
| 11:CL:29:LYS:O    | 11:CL:81:ILE:HG22 | 2.04                     | 0.57              |
| 18:CS:28:LYS:O    | 18:CS:30:LEU:HD12 | 2.04                     | 0.57              |
| 24:DA:30:G:H4'    | 24:DA:1214:A:O2'  | 2.04                     | 0.57              |
| 24:DA:121:G:N2    | 24:DA:131:A:C4    | 2.72                     | 0.57              |
| 24:DA:233:A:O2'   | 24:DA:234:U:C6    | 2.57                     | 0.57              |
| 24:DA:2595:G:N1   | 24:DA:2599:G:C6   | 2.72                     | 0.57              |
| 24:DA:45:G:H4'    | 24:DA:46:G:H5'    | 1.85                     | 0.57              |
| 24:DA:719:C:H2'   | 24:DA:720:U:H6    | 1.69                     | 0.57              |
| 24:DA:777:G:N7    | 24:DA:793:A:H2    | 2.02                     | 0.57              |
| 24:DA:2227:A:H5'' | 26:DC:260:LYS:CD  | 2.34                     | 0.57              |
| 29:DF:16:MET:HA   | 29:DF:21:TYR:HB2  | 1.86                     | 0.57              |
| 24:DA:2358:A:N6   | 35:DL:54:GLN:HE22 | 1.97                     | 0.57              |
| 34:DK:76:VAL:HB   | 39:DP:72:VAL:CG2  | 2.33                     | 0.57              |
| 46:DW:18:LYS:HD3  | 46:DW:19:ARG:HG2  | 1.85                     | 0.57              |
| 47:DX:31:ASN:HD22 | 47:DX:31:ASN:H    | 1.52                     | 0.57              |
| 21:AA:1140:C:HO2' | 21:AA:1141:C:H6   | 1.53                     | 0.57              |
| 21:AA:1305:G:O2'  | 21:AA:1306:A:H8   | 1.87                     | 0.57              |
| 21:AA:324:G:N2    | 21:AA:326:G:H3'   | 2.19                     | 0.57              |
| 14:AO:23:SER:HA   | 21:AA:751:U:H4'   | 1.86                     | 0.57              |
| 12:AM:22:TYR:HB2  | 12:AM:65:GLU:HA   | 1.85                     | 0.57              |
| 20:AU:33:ARG:HE   | 20:AU:34:ARG:HG3  | 1.70                     | 0.57              |
| 22:AX:39:U:H2'    | 22:AX:40:C:H6     | 1.69                     | 0.57              |
| 24:BA:1005:C:H1'  | 24:BA:1012:U:N3   | 2.19                     | 0.57              |
| 24:BA:1016:G:H2'  | 24:BA:1017:G:O4'  | 2.04                     | 0.57              |
| 24:BA:141:G:H5'   | 24:BA:142:A:C8    | 2.39                     | 0.57              |
| 24:BA:2828:G:C2'  | 24:BA:2829:A:H5'  | 2.33                     | 0.57              |
| 24:BA:619:G:H5''  | 24:BA:620:G:OP2   | 2.03                     | 0.57              |
| 24:BA:653:U:H6    | 24:BA:653:U:H5''  | 1.69                     | 0.57              |
| 24:BA:827:U:OP2   | 24:BA:828:U:N3    | 2.37                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:838:C:C5    | 24:BA:941:A:N6    | 2.72                     | 0.57              |
| 24:BA:954:G:N7    | 24:BA:955:U:C5    | 2.72                     | 0.57              |
| 25:BB:76:G:H5'    | 45:BV:9:ARG:HH12  | 1.70                     | 0.57              |
| 33:BJ:88:THR:HG23 | 33:BJ:90:GLU:HG3  | 1.86                     | 0.57              |
| 38:BO:103:VAL:O   | 38:BO:105:ALA:O   | 2.22                     | 0.57              |
| 40:BQ:82:LEU:HB3  | 40:BQ:88:GLU:OE2  | 2.03                     | 0.57              |
| 55:CA:1102:A:O2'  | 55:CA:1103:C:H5'  | 2.04                     | 0.57              |
| 55:CA:1299:A:C8   | 55:CA:1301:U:H1'  | 2.39                     | 0.57              |
| 6:CG:27:ASN:HB3   | 55:CA:1374:A:O3'  | 2.03                     | 0.57              |
| 4:CE:95:MET:HA    | 4:CE:124:ALA:CB   | 2.34                     | 0.57              |
| 6:CG:59:GLU:HG3   | 6:CG:60:ALA:N     | 2.20                     | 0.57              |
| 8:CI:61:ASP:C     | 8:CI:62:LEU:HD22  | 2.25                     | 0.57              |
| 12:CM:1:ALA:H3    | 12:CM:8:ILE:HG23  | 1.68                     | 0.57              |
| 24:DA:1548:A:H2'  | 24:DA:1549:A:C8   | 2.38                     | 0.57              |
| 24:DA:2241:A:H2'  | 24:DA:2242:G:C8   | 2.38                     | 0.57              |
| 24:DA:250:G:H2'   | 24:DA:251:A:N7    | 2.20                     | 0.57              |
| 24:DA:2601:C:C2   | 24:DA:2603:G:N7   | 2.72                     | 0.57              |
| 24:DA:866:A:HO2'  | 24:DA:867:C:H6    | 1.44                     | 0.57              |
| 26:DC:124:LYS:NZ  | 26:DC:124:LYS:HB3 | 2.20                     | 0.57              |
| 26:DC:131:MET:HE2 | 26:DC:187:CYS:O   | 2.04                     | 0.57              |
| 28:DE:29:HIS:HA   | 28:DE:32:VAL:HG22 | 1.86                     | 0.57              |
| 38:DO:57:ALA:C    | 38:DO:58:ILE:HD12 | 2.24                     | 0.57              |
| 42:DS:29:VAL:HG23 | 42:DS:69:LEU:O    | 2.04                     | 0.57              |
| 21:AA:1023:U:H2'  | 21:AA:1024:G:C8   | 2.39                     | 0.57              |
| 21:AA:1099:G:C6   | 21:AA:1100:C:C4   | 2.92                     | 0.57              |
| 21:AA:1394:A:O2'  | 21:AA:1395:C:P    | 2.62                     | 0.57              |
| 21:AA:744:C:H2'   | 21:AA:745:G:C8    | 2.39                     | 0.57              |
| 3:AD:61:ARG:HH21  | 3:AD:67:LEU:HA    | 1.70                     | 0.57              |
| 7:AH:99:GLY:HA3   | 7:AH:129:ALA:CB   | 2.33                     | 0.57              |
| 8:AI:104:THR:HG23 | 21:AA:1179:A:O3'  | 2.04                     | 0.57              |
| 9:AJ:5:ARG:HG2    | 9:AJ:79:PRO:HD3   | 1.84                     | 0.57              |
| 11:AL:45:ASN:ND2  | 21:AA:528:C:N4    | 2.53                     | 0.57              |
| 15:AP:28:ARG:NH1  | 15:AP:29:ASN:HD21 | 2.01                     | 0.57              |
| 24:BA:1050:A:H2'  | 24:BA:1051:G:O4'  | 2.05                     | 0.57              |
| 24:BA:1847:A:H2'  | 24:BA:1848:A:C8   | 2.39                     | 0.57              |
| 24:BA:2297:A:C5   | 24:BA:2320:U:C2   | 2.92                     | 0.57              |
| 24:BA:2450:A:O2'  | 24:BA:2451:A:H5'  | 2.03                     | 0.57              |
| 24:BA:2505:G:O2'  | 24:BA:2506:U:H5'' | 2.04                     | 0.57              |
| 24:BA:2557:G:H2'  | 24:BA:2558:C:C6   | 2.39                     | 0.57              |
| 24:BA:447:A:N1    | 24:BA:454:A:C8    | 2.72                     | 0.57              |
| 26:BC:103:ILE:O   | 26:BC:104:LEU:O   | 2.23                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:1064:C:H5'  | 32:BI:88:GLY:HA3  | 1.87                     | 0.57              |
| 33:BJ:56:VAL:CG1  | 33:BJ:57:LEU:N    | 2.67                     | 0.57              |
| 36:BM:78:LEU:O    | 36:BM:80:VAL:N    | 2.37                     | 0.57              |
| 39:BP:37:LYS:HG2  | 39:BP:37:LYS:O    | 2.03                     | 0.57              |
| 55:CA:1054:C:HO2' | 55:CA:1055:A:H5'' | 1.67                     | 0.57              |
| 55:CA:428:G:H1'   | 55:CA:430:A:C8    | 2.40                     | 0.57              |
| 55:CA:60:A:H62    | 55:CA:110:C:N4    | 2.02                     | 0.57              |
| 55:CA:731:G:H5'   | 55:CA:766:A:H4'   | 1.86                     | 0.57              |
| 4:CE:25:LYS:HB2   | 4:CE:25:LYS:NZ    | 2.20                     | 0.57              |
| 5:CF:68:GLN:HG2   | 5:CF:69:GLU:H     | 1.68                     | 0.57              |
| 9:CJ:80:THR:C     | 9:CJ:84:VAL:HG22  | 2.25                     | 0.57              |
| 16:CQ:27:PHE:CE1  | 16:CQ:36:PHE:HB3  | 2.39                     | 0.57              |
| 51:D1:25:ASN:HB3  | 51:D1:28:THR:OG1  | 2.04                     | 0.57              |
| 24:DA:740:C:C5'   | 24:DA:1784:A:H3'  | 2.23                     | 0.57              |
| 24:DA:2038:G:H2'  | 24:DA:2039:U:O4'  | 2.02                     | 0.57              |
| 24:DA:2179:C:H6   | 24:DA:2179:C:H5'  | 1.70                     | 0.57              |
| 24:DA:2440:C:H2'  | 24:DA:2441:U:O4'  | 2.04                     | 0.57              |
| 24:DA:2461:A:N1   | 24:DA:2490:G:N2   | 2.52                     | 0.57              |
| 24:DA:224:U:H5    | 24:DA:420:C:H4'   | 1.68                     | 0.57              |
| 24:DA:931:U:H5''  | 24:DA:932:U:OP2   | 2.04                     | 0.57              |
| 56:DB:35:C:H2'    | 56:DB:36:C:H4'    | 1.86                     | 0.57              |
| 26:DC:33:LEU:O    | 26:DC:34:GLU:HB3  | 2.04                     | 0.57              |
| 39:DP:88:ARG:HH11 | 39:DP:112:ARG:NH2 | 2.02                     | 0.57              |
| 39:DP:63:ILE:HA   | 39:DP:68:GLY:CA   | 2.31                     | 0.57              |
| 40:DQ:57:ARG:C    | 40:DQ:59:LEU:H    | 2.07                     | 0.57              |
| 44:DU:32:LYS:HE2  | 44:DU:65:GLN:OE1  | 2.04                     | 0.57              |
| 56:DB:76:G:OP1    | 45:DV:12:GLN:HA   | 2.05                     | 0.57              |
| 47:DX:26:ARG:NH1  | 47:DX:28:PHE:CD2  | 2.72                     | 0.57              |
| 48:DY:60:LYS:HG2  | 48:DY:60:LYS:O    | 2.05                     | 0.57              |
| 21:AA:182:A:N3    | 21:AA:184:G:C8    | 2.73                     | 0.57              |
| 21:AA:903:G:C5    | 21:AA:904:U:C4    | 2.92                     | 0.57              |
| 21:AA:903:G:C5    | 21:AA:904:U:C5    | 2.93                     | 0.57              |
| 2:AC:15:LYS:HD2   | 2:AC:16:PRO:HD2   | 1.86                     | 0.57              |
| 11:AL:98:ARG:HD2  | 11:AL:103:CYS:SG  | 2.43                     | 0.57              |
| 22:AX:34:G:H8     | 22:AX:34:G:OP1    | 1.88                     | 0.57              |
| 24:BA:1165:A:C2   | 24:BA:1185:G:C2   | 2.92                     | 0.57              |
| 24:BA:126:A:O2'   | 24:BA:127:A:H5'   | 2.05                     | 0.57              |
| 24:BA:1579:A:H2'  | 24:BA:1580:A:C8   | 2.40                     | 0.57              |
| 24:BA:1782:U:C4   | 24:BA:2587:A:C2   | 2.92                     | 0.57              |
| 24:BA:2049:G:N2   | 24:BA:2620:C:C2   | 2.73                     | 0.57              |
| 24:BA:31:C:O3'    | 24:BA:1238:G:C5'  | 2.52                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:475:C:N3    | 24:BA:481:G:C6     | 2.72                     | 0.57              |
| 24:BA:514:A:H2'   | 24:BA:515:A:C8     | 2.39                     | 0.57              |
| 28:BE:72:SER:C    | 28:BE:74:LYS:H     | 2.08                     | 0.57              |
| 31:BH:8:LYS:O     | 31:BH:13:GLY:HA3   | 2.03                     | 0.57              |
| 32:BI:109:ALA:HB2 | 32:BI:128:ILE:HG13 | 1.85                     | 0.57              |
| 37:BN:67:PHE:O    | 37:BN:71:ARG:HA    | 2.05                     | 0.57              |
| 46:BW:39:GLN:NE2  | 46:BW:43:LYS:N     | 2.49                     | 0.57              |
| 55:CA:1228:C:O2'  | 55:CA:1229:A:C5'   | 2.52                     | 0.57              |
| 55:CA:1376:U:C2   | 55:CA:1377:A:N7    | 2.73                     | 0.57              |
| 55:CA:1387:G:C4   | 55:CA:1388:C:C5    | 2.92                     | 0.57              |
| 55:CA:587:G:C2    | 55:CA:755:G:C5     | 2.92                     | 0.57              |
| 55:CA:724:G:O2'   | 55:CA:725:G:H5'    | 2.04                     | 0.57              |
| 1:CB:27:LYS:N     | 1:CB:28:PRO:CD     | 2.68                     | 0.57              |
| 2:CC:113:LYS:HG3  | 2:CC:184:ASN:ND2   | 2.19                     | 0.57              |
| 3:CD:104:MET:O    | 3:CD:104:MET:HG2   | 2.04                     | 0.57              |
| 6:CG:102:TRP:O    | 6:CG:105:GLU:HB2   | 2.04                     | 0.57              |
| 7:CH:115:ALA:HA   | 7:CH:120:LEU:HD12  | 1.85                     | 0.57              |
| 8:CI:49:GLN:HA    | 8:CI:52:GLU:HG2    | 1.85                     | 0.57              |
| 24:DA:100:U:O2'   | 24:DA:101:A:O5'    | 2.21                     | 0.57              |
| 24:DA:1087:G:H1'  | 24:DA:1089:A:H1'   | 1.87                     | 0.57              |
| 24:DA:1387:A:H2'  | 24:DA:1388:G:H8    | 1.70                     | 0.57              |
| 24:DA:1341:G:H3'  | 24:DA:1397:U:O2    | 2.05                     | 0.57              |
| 24:DA:1586:A:OP2  | 24:DA:1586:A:H3'   | 2.04                     | 0.57              |
| 24:DA:2097:A:H2'  | 24:DA:2098:U:C6    | 2.39                     | 0.57              |
| 24:DA:2135:A:H8   | 24:DA:2135:A:OP2   | 1.88                     | 0.57              |
| 24:DA:2336:A:N7   | 46:DW:40:ARG:CZ    | 2.67                     | 0.57              |
| 24:DA:379:G:C6    | 24:DA:380:G:C5     | 2.92                     | 0.57              |
| 24:DA:534:U:H2'   | 24:DA:535:G:H8     | 1.68                     | 0.57              |
| 24:DA:673:C:H5'   | 28:DE:76:PRO:HD2   | 1.87                     | 0.57              |
| 24:DA:849:A:H2'   | 24:DA:850:U:C6     | 2.40                     | 0.57              |
| 56:DB:17:C:O2'    | 56:DB:18:G:O4'     | 2.22                     | 0.57              |
| 56:DB:43:C:H2'    | 56:DB:45:A:N7      | 2.20                     | 0.57              |
| 26:DC:220:ARG:O   | 26:DC:223:ALA:HB3  | 2.04                     | 0.57              |
| 30:DG:19:ASN:HD22 | 30:DG:19:ASN:N     | 2.02                     | 0.57              |
| 31:DH:1:MET:HB3   | 31:DH:21:VAL:O     | 2.04                     | 0.57              |
| 31:DH:2:GLN:O     | 31:DH:3:VAL:O      | 2.23                     | 0.57              |
| 32:DI:98:GLY:HA3  | 32:DI:137:LEU:HA   | 1.86                     | 0.57              |
| 32:DI:50:LYS:HE2  | 32:DI:50:LYS:HA    | 1.85                     | 0.57              |
| 21:AA:1065:U:H5'' | 21:AA:1190:G:N2    | 2.19                     | 0.57              |
| 21:AA:428:G:C4    | 21:AA:430:A:C6     | 2.93                     | 0.57              |
| 21:AA:695:A:H2'   | 21:AA:696:A:C8     | 2.39                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 21:AA:744:C:H2'  | 21:AA:745:G:H8    | 1.69                     | 0.57              |
| 1:AB:24:PRO:HG3  | 21:AA:830:G:C5'   | 2.29                     | 0.57              |
| 9:AJ:28:THR:HG22 | 9:AJ:28:THR:O     | 2.04                     | 0.57              |
| 51:B1:8:ILE:CG2  | 51:B1:9:LYS:N     | 2.68                     | 0.57              |
| 24:BA:1050:A:C2  | 24:BA:2751:G:C4   | 2.93                     | 0.57              |
| 24:BA:1490:A:C8  | 26:BC:73:ILE:HD13 | 2.39                     | 0.57              |
| 24:BA:1917:U:H2' | 24:BA:1918:A:O4'  | 2.05                     | 0.57              |
| 30:BG:163:TYR:O  | 30:BG:164:ALA:HB2 | 2.04                     | 0.57              |
| 43:BT:44:LYS:O   | 43:BT:48:GLN:HG2  | 2.05                     | 0.57              |
| 48:BY:32:ALA:HB2 | 48:BY:37:LEU:HD12 | 1.85                     | 0.57              |
| 55:CA:1065:U:O4  | 55:CA:1189:U:C2   | 2.58                     | 0.57              |
| 55:CA:1333:A:N6  | 55:CA:1334:G:C2   | 2.73                     | 0.57              |
| 55:CA:52:C:N4    | 55:CA:360:G:N2    | 2.53                     | 0.57              |
| 55:CA:551:U:C4   | 55:CA:552:U:C4    | 2.93                     | 0.57              |
| 55:CA:695:A:H2'  | 55:CA:696:A:C8    | 2.39                     | 0.57              |
| 55:CA:79:G:N1    | 55:CA:80:A:N6     | 2.53                     | 0.57              |
| 55:CA:818:G:C3'  | 55:CA:819:A:H5''  | 2.35                     | 0.57              |
| 6:CG:19:SER:O    | 6:CG:23:ALA:HB2   | 2.05                     | 0.57              |
| 8:CI:40:ARG:H    | 8:CI:44:ARG:HD3   | 1.69                     | 0.57              |
| 24:DA:2886:A:N7  | 50:D0:39:ARG:NE   | 2.53                     | 0.57              |
| 24:DA:1207:C:H2' | 24:DA:1208:C:C6   | 2.40                     | 0.57              |
| 24:DA:1974:C:C2  | 24:DA:1975:G:C8   | 2.92                     | 0.57              |
| 24:DA:2136:G:H2' | 24:DA:2137:U:C6   | 2.38                     | 0.57              |
| 24:DA:2149:U:H2' | 24:DA:2150:C:H6   | 1.69                     | 0.57              |
| 24:DA:2543:G:N1  | 24:DA:2765:A:C8   | 2.72                     | 0.57              |
| 24:DA:442:G:O6   | 24:DA:444:C:N4    | 2.37                     | 0.57              |
| 24:DA:59:U:O2'   | 24:DA:73:A:H2'    | 2.03                     | 0.57              |
| 24:DA:682:G:O2'  | 24:DA:683:U:H5'   | 2.04                     | 0.57              |
| 24:DA:972:A:C6   | 24:DA:973:A:C6    | 2.93                     | 0.57              |
| 26:DC:66:PHE:HB3 | 26:DC:150:GLY:O   | 2.05                     | 0.57              |
| 27:DD:29:VAL:HB  | 27:DD:98:VAL:HG12 | 1.85                     | 0.57              |
| 33:DJ:13:ARG:HG2 | 33:DJ:51:GLY:O    | 2.05                     | 0.57              |
| 15:AP:1:MET:HB2  | 21:AA:135:C:N3    | 2.19                     | 0.57              |
| 21:AA:142:G:C5   | 21:AA:143:A:C8    | 2.93                     | 0.57              |
| 21:AA:229:U:H2'  | 21:AA:230:G:O4'   | 2.05                     | 0.57              |
| 21:AA:252:U:H5'' | 21:AA:252:U:H6    | 1.69                     | 0.57              |
| 1:AB:206:ILE:H   | 1:AB:206:ILE:HD13 | 1.69                     | 0.57              |
| 10:AK:60:PHE:O   | 10:AK:64:VAL:HG12 | 2.04                     | 0.57              |
| 20:AU:24:LYS:NZ  | 20:AU:25:ALA:HB2  | 2.19                     | 0.57              |
| 50:B0:16:ARG:HG2 | 50:B0:19:ASP:OD1  | 2.03                     | 0.57              |
| 54:B4:9:LYS:H    | 54:B4:9:LYS:HD3   | 1.70                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:1063:G:C6   | 24:BA:1064:C:N3    | 2.72                     | 0.57              |
| 24:BA:2383:G:C5   | 24:BA:2384:U:C5    | 2.93                     | 0.57              |
| 24:BA:2592:G:C6   | 24:BA:2593:U:C4    | 2.93                     | 0.57              |
| 24:BA:2721:A:H2'  | 24:BA:2722:G:O4'   | 2.04                     | 0.57              |
| 24:BA:587:C:H2'   | 35:BL:19:LEU:HD22  | 1.86                     | 0.57              |
| 24:BA:704:G:H1'   | 24:BA:727:A:H61    | 1.68                     | 0.57              |
| 29:BF:84:ILE:HG13 | 29:BF:84:ILE:O     | 2.05                     | 0.57              |
| 32:BI:24:GLY:O    | 32:BI:27:LEU:HG    | 2.05                     | 0.57              |
| 36:BM:54:THR:O    | 36:BM:57:VAL:HG22  | 2.05                     | 0.57              |
| 41:BR:90:ARG:O    | 41:BR:91:GLN:HB3   | 2.04                     | 0.57              |
| 42:BS:71:VAL:HG22 | 42:BS:71:VAL:O     | 2.03                     | 0.57              |
| 46:BW:17:ALA:O    | 46:BW:18:LYS:HB3   | 2.04                     | 0.57              |
| 55:CA:160:A:H2'   | 55:CA:161:A:O4'    | 2.03                     | 0.57              |
| 55:CA:794:A:H2'   | 55:CA:795:C:H6     | 1.69                     | 0.57              |
| 3:CD:148:ALA:O    | 3:CD:151:GLN:HB2   | 2.04                     | 0.57              |
| 5:CF:64:VAL:HG23  | 5:CF:66:ALA:H      | 1.70                     | 0.57              |
| 12:CM:32:ILE:O    | 12:CM:32:ILE:HD13  | 2.05                     | 0.57              |
| 12:CM:94:LEU:HD21 | 55:CA:1226:C:H5''  | 1.85                     | 0.57              |
| 24:DA:1022:G:H22  | 24:DA:1142:A:H2    | 1.51                     | 0.57              |
| 24:DA:976:G:H5'   | 24:DA:1156:A:N6    | 2.18                     | 0.57              |
| 24:DA:1696:G:H2'  | 24:DA:1697:G:C8    | 2.40                     | 0.57              |
| 24:DA:1731:G:N3   | 24:DA:1733:G:C8    | 2.73                     | 0.57              |
| 24:DA:2193:G:H2'  | 24:DA:2194:U:H6    | 1.70                     | 0.57              |
| 24:DA:2420:C:OP1  | 53:D3:33:THR:HB    | 2.04                     | 0.57              |
| 24:DA:277:G:H2'   | 24:DA:361:G:O6     | 2.04                     | 0.57              |
| 24:DA:447:A:H5'   | 24:DA:449:A:C5     | 2.39                     | 0.57              |
| 24:DA:468:G:H4'   | 28:DE:57:LYS:CG    | 2.34                     | 0.57              |
| 24:DA:593:U:H2'   | 24:DA:594:U:C6     | 2.40                     | 0.57              |
| 24:DA:862:G:H2'   | 24:DA:863:A:O4'    | 2.04                     | 0.57              |
| 24:DA:874:G:H5'   | 24:DA:875:G:OP2    | 2.03                     | 0.57              |
| 26:DC:93:VAL:CG1  | 26:DC:101:ARG:H    | 2.18                     | 0.57              |
| 24:DA:1820:U:H3   | 26:DC:197:ALA:HA   | 1.70                     | 0.57              |
| 33:DJ:35:ARG:NH1  | 33:DJ:140:LEU:HD11 | 2.20                     | 0.57              |
| 37:DN:7:GLY:O     | 37:DN:8:ARG:HB2    | 2.05                     | 0.57              |
| 42:DS:55:ILE:HG23 | 42:DS:66:ILE:HG21  | 1.85                     | 0.57              |
| 43:DT:39:THR:HG21 | 43:DT:42:GLU:CB    | 2.25                     | 0.57              |
| 49:DZ:32:GLY:C    | 49:DZ:34:THR:H     | 2.08                     | 0.57              |
| 21:AA:1342:C:H2'  | 21:AA:1343:G:H8    | 1.67                     | 0.57              |
| 21:AA:22:G:H4'    | 21:AA:885:G:C8     | 2.40                     | 0.57              |
| 21:AA:130:A:C5    | 21:AA:264:C:H1'    | 2.40                     | 0.57              |
| 9:AJ:59:LYS:HE3   | 21:AA:972:C:O5'    | 2.05                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AC:35:ASP:O     | 2:AC:38:VAL:HG22  | 2.05                     | 0.57              |
| 6:AG:108:ARG:HH21 | 6:AG:118:ARG:HH22 | 1.53                     | 0.57              |
| 6:AG:147:ASN:O    | 6:AG:150:PHE:HD1  | 1.88                     | 0.57              |
| 7:AH:1:SER:HB2    | 21:AA:877:G:N2    | 2.19                     | 0.57              |
| 11:AL:89:LEU:HB2  | 11:AL:92:VAL:HG23 | 1.85                     | 0.57              |
| 14:AO:9:LYS:O     | 14:AO:13:GLU:HG3  | 2.05                     | 0.57              |
| 52:B2:21:ARG:HG2  | 52:B2:31:LEU:HG   | 1.85                     | 0.57              |
| 24:BA:1936:A:H2   | 24:BA:1943:U:C4   | 2.22                     | 0.57              |
| 24:BA:1946:U:H2'  | 24:BA:1947:C:C6   | 2.40                     | 0.57              |
| 24:BA:2383:G:C5   | 24:BA:2384:U:H5   | 2.22                     | 0.57              |
| 24:BA:2492:U:HO2' | 24:BA:2493:U:H5'  | 1.69                     | 0.57              |
| 24:BA:2854:G:H2'  | 24:BA:2855:C:H6   | 1.68                     | 0.57              |
| 24:BA:541:A:H2'   | 24:BA:542:C:O4'   | 2.04                     | 0.57              |
| 26:BC:34:GLU:OE1  | 26:BC:63:ILE:HD11 | 2.04                     | 0.57              |
| 55:CA:1181:G:O2'  | 55:CA:1182:G:O4'  | 2.21                     | 0.57              |
| 55:CA:960:U:O4    | 55:CA:1225:A:H1'  | 2.04                     | 0.57              |
| 55:CA:1394:A:N6   | 55:CA:1501:C:H5'  | 2.18                     | 0.57              |
| 55:CA:407:U:H2'   | 55:CA:408:A:C8    | 2.39                     | 0.57              |
| 55:CA:512:U:O2'   | 55:CA:513:C:C5'   | 2.48                     | 0.57              |
| 55:CA:982:U:H1'   | 55:CA:983:A:C5    | 2.40                     | 0.57              |
| 3:CD:34:GLU:O     | 3:CD:36:ALA:N     | 2.37                     | 0.57              |
| 7:CH:97:GLY:C     | 7:CH:98:LEU:HD12  | 2.25                     | 0.57              |
| 17:CR:58:ILE:HG22 | 17:CR:62:ARG:HE   | 1.69                     | 0.57              |
| 24:DA:1066:U:H3   | 24:DA:1069:A:P    | 2.28                     | 0.57              |
| 24:DA:164:C:O2'   | 24:DA:165:A:H5'   | 2.04                     | 0.57              |
| 24:DA:167:A:H2'   | 24:DA:168:G:O4'   | 2.04                     | 0.57              |
| 24:DA:2214:C:O2'  | 24:DA:2215:C:C5'  | 2.52                     | 0.57              |
| 24:DA:23:G:H2'    | 24:DA:24:G:C8     | 2.39                     | 0.57              |
| 24:DA:489:G:H4'   | 24:DA:490:C:OP1   | 2.04                     | 0.57              |
| 24:DA:745:G:C2    | 24:DA:753:A:N6    | 2.73                     | 0.57              |
| 24:DA:807:U:H4'   | 24:DA:2445:G:O3'  | 2.04                     | 0.57              |
| 27:DD:36:GLN:HG3  | 27:DD:38:LYS:HZ1  | 1.70                     | 0.57              |
| 30:DG:84:LYS:HB3  | 30:DG:132:LEU:O   | 2.03                     | 0.57              |
| 30:DG:84:LYS:O    | 30:DG:85:LYS:HB3  | 2.04                     | 0.57              |
| 44:DU:58:VAL:HG13 | 44:DU:60:LYS:HG2  | 1.85                     | 0.57              |
| 21:AA:1201:A:O2'  | 21:AA:1202:U:OP2  | 2.22                     | 0.57              |
| 21:AA:1211:U:H1'  | 21:AA:1213:A:C2   | 2.40                     | 0.57              |
| 21:AA:926:G:C5    | 21:AA:1505:G:O6   | 2.58                     | 0.57              |
| 21:AA:335:C:H2'   | 21:AA:336:A:H8    | 1.69                     | 0.57              |
| 11:AL:119:LYS:HB3 | 21:AA:37:U:OP1    | 2.04                     | 0.57              |
| 21:AA:57:G:C6     | 21:AA:58:C:C4     | 2.93                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:607:A:H2'    | 21:AA:608:A:C8     | 2.40                     | 0.57              |
| 21:AA:725:G:H2'    | 21:AA:726:C:C6     | 2.40                     | 0.57              |
| 3:AD:117:VAL:CA    | 3:AD:122:ILE:HD11  | 2.34                     | 0.57              |
| 7:AH:10:LEU:HB3    | 7:AH:74:ILE:CG1    | 2.34                     | 0.57              |
| 9:AJ:44:THR:OG1    | 21:AA:1151:A:H5''  | 2.05                     | 0.57              |
| 12:AM:86:ARG:HH22  | 12:AM:97:ARG:HA    | 1.69                     | 0.57              |
| 14:AO:42:PHE:O     | 14:AO:46:LYS:HG2   | 2.04                     | 0.57              |
| 16:AQ:12:VAL:CG1   | 16:AQ:13:SER:H     | 2.17                     | 0.57              |
| 19:AT:29:THR:HA    | 19:AT:32:LYS:HG3   | 1.86                     | 0.57              |
| 24:BA:2307:G:N2    | 24:BA:2311:A:C8    | 2.72                     | 0.57              |
| 24:BA:1669:A:O3'   | 24:BA:2549:G:H5'   | 2.05                     | 0.57              |
| 24:BA:2564:A:OP1   | 24:BA:2648:G:H4'   | 2.05                     | 0.57              |
| 24:BA:435:C:O2'    | 24:BA:436:C:H5'    | 2.05                     | 0.57              |
| 24:BA:657:U:H2'    | 24:BA:658:U:C6     | 2.40                     | 0.57              |
| 26:BC:158:GLY:H    | 26:BC:194:VAL:HG13 | 1.69                     | 0.57              |
| 27:BD:107:VAL:HG21 | 27:BD:177:VAL:CG1  | 2.35                     | 0.57              |
| 24:BA:2531:A:P     | 30:BG:174:LYS:HG3  | 2.44                     | 0.57              |
| 43:BT:43:ILE:HD11  | 43:BT:58:VAL:HG21  | 1.87                     | 0.57              |
| 49:BZ:36:GLU:C     | 49:BZ:37:ARG:HD2   | 2.24                     | 0.57              |
| 55:CA:724:G:H2'    | 55:CA:725:G:C8     | 2.32                     | 0.57              |
| 1:CB:116:LEU:HD13  | 1:CB:140:LEU:HB2   | 1.87                     | 0.57              |
| 2:CC:134:LYS:HG2   | 2:CC:138:GLN:HE22  | 1.70                     | 0.57              |
| 4:CE:24:VAL:HG23   | 4:CE:25:LYS:N      | 2.18                     | 0.57              |
| 6:CG:134:VAL:O     | 6:CG:138:GLU:HB2   | 2.04                     | 0.57              |
| 9:CJ:25:ILE:O      | 9:CJ:25:ILE:HG22   | 2.05                     | 0.57              |
| 10:CK:15:VAL:HG12  | 10:CK:17:ASP:H     | 1.69                     | 0.57              |
| 14:CO:7:THR:O      | 14:CO:11:VAL:HG23  | 2.05                     | 0.57              |
| 17:CR:59:LYS:HA    | 17:CR:62:ARG:HD2   | 1.87                     | 0.57              |
| 24:DA:1651:G:C6    | 24:DA:1652:A:C6    | 2.93                     | 0.57              |
| 24:DA:1773:A:H2'   | 24:DA:1774:C:O4'   | 2.04                     | 0.57              |
| 24:DA:2825:G:H3'   | 24:DA:2826:A:C8    | 2.31                     | 0.57              |
| 24:DA:324:A:H61    | 24:DA:338:G:C2'    | 2.18                     | 0.57              |
| 28:DE:62:GLN:O     | 28:DE:65:THR:HG22  | 2.05                     | 0.57              |
| 29:DF:43:ILE:HG12  | 29:DF:77:LYS:HD3   | 1.87                     | 0.57              |
| 35:DL:63:LYS:HB3   | 53:D3:12:ARG:HD2   | 1.85                     | 0.57              |
| 36:DM:42:THR:HB    | 36:DM:45:GLN:HG3   | 1.85                     | 0.57              |
| 38:DO:30:ARG:HH12  | 38:DO:102:ARG:HB2  | 1.70                     | 0.57              |
| 43:DT:62:VAL:HG12  | 43:DT:63:VAL:N     | 2.20                     | 0.57              |
| 21:AA:116:A:O2'    | 21:AA:117:G:C5'    | 2.52                     | 0.57              |
| 21:AA:1256:A:H1'   | 21:AA:1258:G:N7    | 2.20                     | 0.57              |
| 21:AA:1297:G:H5''  | 21:AA:1298:U:OP1   | 2.05                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:1347:G:N2   | 21:AA:1373:G:H2'  | 2.20                     | 0.57              |
| 21:AA:486:U:C2'   | 21:AA:487:A:H8    | 2.17                     | 0.57              |
| 4:AE:156:ARG:CG   | 7:AH:63:LYS:HZ1   | 2.10                     | 0.57              |
| 10:AK:28:ASN:ND2  | 10:AK:46:ALA:HB3  | 2.20                     | 0.57              |
| 12:AM:10:ASP:CG   | 12:AM:11:HIS:H    | 2.08                     | 0.57              |
| 16:AQ:20:ILE:H    | 16:AQ:47:ASP:CG   | 2.08                     | 0.57              |
| 24:BA:1253:A:C5   | 59:BA:3337:HOH:O  | 2.58                     | 0.57              |
| 24:BA:1328:A:H2'  | 24:BA:1330:C:C4   | 2.39                     | 0.57              |
| 24:BA:1496:A:H2'  | 24:BA:1498:C:H41  | 1.70                     | 0.57              |
| 24:BA:17:G:H2'    | 24:BA:18:U:C6     | 2.39                     | 0.57              |
| 24:BA:2860:A:C3'  | 24:BA:2860:A:C8   | 2.88                     | 0.57              |
| 25:BB:53:A:C2     | 25:BB:54:G:C8     | 2.93                     | 0.57              |
| 30:BG:97:VAL:O    | 30:BG:97:VAL:HG12 | 2.04                     | 0.57              |
| 33:BJ:30:THR:HG22 | 33:BJ:31:GLU:H    | 1.69                     | 0.57              |
| 43:BT:29:THR:HA   | 43:BT:86:THR:HA   | 1.86                     | 0.57              |
| 24:BA:84:A:H5''   | 44:BU:5:ARG:HH21  | 1.70                     | 0.57              |
| 1:CB:94:ARG:HD2   | 55:CA:1100:C:OP1  | 2.05                     | 0.57              |
| 55:CA:1268:G:H21  | 55:CA:1327:C:H1'  | 1.70                     | 0.57              |
| 55:CA:269:C:H2'   | 55:CA:270:A:C8    | 2.39                     | 0.57              |
| 10:CK:127:ARG:NH2 | 55:CA:795:C:H5''  | 2.20                     | 0.57              |
| 1:CB:122:ASP:HB3  | 1:CB:124:THR:HG22 | 1.87                     | 0.57              |
| 1:CB:9:LEU:HG     | 1:CB:10:LYS:N     | 2.18                     | 0.57              |
| 6:CG:148:LYS:HZ2  | 6:CG:148:LYS:HB2  | 1.68                     | 0.57              |
| 19:CT:61:ALA:HA   | 19:CT:67:HIS:HA   | 1.87                     | 0.57              |
| 24:DA:1986:C:H5'' | 59:DA:3444:HOH:O  | 2.05                     | 0.57              |
| 24:DA:2798:U:H5'  | 24:DA:2800:A:N7   | 2.20                     | 0.57              |
| 24:DA:460:A:OP2   | 52:D2:41:ARG:NH1  | 2.33                     | 0.57              |
| 24:DA:592:A:H2'   | 24:DA:593:U:C6    | 2.40                     | 0.57              |
| 24:DA:921:C:C2'   | 24:DA:922:C:H5'   | 2.34                     | 0.57              |
| 24:DA:91:A:H1'    | 24:DA:92:U:C6     | 2.39                     | 0.57              |
| 24:DA:935:C:H2'   | 24:DA:936:A:C8    | 2.40                     | 0.57              |
| 56:DB:11:C:H2'    | 56:DB:15:A:N6     | 2.20                     | 0.57              |
| 29:DF:8:LYS:HB2   | 29:DF:8:LYS:NZ    | 2.20                     | 0.57              |
| 31:DH:109:GLU:OE2 | 31:DH:109:GLU:HA  | 2.05                     | 0.57              |
| 33:DJ:38:GLY:O    | 33:DJ:43:GLU:HB2  | 2.05                     | 0.57              |
| 35:DL:123:ARG:HA  | 35:DL:143:GLU:HB3 | 1.87                     | 0.57              |
| 43:DT:4:GLU:HG3   | 43:DT:6:ARG:HH21  | 1.68                     | 0.57              |
| 46:DW:33:GLY:O    | 46:DW:34:SER:HB2  | 2.05                     | 0.57              |
| 47:DX:39:VAL:O    | 47:DX:40:GLU:HB2  | 2.05                     | 0.57              |
| 48:DY:4:LYS:H     | 48:DY:4:LYS:HD3   | 1.69                     | 0.57              |
| 21:AA:1262:C:H2'  | 21:AA:1263:C:O4'  | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:266:G:O2'   | 21:AA:267:C:H3'   | 2.05                     | 0.56              |
| 7:AH:87:ARG:HB3   | 21:AA:600:A:OP1   | 2.05                     | 0.56              |
| 21:AA:880:C:O2'   | 21:AA:881:G:H5'   | 2.05                     | 0.56              |
| 6:AG:14:ASP:HB3   | 6:AG:18:GLY:N     | 2.11                     | 0.56              |
| 12:AM:28:ARG:HH11 | 12:AM:28:ARG:HB3  | 1.69                     | 0.56              |
| 13:AN:44:VAL:HG23 | 13:AN:45:LEU:N    | 2.16                     | 0.56              |
| 16:AQ:45:VAL:HG13 | 16:AQ:72:TRP:O    | 2.05                     | 0.56              |
| 24:BA:1076:C:H2'  | 24:BA:1077:A:C8   | 2.40                     | 0.56              |
| 24:BA:974:G:C2    | 24:BA:1186:G:N1   | 2.73                     | 0.56              |
| 24:BA:1612:C:H4'  | 52:B2:5:PHE:O     | 2.05                     | 0.56              |
| 24:BA:2063:C:H6   | 24:BA:2063:C:C5'  | 2.18                     | 0.56              |
| 24:BA:2061:G:H5'' | 24:BA:2503:A:C2   | 2.40                     | 0.56              |
| 24:BA:2636:C:O2'  | 27:BD:45:TYR:OH   | 2.21                     | 0.56              |
| 24:BA:593:U:H2'   | 24:BA:594:U:C6    | 2.40                     | 0.56              |
| 24:BA:728:G:HO2'  | 24:BA:730:A:H8    | 1.50                     | 0.56              |
| 24:BA:84:A:N1     | 24:BA:103:A:C6    | 2.72                     | 0.56              |
| 41:BR:38:VAL:HG23 | 41:BR:40:MET:H    | 1.69                     | 0.56              |
| 44:BU:85:ARG:NH1  | 44:BU:91:LYS:HA   | 2.20                     | 0.56              |
| 55:CA:1242:G:H4'  | 55:CA:1304:G:OP1  | 2.05                     | 0.56              |
| 55:CA:979:C:H1'   | 55:CA:1317:C:H41  | 1.69                     | 0.56              |
| 55:CA:769:G:H4'   | 55:CA:1513:A:H4'  | 1.87                     | 0.56              |
| 3:CD:32:LYS:HB3   | 3:CD:35:GLN:OE1   | 2.05                     | 0.56              |
| 7:CH:17:GLN:HE21  | 7:CH:71:VAL:HG23  | 1.70                     | 0.56              |
| 11:CL:109:ARG:NH2 | 11:CL:116:TYR:HE2 | 2.03                     | 0.56              |
| 12:CM:64:VAL:HG12 | 12:CM:65:GLU:HG3  | 1.87                     | 0.56              |
| 24:DA:1088:A:H4'  | 24:DA:1089:A:C8   | 2.40                     | 0.56              |
| 24:DA:1682:G:C8   | 24:DA:1757:A:C2   | 2.92                     | 0.56              |
| 24:DA:1845:G:C6   | 24:DA:1896:G:C6   | 2.93                     | 0.56              |
| 24:DA:1965:C:H5'' | 24:DA:1965:C:H6   | 1.70                     | 0.56              |
| 24:DA:2447:G:O6   | 24:DA:2504:U:O4   | 2.22                     | 0.56              |
| 24:DA:2597:G:H2'  | 24:DA:2598:A:C8   | 2.39                     | 0.56              |
| 24:DA:2822:G:H2'  | 24:DA:2823:A:H5'' | 1.87                     | 0.56              |
| 24:DA:357:C:H2'   | 24:DA:358:U:O4'   | 2.05                     | 0.56              |
| 24:DA:792:A:H1'   | 24:DA:2072:C:O2'  | 2.04                     | 0.56              |
| 24:DA:782:A:C2    | 26:DC:224:MET:SD  | 2.98                     | 0.56              |
| 27:DD:33:ARG:H    | 27:DD:33:ARG:HD2  | 1.70                     | 0.56              |
| 29:DF:58:ALA:HB1  | 29:DF:139:GLU:HG2 | 1.87                     | 0.56              |
| 32:DI:28:GLY:O    | 32:DI:30:GLN:HG3  | 2.05                     | 0.56              |
| 35:DL:79:LEU:CA   | 35:DL:82:LEU:HD11 | 2.31                     | 0.56              |
| 36:DM:26:VAL:HG21 | 36:DM:132:THR:O   | 2.05                     | 0.56              |
| 37:DN:19:ALA:HA   | 37:DN:22:ARG:HB3  | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:DP:1:SER:HB3   | 39:DP:4:ILE:HB    | 1.87                     | 0.56              |
| 43:DT:19:LYS:HE2  | 43:DT:23:ALA:HB3  | 1.86                     | 0.56              |
| 21:AA:577:G:N2    | 21:AA:578:C:C2    | 2.73                     | 0.56              |
| 21:AA:580:C:H2'   | 21:AA:581:G:H8    | 1.65                     | 0.56              |
| 21:AA:70:U:O2'    | 21:AA:71:A:C8     | 2.58                     | 0.56              |
| 21:AA:993:G:H2'   | 21:AA:995:C:H41   | 1.70                     | 0.56              |
| 1:AB:160:LEU:HB3  | 1:AB:182:VAL:HG13 | 1.86                     | 0.56              |
| 6:AG:68:VAL:HG12  | 6:AG:102:TRP:HE3  | 1.69                     | 0.56              |
| 10:AK:18:GLY:O    | 10:AK:81:LEU:HB2  | 2.05                     | 0.56              |
| 15:AP:80:LYS:NZ   | 15:AP:80:LYS:HB2  | 2.21                     | 0.56              |
| 18:AS:36:ARG:O    | 18:AS:69:LYS:HD2  | 2.05                     | 0.56              |
| 24:BA:1022:G:O2'  | 24:BA:1023:U:OP2  | 2.23                     | 0.56              |
| 24:BA:1435:G:N2   | 24:BA:1558:C:H41  | 2.03                     | 0.56              |
| 24:BA:1463:C:H2'  | 24:BA:1464:G:O4'  | 2.05                     | 0.56              |
| 24:BA:163:C:O2'   | 24:BA:164:C:C5'   | 2.52                     | 0.56              |
| 24:BA:1916:A:H2'  | 24:BA:1917:U:O4'  | 2.04                     | 0.56              |
| 24:BA:532:A:C8    | 24:BA:2021:C:C5   | 2.93                     | 0.56              |
| 24:BA:2792:A:C2   | 24:BA:2793:C:C2   | 2.93                     | 0.56              |
| 25:BB:14:U:H3'    | 25:BB:15:A:H5''   | 1.87                     | 0.56              |
| 26:BC:77:VAL:HA   | 26:BC:93:VAL:HA   | 1.87                     | 0.56              |
| 30:BG:30:GLY:HA3  | 30:BG:78:VAL:HG12 | 1.87                     | 0.56              |
| 31:BH:6:LEU:O     | 31:BH:15:LEU:HA   | 2.04                     | 0.56              |
| 33:BJ:55:ILE:HD12 | 33:BJ:56:VAL:O    | 2.05                     | 0.56              |
| 34:BK:78:ARG:NH1  | 39:BP:70:GLU:OE2  | 2.38                     | 0.56              |
| 38:BO:75:GLY:HA2  | 38:BO:106:LEU:CD1 | 2.34                     | 0.56              |
| 55:CA:157:U:O2'   | 55:CA:158:G:H5'   | 2.05                     | 0.56              |
| 55:CA:54:C:N4     | 55:CA:352:C:H2'   | 2.20                     | 0.56              |
| 55:CA:536:C:H2'   | 55:CA:537:G:H8    | 1.69                     | 0.56              |
| 55:CA:926:G:H22   | 23:CW:1:U:P       | 2.28                     | 0.56              |
| 6:CG:20:GLU:O     | 6:CG:23:ALA:HB3   | 2.05                     | 0.56              |
| 19:CT:67:HIS:ND1  | 19:CT:68:LYS:N    | 2.52                     | 0.56              |
| 20:CU:33:ARG:NH1  | 20:CU:34:ARG:HD3  | 2.20                     | 0.56              |
| 20:CU:53:LYS:HB2  | 20:CU:53:LYS:NZ   | 2.20                     | 0.56              |
| 24:DA:1237:A:O2'  | 24:DA:1238:G:H4'  | 2.03                     | 0.56              |
| 24:DA:1331:G:O2'  | 24:DA:1332:G:C5'  | 2.53                     | 0.56              |
| 24:DA:1456:G:O2'  | 24:DA:1457:U:H5'  | 2.04                     | 0.56              |
| 24:DA:1916:A:H8   | 24:DA:1916:A:H5'' | 1.69                     | 0.56              |
| 24:DA:226:A:C2    | 24:DA:230:G:O6    | 2.58                     | 0.56              |
| 24:DA:2287:A:C6   | 24:DA:2289:G:C5   | 2.93                     | 0.56              |
| 24:DA:2287:A:C4   | 24:DA:2289:G:N7   | 2.74                     | 0.56              |
| 24:DA:390:U:O2'   | 24:DA:391:A:H8    | 1.88                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:790:U:H3     | 24:DA:795:C:H5'    | 1.70                     | 0.56              |
| 24:DA:903:C:H2'    | 24:DA:904:G:C8     | 2.40                     | 0.56              |
| 26:DC:66:PHE:CZ    | 26:DC:155:ARG:NH1  | 2.74                     | 0.56              |
| 27:DD:151:THR:HB   | 27:DD:152:PRO:HD3  | 1.86                     | 0.56              |
| 24:DA:600:G:H5'    | 28:DE:27:LEU:HD13  | 1.87                     | 0.56              |
| 29:DF:31:GLU:C     | 29:DF:95:MET:HE1   | 2.26                     | 0.56              |
| 30:DG:44:HIS:HA    | 30:DG:49:LEU:HA    | 1.88                     | 0.56              |
| 30:DG:62:ALA:O     | 30:DG:66:THR:HG23  | 2.05                     | 0.56              |
| 38:DO:30:ARG:CG    | 38:DO:30:ARG:HH11  | 2.17                     | 0.56              |
| 24:DA:112:U:H5'    | 48:DY:58:ASN:HD21  | 1.70                     | 0.56              |
| 21:AA:1130:A:C5    | 21:AA:1146:A:C6    | 2.94                     | 0.56              |
| 21:AA:1425:U:O2'   | 21:AA:1426:G:H5'   | 2.05                     | 0.56              |
| 21:AA:223:A:H2'    | 21:AA:224:U:C6     | 2.40                     | 0.56              |
| 21:AA:734:G:C6     | 21:AA:735:C:C4     | 2.94                     | 0.56              |
| 21:AA:821:G:H4'    | 59:AA:1740:HOH:O   | 2.05                     | 0.56              |
| 1:AB:209:VAL:O     | 1:AB:213:LEU:N     | 2.34                     | 0.56              |
| 1:AB:80:LYS:HG3    | 1:AB:90:PHE:CE1    | 2.40                     | 0.56              |
| 4:AE:154:ALA:HB3   | 7:AH:65:PHE:CE1    | 2.40                     | 0.56              |
| 8:AI:119:LYS:O     | 8:AI:120:ALA:HB3   | 2.05                     | 0.56              |
| 10:AK:35:ASP:OD2   | 10:AK:39:ASN:HB2   | 2.05                     | 0.56              |
| 11:AL:42:LYS:HB3   | 11:AL:43:LYS:NZ    | 2.20                     | 0.56              |
| 24:BA:103:A:H2'    | 24:BA:104:A:H8     | 1.70                     | 0.56              |
| 24:BA:1179:G:N7    | 24:BA:1180:U:H1'   | 2.20                     | 0.56              |
| 24:BA:1459:G:O2'   | 24:BA:1460:U:H5''  | 2.05                     | 0.56              |
| 24:BA:1649:G:O2'   | 24:BA:1650:A:H5'   | 2.05                     | 0.56              |
| 24:BA:2397:G:C2    | 24:BA:2420:C:O2    | 2.58                     | 0.56              |
| 24:BA:2439:A:H4'   | 24:BA:2440:C:O5'   | 2.06                     | 0.56              |
| 24:BA:2617:U:H2'   | 24:BA:2618:G:O4'   | 2.04                     | 0.56              |
| 24:BA:300:A:N1     | 24:BA:333:G:O2'    | 2.38                     | 0.56              |
| 25:BB:51:G:N2      | 25:BB:53:A:N6      | 2.53                     | 0.56              |
| 24:BA:449:A:OP1    | 28:BE:80:SER:HA    | 2.05                     | 0.56              |
| 29:BF:142:TYR:HA   | 29:BF:145:VAL:HG13 | 1.87                     | 0.56              |
| 30:BG:168:VAL:HG23 | 30:BG:168:VAL:O    | 2.05                     | 0.56              |
| 21:AA:346:G:OP1    | 39:BP:33:GLU:OE1   | 2.23                     | 0.56              |
| 39:BP:57:ALA:HB1   | 39:BP:73:PHE:O     | 2.05                     | 0.56              |
| 42:BS:70:LYS:N     | 42:BS:70:LYS:HD2   | 2.21                     | 0.56              |
| 44:BU:85:ARG:HA    | 44:BU:91:LYS:O     | 2.05                     | 0.56              |
| 46:BW:8:SER:O      | 46:BW:9:THR:CB     | 2.53                     | 0.56              |
| 48:BY:7:ARG:H      | 48:BY:60:LYS:HZ1   | 1.53                     | 0.56              |
| 55:CA:193:C:H2'    | 55:CA:194:C:C6     | 2.40                     | 0.56              |
| 55:CA:260:G:H2'    | 55:CA:261:U:H6     | 1.70                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 55:CA:965:U:H1'    | 55:CA:969:A:C5    | 2.40                     | 0.56              |
| 1:CB:125:PHE:CD1   | 1:CB:137:THR:HG22 | 2.40                     | 0.56              |
| 1:CB:161:PHE:CE2   | 1:CB:216:VAL:HG21 | 2.40                     | 0.56              |
| 10:CK:19:VAL:HB    | 10:CK:34:THR:HG23 | 1.86                     | 0.56              |
| 11:CL:83:GLY:HA2   | 11:CL:94:TYR:CD1  | 2.40                     | 0.56              |
| 11:CL:65:TYR:HB3   | 11:CL:95:HIS:CD2  | 2.40                     | 0.56              |
| 24:DA:117:G:C6     | 24:DA:119:A:C6    | 2.93                     | 0.56              |
| 24:DA:1461:C:O2'   | 24:DA:1462:C:C6   | 2.53                     | 0.56              |
| 24:DA:1819:A:OP1   | 26:DC:154:ALA:HA  | 2.05                     | 0.56              |
| 24:DA:2093:G:O2'   | 24:DA:2094:A:H5'  | 2.05                     | 0.56              |
| 24:DA:281:C:H2'    | 24:DA:282:A:H8    | 1.70                     | 0.56              |
| 24:DA:475:C:H6     | 24:DA:475:C:O5'   | 1.88                     | 0.56              |
| 24:DA:656:G:H2'    | 24:DA:657:U:C5    | 2.39                     | 0.56              |
| 34:DK:45:GLU:O     | 34:DK:54:LYS:HE3  | 2.04                     | 0.56              |
| 37:DN:67:PHE:HE2   | 37:DN:73:ASN:HD21 | 1.52                     | 0.56              |
| 38:DO:94:ARG:HD2   | 38:DO:97:PHE:O    | 2.05                     | 0.56              |
| 42:DS:14:ALA:O     | 42:DS:18:ARG:HB2  | 2.05                     | 0.56              |
| 45:DV:27:PRO:O     | 45:DV:88:HIS:HA   | 2.04                     | 0.56              |
| 21:AA:214:C:H2'    | 21:AA:215:C:H6    | 1.70                     | 0.56              |
| 11:AL:8:ARG:NH1    | 21:AA:880:C:OP1   | 2.35                     | 0.56              |
| 1:AB:51:GLU:HG2    | 1:AB:197:PHE:HE1  | 1.69                     | 0.56              |
| 2:AC:100:ILE:O     | 2:AC:100:ILE:HG23 | 2.05                     | 0.56              |
| 4:AE:82:HIS:O      | 4:AE:146:MET:HE2  | 2.05                     | 0.56              |
| 4:AE:83:PRO:HD3    | 4:AE:97:PRO:HD3   | 1.86                     | 0.56              |
| 5:AF:47:LEU:HG     | 5:AF:56:LYS:H     | 1.70                     | 0.56              |
| 6:AG:143:MET:O     | 6:AG:146:ALA:HB3  | 2.06                     | 0.56              |
| 20:AU:38:GLU:OE2   | 20:AU:41:THR:HG21 | 2.06                     | 0.56              |
| 54:B4:9:LYS:N      | 54:B4:9:LYS:HD3   | 2.20                     | 0.56              |
| 24:BA:83:A:N6      | 24:BA:101:A:C4    | 2.74                     | 0.56              |
| 24:BA:2886:A:C2    | 24:BA:2887:A:H1'  | 2.41                     | 0.56              |
| 24:BA:919:U:N3     | 24:BA:920:A:N7    | 2.54                     | 0.56              |
| 26:BC:229:HIS:CG   | 26:BC:230:PRO:HD2 | 2.40                     | 0.56              |
| 29:BF:107:VAL:HG13 | 29:BF:113:PHE:CZ  | 2.40                     | 0.56              |
| 32:BI:126:ARG:HA   | 32:BI:129:GLU:CG  | 2.36                     | 0.56              |
| 39:BP:85:VAL:O     | 39:BP:86:LYS:HB2  | 2.04                     | 0.56              |
| 41:BR:45:GLU:HA    | 41:BR:45:GLU:OE2  | 2.05                     | 0.56              |
| 45:BV:5:ASN:H      | 45:BV:5:ASN:ND2   | 2.01                     | 0.56              |
| 55:CA:1202:U:H2'   | 55:CA:1203:C:C6   | 2.40                     | 0.56              |
| 55:CA:1494:G:H8    | 55:CA:1494:G:OP2  | 1.89                     | 0.56              |
| 55:CA:374:A:OP1    | 55:CA:452:A:N1    | 2.39                     | 0.56              |
| 55:CA:588:G:C2     | 55:CA:589:U:C2    | 2.93                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:CA:920:U:H2'    | 55:CA:921:U:H6     | 1.70                     | 0.56              |
| 6:CG:2:ARG:NH1     | 55:CA:932:C:C5     | 2.74                     | 0.56              |
| 6:CG:77:ARG:NH2    | 55:CA:1381:U:H3    | 2.03                     | 0.56              |
| 12:CM:89:ARG:HB3   | 12:CM:94:LEU:O     | 2.05                     | 0.56              |
| 13:CN:16:ALA:HB2   | 13:CN:59:GLN:HE22  | 1.70                     | 0.56              |
| 14:CO:25:GLU:HA    | 14:CO:80:LEU:HD11  | 1.87                     | 0.56              |
| 24:DA:110:G:C4     | 24:DA:111:A:C8     | 2.93                     | 0.56              |
| 24:DA:1203:U:N3    | 24:DA:1204:A:N6    | 2.53                     | 0.56              |
| 24:DA:1526:C:H2'   | 24:DA:1527:G:O4'   | 2.06                     | 0.56              |
| 24:DA:155:A:H2'    | 24:DA:156:A:H8     | 1.70                     | 0.56              |
| 24:DA:2216:G:H2'   | 24:DA:2217:G:H8    | 1.70                     | 0.56              |
| 24:DA:223:A:C4     | 24:DA:408:G:H1'    | 2.40                     | 0.56              |
| 24:DA:233:A:O2'    | 24:DA:234:U:O5'    | 2.23                     | 0.56              |
| 24:DA:2602:A:H3'   | 24:DA:2602:A:OP1   | 2.06                     | 0.56              |
| 24:DA:265:A:C5     | 24:DA:428:A:C8     | 2.93                     | 0.56              |
| 24:DA:606:U:OP1    | 28:DE:99:LYS:HD3   | 2.05                     | 0.56              |
| 24:DA:621:A:H2'    | 24:DA:622:G:C8     | 2.40                     | 0.56              |
| 56:DB:45:A:C2'     | 56:DB:46:A:H8      | 2.16                     | 0.56              |
| 26:DC:196:ASN:OD1  | 26:DC:199:HIS:HB2  | 2.04                     | 0.56              |
| 27:DD:112:THR:HG22 | 27:DD:113:SER:N    | 2.20                     | 0.56              |
| 29:DF:5:ASP:C      | 29:DF:7:TYR:H      | 2.09                     | 0.56              |
| 24:DA:1650:A:H1'   | 37:DN:108:ALA:HB2  | 1.87                     | 0.56              |
| 37:DN:55:ALA:HA    | 37:DN:80:PHE:CE1   | 2.40                     | 0.56              |
| 24:DA:329:G:O6     | 44:DU:16:LYS:HB2   | 2.05                     | 0.56              |
| 45:DV:9:ARG:HH22   | 45:DV:17:SER:HB2   | 1.69                     | 0.56              |
| 21:AA:1502:A:O2'   | 21:AA:1503:A:OP1   | 2.23                     | 0.56              |
| 21:AA:246:A:H4'    | 21:AA:247:G:OP1    | 2.05                     | 0.56              |
| 21:AA:82:G:N2      | 21:AA:84:U:N3      | 2.50                     | 0.56              |
| 21:AA:71:A:N6      | 21:AA:99:C:H1'     | 2.13                     | 0.56              |
| 1:AB:187:ASP:CG    | 1:AB:188:THR:H     | 2.09                     | 0.56              |
| 1:AB:86:CYS:SG     | 1:AB:221:ARG:HB2   | 2.45                     | 0.56              |
| 4:AE:10:LEU:H      | 4:AE:10:LEU:HD23   | 1.71                     | 0.56              |
| 8:AI:18:VAL:HG22   | 8:AI:64:ILE:HD13   | 1.87                     | 0.56              |
| 24:BA:51:G:N2      | 24:BA:120:U:O2     | 2.37                     | 0.56              |
| 24:BA:119:A:H4'    | 24:BA:120:U:O5'    | 2.05                     | 0.56              |
| 24:BA:1731:G:H2'   | 24:BA:1732:C:H5''  | 1.88                     | 0.56              |
| 24:BA:950:G:C5     | 24:BA:951:C:C5     | 2.93                     | 0.56              |
| 26:BC:106:PRO:CA   | 26:BC:141:HIS:CE1  | 2.87                     | 0.56              |
| 27:BD:4:LEU:HD13   | 27:BD:100:LEU:HD23 | 1.86                     | 0.56              |
| 28:BE:31:VAL:HG21  | 28:BE:104:ALA:CB   | 2.35                     | 0.56              |
| 29:BF:129:MET:HG3  | 29:BF:153:ILE:HD11 | 1.87                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:BF:148:VAL:O   | 29:BF:150:GLY:N    | 2.38                     | 0.56              |
| 38:BO:54:VAL:HG22 | 38:BO:54:VAL:O     | 2.04                     | 0.56              |
| 55:CA:1092:A:C6   | 55:CA:1183:U:O2    | 2.59                     | 0.56              |
| 55:CA:536:C:H2'   | 55:CA:537:G:C8     | 2.40                     | 0.56              |
| 1:CB:114:LYS:HE3  | 1:CB:151:LYS:HB2   | 1.87                     | 0.56              |
| 2:CC:31:ASN:O     | 2:CC:35:ASP:HB2    | 2.04                     | 0.56              |
| 6:CG:142:ARG:O    | 6:CG:146:ALA:HB3   | 2.05                     | 0.56              |
| 7:CH:24:VAL:HG22  | 7:CH:25:THR:H      | 1.70                     | 0.56              |
| 7:CH:24:VAL:HG22  | 7:CH:25:THR:N      | 2.20                     | 0.56              |
| 9:CJ:9:ARG:HH21   | 9:CJ:71:LEU:HD21   | 1.69                     | 0.56              |
| 12:CM:94:LEU:HD22 | 55:CA:1226:C:OP2   | 2.06                     | 0.56              |
| 15:CP:22:ALA:HA   | 15:CP:33:ILE:HG13  | 1.88                     | 0.56              |
| 17:CR:37:LYS:HD2  | 20:CU:22:CYS:HB3   | 1.86                     | 0.56              |
| 22:CV:34:G:H2'    | 22:CV:35:A:C8      | 2.38                     | 0.56              |
| 24:DA:1265:A:H1'  | 24:DA:1267:U:C5    | 2.41                     | 0.56              |
| 24:DA:1874:C:H2'  | 24:DA:1875:G:O4'   | 2.05                     | 0.56              |
| 24:DA:2001:C:H1'  | 24:DA:2689:U:N3    | 2.20                     | 0.56              |
| 24:DA:2226:C:O2'  | 24:DA:2227:A:H5'   | 2.05                     | 0.56              |
| 24:DA:250:G:C2'   | 24:DA:251:A:C8     | 2.87                     | 0.56              |
| 24:DA:277:G:H4'   | 24:DA:278:A:C8     | 2.41                     | 0.56              |
| 24:DA:2823:A:C5   | 24:DA:2824:C:C5    | 2.93                     | 0.56              |
| 24:DA:538:A:H2'   | 24:DA:539:G:H8     | 1.68                     | 0.56              |
| 24:DA:576:U:O2'   | 24:DA:577:G:H5'    | 2.05                     | 0.56              |
| 27:DD:116:LYS:HD3 | 37:DN:1:MET:HE1    | 1.87                     | 0.56              |
| 39:DP:67:GLU:CD   | 39:DP:68:GLY:H     | 2.09                     | 0.56              |
| 44:DU:95:PHE:O    | 44:DU:97:SER:N     | 2.38                     | 0.56              |
| 4:AE:134:ASN:OD1  | 21:AA:1078:U:H1'   | 2.06                     | 0.56              |
| 21:AA:1206:G:C6   | 21:AA:1207:G:C5    | 2.93                     | 0.56              |
| 21:AA:92:U:H2'    | 21:AA:93:U:O4'     | 2.06                     | 0.56              |
| 3:AD:131:ILE:HG22 | 21:AA:403:C:H5'    | 1.88                     | 0.56              |
| 5:AF:51:ILE:HG13  | 21:AA:674:G:OP1    | 2.06                     | 0.56              |
| 6:AG:3:ARG:HG3    | 6:AG:4:ARG:N       | 2.14                     | 0.56              |
| 24:BA:2635:A:O2'  | 27:BD:81:GLU:HG3   | 2.05                     | 0.56              |
| 24:BA:2656:U:C5   | 24:BA:2664:G:N2    | 2.73                     | 0.56              |
| 24:BA:288:U:O2'   | 24:BA:289:G:H5'    | 2.05                     | 0.56              |
| 24:BA:48:G:N2     | 24:BA:177:G:H21    | 2.03                     | 0.56              |
| 24:BA:831:G:C6    | 24:BA:832:U:C4     | 2.93                     | 0.56              |
| 28:BE:105:LEU:O   | 28:BE:109:LEU:HB2  | 2.06                     | 0.56              |
| 29:BF:47:LYS:NZ   | 29:BF:47:LYS:HB3   | 2.21                     | 0.56              |
| 30:BG:82:PHE:CZ   | 30:BG:137:LYS:HB2  | 2.40                     | 0.56              |
| 35:BL:95:LEU:HD11 | 35:BL:125:LEU:HD11 | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 49:BZ:15:ARG:NH1  | 49:BZ:15:ARG:HG3  | 2.21                     | 0.56              |
| 55:CA:102:G:H2'   | 55:CA:103:U:C6    | 2.41                     | 0.56              |
| 55:CA:1087:G:H2'  | 55:CA:1088:G:H8   | 1.71                     | 0.56              |
| 55:CA:1151:A:H2'  | 55:CA:1152:A:H8   | 1.71                     | 0.56              |
| 55:CA:977:A:C8    | 55:CA:1223:C:C2   | 2.85                     | 0.56              |
| 55:CA:1395:C:H6   | 55:CA:1395:C:O5'  | 1.88                     | 0.56              |
| 55:CA:316:C:O2'   | 55:CA:317:U:H5'   | 2.06                     | 0.56              |
| 55:CA:549:C:H2'   | 55:CA:550:G:H8    | 1.71                     | 0.56              |
| 55:CA:649:A:C2    | 55:CA:650:G:H1'   | 2.41                     | 0.56              |
| 55:CA:692:U:H2'   | 55:CA:694:A:OP2   | 2.06                     | 0.56              |
| 55:CA:709:U:H2'   | 55:CA:710:G:H8    | 1.71                     | 0.56              |
| 5:CF:14:GLN:HB3   | 5:CF:17:GLN:NE2   | 2.20                     | 0.56              |
| 8:CI:59:LYS:HE3   | 8:CI:60:LEU:HG    | 1.86                     | 0.56              |
| 17:CR:25:ILE:O    | 17:CR:29:LYS:HG2  | 2.06                     | 0.56              |
| 52:D2:22:MET:O    | 52:D2:22:MET:HG2  | 2.06                     | 0.56              |
| 52:D2:35:ARG:HG3  | 52:D2:42:LEU:HD21 | 1.86                     | 0.56              |
| 24:DA:104:A:H2'   | 24:DA:105:C:C6    | 2.39                     | 0.56              |
| 24:DA:1136:G:HO2' | 24:DA:1137:G:H8   | 1.52                     | 0.56              |
| 24:DA:133:U:H2'   | 24:DA:134:G:O4'   | 2.06                     | 0.56              |
| 24:DA:1351:C:H2'  | 24:DA:1352:U:O4'  | 2.04                     | 0.56              |
| 24:DA:1840:G:H2'  | 24:DA:1841:U:H6   | 1.71                     | 0.56              |
| 24:DA:2332:C:H4'  | 46:DW:40:ARG:CZ   | 2.35                     | 0.56              |
| 24:DA:2540:C:C2   | 24:DA:2541:A:C8   | 2.94                     | 0.56              |
| 24:DA:2547:A:C1'  | 24:DA:2566:A:C6   | 2.88                     | 0.56              |
| 24:DA:732:C:H2'   | 24:DA:733:G:O4'   | 2.06                     | 0.56              |
| 24:DA:996:A:H2'   | 24:DA:997:G:H8    | 1.69                     | 0.56              |
| 56:DB:42:C:O2     | 29:DF:89:THR:HB   | 2.06                     | 0.56              |
| 35:DL:56:PRO:O    | 35:DL:60:ARG:HG3  | 2.06                     | 0.56              |
| 39:DP:25:VAL:HA   | 39:DP:85:VAL:HA   | 1.88                     | 0.56              |
| 40:DQ:4:LYS:HG2   | 40:DQ:6:GLY:N     | 2.21                     | 0.56              |
| 36:DM:34:LYS:NZ   | 45:DV:82:TYR:HA   | 2.20                     | 0.56              |
| 21:AA:1052:U:H5'  | 21:AA:1053:G:OP2  | 2.06                     | 0.56              |
| 21:AA:1504:G:H5'  | 21:AA:1505:G:N2   | 2.20                     | 0.56              |
| 21:AA:923:A:H2'   | 21:AA:924:C:C6    | 2.40                     | 0.56              |
| 1:AB:113:LEU:HD13 | 1:AB:143:LEU:CD2  | 2.36                     | 0.56              |
| 1:AB:71:THR:HG22  | 1:AB:72:LYS:N     | 2.18                     | 0.56              |
| 4:AE:25:LYS:CB    | 4:AE:25:LYS:NZ    | 2.68                     | 0.56              |
| 7:AH:88:LYS:HG3   | 7:AH:89:ASP:N     | 2.20                     | 0.56              |
| 10:AK:95:THR:HG23 | 10:AK:96:ILE:HG23 | 1.88                     | 0.56              |
| 11:AL:88:ASP:O    | 11:AL:90:PRO:HD3  | 2.06                     | 0.56              |
| 12:AM:10:ASP:OD1  | 12:AM:44:ILE:HD13 | 2.06                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:B1:49:LYS:O    | 51:B1:50:GLU:HB3   | 2.05                     | 0.56              |
| 24:BA:1243:C:H2'  | 24:BA:1244:A:O4'   | 2.06                     | 0.56              |
| 24:BA:1509:A:O2'  | 24:BA:1510:G:OP2   | 2.23                     | 0.56              |
| 24:BA:1989:G:H2'  | 24:BA:1990:C:H5'   | 1.87                     | 0.56              |
| 24:BA:27:G:O2'    | 24:BA:28:A:P       | 2.64                     | 0.56              |
| 24:BA:653:U:H3'   | 24:BA:654:A:H5'    | 1.86                     | 0.56              |
| 24:BA:821:A:H5''  | 24:BA:822:G:O5'    | 2.04                     | 0.56              |
| 29:BF:35:LEU:CD1  | 29:BF:88:VAL:HB    | 2.36                     | 0.56              |
| 29:BF:46:LYS:H    | 29:BF:46:LYS:HD2   | 1.70                     | 0.56              |
| 35:BL:95:LEU:HB3  | 35:BL:100:ILE:CD1  | 2.36                     | 0.56              |
| 39:BP:112:ARG:C   | 39:BP:113:LEU:HD23 | 2.26                     | 0.56              |
| 43:BT:2:ILE:HG13  | 43:BT:3:ARG:CZ     | 2.35                     | 0.56              |
| 24:BA:309:A:H4'   | 44:BU:15:GLY:HA2   | 1.87                     | 0.56              |
| 46:BW:18:LYS:HA   | 46:BW:36:ILE:HG12  | 1.87                     | 0.56              |
| 55:CA:1233:G:H2'  | 55:CA:1234:C:H6    | 1.70                     | 0.56              |
| 55:CA:1366:C:H2'  | 55:CA:1367:C:C6    | 2.39                     | 0.56              |
| 55:CA:1483:A:H8   | 55:CA:1483:A:O5'   | 1.89                     | 0.56              |
| 55:CA:1507:A:C6   | 55:CA:1530:G:C6    | 2.94                     | 0.56              |
| 55:CA:825:A:H2'   | 55:CA:826:C:H6     | 1.70                     | 0.56              |
| 55:CA:872:A:C4    | 55:CA:874:G:N7     | 2.73                     | 0.56              |
| 3:CD:57:LYS:HA    | 3:CD:199:ILE:HG22  | 1.88                     | 0.56              |
| 8:CI:122:ARG:NH1  | 55:CA:1343:G:H1'   | 2.21                     | 0.56              |
| 51:D1:8:ILE:CD1   | 51:D1:52:LYS:HG3   | 2.36                     | 0.56              |
| 24:DA:1168:G:C6   | 24:DA:1182:G:C6    | 2.93                     | 0.56              |
| 24:DA:117:G:N1    | 24:DA:119:A:N6     | 2.53                     | 0.56              |
| 24:DA:2198:A:O2'  | 24:DA:2199:A:H8    | 1.87                     | 0.56              |
| 24:DA:2287:A:C5   | 24:DA:2289:G:N7    | 2.74                     | 0.56              |
| 24:DA:2394:C:H41  | 53:D3:30:HIS:CE1   | 2.24                     | 0.56              |
| 24:DA:2543:G:C6   | 24:DA:2765:A:C4    | 2.94                     | 0.56              |
| 24:DA:476:G:O2'   | 24:DA:477:A:O5'    | 2.12                     | 0.56              |
| 24:DA:822:G:O6    | 24:DA:943:A:H2     | 1.89                     | 0.56              |
| 24:DA:91:A:HO2'   | 24:DA:92:U:H6      | 1.48                     | 0.56              |
| 26:DC:99:GLU:HG2  | 26:DC:100:ARG:N    | 2.21                     | 0.56              |
| 28:DE:29:HIS:ND1  | 35:DL:6:LEU:HD22   | 2.20                     | 0.56              |
| 24:DA:469:G:OP2   | 28:DE:55:SER:HB3   | 2.06                     | 0.56              |
| 29:DF:139:GLU:HB3 | 29:DF:142:TYR:HB3  | 1.87                     | 0.56              |
| 45:DV:31:TYR:O    | 45:DV:31:TYR:HD1   | 1.89                     | 0.56              |
| 21:AA:1160:G:O6   | 21:AA:1181:G:C6    | 2.58                     | 0.56              |
| 21:AA:1391:U:H2'  | 21:AA:1392:G:C8    | 2.41                     | 0.56              |
| 21:AA:486:U:C5'   | 21:AA:486:U:H6     | 2.17                     | 0.56              |
| 21:AA:687:A:C2    | 21:AA:704:A:C5     | 2.93                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:720:C:N4    | 21:AA:721:G:C2     | 2.73                     | 0.56              |
| 4:AE:11:GLN:O     | 4:AE:11:GLN:HG3    | 2.05                     | 0.56              |
| 4:AE:82:HIS:CE1   | 4:AE:146:MET:HG3   | 2.41                     | 0.56              |
| 5:AF:40:GLU:O     | 5:AF:42:TRP:CD1    | 2.58                     | 0.56              |
| 8:AI:21:LYS:HZ2   | 8:AI:23:GLY:HA3    | 1.70                     | 0.56              |
| 8:AI:27:ILE:HD13  | 8:AI:34:LEU:HB2    | 1.86                     | 0.56              |
| 8:AI:51:LEU:HB3   | 8:AI:56:MET:CG     | 2.36                     | 0.56              |
| 11:AL:65:TYR:HE1  | 11:AL:67:GLY:HA2   | 1.69                     | 0.56              |
| 16:AQ:16:MET:O    | 16:AQ:19:SER:N     | 2.37                     | 0.56              |
| 24:BA:1572:A:H2'  | 24:BA:1573:G:O4'   | 2.06                     | 0.56              |
| 24:BA:735:A:H3'   | 24:BA:736:C:C6     | 2.40                     | 0.56              |
| 24:BA:994:C:O3'   | 24:BA:995:C:H3'    | 2.06                     | 0.56              |
| 28:BE:137:LYS:O   | 28:BE:141:MET:HG3  | 2.05                     | 0.56              |
| 28:BE:48:THR:C    | 28:BE:50:ALA:H     | 2.08                     | 0.56              |
| 29:BF:142:TYR:O   | 29:BF:145:VAL:HG22 | 2.06                     | 0.56              |
| 30:BG:84:LYS:HZ2  | 30:BG:133:LYS:HE3  | 1.70                     | 0.56              |
| 31:BH:21:VAL:HG21 | 31:BH:25:TYR:CD2   | 2.41                     | 0.56              |
| 33:BJ:77:HIS:HD2  | 33:BJ:79:GLY:H     | 1.51                     | 0.56              |
| 36:BM:69:PRO:HA   | 36:BM:94:ALA:HB2   | 1.87                     | 0.56              |
| 41:BR:27:ILE:HG13 | 41:BR:33:VAL:HG12  | 1.87                     | 0.56              |
| 42:BS:18:ARG:HA   | 42:BS:21:ALA:HB3   | 1.88                     | 0.56              |
| 44:BU:86:PHE:CE1  | 44:BU:101:THR:HG21 | 2.41                     | 0.56              |
| 55:CA:1123:U:H2'  | 55:CA:1124:G:O4'   | 2.06                     | 0.56              |
| 55:CA:1386:G:H2'  | 55:CA:1387:G:H8    | 1.71                     | 0.56              |
| 55:CA:438:U:C5    | 55:CA:494:G:N7     | 2.74                     | 0.56              |
| 55:CA:728:A:H2'   | 55:CA:729:A:C8     | 2.41                     | 0.56              |
| 6:CG:143:MET:HA   | 6:CG:147:ASN:HB3   | 1.88                     | 0.56              |
| 9:CJ:5:ARG:HG2    | 9:CJ:79:PRO:HG3    | 1.87                     | 0.56              |
| 11:CL:22:ALA:HB3  | 11:CL:94:TYR:OH    | 2.06                     | 0.56              |
| 24:DA:1203:U:N3   | 24:DA:1204:A:C6    | 2.73                     | 0.56              |
| 24:DA:1290:C:HO2' | 24:DA:1291:C:H6    | 1.51                     | 0.56              |
| 24:DA:2028:U:H2'  | 24:DA:2029:G:C8    | 2.41                     | 0.56              |
| 24:DA:573:U:N3    | 24:DA:2030:A:H3'   | 2.21                     | 0.56              |
| 24:DA:258:G:H2'   | 24:DA:259:G:C8     | 2.40                     | 0.56              |
| 24:DA:2893:A:H5'' | 24:DA:2894:G:H5'   | 1.88                     | 0.56              |
| 24:DA:356:G:H2'   | 24:DA:357:C:O4'    | 2.05                     | 0.56              |
| 24:DA:443:A:H61   | 28:DE:36:ALA:HB1   | 1.70                     | 0.56              |
| 24:DA:502:A:H5'   | 24:DA:503:A:OP2    | 2.06                     | 0.56              |
| 24:DA:56:A:H2'    | 24:DA:57:C:C6      | 2.41                     | 0.56              |
| 24:DA:800:A:O2'   | 24:DA:801:G:H5''   | 2.06                     | 0.56              |
| 24:DA:320:A:C5    | 28:DE:132:LYS:HB2  | 2.41                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:DS:66:ILE:H    | 42:DS:66:ILE:HD13 | 1.70                     | 0.56              |
| 43:DT:45:ALA:HA   | 43:DT:48:GLN:CG   | 2.36                     | 0.56              |
| 48:DY:57:LEU:HD13 | 48:DY:60:LYS:HE3  | 1.87                     | 0.56              |
| 21:AA:369:G:OP2   | 21:AA:388:G:N2    | 2.29                     | 0.56              |
| 21:AA:366:A:O2'   | 21:AA:394:G:N2    | 2.39                     | 0.56              |
| 13:AN:30:ILE:HG23 | 13:AN:44:VAL:HG12 | 1.87                     | 0.56              |
| 24:BA:100:U:C2    | 24:BA:101:A:N6    | 2.73                     | 0.56              |
| 24:BA:1021:A:N6   | 24:BA:1142:A:N6   | 2.54                     | 0.56              |
| 24:BA:1419:A:N7   | 24:BA:1421:G:C6   | 2.74                     | 0.56              |
| 24:BA:2067:G:H4'  | 24:BA:2068:U:OP2  | 2.05                     | 0.56              |
| 24:BA:646:U:O4    | 24:BA:2368:C:H1'  | 2.06                     | 0.56              |
| 24:BA:2516:A:C4   | 24:BA:2569:G:N2   | 2.73                     | 0.56              |
| 24:BA:271:G:O2'   | 24:BA:272:A:C5'   | 2.53                     | 0.56              |
| 24:BA:2816:G:C4   | 24:BA:2817:U:C5   | 2.93                     | 0.56              |
| 24:BA:315:G:H2'   | 24:BA:316:C:C6    | 2.41                     | 0.56              |
| 24:BA:358:U:H2'   | 24:BA:359:G:O4'   | 2.06                     | 0.56              |
| 24:BA:35:G:HO2'   | 24:BA:36:G:P      | 2.28                     | 0.56              |
| 24:BA:623:C:H2'   | 24:BA:624:C:C6    | 2.40                     | 0.56              |
| 24:BA:706:A:H2'   | 24:BA:707:G:O4'   | 2.06                     | 0.56              |
| 24:BA:705:A:H62   | 24:BA:726:G:H1'   | 1.68                     | 0.56              |
| 24:BA:864:G:C6    | 24:BA:865:C:N4    | 2.74                     | 0.56              |
| 24:BA:947:A:H2'   | 24:BA:948:C:H6    | 1.70                     | 0.56              |
| 26:BC:263:ASP:O   | 26:BC:264:LYS:C   | 2.44                     | 0.56              |
| 26:BC:61:TYR:HD2  | 26:BC:85:ASN:ND2  | 2.04                     | 0.56              |
| 29:BF:127:TYR:CE2 | 29:BF:129:MET:HG2 | 2.40                     | 0.56              |
| 30:BG:59:ASP:O    | 30:BG:62:ALA:HB3  | 2.06                     | 0.56              |
| 30:BG:59:ASP:HB2  | 30:BG:63:GLN:HG2  | 1.88                     | 0.56              |
| 34:BK:121:GLU:OE2 | 39:BP:64:SER:OG   | 2.19                     | 0.56              |
| 40:BQ:13:HIS:HD2  | 40:BQ:31:TYR:CE1  | 2.23                     | 0.56              |
| 43:BT:12:ARG:O    | 43:BT:13:ALA:HB2  | 2.06                     | 0.56              |
| 48:BY:17:GLU:HB2  | 48:BY:53:VAL:HG11 | 1.88                     | 0.56              |
| 55:CA:177:G:H2'   | 55:CA:178:C:H5'   | 1.88                     | 0.56              |
| 55:CA:324:G:N2    | 55:CA:326:G:H3'   | 2.21                     | 0.56              |
| 55:CA:652:U:H1'   | 55:CA:653:U:C5    | 2.40                     | 0.56              |
| 55:CA:65:A:H4'    | 55:CA:66:A:O5'    | 2.06                     | 0.56              |
| 55:CA:734:G:H2'   | 55:CA:735:C:C6    | 2.41                     | 0.56              |
| 55:CA:764:C:H2'   | 55:CA:765:G:H5'   | 1.88                     | 0.56              |
| 6:CG:3:ARG:HG2    | 55:CA:932:C:H5'   | 1.86                     | 0.56              |
| 1:CB:160:LEU:O    | 1:CB:183:PHE:HD1  | 1.89                     | 0.56              |
| 10:CK:15:VAL:O    | 10:CK:16:SER:HB2  | 2.05                     | 0.56              |
| 24:DA:2080:A:C2   | 24:DA:2081:U:C2   | 2.94                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:2592:G:C4   | 24:DA:2593:U:C5    | 2.94                     | 0.56              |
| 24:DA:673:C:C5'   | 28:DE:75:SER:HB2   | 2.35                     | 0.56              |
| 24:DA:322:A:H5''  | 28:DE:163:ASN:ND2  | 2.20                     | 0.56              |
| 29:DF:113:PHE:CE2 | 29:DF:116:LEU:HD22 | 2.41                     | 0.56              |
| 31:DH:9:VAL:CG1   | 31:DH:10:ALA:N     | 2.68                     | 0.56              |
| 37:DN:103:ARG:HB2 | 37:DN:110:MET:CG   | 2.35                     | 0.56              |
| 24:DA:2849:U:OP1  | 39:DP:92:ARG:NH1   | 2.39                     | 0.56              |
| 43:DT:9:LYS:HG3   | 48:DY:21:LEU:HD13  | 1.87                     | 0.56              |
| 13:AN:74:ARG:HG2  | 21:AA:1358:U:OP1   | 2.06                     | 0.56              |
| 1:AB:20:ARG:HA    | 1:AB:20:ARG:NH1    | 2.21                     | 0.56              |
| 2:AC:36:PHE:HD1   | 2:AC:36:PHE:O      | 1.89                     | 0.56              |
| 8:AI:49:GLN:N     | 8:AI:50:PRO:HD2    | 2.20                     | 0.56              |
| 20:AU:40:PRO:HB3  | 20:AU:44:ARG:HD3   | 1.88                     | 0.56              |
| 54:B4:9:LYS:N     | 54:B4:9:LYS:CD     | 2.68                     | 0.56              |
| 24:BA:1021:A:H2'  | 24:BA:1021:A:N3    | 2.21                     | 0.56              |
| 24:BA:1116:G:O2'  | 24:BA:1117:C:H5'   | 2.05                     | 0.56              |
| 24:BA:1229:C:H2'  | 24:BA:1230:A:C8    | 2.41                     | 0.56              |
| 24:BA:1278:C:H2'  | 24:BA:1279:G:C8    | 2.40                     | 0.56              |
| 24:BA:1383:A:C6   | 24:BA:1384:A:N1    | 2.74                     | 0.56              |
| 24:BA:1411:U:O2'  | 24:BA:1412:U:H5'   | 2.06                     | 0.56              |
| 24:BA:1556:C:O2'  | 24:BA:1557:C:H5'   | 2.06                     | 0.56              |
| 24:BA:231:A:N6    | 24:BA:232:G:N2     | 2.54                     | 0.56              |
| 24:BA:2473:U:H5'' | 24:BA:2474:U:OP2   | 2.06                     | 0.56              |
| 24:BA:417:C:H2'   | 24:BA:418:C:C6     | 2.38                     | 0.56              |
| 24:BA:588:U:H2'   | 24:BA:589:U:H6     | 1.71                     | 0.56              |
| 26:BC:16:VAL:H    | 26:BC:203:VAL:HG12 | 1.70                     | 0.56              |
| 29:BF:10:GLU:O    | 29:BF:11:VAL:HB    | 2.06                     | 0.56              |
| 29:BF:128:SER:OG  | 29:BF:154:THR:HB   | 2.06                     | 0.56              |
| 35:BL:77:ILE:CD1  | 35:BL:108:ALA:HB1  | 2.35                     | 0.56              |
| 44:BU:6:ARG:O     | 44:BU:24:VAL:HB    | 2.05                     | 0.56              |
| 55:CA:13:U:O2'    | 55:CA:14:U:P       | 2.63                     | 0.56              |
| 55:CA:593:U:C4    | 55:CA:594:U:C5     | 2.93                     | 0.56              |
| 55:CA:637:C:H2'   | 55:CA:638:U:H6     | 1.71                     | 0.56              |
| 55:CA:79:G:H2'    | 55:CA:80:A:H8      | 1.71                     | 0.56              |
| 55:CA:82:G:N7     | 55:CA:89:U:C4      | 2.74                     | 0.56              |
| 55:CA:966:G:C2    | 55:CA:967:C:C2     | 2.94                     | 0.56              |
| 55:CA:96:U:HO2'   | 55:CA:97:G:H8      | 1.53                     | 0.56              |
| 9:CJ:71:LEU:O     | 9:CJ:72:ARG:HD3    | 2.05                     | 0.56              |
| 13:CN:30:ILE:O    | 13:CN:45:LEU:HD11  | 2.06                     | 0.56              |
| 18:CS:35:ARG:NH1  | 18:CS:52:ASN:HA    | 2.21                     | 0.56              |
| 50:D0:28:SER:HB3  | 50:D0:39:ARG:NE    | 2.21                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:1128:G:O6    | 24:DA:2491:U:C5    | 2.59                     | 0.56              |
| 24:DA:1854:A:H62   | 24:DA:1888:G:H8    | 1.53                     | 0.56              |
| 24:DA:234:U:O2'    | 24:DA:235:U:H6     | 1.88                     | 0.56              |
| 24:DA:374:A:C6     | 24:DA:401:A:C8     | 2.94                     | 0.56              |
| 24:DA:547:A:H2'    | 24:DA:548:G:H5'    | 1.88                     | 0.56              |
| 24:DA:655:A:H4'    | 24:DA:656:G:O5'    | 2.04                     | 0.56              |
| 24:DA:822:G:H5''   | 59:DA:3360:HOH:O   | 2.06                     | 0.56              |
| 26:DC:68:ARG:HD3   | 26:DC:103:ILE:HD13 | 1.86                     | 0.56              |
| 26:DC:52:HIS:NE2   | 26:DC:218:THR:HG23 | 2.21                     | 0.56              |
| 28:DE:128:ALA:HB1  | 28:DE:129:PRO:CD   | 2.34                     | 0.56              |
| 29:DF:48:LEU:HG    | 29:DF:49:LEU:HD22  | 1.88                     | 0.56              |
| 33:DJ:77:HIS:CE1   | 33:DJ:83:GLY:HA3   | 2.40                     | 0.56              |
| 33:DJ:86:GLN:O     | 33:DJ:87:ALA:HB2   | 2.06                     | 0.56              |
| 56:DB:51:G:H5''    | 38:DO:64:TYR:CG    | 2.40                     | 0.56              |
| 39:DP:88:ARG:NE    | 39:DP:112:ARG:HH21 | 2.01                     | 0.56              |
| 39:DP:59:THR:OG1   | 39:DP:72:VAL:HG12  | 2.06                     | 0.56              |
| 39:DP:5:LYS:O      | 39:DP:9:GLN:HG2    | 2.04                     | 0.56              |
| 42:DS:14:ALA:HB1   | 42:DS:18:ARG:NH2   | 2.21                     | 0.56              |
| 42:DS:18:ARG:HH21  | 42:DS:76:VAL:HG22  | 1.71                     | 0.56              |
| 21:AA:2:A:N6       | 21:AA:3:A:N1       | 2.54                     | 0.56              |
| 7:AH:29:SER:HB2    | 7:AH:32:LYS:HZ3    | 1.69                     | 0.56              |
| 10:AK:106:ILE:HD13 | 10:AK:107:THR:N    | 2.20                     | 0.56              |
| 11:AL:41:PRO:HB3   | 11:AL:49:ARG:NH1   | 2.21                     | 0.56              |
| 14:AO:45:HIS:HB3   | 21:AA:668:G:O2'    | 2.06                     | 0.56              |
| 22:AX:39:U:H2'     | 22:AX:40:C:C6      | 2.41                     | 0.56              |
| 24:BA:2286:G:O6    | 51:B1:22:THR:HG21  | 2.05                     | 0.56              |
| 51:B1:27:ARG:O     | 51:B1:30:PRO:HD3   | 2.06                     | 0.56              |
| 24:BA:1065:U:H5    | 24:BA:1074:G:H21   | 1.54                     | 0.56              |
| 24:BA:2426:A:H3'   | 24:BA:2427:C:H5'   | 1.88                     | 0.56              |
| 24:BA:463:G:N1     | 24:BA:467:G:C6     | 2.74                     | 0.56              |
| 24:BA:90:U:H2'     | 24:BA:91:A:C8      | 2.41                     | 0.56              |
| 24:BA:960:A:N7     | 24:BA:962:G:C8     | 2.74                     | 0.56              |
| 27:BD:9:VAL:HG22   | 27:BD:10:GLY:N     | 2.20                     | 0.56              |
| 30:BG:54:ARG:C     | 30:BG:54:ARG:HD3   | 2.27                     | 0.56              |
| 33:BJ:112:GLY:O    | 33:BJ:113:PRO:C    | 2.45                     | 0.56              |
| 33:BJ:13:ARG:O     | 33:BJ:14:ASP:CB    | 2.54                     | 0.56              |
| 37:BN:75:ILE:HG13  | 37:BN:76:VAL:N     | 2.20                     | 0.56              |
| 55:CA:1310:G:H2'   | 55:CA:1311:A:O4'   | 2.06                     | 0.56              |
| 55:CA:1381:U:O2'   | 55:CA:1382:C:C5'   | 2.54                     | 0.56              |
| 55:CA:481:G:H4'    | 55:CA:482:A:OP1    | 2.06                     | 0.56              |
| 55:CA:914:A:O2'    | 55:CA:915:A:C5'    | 2.54                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CB:86:CYS:SG     | 1:CB:220:VAL:HB    | 2.45                     | 0.56              |
| 12:CM:62:PHE:O     | 12:CM:64:VAL:HG23  | 2.04                     | 0.56              |
| 20:CU:14:ALA:O     | 20:CU:15:LEU:HG    | 2.06                     | 0.56              |
| 53:D3:57:VAL:HA    | 53:D3:60:CYS:SG    | 2.46                     | 0.56              |
| 24:DA:1916:A:C8    | 24:DA:1916:A:H5''  | 2.41                     | 0.56              |
| 24:DA:2248:C:H2'   | 24:DA:2249:U:O4'   | 2.06                     | 0.56              |
| 24:DA:2261:C:O2'   | 24:DA:2262:U:H5'   | 2.06                     | 0.56              |
| 24:DA:333:G:O2'    | 24:DA:334:C:C5'    | 2.54                     | 0.56              |
| 24:DA:45:G:C5'     | 24:DA:46:G:H5'     | 2.35                     | 0.56              |
| 24:DA:600:G:C5'    | 28:DE:27:LEU:HD22  | 2.35                     | 0.56              |
| 29:DF:136:ILE:HG23 | 29:DF:142:TYR:HB2  | 1.87                     | 0.56              |
| 29:DF:136:ILE:CD1  | 29:DF:145:VAL:HG11 | 2.34                     | 0.56              |
| 29:DF:147:ARG:H    | 29:DF:147:ARG:HD2  | 1.71                     | 0.56              |
| 30:DG:85:LYS:HG3   | 30:DG:163:TYR:HB2  | 1.87                     | 0.56              |
| 31:DH:41:LYS:HA    | 31:DH:44:ILE:CG1   | 2.35                     | 0.56              |
| 39:DP:9:GLN:HB3    | 39:DP:12:MET:CE    | 2.36                     | 0.56              |
| 21:AA:1089:G:N2    | 21:AA:1090:U:H1'   | 2.20                     | 0.55              |
| 21:AA:1295:U:H2'   | 21:AA:1296:C:C6    | 2.40                     | 0.55              |
| 21:AA:1239:A:C5    | 21:AA:1298:U:C5    | 2.93                     | 0.55              |
| 21:AA:1468:A:H8    | 21:AA:1468:A:O5'   | 1.89                     | 0.55              |
| 21:AA:205:A:H62    | 21:AA:214:C:H1'    | 1.70                     | 0.55              |
| 21:AA:985:C:O2'    | 21:AA:986:U:H5'    | 2.06                     | 0.55              |
| 21:AA:98:A:H2'     | 21:AA:99:C:H6      | 1.71                     | 0.55              |
| 3:AD:25:ARG:NH1    | 3:AD:30:LYS:HE3    | 2.21                     | 0.55              |
| 10:AK:85:VAL:HG12  | 10:AK:86:LYS:N     | 2.21                     | 0.55              |
| 11:AL:23:LEU:C     | 11:AL:25:ALA:H     | 2.09                     | 0.55              |
| 11:AL:42:LYS:HA    | 21:AA:1492:A:OP1   | 2.06                     | 0.55              |
| 11:AL:43:LYS:N     | 21:AA:1492:A:OP1   | 2.39                     | 0.55              |
| 13:AN:48:GLN:NE2   | 13:AN:48:GLN:HA    | 2.20                     | 0.55              |
| 50:B0:32:THR:OG1   | 50:B0:50:GLY:HA2   | 2.06                     | 0.55              |
| 52:B2:30:VAL:HG22  | 52:B2:33:ARG:NH1   | 2.21                     | 0.55              |
| 53:B3:28:LEU:CD1   | 53:B3:40:LYS:HG2   | 2.36                     | 0.55              |
| 24:BA:1256:G:C2'   | 28:BE:77:ILE:HD11  | 2.35                     | 0.55              |
| 24:BA:1468:U:C2    | 24:BA:1522:A:C2    | 2.95                     | 0.55              |
| 24:BA:1498:C:H2'   | 24:BA:1499:C:C6    | 2.41                     | 0.55              |
| 24:BA:1313:U:C6    | 24:BA:1610:A:N3    | 2.74                     | 0.55              |
| 24:BA:1683:U:H2'   | 24:BA:1684:G:H8    | 1.69                     | 0.55              |
| 24:BA:2305:U:C5    | 24:BA:2306:C:C4    | 2.94                     | 0.55              |
| 24:BA:503:A:C2     | 24:BA:505:A:C4     | 2.95                     | 0.55              |
| 24:BA:809:G:H2'    | 24:BA:810:U:O5'    | 2.05                     | 0.55              |
| 24:BA:784:G:O6     | 26:BC:227:VAL:HG11 | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:BJ:114:LEU:O   | 33:BJ:118:MET:HG3 | 2.05                     | 0.55              |
| 24:BA:1649:G:O2'  | 37:BN:106:ASP:OD2 | 2.23                     | 0.55              |
| 46:BW:23:LYS:HE3  | 46:BW:24:ARG:O    | 2.06                     | 0.55              |
| 55:CA:1134:G:C2   | 55:CA:1141:C:C2   | 2.94                     | 0.55              |
| 55:CA:720:C:H2'   | 55:CA:721:G:C8    | 2.41                     | 0.55              |
| 4:CE:28:ARG:HG2   | 4:CE:29:ILE:N     | 2.21                     | 0.55              |
| 7:CH:36:ALA:HA    | 7:CH:39:LEU:HD12  | 1.88                     | 0.55              |
| 12:CM:52:ILE:HD12 | 12:CM:55:LEU:HB2  | 1.88                     | 0.55              |
| 16:CQ:18:LYS:HD3  | 16:CQ:48:GLU:OE2  | 2.05                     | 0.55              |
| 24:DA:1055:G:C3'  | 24:DA:1056:G:H5'  | 2.36                     | 0.55              |
| 24:DA:1439:A:N6   | 24:DA:1440:U:C2   | 2.74                     | 0.55              |
| 24:DA:1717:A:H2'  | 24:DA:1718:G:O4'  | 2.06                     | 0.55              |
| 24:DA:2147:A:N3   | 24:DA:2147:A:H2'  | 2.20                     | 0.55              |
| 24:DA:216:A:C2'   | 24:DA:217:A:H8    | 2.18                     | 0.55              |
| 24:DA:2230:G:C6   | 24:DA:2231:U:C4   | 2.95                     | 0.55              |
| 24:DA:2299:U:H2'  | 24:DA:2300:C:C6   | 2.41                     | 0.55              |
| 24:DA:2307:G:H1'  | 24:DA:2308:G:C8   | 2.40                     | 0.55              |
| 24:DA:2458:G:H5'' | 24:DA:2459:A:OP1  | 2.06                     | 0.55              |
| 24:DA:604:G:C6    | 24:DA:625:G:C6    | 2.94                     | 0.55              |
| 24:DA:695:G:C4    | 24:DA:768:G:C2    | 2.95                     | 0.55              |
| 56:DB:43:C:H4'    | 29:DF:91:ARG:NH2  | 2.22                     | 0.55              |
| 26:DC:78:GLU:OE2  | 26:DC:94:LEU:HD22 | 2.06                     | 0.55              |
| 24:DA:1070:A:H61  | 32:DI:8:VAL:HG12  | 1.69                     | 0.55              |
| 24:DA:17:G:H4'    | 40:DQ:24:TYR:HE1  | 1.71                     | 0.55              |
| 24:DA:508:A:N6    | 42:DS:9:HIS:CE1   | 2.74                     | 0.55              |
| 48:DY:28:LEU:HD23 | 48:DY:42:LEU:HD13 | 1.87                     | 0.55              |
| 21:AA:115:G:H4'   | 21:AA:116:A:O5'   | 2.04                     | 0.55              |
| 21:AA:123:U:H5''  | 21:AA:311:C:O2'   | 2.06                     | 0.55              |
| 21:AA:1419:G:C6   | 21:AA:1420:U:C4   | 2.94                     | 0.55              |
| 3:AD:196:GLU:O    | 3:AD:198:LEU:N    | 2.39                     | 0.55              |
| 7:AH:6:ILE:O      | 7:AH:9:MET:HB3    | 2.06                     | 0.55              |
| 11:AL:118:VAL:O   | 21:AA:36:C:H4'    | 2.06                     | 0.55              |
| 11:AL:89:LEU:HD22 | 11:AL:89:LEU:H    | 1.72                     | 0.55              |
| 53:B3:40:LYS:O    | 53:B3:43:LEU:N    | 2.35                     | 0.55              |
| 24:BA:1303:G:O2'  | 24:BA:1304:A:H5'  | 2.05                     | 0.55              |
| 24:BA:1796:U:H2'  | 24:BA:1797:G:H8   | 1.70                     | 0.55              |
| 24:BA:1831:G:C4   | 24:BA:1832:C:C5   | 2.94                     | 0.55              |
| 24:BA:1849:G:O2'  | 24:BA:1850:G:H5'  | 2.05                     | 0.55              |
| 24:BA:1891:G:H8   | 24:BA:1891:G:O5'  | 1.89                     | 0.55              |
| 24:BA:1998:A:P    | 27:BD:141:ARG:NH2 | 2.79                     | 0.55              |
| 24:BA:2540:C:H2'  | 24:BA:2541:A:C5'  | 2.36                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:2657:A:C2   | 24:BA:2665:A:C4    | 2.94                     | 0.55              |
| 24:BA:2697:G:C5   | 24:BA:2698:U:C5    | 2.94                     | 0.55              |
| 24:BA:682:G:H5'   | 52:B2:26:ASN:OD1   | 2.07                     | 0.55              |
| 24:BA:827:U:H5'   | 24:BA:828:U:OP1    | 2.07                     | 0.55              |
| 27:BD:150:GLN:HG3 | 27:BD:150:GLN:O    | 2.06                     | 0.55              |
| 28:BE:79:ARG:CG   | 28:BE:80:SER:N     | 2.67                     | 0.55              |
| 24:BA:2305:U:C5'  | 29:BF:130:GLY:HA3  | 2.33                     | 0.55              |
| 33:BJ:17:VAL:HG23 | 33:BJ:137:PRO:HB2  | 1.88                     | 0.55              |
| 42:BS:20:VAL:HG21 | 42:BS:43:ALA:HB3   | 1.87                     | 0.55              |
| 43:BT:54:GLU:O    | 43:BT:55:VAL:HB    | 2.06                     | 0.55              |
| 55:CA:1060:U:O2   | 55:CA:1198:G:C2    | 2.58                     | 0.55              |
| 55:CA:1250:A:N3   | 55:CA:1287:A:N6    | 2.54                     | 0.55              |
| 55:CA:1300:G:N1   | 55:CA:1334:G:C8    | 2.74                     | 0.55              |
| 55:CA:275:G:O2'   | 55:CA:276:G:C5'    | 2.53                     | 0.55              |
| 55:CA:79:G:H2'    | 55:CA:80:A:C8      | 2.41                     | 0.55              |
| 2:CC:181:ILE:HA   | 2:CC:201:ILE:O     | 2.06                     | 0.55              |
| 24:DA:1236:G:O2'  | 24:DA:1237:A:C8    | 2.58                     | 0.55              |
| 24:DA:1809:A:H2'  | 24:DA:1810:A:C8    | 2.41                     | 0.55              |
| 24:DA:1965:C:H3'  | 24:DA:1966:A:C5'   | 2.31                     | 0.55              |
| 24:DA:2332:C:H4'  | 46:DW:40:ARG:NH2   | 2.21                     | 0.55              |
| 24:DA:2542:A:H4'  | 24:DA:2543:G:H5'   | 1.87                     | 0.55              |
| 24:DA:275:C:H2'   | 24:DA:276:U:O4'    | 2.06                     | 0.55              |
| 24:DA:682:G:H2'   | 24:DA:683:U:C6     | 2.41                     | 0.55              |
| 24:DA:822:G:N7    | 24:DA:944:C:H1'    | 2.21                     | 0.55              |
| 27:DD:119:ALA:HB3 | 27:DD:163:GLY:N    | 2.18                     | 0.55              |
| 28:DE:147:LEU:O   | 28:DE:148:ILE:HB   | 2.05                     | 0.55              |
| 28:DE:105:LEU:HB3 | 28:DE:200:LEU:HD11 | 1.88                     | 0.55              |
| 30:DG:86:LEU:HD12 | 30:DG:132:LEU:HD11 | 1.88                     | 0.55              |
| 31:DH:132:PHE:CZ  | 31:DH:134:VAL:HB   | 2.42                     | 0.55              |
| 31:DH:8:LYS:HD2   | 31:DH:9:VAL:N      | 2.21                     | 0.55              |
| 37:DN:37:THR:HB   | 37:DN:40:LYS:HB2   | 1.88                     | 0.55              |
| 39:DP:105:LYS:HA  | 39:DP:108:ARG:NE   | 2.22                     | 0.55              |
| 44:DU:11:ILE:HG21 | 44:DU:79:ALA:HB2   | 1.88                     | 0.55              |
| 45:DV:57:TYR:HD2  | 45:DV:74:ALA:HB1   | 1.72                     | 0.55              |
| 24:DA:396:G:OP2   | 47:DX:9:LYS:NZ     | 2.35                     | 0.55              |
| 48:DY:19:LEU:HG   | 48:DY:22:LEU:HD22  | 1.89                     | 0.55              |
| 21:AA:1461:G:H2'  | 21:AA:1462:C:H6    | 1.72                     | 0.55              |
| 21:AA:271:C:O2'   | 21:AA:272:C:H5'    | 2.06                     | 0.55              |
| 21:AA:630:A:H2'   | 21:AA:631:C:O4'    | 2.07                     | 0.55              |
| 21:AA:830:G:H2'   | 21:AA:831:A:C8     | 2.42                     | 0.55              |
| 1:AB:9:LEU:HD12   | 1:AB:42:LEU:CD1    | 2.36                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AC:78:LYS:HG3    | 2:AC:79:LYS:HD2    | 1.88                     | 0.55              |
| 4:AE:96:GLN:CD     | 4:AE:97:PRO:HD2    | 2.27                     | 0.55              |
| 16:AQ:20:ILE:HG22  | 16:AQ:47:ASP:OD1   | 2.06                     | 0.55              |
| 19:AT:73:ARG:HH11  | 19:AT:73:ARG:HG3   | 1.71                     | 0.55              |
| 24:BA:1006:C:C6    | 24:BA:1138:G:N2    | 2.74                     | 0.55              |
| 24:BA:1026:G:C2'   | 24:BA:1027:A:H8    | 2.18                     | 0.55              |
| 24:BA:1734:G:C4    | 24:BA:1735:A:C8    | 2.94                     | 0.55              |
| 24:BA:790:U:O2'    | 24:BA:791:C:H5'    | 2.06                     | 0.55              |
| 24:BA:7:G:C6       | 24:BA:8:C:C4       | 2.94                     | 0.55              |
| 24:BA:977:G:C2     | 24:BA:978:G:C8     | 2.94                     | 0.55              |
| 27:BD:107:VAL:HG21 | 27:BD:177:VAL:HG13 | 1.87                     | 0.55              |
| 32:BI:85:ILE:HD13  | 32:BI:88:GLY:HA2   | 1.89                     | 0.55              |
| 36:BM:46:ILE:CG1   | 36:BM:47:GLU:H     | 2.19                     | 0.55              |
| 36:BM:96:ILE:O     | 36:BM:96:ILE:HD12  | 2.06                     | 0.55              |
| 39:BP:50:ARG:CG    | 39:BP:57:ALA:H     | 2.19                     | 0.55              |
| 39:BP:59:THR:HG23  | 39:BP:72:VAL:CG1   | 2.35                     | 0.55              |
| 55:CA:1010:U:C2    | 55:CA:1020:G:N2    | 2.74                     | 0.55              |
| 55:CA:1446:A:H61   | 55:CA:1447:A:N6    | 2.04                     | 0.55              |
| 55:CA:542:G:H2'    | 55:CA:543:U:H6     | 1.71                     | 0.55              |
| 55:CA:689:C:H2'    | 55:CA:690:G:O4'    | 2.06                     | 0.55              |
| 55:CA:765:G:O6     | 55:CA:811:C:C5     | 2.59                     | 0.55              |
| 55:CA:881:G:H2'    | 55:CA:882:C:O4'    | 2.07                     | 0.55              |
| 3:CD:10:LEU:HD23   | 3:CD:62:ARG:HD3    | 1.87                     | 0.55              |
| 3:CD:69:ARG:O      | 3:CD:70:GLN:C      | 2.44                     | 0.55              |
| 4:CE:80:LEU:HB3    | 4:CE:97:PRO:CB     | 2.37                     | 0.55              |
| 6:CG:137:ARG:NH1   | 6:CG:138:GLU:OE2   | 2.40                     | 0.55              |
| 13:CN:30:ILE:HB    | 13:CN:45:LEU:HD21  | 1.89                     | 0.55              |
| 16:CQ:17:GLU:HG3   | 55:CA:254:G:H21    | 1.71                     | 0.55              |
| 13:CN:46:LYS:HE3   | 18:CS:10:ILE:HB    | 1.89                     | 0.55              |
| 54:D4:19:ARG:O     | 54:D4:20:ASP:CB    | 2.54                     | 0.55              |
| 24:DA:1011:G:C6    | 24:DA:1013:C:C4    | 2.94                     | 0.55              |
| 24:DA:1054:A:C4    | 24:DA:1055:G:H1'   | 2.41                     | 0.55              |
| 24:DA:155:A:H2'    | 24:DA:156:A:C8     | 2.41                     | 0.55              |
| 24:DA:233:A:H2'    | 24:DA:234:U:C6     | 2.42                     | 0.55              |
| 24:DA:2542:A:H5''  | 24:DA:2543:G:OP1   | 2.06                     | 0.55              |
| 24:DA:2693:G:H2'   | 24:DA:2694:G:H8    | 1.71                     | 0.55              |
| 24:DA:74:A:O2'     | 24:DA:88:G:C8      | 2.60                     | 0.55              |
| 24:DA:955:U:OP1    | 36:DM:86:LYS:HE3   | 2.07                     | 0.55              |
| 27:DD:10:GLY:O     | 27:DD:11:MET:CB    | 2.54                     | 0.55              |
| 42:DS:32:ALA:HA    | 42:DS:35:ILE:HD11  | 1.86                     | 0.55              |
| 21:AA:1138:G:O2'   | 21:AA:1139:G:H4'   | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:1324:A:H2'  | 21:AA:1325:C:C6   | 2.41                     | 0.55              |
| 21:AA:192:A:C5    | 21:AA:193:C:C5    | 2.95                     | 0.55              |
| 2:AC:78:LYS:CG    | 2:AC:79:LYS:HD2   | 2.35                     | 0.55              |
| 4:AE:11:GLN:HG2   | 4:AE:116:VAL:HA   | 1.87                     | 0.55              |
| 9:AJ:14:ASP:HB2   | 9:AJ:17:LEU:HB3   | 1.88                     | 0.55              |
| 19:AT:19:HIS:O    | 19:AT:23:ARG:HG2  | 2.06                     | 0.55              |
| 24:BA:1455:G:O2'  | 24:BA:1456:G:H5'  | 2.05                     | 0.55              |
| 24:BA:1833:C:C2   | 24:BA:1834:U:C6   | 2.95                     | 0.55              |
| 24:BA:2426:A:H3'  | 24:BA:2427:C:C5'  | 2.36                     | 0.55              |
| 30:BG:33:THR:C    | 30:BG:34:ARG:HD3  | 2.26                     | 0.55              |
| 33:BJ:25:LEU:HB2  | 33:BJ:62:VAL:CG2  | 2.36                     | 0.55              |
| 34:BK:61:VAL:HG21 | 34:BK:112:PHE:CE2 | 2.42                     | 0.55              |
| 38:BO:104:GLN:O   | 38:BO:107:ALA:HB3 | 2.07                     | 0.55              |
| 39:BP:33:GLU:HB2  | 39:BP:38:ARG:NH1  | 2.18                     | 0.55              |
| 40:BQ:91:ARG:NH1  | 41:BR:10:LYS:HB3  | 2.21                     | 0.55              |
| 49:BZ:37:ARG:N    | 49:BZ:37:ARG:HD2  | 2.20                     | 0.55              |
| 55:CA:1347:G:N2   | 55:CA:1373:G:H2'  | 2.21                     | 0.55              |
| 55:CA:1531:A:O2'  | 55:CA:1532:U:H5'  | 2.06                     | 0.55              |
| 55:CA:369:G:N2    | 55:CA:370:C:C2    | 2.75                     | 0.55              |
| 55:CA:688:G:N2    | 55:CA:689:C:C2    | 2.75                     | 0.55              |
| 55:CA:880:C:C2'   | 55:CA:881:G:H5'   | 2.37                     | 0.55              |
| 1:CB:49:PHE:HB3   | 1:CB:199:ILE:HG22 | 1.88                     | 0.55              |
| 1:CB:80:LYS:HB3   | 1:CB:90:PHE:CE2   | 2.41                     | 0.55              |
| 2:CC:115:VAL:O    | 2:CC:118:SER:HB3  | 2.07                     | 0.55              |
| 2:CC:179:ALA:O    | 2:CC:181:ILE:HG13 | 2.06                     | 0.55              |
| 5:CF:3:HIS:NE2    | 5:CF:95:ALA:HB2   | 2.22                     | 0.55              |
| 8:CI:24:ASN:HD22  | 8:CI:26:LYS:CD    | 2.18                     | 0.55              |
| 8:CI:20:ILE:HD11  | 8:CI:62:LEU:HD13  | 1.88                     | 0.55              |
| 9:CJ:11:LYS:N     | 9:CJ:11:LYS:HD3   | 2.18                     | 0.55              |
| 12:CM:1:ALA:N     | 12:CM:2:ARG:HD3   | 2.21                     | 0.55              |
| 12:CM:69:ARG:HH21 | 55:CA:1330:U:H5'  | 1.70                     | 0.55              |
| 12:CM:68:LEU:HD22 | 12:CM:69:ARG:NH1  | 2.21                     | 0.55              |
| 13:CN:16:ALA:HB2  | 13:CN:59:GLN:NE2  | 2.21                     | 0.55              |
| 19:CT:17:ARG:HG2  | 55:CA:322:C:O3'   | 2.06                     | 0.55              |
| 24:DA:2466:C:OP1  | 54:D4:4:ARG:HB3   | 2.06                     | 0.55              |
| 24:DA:1439:A:N6   | 24:DA:1551:A:N1   | 2.54                     | 0.55              |
| 24:DA:1663:G:C6   | 24:DA:1992:G:N7   | 2.75                     | 0.55              |
| 24:DA:2065:C:N4   | 24:DA:2066:C:N4   | 2.55                     | 0.55              |
| 24:DA:2656:U:HO2' | 24:DA:2657:A:H8   | 1.55                     | 0.55              |
| 24:DA:482:A:C6    | 24:DA:506:G:C4    | 2.95                     | 0.55              |
| 24:DA:511:U:H5''  | 24:DA:1235:G:H4'  | 1.87                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:54:G:C4     | 24:DA:55:G:C8     | 2.95                     | 0.55              |
| 24:DA:76:C:N3     | 24:DA:111:A:C2    | 2.74                     | 0.55              |
| 24:DA:828:U:H4'   | 24:DA:831:G:N1    | 2.22                     | 0.55              |
| 56:DB:45:A:HO2'   | 56:DB:46:A:H8     | 1.54                     | 0.55              |
| 31:DH:83:LYS:HE2  | 31:DH:149:GLU:HB3 | 1.88                     | 0.55              |
| 36:DM:133:LYS:NZ  | 36:DM:133:LYS:HB3 | 2.21                     | 0.55              |
| 38:DO:70:ALA:O    | 38:DO:74:VAL:HG23 | 2.07                     | 0.55              |
| 41:DR:2:TYR:CE1   | 41:DR:13:ARG:HD2  | 2.41                     | 0.55              |
| 41:DR:90:ARG:O    | 41:DR:91:GLN:HB3  | 2.06                     | 0.55              |
| 49:DZ:28:LEU:HD23 | 49:DZ:28:LEU:N    | 2.22                     | 0.55              |
| 21:AA:1242:G:O2'  | 21:AA:1243:C:H5'  | 2.06                     | 0.55              |
| 21:AA:1345:U:H4'  | 21:AA:1346:A:O5'  | 2.05                     | 0.55              |
| 21:AA:922:G:N3    | 21:AA:1398:A:H2   | 2.04                     | 0.55              |
| 21:AA:161:A:H2'   | 21:AA:162:A:C8    | 2.41                     | 0.55              |
| 21:AA:235:C:H2'   | 21:AA:236:A:C8    | 2.41                     | 0.55              |
| 21:AA:466:A:C5'   | 21:AA:467:U:OP2   | 2.55                     | 0.55              |
| 21:AA:828:U:H5'   | 21:AA:870:U:O4    | 2.07                     | 0.55              |
| 1:AB:209:VAL:HG23 | 1:AB:210:THR:H    | 1.71                     | 0.55              |
| 3:AD:1:ALA:O      | 3:AD:67:LEU:HD11  | 2.07                     | 0.55              |
| 4:AE:72:ASN:N     | 4:AE:72:ASN:HD22  | 2.04                     | 0.55              |
| 6:AG:65:LEU:HD11  | 6:AG:100:MET:HG2  | 1.86                     | 0.55              |
| 8:AI:75:ALA:HA    | 8:AI:78:ILE:HD12  | 1.88                     | 0.55              |
| 11:AL:23:LEU:O    | 11:AL:25:ALA:N    | 2.40                     | 0.55              |
| 15:AP:51:ARG:HG2  | 15:AP:52:LEU:H    | 1.71                     | 0.55              |
| 51:B1:33:LEU:N    | 51:B1:51:ALA:HB3  | 2.21                     | 0.55              |
| 24:BA:1477:A:H61  | 24:BA:1514:G:H1'  | 1.71                     | 0.55              |
| 24:BA:1805:A:N3   | 26:BC:49:THR:CG2  | 2.70                     | 0.55              |
| 24:BA:2417:C:C2   | 24:BA:2418:A:C8   | 2.94                     | 0.55              |
| 24:BA:324:A:N6    | 24:BA:338:G:H2'   | 2.21                     | 0.55              |
| 24:BA:370:G:C6    | 24:BA:424:G:C8    | 2.94                     | 0.55              |
| 24:BA:77:G:C6     | 24:BA:78:U:C4     | 2.95                     | 0.55              |
| 24:BA:85:G:O6     | 24:BA:98:G:C6     | 2.59                     | 0.55              |
| 24:BA:949:G:N2    | 24:BA:969:G:C4    | 2.75                     | 0.55              |
| 24:BA:983:A:C6    | 24:BA:984:A:C2    | 2.95                     | 0.55              |
| 31:BH:40:THR:O    | 31:BH:42:LYS:N    | 2.35                     | 0.55              |
| 31:BH:78:VAL:HG11 | 31:BH:145:ASN:HB3 | 1.87                     | 0.55              |
| 33:BJ:38:GLY:O    | 33:BJ:40:HIS:N    | 2.39                     | 0.55              |
| 34:BK:69:VAL:O    | 34:BK:76:VAL:HA   | 2.06                     | 0.55              |
| 36:BM:70:ASP:C    | 36:BM:70:ASP:OD1  | 2.45                     | 0.55              |
| 42:BS:9:HIS:H     | 42:BS:102:HIS:CE1 | 2.24                     | 0.55              |
| 24:BA:2386:A:C2   | 46:BW:38:ARG:HD2  | 2.41                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:BW:43:LYS:HE2  | 46:BW:68:PHE:HE1  | 1.71                     | 0.55              |
| 55:CA:1067:A:O2'  | 55:CA:1094:G:H3'  | 2.07                     | 0.55              |
| 55:CA:171:A:H2'   | 55:CA:172:A:C8    | 2.41                     | 0.55              |
| 55:CA:832:G:C2    | 55:CA:855:U:C2    | 2.94                     | 0.55              |
| 55:CA:844:G:O6    | 55:CA:847:G:H1'   | 2.07                     | 0.55              |
| 55:CA:914:A:HO2'  | 55:CA:915:A:H8    | 1.53                     | 0.55              |
| 1:CB:95:TRP:HZ3   | 1:CB:170:ILE:HG22 | 1.71                     | 0.55              |
| 2:CC:15:LYS:HG3   | 2:CC:16:PRO:HD2   | 1.88                     | 0.55              |
| 2:CC:19:SER:HB3   | 2:CC:21:TRP:HE1   | 1.71                     | 0.55              |
| 2:CC:25:THR:HB    | 2:CC:26:LYS:NZ    | 2.21                     | 0.55              |
| 11:CL:11:ARG:HD2  | 55:CA:562:U:H1'   | 1.88                     | 0.55              |
| 18:CS:36:ARG:HD3  | 55:CA:1318:A:O2'  | 2.07                     | 0.55              |
| 24:DA:1049:C:O2'  | 24:DA:1050:A:C5'  | 2.54                     | 0.55              |
| 24:DA:1558:C:H1'  | 24:DA:1560:G:C5   | 2.41                     | 0.55              |
| 24:DA:1776:G:N2   | 24:DA:1789:A:H1'  | 2.20                     | 0.55              |
| 24:DA:2447:G:C8   | 24:DA:2500:U:C6   | 2.94                     | 0.55              |
| 24:DA:2616:C:O2'  | 24:DA:2617:U:O4'  | 2.24                     | 0.55              |
| 56:DB:24:G:H5'    | 56:DB:25:U:H5     | 1.71                     | 0.55              |
| 33:DJ:80:HIS:HB3  | 33:DJ:81:ILE:HG13 | 1.87                     | 0.55              |
| 56:DB:76:G:H21    | 45:DV:78:GLN:HE22 | 1.53                     | 0.55              |
| 21:AA:329:A:C8    | 21:AA:332:G:C6    | 2.94                     | 0.55              |
| 21:AA:35:G:H2'    | 21:AA:36:C:H6     | 1.72                     | 0.55              |
| 21:AA:461:A:H3'   | 21:AA:461:A:N3    | 2.22                     | 0.55              |
| 4:AE:33:THR:HG22  | 4:AE:51:LYS:HE2   | 1.87                     | 0.55              |
| 7:AH:8:ASP:O      | 7:AH:12:ARG:HB2   | 2.07                     | 0.55              |
| 24:BA:1797:G:C6   | 24:BA:1798:U:C4   | 2.94                     | 0.55              |
| 24:BA:1812:U:H2'  | 24:BA:1813:G:H8   | 1.70                     | 0.55              |
| 24:BA:2037:A:C2   | 24:BA:2038:G:C4   | 2.94                     | 0.55              |
| 24:BA:2251:G:H2'  | 24:BA:2252:G:H8   | 1.67                     | 0.55              |
| 24:BA:60:G:O2'    | 24:BA:61:C:P      | 2.64                     | 0.55              |
| 26:BC:171:VAL:CG2 | 26:BC:185:ALA:HA  | 2.37                     | 0.55              |
| 30:BG:61:TRP:CE3  | 30:BG:61:TRP:HA   | 2.40                     | 0.55              |
| 24:BA:1059:G:H2'  | 32:BI:131:THR:OG1 | 2.06                     | 0.55              |
| 46:BW:39:GLN:HG2  | 46:BW:41:GLY:N    | 2.17                     | 0.55              |
| 55:CA:106:C:H2'   | 55:CA:107:G:O4'   | 2.07                     | 0.55              |
| 55:CA:1245:C:H2'  | 55:CA:1246:A:C8   | 2.41                     | 0.55              |
| 55:CA:93:U:O5'    | 55:CA:93:U:H6     | 1.89                     | 0.55              |
| 11:CL:122:LYS:O   | 11:CL:123:ALA:HB3 | 2.07                     | 0.55              |
| 11:CL:23:LEU:HD11 | 11:CL:94:TYR:CE1  | 2.42                     | 0.55              |
| 19:CT:32:LYS:HA   | 19:CT:35:TYR:HB3  | 1.89                     | 0.55              |
| 24:DA:1098:A:H3'  | 24:DA:1099:G:H8   | 1.71                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:1238:G:N3   | 24:DA:1239:G:C8   | 2.74                     | 0.55              |
| 24:DA:123:G:C2    | 24:DA:124:G:H1'   | 2.41                     | 0.55              |
| 24:DA:1333:G:O2'  | 24:DA:1334:G:H5'  | 2.06                     | 0.55              |
| 24:DA:1668:A:N6   | 24:DA:1676:A:H61  | 2.04                     | 0.55              |
| 24:DA:1788:C:H2'  | 24:DA:1789:A:H8   | 1.71                     | 0.55              |
| 24:DA:52:A:H2     | 24:DA:179:C:O4'   | 1.90                     | 0.55              |
| 24:DA:605:G:H2'   | 24:DA:606:U:H6    | 1.71                     | 0.55              |
| 24:DA:752:A:HO2'  | 24:DA:753:A:P     | 2.30                     | 0.55              |
| 24:DA:672:C:C2    | 24:DA:809:G:N2    | 2.75                     | 0.55              |
| 24:DA:825:A:C2    | 24:DA:826:U:C2    | 2.94                     | 0.55              |
| 26:DC:146:LYS:O   | 26:DC:148:GLY:N   | 2.39                     | 0.55              |
| 27:DD:148:GLN:HG2 | 27:DD:152:PRO:HG2 | 1.86                     | 0.55              |
| 28:DE:6:LYS:HE3   | 28:DE:7:ASP:OD2   | 2.07                     | 0.55              |
| 31:DH:8:LYS:C     | 31:DH:8:LYS:HD2   | 2.26                     | 0.55              |
| 35:DL:23:ILE:HD13 | 41:DR:84:ARG:CZ   | 2.36                     | 0.55              |
| 43:DT:4:GLU:HG3   | 43:DT:6:ARG:NH2   | 2.22                     | 0.55              |
| 1:AB:40:ILE:HG21  | 1:AB:201:GLY:CA   | 2.36                     | 0.55              |
| 5:AF:18:VAL:HB    | 5:AF:19:PRO:CD    | 2.36                     | 0.55              |
| 6:AG:75:LYS:HE3   | 21:AA:1378:C:O2   | 2.07                     | 0.55              |
| 8:AI:40:ARG:CA    | 8:AI:44:ARG:HB3   | 2.37                     | 0.55              |
| 20:AU:36:PHE:HD1  | 20:AU:39:LYS:HB3  | 1.70                     | 0.55              |
| 53:B3:56:LEU:H    | 53:B3:56:LEU:CD2  | 2.19                     | 0.55              |
| 24:BA:1649:G:C6   | 24:BA:2009:A:C6   | 2.94                     | 0.55              |
| 24:BA:1716:U:O2'  | 24:BA:1717:A:H5'  | 2.07                     | 0.55              |
| 24:BA:1747:U:O2'  | 24:BA:1748:C:H5'  | 2.06                     | 0.55              |
| 24:BA:1764:C:O2'  | 24:BA:1765:U:H5'  | 2.07                     | 0.55              |
| 24:BA:1915:U:H2'  | 24:BA:1916:A:C8   | 2.42                     | 0.55              |
| 24:BA:2328:A:H2'  | 24:BA:2329:U:H6   | 1.71                     | 0.55              |
| 24:BA:2484:G:C2   | 24:BA:2485:G:C8   | 2.94                     | 0.55              |
| 24:BA:2492:U:H2'  | 24:BA:2493:U:H6   | 1.70                     | 0.55              |
| 24:BA:432:A:C5    | 24:BA:433:C:C5    | 2.94                     | 0.55              |
| 24:BA:469:G:O6    | 52:B2:39:ARG:NH1  | 2.39                     | 0.55              |
| 25:BB:46:A:H2'    | 25:BB:47:C:O4'    | 2.06                     | 0.55              |
| 26:BC:90:ILE:CG2  | 26:BC:102:TYR:CD1 | 2.90                     | 0.55              |
| 29:BF:134:GLN:CG  | 29:BF:135:ILE:H   | 2.04                     | 0.55              |
| 29:BF:129:MET:HG3 | 29:BF:153:ILE:CD1 | 2.37                     | 0.55              |
| 34:BK:76:VAL:HB   | 39:BP:72:VAL:CG2  | 2.36                     | 0.55              |
| 24:BA:2330:G:H21  | 46:BW:38:ARG:HA   | 1.71                     | 0.55              |
| 48:BY:18:LEU:HD13 | 48:BY:18:LEU:O    | 2.07                     | 0.55              |
| 55:CA:1124:G:O2'  | 55:CA:1127:G:O6   | 2.18                     | 0.55              |
| 55:CA:55:A:H2'    | 55:CA:56:U:H5'    | 1.88                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:CA:78:A:H2'    | 55:CA:79:G:H8      | 1.70                     | 0.55              |
| 12:CM:90:HIS:HA   | 12:CM:108:ARG:NH2  | 2.22                     | 0.55              |
| 24:DA:1035:U:H2'  | 24:DA:1036:G:C8    | 2.42                     | 0.55              |
| 24:DA:1249:U:H4'  | 40:DQ:3:VAL:HG21   | 1.87                     | 0.55              |
| 24:DA:1352:U:H5   | 24:DA:1377:G:C6    | 2.24                     | 0.55              |
| 24:DA:2902:C:H6   | 24:DA:2902:C:OP2   | 1.90                     | 0.55              |
| 24:DA:553:G:H2'   | 24:DA:554:U:O4'    | 2.07                     | 0.55              |
| 24:DA:815:C:P     | 41:DR:85:LYS:HE2   | 2.46                     | 0.55              |
| 26:DC:158:GLY:N   | 26:DC:194:VAL:HG13 | 2.20                     | 0.55              |
| 29:DF:129:MET:HG3 | 29:DF:153:ILE:HD12 | 1.88                     | 0.55              |
| 29:DF:66:ILE:HG13 | 29:DF:83:PRO:HB3   | 1.89                     | 0.55              |
| 31:DH:50:ARG:CZ   | 31:DH:50:ARG:HB2   | 2.30                     | 0.55              |
| 33:DJ:4:PHE:O     | 33:DJ:44:TYR:CZ    | 2.60                     | 0.55              |
| 42:DS:84:ARG:HB3  | 42:DS:96:ILE:HG23  | 1.87                     | 0.55              |
| 47:DX:36:ARG:HG2  | 47:DX:47:THR:HB    | 1.88                     | 0.55              |
| 21:AA:1006:G:H2'  | 21:AA:1007:U:O4'   | 2.07                     | 0.55              |
| 8:AI:105:ARG:NE   | 21:AA:1117:A:O3'   | 2.39                     | 0.55              |
| 21:AA:1237:C:OP1  | 21:AA:1238:A:H1'   | 2.07                     | 0.55              |
| 21:AA:1422:G:C2   | 21:AA:1423:G:C8    | 2.95                     | 0.55              |
| 21:AA:317:U:C2    | 21:AA:337:G:N2     | 2.74                     | 0.55              |
| 3:AD:8:LEU:HB2    | 21:AA:430:A:OP1    | 2.07                     | 0.55              |
| 21:AA:78:A:N6     | 21:AA:79:G:N1      | 2.54                     | 0.55              |
| 21:AA:914:A:C2'   | 21:AA:915:A:H8     | 2.19                     | 0.55              |
| 1:AB:51:GLU:CD    | 1:AB:197:PHE:HE1   | 2.10                     | 0.55              |
| 2:AC:10:ARG:O     | 2:AC:11:LEU:C      | 2.46                     | 0.55              |
| 9:AJ:15:HIS:O     | 9:AJ:18:ILE:HG22   | 2.06                     | 0.55              |
| 14:AO:27:GLN:O    | 14:AO:30:LEU:HB2   | 2.06                     | 0.55              |
| 24:BA:1017:G:C5   | 24:BA:1018:U:C5    | 2.95                     | 0.55              |
| 24:BA:1220:G:H2'  | 24:BA:1221:C:O4'   | 2.07                     | 0.55              |
| 24:BA:121:G:HO2'  | 24:BA:122:G:H8     | 1.51                     | 0.55              |
| 24:BA:1385:A:C6   | 24:BA:1403:A:C5    | 2.95                     | 0.55              |
| 24:BA:1456:G:C2'  | 24:BA:1457:U:H5'   | 2.36                     | 0.55              |
| 24:BA:324:A:H61   | 24:BA:338:G:H2'    | 1.72                     | 0.55              |
| 24:BA:60:G:C2     | 24:BA:74:A:C2      | 2.95                     | 0.55              |
| 27:BD:151:THR:CB  | 27:BD:152:PRO:HD3  | 2.37                     | 0.55              |
| 32:BI:104:GLN:O   | 32:BI:105:LEU:CB   | 2.55                     | 0.55              |
| 41:BR:39:LEU:HA   | 41:BR:49:ILE:HG21  | 1.88                     | 0.55              |
| 46:BW:40:ARG:HD3  | 46:BW:45:HIS:CE1   | 2.42                     | 0.55              |
| 55:CA:1124:G:O2'  | 55:CA:1125:U:C5    | 2.59                     | 0.55              |
| 55:CA:1160:G:O6   | 55:CA:1181:G:C6    | 2.60                     | 0.55              |
| 55:CA:812:G:H2'   | 55:CA:812:G:N3     | 2.21                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CB:92:ASN:H     | 1:CB:92:ASN:ND2    | 2.04                     | 0.55              |
| 5:CF:27:ALA:O     | 5:CF:31:GLY:HA3    | 2.06                     | 0.55              |
| 6:CG:69:ARG:HD3   | 6:CG:70:PRO:HD2    | 1.89                     | 0.55              |
| 7:CH:77:VAL:HG12  | 7:CH:84:ILE:HG13   | 1.87                     | 0.55              |
| 13:CN:66:THR:HG23 | 13:CN:82:LYS:HE3   | 1.88                     | 0.55              |
| 14:CO:24:THR:HG21 | 14:CO:69:LEU:HB2   | 1.88                     | 0.55              |
| 16:CQ:75:VAL:O    | 16:CQ:76:ARG:HB3   | 2.06                     | 0.55              |
| 19:CT:54:GLN:N    | 19:CT:55:PRO:HD2   | 2.22                     | 0.55              |
| 24:DA:999:U:O2'   | 24:DA:1000:A:H5'   | 2.07                     | 0.55              |
| 24:DA:1183:U:H2'  | 24:DA:1184:U:C6    | 2.42                     | 0.55              |
| 24:DA:1286:A:C5   | 24:DA:1289:C:N4    | 2.75                     | 0.55              |
| 24:DA:216:A:O2'   | 24:DA:217:A:O5'    | 2.24                     | 0.55              |
| 24:DA:2276:G:O2'  | 24:DA:2277:G:H5'   | 2.07                     | 0.55              |
| 24:DA:2459:A:H2'  | 24:DA:2460:U:H6    | 1.72                     | 0.55              |
| 24:DA:301:G:C6    | 24:DA:302:C:N4     | 2.75                     | 0.55              |
| 24:DA:572:A:H2'   | 24:DA:573:U:O4'    | 2.07                     | 0.55              |
| 24:DA:629:G:H2'   | 24:DA:630:G:C8     | 2.42                     | 0.55              |
| 24:DA:804:A:H2'   | 24:DA:806:C:N4     | 2.22                     | 0.55              |
| 24:DA:804:A:H5''  | 24:DA:805:G:OP1    | 2.07                     | 0.55              |
| 56:DB:86:G:H2'    | 56:DB:87:U:H5''    | 1.89                     | 0.55              |
| 26:DC:255:LYS:C   | 26:DC:256:THR:HG23 | 2.27                     | 0.55              |
| 27:DD:38:LYS:HB3  | 27:DD:38:LYS:NZ    | 2.21                     | 0.55              |
| 28:DE:129:PRO:HD3 | 28:DE:156:ASN:OD1  | 2.07                     | 0.55              |
| 28:DE:79:ARG:CG   | 28:DE:80:SER:H     | 2.19                     | 0.55              |
| 30:DG:43:LYS:O    | 30:DG:49:LEU:HD12  | 2.07                     | 0.55              |
| 30:DG:84:LYS:HB2  | 30:DG:132:LEU:H    | 1.72                     | 0.55              |
| 38:DO:23:ALA:O    | 38:DO:42:PRO:HG3   | 2.06                     | 0.55              |
| 39:DP:91:VAL:HG21 | 39:DP:96:LEU:HD21  | 1.89                     | 0.55              |
| 44:DU:95:PHE:N    | 44:DU:95:PHE:CD1   | 2.74                     | 0.55              |
| 46:DW:18:LYS:H    | 46:DW:36:ILE:CG1   | 2.20                     | 0.55              |
| 21:AA:1101:A:O2'  | 21:AA:1102:A:C8    | 2.59                     | 0.55              |
| 21:AA:266:G:O2'   | 21:AA:267:C:O5'    | 2.25                     | 0.55              |
| 3:AD:109:THR:HG21 | 21:AA:408:A:P      | 2.47                     | 0.55              |
| 21:AA:950:U:H2'   | 21:AA:951:G:C8     | 2.42                     | 0.55              |
| 8:AI:129:ARG:HH22 | 21:AA:967:C:C1'    | 2.20                     | 0.55              |
| 9:AJ:35:GLN:HG2   | 9:AJ:77:VAL:HB     | 1.89                     | 0.55              |
| 11:AL:6:LEU:HD21  | 11:AL:11:ARG:HE    | 1.72                     | 0.55              |
| 52:B2:42:LEU:H    | 52:B2:42:LEU:HD22  | 1.70                     | 0.55              |
| 24:BA:1124:G:H1'  | 54:B4:38:GLY:OXT   | 2.06                     | 0.55              |
| 24:BA:1641:A:N6   | 24:BA:1642:G:C2    | 2.74                     | 0.55              |
| 24:BA:1647:U:H3'  | 24:BA:1647:U:P     | 2.46                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:2093:G:N7   | 24:BA:2225:A:H2'  | 2.21                     | 0.55              |
| 24:BA:229:C:C5    | 24:BA:230:G:C8    | 2.95                     | 0.55              |
| 24:BA:10:A:C5     | 24:BA:2800:A:C6   | 2.95                     | 0.55              |
| 24:BA:2896:C:O2'  | 24:BA:2897:U:H5'  | 2.07                     | 0.55              |
| 24:BA:88:G:C6     | 24:BA:89:A:N7     | 2.75                     | 0.55              |
| 24:BA:2222:C:H4'  | 26:BC:184:GLU:OE1 | 2.07                     | 0.55              |
| 33:BJ:25:LEU:HB2  | 33:BJ:62:VAL:HG22 | 1.89                     | 0.55              |
| 34:BK:18:ARG:N    | 34:BK:45:GLU:HB2  | 2.21                     | 0.55              |
| 40:BQ:96:ASP:C    | 40:BQ:98:ALA:H    | 2.10                     | 0.55              |
| 45:BV:40:ILE:HG22 | 45:BV:41:GLU:H    | 1.71                     | 0.55              |
| 46:BW:42:THR:O    | 46:BW:43:LYS:HD3  | 2.07                     | 0.55              |
| 55:CA:1026:G:H22  | 55:CA:1036:A:H61  | 1.52                     | 0.55              |
| 55:CA:1043:G:O6   | 55:CA:1044:A:N6   | 2.40                     | 0.55              |
| 55:CA:1136:C:C5   | 55:CA:1138:G:O6   | 2.59                     | 0.55              |
| 55:CA:315:A:H5''  | 55:CA:317:U:OP2   | 2.07                     | 0.55              |
| 55:CA:908:A:H2'   | 55:CA:909:A:C8    | 2.42                     | 0.55              |
| 55:CA:976:G:O5'   | 55:CA:1358:U:O2'  | 2.25                     | 0.55              |
| 2:CC:156:LEU:C    | 2:CC:158:GLY:H    | 2.10                     | 0.55              |
| 9:CJ:80:THR:O     | 9:CJ:84:VAL:HG22  | 2.06                     | 0.55              |
| 12:CM:2:ARG:N     | 12:CM:2:ARG:CD    | 2.59                     | 0.55              |
| 24:DA:2350:C:H5   | 53:D3:41:ARG:CZ   | 2.20                     | 0.55              |
| 24:DA:1079:C:N4   | 24:DA:1088:A:C2   | 2.75                     | 0.55              |
| 24:DA:1838:C:C6   | 24:DA:1899:A:C6   | 2.95                     | 0.55              |
| 24:DA:2278:A:H2'  | 24:DA:2279:G:H5'' | 1.89                     | 0.55              |
| 24:DA:2539:C:C4   | 24:DA:2540:C:C5   | 2.94                     | 0.55              |
| 24:DA:2770:G:C8   | 24:DA:2770:G:O5'  | 2.60                     | 0.55              |
| 24:DA:364:C:H2'   | 24:DA:365:U:C5    | 2.41                     | 0.55              |
| 30:DG:115:GLN:HG2 | 30:DG:116:LEU:H   | 1.70                     | 0.55              |
| 24:DA:2751:G:H4'  | 30:DG:3:VAL:HG11  | 1.87                     | 0.55              |
| 37:DN:24:MET:HG2  | 37:DN:44:LEU:HD22 | 1.87                     | 0.55              |
| 43:DT:68:LYS:O    | 43:DT:74:ILE:HG13 | 2.05                     | 0.55              |
| 45:DV:30:ILE:HG12 | 45:DV:91:PHE:HB2  | 1.89                     | 0.55              |
| 45:DV:82:TYR:CE1  | 45:DV:83:LYS:HG2  | 2.41                     | 0.55              |
| 21:AA:1117:A:C6   | 21:AA:1184:G:O6   | 2.59                     | 0.55              |
| 21:AA:113:G:H2'   | 21:AA:114:U:H6    | 1.72                     | 0.55              |
| 21:AA:597:G:C5    | 21:AA:598:U:C5    | 2.95                     | 0.55              |
| 1:AB:20:ARG:CZ    | 1:AB:20:ARG:HA    | 2.36                     | 0.55              |
| 2:AC:34:SER:O     | 2:AC:38:VAL:HG13  | 2.07                     | 0.55              |
| 6:AG:86:VAL:HG22  | 6:AG:150:PHE:HB3  | 1.89                     | 0.55              |
| 11:AL:45:ASN:HA   | 21:AA:529:G:O6    | 2.07                     | 0.55              |
| 22:AX:30:G:O2'    | 22:AX:31:A:H5'    | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:1115:G:O2'  | 24:BA:1116:G:O5'  | 2.23                     | 0.55              |
| 24:BA:1495:A:O2'  | 24:BA:1496:A:C8   | 2.58                     | 0.55              |
| 24:BA:1847:A:H2'  | 24:BA:1848:A:H8   | 1.72                     | 0.55              |
| 24:BA:195:A:C6    | 24:BA:198:C:C5    | 2.95                     | 0.55              |
| 24:BA:2063:C:O2   | 24:BA:2450:A:N1   | 2.40                     | 0.55              |
| 24:BA:2209:G:C5   | 24:BA:2210:U:C4   | 2.95                     | 0.55              |
| 24:BA:2680:U:OP1  | 27:BD:114:LYS:HE2 | 2.07                     | 0.55              |
| 24:BA:515:A:C8    | 24:BA:516:C:C5    | 2.95                     | 0.55              |
| 24:BA:639:U:C2    | 24:BA:640:C:C5    | 2.95                     | 0.55              |
| 27:BD:120:GLY:HA2 | 27:BD:162:ALA:CB  | 2.36                     | 0.55              |
| 27:BD:97:SER:H    | 27:BD:99:GLU:CD   | 2.10                     | 0.55              |
| 29:BF:68:LYS:HA   | 29:BF:83:PRO:HA   | 1.89                     | 0.55              |
| 30:BG:32:LEU:O    | 30:BG:33:THR:HG23 | 2.07                     | 0.55              |
| 36:BM:42:THR:O    | 36:BM:43:ALA:HB3  | 2.06                     | 0.55              |
| 40:BQ:86:SER:HB3  | 41:BR:51:VAL:HG12 | 1.89                     | 0.55              |
| 40:BQ:91:ARG:CZ   | 41:BR:11:GLN:H    | 2.20                     | 0.55              |
| 46:BW:40:ARG:HH11 | 46:BW:45:HIS:CE1  | 2.25                     | 0.55              |
| 55:CA:1287:A:O2'  | 55:CA:1288:A:C8   | 2.55                     | 0.55              |
| 55:CA:942:G:C2    | 55:CA:1342:C:C2   | 2.95                     | 0.55              |
| 55:CA:229:U:H2'   | 55:CA:230:G:O4'   | 2.06                     | 0.55              |
| 55:CA:860:A:H2'   | 55:CA:861:G:O4'   | 2.05                     | 0.55              |
| 2:CC:61:LYS:O     | 2:CC:97:PRO:HD2   | 2.06                     | 0.55              |
| 5:CF:68:GLN:HG2   | 5:CF:69:GLU:N     | 2.22                     | 0.55              |
| 6:CG:134:VAL:HB   | 6:CG:137:ARG:HH21 | 1.72                     | 0.55              |
| 19:CT:30:PHE:CE2  | 19:CT:52:GLU:HG2  | 2.41                     | 0.55              |
| 24:DA:1010:A:OP1  | 40:DQ:61:ILE:HG22 | 2.07                     | 0.55              |
| 24:DA:2240:U:O2'  | 24:DA:2241:A:O5'  | 2.25                     | 0.55              |
| 24:DA:2287:A:O2'  | 24:DA:2288:A:O5'  | 2.20                     | 0.55              |
| 24:DA:241:A:H4'   | 24:DA:242:G:OP1   | 2.07                     | 0.55              |
| 24:DA:2611:C:O2'  | 24:DA:2612:C:C5'  | 2.55                     | 0.55              |
| 24:DA:2868:A:O2'  | 24:DA:2869:G:H5'  | 2.07                     | 0.55              |
| 26:DC:106:PRO:HB3 | 26:DC:141:HIS:CE1 | 2.41                     | 0.55              |
| 26:DC:140:VAL:CG2 | 26:DC:161:VAL:HB  | 2.37                     | 0.55              |
| 26:DC:245:THR:C   | 26:DC:247:TRP:H   | 2.11                     | 0.55              |
| 30:DG:106:LEU:HB2 | 30:DG:108:PHE:CE1 | 2.42                     | 0.55              |
| 24:DA:2751:G:H4'  | 30:DG:3:VAL:CG1   | 2.36                     | 0.55              |
| 33:DJ:45:THR:H    | 33:DJ:46:PRO:HD3  | 1.71                     | 0.55              |
| 34:DK:87:LEU:HD23 | 34:DK:87:LEU:H    | 1.71                     | 0.55              |
| 37:DN:71:ARG:HB2  | 37:DN:71:ARG:NH2  | 2.21                     | 0.55              |
| 56:DB:50:A:H5''   | 38:DO:67:ASN:OD1  | 2.07                     | 0.55              |
| 24:DA:1251:C:C6   | 40:DQ:5:ARG:NH1   | 2.75                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:DT:55:VAL:HG21 | 43:DT:85:VAL:O    | 2.07                     | 0.55              |
| 2:AC:177:LEU:HD23 | 21:AA:1112:C:N4   | 2.22                     | 0.54              |
| 21:AA:115:G:C2    | 21:AA:313:A:C2    | 2.95                     | 0.54              |
| 21:AA:1322:C:O2'  | 21:AA:1323:G:C5'  | 2.53                     | 0.54              |
| 21:AA:181:A:H5''  | 21:AA:182:A:OP1   | 2.07                     | 0.54              |
| 16:AQ:15:LYS:HE2  | 21:AA:274:A:H5'   | 1.88                     | 0.54              |
| 21:AA:519:C:O2'   | 21:AA:520:A:H5'   | 2.07                     | 0.54              |
| 1:AB:24:PRO:C     | 1:AB:26:MET:H     | 2.10                     | 0.54              |
| 1:AB:95:TRP:CH2   | 1:AB:99:MET:HG2   | 2.42                     | 0.54              |
| 2:AC:52:SER:HB2   | 2:AC:111:ASP:OD2  | 2.07                     | 0.54              |
| 5:AF:6:ILE:HB     | 5:AF:62:MET:CB    | 2.37                     | 0.54              |
| 6:AG:99:ALA:HA    | 6:AG:102:TRP:CE3  | 2.41                     | 0.54              |
| 14:AO:69:LEU:HD21 | 14:AO:76:ARG:HB2  | 1.89                     | 0.54              |
| 24:BA:1045:C:H1'  | 24:BA:1047:G:C2   | 2.41                     | 0.54              |
| 24:BA:1073:A:C3'  | 24:BA:1074:G:C5'  | 2.80                     | 0.54              |
| 24:BA:1079:C:C4   | 24:BA:1088:A:C2   | 2.95                     | 0.54              |
| 24:BA:1300:G:H5'' | 24:BA:1301:A:H5'' | 1.89                     | 0.54              |
| 24:BA:1730:C:H2'  | 24:BA:1731:G:H5'' | 1.89                     | 0.54              |
| 24:BA:1784:A:H4'  | 24:BA:1785:A:C5'  | 2.37                     | 0.54              |
| 24:BA:1667:G:O2'  | 24:BA:1991:U:O4   | 2.24                     | 0.54              |
| 24:BA:2025:C:H2'  | 24:BA:2026:U:C6   | 2.41                     | 0.54              |
| 24:BA:2144:G:H3'  | 24:BA:2144:G:N3   | 2.21                     | 0.54              |
| 24:BA:470:A:H61   | 43:BT:72:GLN:NE2  | 2.04                     | 0.54              |
| 25:BB:74:U:O2     | 45:BV:29:ILE:HD12 | 2.07                     | 0.54              |
| 26:BC:199:HIS:O   | 26:BC:202:ARG:HG3 | 2.07                     | 0.54              |
| 27:BD:14:ILE:O    | 27:BD:14:ILE:CG1  | 2.55                     | 0.54              |
| 28:BE:1:MET:CG    | 28:BE:14:VAL:HG23 | 2.36                     | 0.54              |
| 31:BH:131:SER:HB2 | 31:BH:139:PHE:HD2 | 1.72                     | 0.54              |
| 34:BK:2:ILE:HG21  | 34:BK:39:ILE:HD12 | 1.90                     | 0.54              |
| 36:BM:71:LYS:HD3  | 36:BM:95:LEU:CD1  | 2.37                     | 0.54              |
| 45:BV:51:GLN:NE2  | 45:BV:51:GLN:O    | 2.40                     | 0.54              |
| 49:BZ:39:ASP:CG   | 49:BZ:44:ARG:HH11 | 2.11                     | 0.54              |
| 55:CA:51:A:O2'    | 55:CA:116:A:H4'   | 2.07                     | 0.54              |
| 55:CA:1493:A:H2   | 22:CX:36:A:N3     | 2.05                     | 0.54              |
| 55:CA:330:C:H2'   | 55:CA:331:G:C8    | 2.42                     | 0.54              |
| 55:CA:436:C:N3    | 55:CA:437:U:C5    | 2.75                     | 0.54              |
| 55:CA:988:G:H2'   | 55:CA:989:U:O4'   | 2.07                     | 0.54              |
| 55:CA:9:G:N3      | 55:CA:10:A:C8     | 2.74                     | 0.54              |
| 2:CC:75:VAL:HG12  | 2:CC:83:VAL:HG12  | 1.89                     | 0.54              |
| 5:CF:6:ILE:HG12   | 5:CF:74:LEU:HD23  | 1.89                     | 0.54              |
| 13:CN:20:PHE:CE1  | 13:CN:54:SER:HB2  | 2.42                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:100:U:HO2'  | 24:DA:101:A:C5'   | 2.21                     | 0.54              |
| 24:DA:1074:G:OP2  | 24:DA:1074:G:H8   | 1.90                     | 0.54              |
| 24:DA:1276:A:C2   | 24:DA:1277:G:C5   | 2.95                     | 0.54              |
| 24:DA:1455:G:H2'  | 24:DA:1456:G:H8   | 1.72                     | 0.54              |
| 24:DA:2079:U:H2'  | 24:DA:2080:A:C8   | 2.42                     | 0.54              |
| 24:DA:2346:A:H3'  | 24:DA:2347:C:H5'' | 1.88                     | 0.54              |
| 24:DA:241:A:H1'   | 24:DA:243:U:C4    | 2.42                     | 0.54              |
| 24:DA:9:G:N1      | 24:DA:2629:U:H2'  | 2.19                     | 0.54              |
| 24:DA:324:A:N6    | 24:DA:338:G:H2'   | 2.22                     | 0.54              |
| 24:DA:807:U:O4'   | 24:DA:2445:G:H5'  | 2.08                     | 0.54              |
| 24:DA:874:G:C2    | 24:DA:904:G:C2    | 2.95                     | 0.54              |
| 35:DL:33:ARG:HD3  | 35:DL:40:SER:HA   | 1.87                     | 0.54              |
| 33:DJ:3:THR:HG21  | 40:DQ:60:TRP:HE1  | 1.72                     | 0.54              |
| 21:AA:1143:G:H2'  | 21:AA:1144:G:H8   | 1.73                     | 0.54              |
| 21:AA:250:A:H4'   | 21:AA:251:G:O5'   | 2.08                     | 0.54              |
| 21:AA:368:U:H3'   | 21:AA:369:G:H5'   | 1.89                     | 0.54              |
| 21:AA:84:U:O2     | 21:AA:84:U:H2'    | 2.07                     | 0.54              |
| 1:AB:160:LEU:C    | 1:AB:182:VAL:HG13 | 2.28                     | 0.54              |
| 3:AD:11:SER:OG    | 3:AD:17:ASP:HA    | 2.07                     | 0.54              |
| 8:AI:17:ARG:HH22  | 21:AA:1129:C:H5'' | 1.71                     | 0.54              |
| 10:AK:30:ILE:HD12 | 10:AK:30:ILE:O    | 2.07                     | 0.54              |
| 2:AC:5:HIS:HB3    | 13:AN:88:MET:CE   | 2.37                     | 0.54              |
| 20:AU:52:VAL:HG13 | 20:AU:53:LYS:N    | 2.18                     | 0.54              |
| 51:B1:33:LEU:H    | 51:B1:51:ALA:HB3  | 1.72                     | 0.54              |
| 24:BA:1494:A:H2'  | 24:BA:1495:A:C8   | 2.42                     | 0.54              |
| 24:BA:1522:A:HO2' | 24:BA:1523:U:P    | 2.30                     | 0.54              |
| 24:BA:1274:A:C2   | 24:BA:1645:G:O4'  | 2.60                     | 0.54              |
| 24:BA:1855:U:H2'  | 24:BA:1856:U:O4'  | 2.07                     | 0.54              |
| 24:BA:187:G:C2    | 24:BA:210:C:O2    | 2.61                     | 0.54              |
| 24:BA:2287:A:C5   | 24:BA:2289:G:C8   | 2.96                     | 0.54              |
| 24:BA:2808:G:N2   | 24:BA:2891:U:C6   | 2.76                     | 0.54              |
| 25:BB:29:A:H2'    | 25:BB:30:C:H6     | 1.69                     | 0.54              |
| 25:BB:52:A:N7     | 38:BO:64:TYR:OH   | 2.27                     | 0.54              |
| 32:BI:23:VAL:HG23 | 32:BI:24:GLY:H    | 1.72                     | 0.54              |
| 39:BP:23:ASP:HA   | 39:BP:89:GLY:H    | 1.73                     | 0.54              |
| 48:BY:7:ARG:HG3   | 48:BY:7:ARG:O     | 2.07                     | 0.54              |
| 55:CA:1140:C:H2'  | 55:CA:1141:C:C5   | 2.43                     | 0.54              |
| 55:CA:1401:G:C2   | 55:CA:1402:C:H1'  | 2.42                     | 0.54              |
| 55:CA:1523:G:C5   | 55:CA:1524:C:C5   | 2.95                     | 0.54              |
| 55:CA:815:A:N7    | 55:CA:1509:C:O2'  | 2.26                     | 0.54              |
| 55:CA:825:A:H2'   | 55:CA:826:C:C6    | 2.43                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:914:A:O2'   | 55:CA:915:A:H8    | 1.91                     | 0.54              |
| 7:CH:15:ASN:HD21  | 55:CA:875:U:H1'   | 1.71                     | 0.54              |
| 9:CJ:10:LEU:O     | 9:CJ:18:ILE:HD11  | 2.06                     | 0.54              |
| 9:CJ:57:VAL:HG13  | 9:CJ:58:ASN:N     | 2.23                     | 0.54              |
| 9:CJ:17:LEU:HG    | 9:CJ:96:VAL:HG13  | 1.89                     | 0.54              |
| 24:DA:1032:A:H1'  | 54:D4:23:ILE:HD13 | 1.90                     | 0.54              |
| 24:DA:1114:C:H2'  | 24:DA:1115:G:C8   | 2.41                     | 0.54              |
| 24:DA:1353:A:H2'  | 24:DA:1354:A:C8   | 2.41                     | 0.54              |
| 24:DA:1425:G:H2'  | 24:DA:1426:G:C8   | 2.42                     | 0.54              |
| 24:DA:1431:A:H2'  | 24:DA:1432:G:O4'  | 2.05                     | 0.54              |
| 24:DA:1507:C:H3'  | 24:DA:1508:A:O4'  | 2.05                     | 0.54              |
| 24:DA:1681:G:O2'  | 24:DA:1762:A:H2'  | 2.08                     | 0.54              |
| 24:DA:258:G:H2'   | 24:DA:259:G:H8    | 1.72                     | 0.54              |
| 24:DA:271:G:C6    | 24:DA:272:A:N6    | 2.75                     | 0.54              |
| 24:DA:839:U:H2'   | 24:DA:840:C:C6    | 2.42                     | 0.54              |
| 24:DA:973:A:O4'   | 24:DA:973:A:OP1   | 2.24                     | 0.54              |
| 27:DD:148:GLN:OE1 | 27:DD:152:PRO:HG2 | 2.06                     | 0.54              |
| 36:DM:27:SER:N    | 36:DM:66:ARG:NH2  | 2.43                     | 0.54              |
| 40:DQ:16:ILE:HG23 | 40:DQ:38:VAL:HG21 | 1.89                     | 0.54              |
| 21:AA:1333:A:H2'  | 21:AA:1334:G:O4'  | 2.08                     | 0.54              |
| 21:AA:1413:A:C2   | 21:AA:1488:G:C2   | 2.95                     | 0.54              |
| 21:AA:206:C:C2    | 21:AA:207:C:H1'   | 2.43                     | 0.54              |
| 21:AA:211:G:N2    | 21:AA:212:G:C4    | 2.74                     | 0.54              |
| 21:AA:455:G:H2'   | 21:AA:456:A:C8    | 2.39                     | 0.54              |
| 21:AA:577:G:H4'   | 21:AA:816:A:H2'   | 1.88                     | 0.54              |
| 6:AG:101:ARG:NH2  | 21:AA:939:G:H5'   | 2.21                     | 0.54              |
| 13:AN:14:ALA:O    | 13:AN:18:LYS:HG3  | 2.07                     | 0.54              |
| 24:BA:684:G:OP1   | 52:B2:16:HIS:HD2  | 1.90                     | 0.54              |
| 54:B4:1:MET:CE    | 54:B4:34:LYS:HG2  | 2.37                     | 0.54              |
| 24:BA:1017:G:C6   | 24:BA:1018:U:C5   | 2.95                     | 0.54              |
| 24:BA:1019:U:C4   | 24:BA:1020:A:N6   | 2.75                     | 0.54              |
| 24:BA:1385:A:C6   | 24:BA:1403:A:C6   | 2.96                     | 0.54              |
| 24:BA:1416:G:O2'  | 24:BA:1417:C:O4'  | 2.25                     | 0.54              |
| 24:BA:155:A:H2'   | 24:BA:156:A:C8    | 2.43                     | 0.54              |
| 24:BA:1900:A:C2   | 24:BA:1970:A:C4   | 2.96                     | 0.54              |
| 24:BA:1131:G:N2   | 24:BA:2024:G:H21  | 2.05                     | 0.54              |
| 24:BA:232:G:H4'   | 24:BA:233:A:OP1   | 2.06                     | 0.54              |
| 24:BA:2497:A:H4'  | 24:BA:2498:C:OP1  | 2.06                     | 0.54              |
| 24:BA:685:A:C2    | 24:BA:689:A:C6    | 2.95                     | 0.54              |
| 24:BA:790:U:O2'   | 24:BA:791:C:O5'   | 2.24                     | 0.54              |
| 25:BB:37:C:C5     | 25:BB:38:C:C4     | 2.96                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:BB:45:A:H2'     | 25:BB:46:A:C8     | 2.41                     | 0.54              |
| 26:BC:12:ARG:CG    | 26:BC:12:ARG:NH1  | 2.55                     | 0.54              |
| 33:BJ:81:ILE:CG2   | 33:BJ:82:GLY:H    | 2.05                     | 0.54              |
| 43:BT:28:ASN:HA    | 43:BT:91:GLN:OE1  | 2.07                     | 0.54              |
| 55:CA:1106:G:H2'   | 55:CA:1107:C:C6   | 2.42                     | 0.54              |
| 55:CA:1244:G:C6    | 55:CA:1245:C:N4   | 2.76                     | 0.54              |
| 55:CA:520:A:O2'    | 55:CA:521:G:O5'   | 2.25                     | 0.54              |
| 55:CA:920:U:H2'    | 55:CA:921:U:C6    | 2.42                     | 0.54              |
| 3:CD:10:LEU:HD23   | 3:CD:62:ARG:HB3   | 1.89                     | 0.54              |
| 13:CN:89:ARG:HG3   | 13:CN:91:GLU:HG3  | 1.89                     | 0.54              |
| 24:DA:1213:A:O2'   | 24:DA:1214:A:C5'  | 2.55                     | 0.54              |
| 24:DA:2615:U:C4    | 50:D0:2:VAL:C     | 2.80                     | 0.54              |
| 24:DA:2884:U:O2    | 50:D0:49:ARG:HB3  | 2.08                     | 0.54              |
| 24:DA:2902:C:O2'   | 24:DA:2903:U:O5'  | 2.26                     | 0.54              |
| 24:DA:492:A:H2'    | 24:DA:493:G:O4'   | 2.07                     | 0.54              |
| 24:DA:54:G:C5      | 24:DA:55:G:C8     | 2.96                     | 0.54              |
| 24:DA:969:G:H2'    | 24:DA:970:U:C6    | 2.42                     | 0.54              |
| 30:DG:112:VAL:HG12 | 30:DG:114:HIS:N   | 2.22                     | 0.54              |
| 35:DL:73:ILE:O     | 35:DL:105:ILE:HA  | 2.07                     | 0.54              |
| 24:DA:508:A:N6     | 42:DS:9:HIS:NE2   | 2.56                     | 0.54              |
| 49:DZ:4:ILE:CG2    | 49:DZ:56:VAL:HG13 | 2.37                     | 0.54              |
| 21:AA:1413:A:H2'   | 21:AA:1414:U:O4'  | 2.08                     | 0.54              |
| 21:AA:1416:G:H2'   | 21:AA:1417:G:H5'  | 1.89                     | 0.54              |
| 21:AA:91:U:H2'     | 21:AA:92:U:H1'    | 1.87                     | 0.54              |
| 21:AA:996:A:C4     | 21:AA:997:U:C5    | 2.95                     | 0.54              |
| 3:AD:43:ARG:O      | 3:AD:45:PRO:HD3   | 2.07                     | 0.54              |
| 5:AF:42:TRP:CD1    | 5:AF:42:TRP:N     | 2.74                     | 0.54              |
| 4:AE:155:LYS:HG2   | 7:AH:65:PHE:HB2   | 1.88                     | 0.54              |
| 10:AK:125:LYS:H    | 10:AK:125:LYS:HD3 | 1.72                     | 0.54              |
| 15:AP:33:ILE:HG21  | 15:AP:60:TRP:CZ2  | 2.43                     | 0.54              |
| 51:B1:8:ILE:HG23   | 51:B1:51:ALA:HA   | 1.90                     | 0.54              |
| 24:BA:1298:C:C2    | 24:BA:1643:G:N2   | 2.75                     | 0.54              |
| 24:BA:2210:U:H4'   | 24:BA:2211:A:C5'  | 2.36                     | 0.54              |
| 24:BA:233:A:H61    | 24:BA:428:A:H61   | 1.54                     | 0.54              |
| 24:BA:2289:G:O2'   | 24:BA:2346:A:OP2  | 2.25                     | 0.54              |
| 24:BA:2720:U:C2    | 24:BA:2872:A:C5   | 2.95                     | 0.54              |
| 24:BA:976:G:C2     | 24:BA:977:G:C5    | 2.96                     | 0.54              |
| 25:BB:61:G:C6      | 25:BB:62:C:C4     | 2.96                     | 0.54              |
| 26:BC:69:ASN:O     | 26:BC:117:SER:OG  | 2.25                     | 0.54              |
| 31:BH:8:LYS:O      | 31:BH:9:VAL:CB    | 2.55                     | 0.54              |
| 36:BM:43:ALA:O     | 36:BM:46:ILE:HG13 | 2.08                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BS:42:LYS:O     | 42:BS:42:LYS:HD3   | 2.07                     | 0.54              |
| 47:BX:73:ARG:HG2   | 47:BX:75:GLU:HG3   | 1.88                     | 0.54              |
| 55:CA:10:A:N6      | 55:CA:25:C:H42     | 2.05                     | 0.54              |
| 55:CA:1411:C:OP2   | 55:CA:1411:C:H6    | 1.90                     | 0.54              |
| 55:CA:248:C:O2'    | 55:CA:249:U:O5'    | 2.24                     | 0.54              |
| 55:CA:373:A:O2'    | 55:CA:374:A:C5'    | 2.54                     | 0.54              |
| 1:CB:161:PHE:CZ    | 1:CB:216:VAL:HG21  | 2.43                     | 0.54              |
| 1:CB:185:ILE:HD12  | 1:CB:202:ASN:H     | 1.72                     | 0.54              |
| 2:CC:9:ILE:HG23    | 2:CC:10:ARG:HG3    | 1.88                     | 0.54              |
| 5:CF:18:VAL:N      | 5:CF:19:PRO:HD2    | 2.23                     | 0.54              |
| 11:CL:23:LEU:HD11  | 11:CL:94:TYR:HE1   | 1.71                     | 0.54              |
| 13:CN:96:LYS:HD2   | 13:CN:96:LYS:H     | 1.73                     | 0.54              |
| 20:CU:3:ILE:O      | 20:CU:3:ILE:HG23   | 2.08                     | 0.54              |
| 22:CV:33:U:H5'     | 22:CV:34:G:OP2     | 2.07                     | 0.54              |
| 24:DA:1527:G:H5''  | 24:DA:1528:A:OP1   | 2.07                     | 0.54              |
| 24:DA:161:A:C5     | 24:DA:162:U:C4     | 2.96                     | 0.54              |
| 24:DA:1665:A:H2'   | 24:DA:1666:G:O4'   | 2.08                     | 0.54              |
| 24:DA:2052:A:N7    | 27:DD:146:ILE:HD11 | 2.22                     | 0.54              |
| 24:DA:2304:G:H22   | 24:DA:2312:U:H3    | 1.54                     | 0.54              |
| 24:DA:657:U:O2'    | 24:DA:658:U:C6     | 2.57                     | 0.54              |
| 24:DA:664:G:H2'    | 24:DA:665:U:O4'    | 2.07                     | 0.54              |
| 26:DC:239:PHE:HD1  | 26:DC:240:GLY:H    | 1.55                     | 0.54              |
| 27:DD:133:THR:HG23 | 27:DD:134:HIS:N    | 2.23                     | 0.54              |
| 28:DE:112:LEU:HD11 | 28:DE:186:VAL:HG11 | 1.89                     | 0.54              |
| 28:DE:149:ILE:HG23 | 28:DE:188:MET:N    | 2.21                     | 0.54              |
| 29:DF:109:ARG:NH1  | 29:DF:135:ILE:HG22 | 2.23                     | 0.54              |
| 31:DH:7:ASP:O      | 31:DH:15:LEU:HA    | 2.08                     | 0.54              |
| 32:DI:90:GLY:O     | 32:DI:92:PRO:HD3   | 2.07                     | 0.54              |
| 34:DK:7:MET:HG3    | 34:DK:17:ARG:HH12  | 1.71                     | 0.54              |
| 38:DO:30:ARG:HA    | 38:DO:35:ILE:HD13  | 1.87                     | 0.54              |
| 42:DS:49:LYS:HB3   | 42:DS:49:LYS:NZ    | 2.23                     | 0.54              |
| 21:AA:1202:U:O2'   | 21:AA:1203:C:C5'   | 2.56                     | 0.54              |
| 21:AA:63:C:O2'     | 21:AA:380:G:H4'    | 2.08                     | 0.54              |
| 21:AA:441:A:C2     | 21:AA:497:G:C6     | 2.95                     | 0.54              |
| 21:AA:820:U:H4'    | 21:AA:821:G:OP2    | 2.07                     | 0.54              |
| 1:AB:40:ILE:HG21   | 1:AB:201:GLY:H     | 1.73                     | 0.54              |
| 5:AF:47:LEU:HD22   | 17:AR:65:SER:CB    | 2.37                     | 0.54              |
| 13:AN:14:ALA:HB1   | 13:AN:18:LYS:NZ    | 2.23                     | 0.54              |
| 19:AT:26:MET:SD    | 19:AT:27:MET:N     | 2.81                     | 0.54              |
| 51:B1:46:VAL:HG12  | 51:B1:47:ILE:H     | 1.71                     | 0.54              |
| 24:BA:1088:A:N3    | 24:BA:1088:A:O4'   | 2.39                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:1442:U:H2'   | 24:BA:1443:U:H6    | 1.72                     | 0.54              |
| 24:BA:1759:A:H2'   | 24:BA:1760:C:C6    | 2.42                     | 0.54              |
| 24:BA:151:C:O2     | 24:BA:176:A:C2     | 2.61                     | 0.54              |
| 24:BA:1936:A:H5''  | 24:BA:1937:A:C5'   | 2.36                     | 0.54              |
| 24:BA:215:G:H4'    | 24:BA:216:A:OP1    | 2.07                     | 0.54              |
| 24:BA:2393:U:H2'   | 24:BA:2394:C:H6    | 1.72                     | 0.54              |
| 24:BA:2663:G:H2'   | 24:BA:2664:G:O5'   | 2.08                     | 0.54              |
| 24:BA:769:U:H2'    | 24:BA:770:G:C8     | 2.42                     | 0.54              |
| 24:BA:827:U:C4     | 24:BA:2430:A:C6    | 2.95                     | 0.54              |
| 30:BG:15:ASP:CG    | 30:BG:16:VAL:N     | 2.61                     | 0.54              |
| 35:BL:101:ILE:HG22 | 35:BL:102:GLY:N    | 2.23                     | 0.54              |
| 39:BP:20:ARG:HD2   | 39:BP:112:ARG:HH11 | 1.71                     | 0.54              |
| 24:BA:2331:G:O2'   | 46:BW:39:GLN:O     | 2.19                     | 0.54              |
| 46:BW:46:ALA:HB3   | 46:BW:79:ILE:O     | 2.08                     | 0.54              |
| 48:BY:6:LEU:O      | 48:BY:7:ARG:HB3    | 2.07                     | 0.54              |
| 55:CA:1452:C:H4'   | 55:CA:1453:G:O5'   | 2.06                     | 0.54              |
| 55:CA:370:C:H2'    | 55:CA:371:A:H8     | 1.70                     | 0.54              |
| 55:CA:372:C:O2'    | 55:CA:373:A:OP2    | 2.23                     | 0.54              |
| 7:CH:121:GLY:HA3   | 55:CA:599:C:H4'    | 1.89                     | 0.54              |
| 55:CA:973:G:OP2    | 55:CA:975:A:OP1    | 2.24                     | 0.54              |
| 3:CD:25:ARG:HB3    | 3:CD:30:LYS:NZ     | 2.23                     | 0.54              |
| 8:CI:79:ARG:HD2    | 8:CI:102:PHE:CE1   | 2.43                     | 0.54              |
| 8:CI:9:GLY:HA3     | 8:CI:77:ALA:O      | 2.08                     | 0.54              |
| 10:CK:81:LEU:HD11  | 10:CK:104:PHE:HB3  | 1.90                     | 0.54              |
| 13:CN:80:ARG:HG2   | 13:CN:81:ILE:H     | 1.73                     | 0.54              |
| 19:CT:4:LYS:C      | 19:CT:6:ALA:H      | 2.10                     | 0.54              |
| 24:DA:1022:G:N2    | 24:DA:1142:A:C2    | 2.76                     | 0.54              |
| 24:DA:1474:U:H2'   | 24:DA:1475:G:C5'   | 2.33                     | 0.54              |
| 24:DA:1984:G:C6    | 24:DA:1985:C:C4    | 2.96                     | 0.54              |
| 24:DA:2312:U:OP1   | 24:DA:2312:U:H4'   | 2.08                     | 0.54              |
| 24:DA:2627:G:N3    | 24:DA:2781:A:H2    | 2.05                     | 0.54              |
| 24:DA:310:A:H2'    | 24:DA:312:G:N7     | 2.21                     | 0.54              |
| 24:DA:586:A:O5'    | 24:DA:586:A:H8     | 1.90                     | 0.54              |
| 24:DA:617:G:O2'    | 24:DA:618:G:O4'    | 2.21                     | 0.54              |
| 24:DA:70:G:O2'     | 24:DA:71:A:C5'     | 2.56                     | 0.54              |
| 26:DC:93:VAL:HG12  | 26:DC:101:ARG:H    | 1.72                     | 0.54              |
| 27:DD:181:ASP:C    | 27:DD:183:GLU:H    | 2.10                     | 0.54              |
| 29:DF:32:LYS:HB3   | 29:DF:156:THR:HB   | 1.88                     | 0.54              |
| 36:DM:119:LEU:HD23 | 36:DM:119:LEU:O    | 2.08                     | 0.54              |
| 48:DY:17:GLU:OE1   | 48:DY:53:VAL:HB    | 2.08                     | 0.54              |
| 48:DY:57:LEU:O     | 48:DY:60:LYS:HB3   | 2.07                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 49:DZ:16:LEU:N    | 49:DZ:16:LEU:HD22  | 2.19                     | 0.54              |
| 21:AA:99:C:H2'    | 21:AA:100:G:OP2    | 2.08                     | 0.54              |
| 21:AA:1125:U:HO2' | 21:AA:1126:U:P     | 2.30                     | 0.54              |
| 21:AA:1129:C:H2'  | 21:AA:1139:G:N7    | 2.22                     | 0.54              |
| 21:AA:1305:G:N2   | 21:AA:1332:A:OP2   | 2.40                     | 0.54              |
| 21:AA:1498:U:H5'' | 21:AA:1499:A:OP1   | 2.06                     | 0.54              |
| 10:AK:34:THR:HA   | 10:AK:41:LEU:HG    | 1.90                     | 0.54              |
| 51:B1:46:VAL:HG12 | 51:B1:47:ILE:N     | 2.23                     | 0.54              |
| 24:BA:1380:G:C2   | 24:BA:1381:G:C8    | 2.95                     | 0.54              |
| 24:BA:145:C:H2'   | 24:BA:146:A:H8     | 1.72                     | 0.54              |
| 24:BA:1783:A:H2   | 24:BA:2587:A:C5    | 2.26                     | 0.54              |
| 24:BA:1923:U:H2'  | 24:BA:1924:C:H6    | 1.72                     | 0.54              |
| 24:BA:1905:C:HO2' | 24:BA:1929:G:HO2'  | 1.51                     | 0.54              |
| 24:BA:1950:G:C8   | 24:BA:1951:U:H5    | 2.25                     | 0.54              |
| 24:BA:2144:G:C2'  | 24:BA:2148:G:O6    | 2.54                     | 0.54              |
| 24:BA:243:U:OP1   | 53:B3:5:THR:CG2    | 2.55                     | 0.54              |
| 24:BA:2846:G:OP1  | 39:BP:50:ARG:O     | 2.25                     | 0.54              |
| 24:BA:587:C:H42   | 35:BL:33:ARG:HD3   | 1.72                     | 0.54              |
| 24:BA:776:G:C5    | 24:BA:793:A:C8     | 2.95                     | 0.54              |
| 24:BA:1797:G:O3'  | 26:BC:255:LYS:O    | 2.25                     | 0.54              |
| 28:BE:28:VAL:HA   | 28:BE:104:ALA:HB1  | 1.90                     | 0.54              |
| 29:BF:129:MET:CG  | 29:BF:153:ILE:HD11 | 2.37                     | 0.54              |
| 30:BG:164:ALA:C   | 30:BG:166:GLU:H    | 2.10                     | 0.54              |
| 39:BP:83:ILE:HD13 | 39:BP:84:SER:N     | 2.22                     | 0.54              |
| 42:BS:13:SER:O    | 42:BS:14:ALA:CB    | 2.55                     | 0.54              |
| 43:BT:2:ILE:HG13  | 43:BT:3:ARG:NH2    | 2.22                     | 0.54              |
| 47:BX:34:SER:HA   | 47:BX:48:LEU:O     | 2.06                     | 0.54              |
| 55:CA:1050:G:O2'  | 55:CA:1051:C:H6    | 1.89                     | 0.54              |
| 55:CA:1501:C:N4   | 55:CA:1504:G:C2    | 2.76                     | 0.54              |
| 55:CA:253:A:O2'   | 55:CA:254:G:H8     | 1.89                     | 0.54              |
| 55:CA:555:U:C2    | 55:CA:556:C:C5     | 2.96                     | 0.54              |
| 55:CA:649:A:N3    | 55:CA:650:G:H1'    | 2.23                     | 0.54              |
| 1:CB:128:LEU:HD22 | 1:CB:132:GLU:HG2   | 1.89                     | 0.54              |
| 2:CC:22:PHE:HD1   | 9:CJ:13:PHE:CE1    | 2.25                     | 0.54              |
| 3:CD:2:ARG:NH2    | 3:CD:114:ARG:HH11  | 2.06                     | 0.54              |
| 8:CI:44:ARG:NH1   | 8:CI:44:ARG:HB3    | 2.23                     | 0.54              |
| 10:CK:86:LYS:HE2  | 10:CK:112:VAL:O    | 2.07                     | 0.54              |
| 10:CK:62:ALA:O    | 10:CK:66:ALA:N     | 2.40                     | 0.54              |
| 17:CR:53:GLN:O    | 17:CR:56:ARG:HB2   | 2.07                     | 0.54              |
| 24:DA:466:A:P     | 52:D2:34:ARG:HH21  | 2.31                     | 0.54              |
| 24:DA:1147:A:H2'  | 24:DA:1148:U:C6    | 2.40                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:1353:A:H2'  | 24:DA:1354:A:H8   | 1.73                     | 0.54              |
| 24:DA:287:G:O2'   | 24:DA:288:U:H5'   | 2.08                     | 0.54              |
| 24:DA:53:A:C2     | 52:D2:35:ARG:NH1  | 2.76                     | 0.54              |
| 29:DF:137:PHE:CB  | 29:DF:138:PRO:HD2 | 2.30                     | 0.54              |
| 34:DK:88:ASN:HB2  | 34:DK:91:SER:HB2  | 1.89                     | 0.54              |
| 24:DA:1287:A:OP1  | 37:DN:103:ARG:HG3 | 2.07                     | 0.54              |
| 40:DQ:8:ILE:O     | 40:DQ:8:ILE:HG12  | 2.07                     | 0.54              |
| 45:DV:44:HIS:CD2  | 45:DV:85:LYS:HB2  | 2.42                     | 0.54              |
| 47:DX:6:VAL:HG13  | 47:DX:7:THR:N     | 2.22                     | 0.54              |
| 21:AA:1131:G:C2'  | 21:AA:1132:C:O5'  | 2.56                     | 0.54              |
| 21:AA:844:G:H21   | 21:AA:845:A:H62   | 1.55                     | 0.54              |
| 1:AB:61:SER:O     | 1:AB:224:ARG:HB3  | 2.08                     | 0.54              |
| 4:AE:132:PRO:O    | 4:AE:135:VAL:HG12 | 2.08                     | 0.54              |
| 8:AI:128:LYS:HD2  | 8:AI:129:ARG:H    | 1.73                     | 0.54              |
| 10:AK:22:ILE:CD1  | 10:AK:95:THR:HG21 | 2.37                     | 0.54              |
| 11:AL:114:SER:HB3 | 21:AA:502:A:OP1   | 2.07                     | 0.54              |
| 15:AP:57:ILE:HG22 | 15:AP:58:ALA:N    | 2.22                     | 0.54              |
| 20:AU:4:LYS:O     | 20:AU:4:LYS:HD2   | 2.07                     | 0.54              |
| 24:BA:1179:G:H3'  | 24:BA:1180:U:C4'  | 2.25                     | 0.54              |
| 24:BA:136:G:C6    | 24:BA:142:A:N6    | 2.75                     | 0.54              |
| 24:BA:1555:G:N2   | 24:BA:1556:C:C2   | 2.75                     | 0.54              |
| 24:BA:1779:U:C5   | 24:BA:1783:A:C8   | 2.95                     | 0.54              |
| 24:BA:2018:G:C2   | 24:BA:2019:A:C4   | 2.96                     | 0.54              |
| 24:BA:2109:U:H2'  | 24:BA:2110:G:H5'  | 1.89                     | 0.54              |
| 24:BA:2473:U:O2   | 24:BA:2473:U:H2'  | 2.08                     | 0.54              |
| 24:BA:570:G:OP1   | 24:BA:972:A:O2'   | 2.23                     | 0.54              |
| 24:BA:613:A:H8    | 24:BA:616:A:N1    | 2.05                     | 0.54              |
| 26:BC:5:CYS:SG    | 26:BC:15:VAL:HB   | 2.47                     | 0.54              |
| 24:BA:2091:C:O2   | 47:BX:33:HIS:CE1  | 2.61                     | 0.54              |
| 18:CS:4:LEU:HD11  | 55:CA:1319:A:OP2  | 2.06                     | 0.54              |
| 55:CA:1394:A:C5   | 55:CA:1501:C:H4'  | 2.43                     | 0.54              |
| 55:CA:32:A:N6     | 55:CA:553:A:C6    | 2.76                     | 0.54              |
| 55:CA:501:C:H2'   | 55:CA:502:A:C8    | 2.43                     | 0.54              |
| 55:CA:618:C:C6    | 55:CA:620:C:OP2   | 2.60                     | 0.54              |
| 55:CA:652:U:O2'   | 55:CA:653:U:O5'   | 2.25                     | 0.54              |
| 55:CA:81:A:C2     | 55:CA:89:U:O4     | 2.61                     | 0.54              |
| 1:CB:128:LEU:O    | 1:CB:129:THR:C    | 2.46                     | 0.54              |
| 5:CF:17:GLN:O     | 5:CF:21:MET:HG3   | 2.07                     | 0.54              |
| 15:CP:78:VAL:O    | 15:CP:78:VAL:HG12 | 2.08                     | 0.54              |
| 19:CT:78:LEU:O    | 19:CT:82:ILE:HG12 | 2.07                     | 0.54              |
| 24:DA:1067:A:H2'  | 24:DA:1068:G:H5'' | 1.90                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:1290:C:O2'   | 24:DA:1291:C:O4'   | 2.26                     | 0.54              |
| 24:DA:1590:A:H2'   | 24:DA:1591:A:H8    | 1.73                     | 0.54              |
| 24:DA:2015:A:N1    | 50:D0:2:VAL:HG11   | 2.23                     | 0.54              |
| 24:DA:2783:U:H2'   | 24:DA:2784:U:C6    | 2.42                     | 0.54              |
| 24:DA:2835:A:N7    | 24:DA:2879:A:C2    | 2.76                     | 0.54              |
| 24:DA:449:A:HO2'   | 24:DA:450:G:H5'    | 1.68                     | 0.54              |
| 24:DA:860:U:O2'    | 24:DA:861:A:H5'    | 2.08                     | 0.54              |
| 24:DA:90:U:C4      | 24:DA:91:A:C5      | 2.96                     | 0.54              |
| 26:DC:120:ASP:CG   | 26:DC:121:ALA:H    | 2.11                     | 0.54              |
| 26:DC:259:ASN:C    | 26:DC:261:ARG:H    | 2.11                     | 0.54              |
| 27:DD:51:THR:HG21  | 27:DD:75:ALA:O     | 2.08                     | 0.54              |
| 28:DE:196:VAL:HG13 | 28:DE:200:LEU:HD23 | 1.90                     | 0.54              |
| 30:DG:28:LYS:HG3   | 30:DG:79:THR:HG22  | 1.89                     | 0.54              |
| 33:DJ:106:LYS:HD2  | 33:DJ:119:PHE:CD2  | 2.42                     | 0.54              |
| 34:DK:113:MET:O    | 34:DK:116:ILE:HG13 | 2.08                     | 0.54              |
| 35:DL:48:ARG:HG3   | 35:DL:48:ARG:HH11  | 1.73                     | 0.54              |
| 42:DS:47:VAL:HG12  | 42:DS:103:ILE:HG12 | 1.89                     | 0.54              |
| 43:DT:29:THR:CB    | 43:DT:86:THR:H     | 2.21                     | 0.54              |
| 21:AA:1102:A:H2'   | 21:AA:1103:C:C5    | 2.43                     | 0.54              |
| 21:AA:1125:U:OP2   | 21:AA:1145:A:N6    | 2.41                     | 0.54              |
| 21:AA:1181:G:C2    | 21:AA:1182:G:N2    | 2.76                     | 0.54              |
| 16:AQ:26:ARG:NH2   | 21:AA:237:G:H5''   | 2.22                     | 0.54              |
| 21:AA:430:A:O2'    | 21:AA:431:A:C5'    | 2.49                     | 0.54              |
| 21:AA:780:A:C8     | 21:AA:800:G:C6     | 2.95                     | 0.54              |
| 21:AA:802:A:H3'    | 21:AA:803:G:H8     | 1.72                     | 0.54              |
| 21:AA:87:C:H2'     | 21:AA:88:U:O4'     | 2.07                     | 0.54              |
| 1:AB:67:LEU:HD22   | 1:AB:69:VAL:HG22   | 1.89                     | 0.54              |
| 3:AD:191:SER:O     | 3:AD:192:ALA:HB2   | 2.06                     | 0.54              |
| 4:AE:79:THR:CA     | 4:AE:119:VAL:HG12  | 2.35                     | 0.54              |
| 5:AF:5:GLU:HG3     | 5:AF:63:ASN:OD1    | 2.08                     | 0.54              |
| 12:AM:67:ASP:O     | 12:AM:70:ARG:CB    | 2.53                     | 0.54              |
| 12:AM:84:CYS:O     | 12:AM:88:LEU:HG    | 2.08                     | 0.54              |
| 15:AP:38:PHE:CZ    | 15:AP:51:ARG:HB2   | 2.42                     | 0.54              |
| 15:AP:51:ARG:HG2   | 15:AP:52:LEU:N     | 2.22                     | 0.54              |
| 54:B4:30:GLU:OE2   | 54:B4:32:LYS:HG3   | 2.08                     | 0.54              |
| 24:BA:1062:G:H1'   | 32:BI:134:SER:CB   | 2.33                     | 0.54              |
| 24:BA:1555:G:N1    | 24:BA:1556:C:C4    | 2.76                     | 0.54              |
| 24:BA:1744:A:H3'   | 24:BA:1745:A:H8    | 1.73                     | 0.54              |
| 24:BA:1783:A:H2    | 24:BA:2587:A:C4    | 2.26                     | 0.54              |
| 24:BA:1797:G:O3'   | 26:BC:255:LYS:HA   | 2.08                     | 0.54              |
| 24:BA:2135:A:C2'   | 24:BA:2136:G:C8    | 2.88                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:2100:G:C6   | 24:BA:2190:G:C6    | 2.95                     | 0.54              |
| 24:BA:2320:U:H4'  | 24:BA:2321:U:C5'   | 2.36                     | 0.54              |
| 24:BA:2377:A:H2'  | 24:BA:2378:A:C8    | 2.42                     | 0.54              |
| 24:BA:2657:A:H2'  | 24:BA:2658:C:O4'   | 2.08                     | 0.54              |
| 24:BA:2675:A:C2'  | 24:BA:2676:C:H5'   | 2.37                     | 0.54              |
| 24:BA:265:A:N7    | 24:BA:428:A:N3     | 2.55                     | 0.54              |
| 24:BA:479:A:C2    | 24:BA:480:A:C4     | 2.95                     | 0.54              |
| 24:BA:734:A:N7    | 24:BA:735:A:N7     | 2.56                     | 0.54              |
| 24:BA:743:A:O2'   | 24:BA:744:U:H5'    | 2.08                     | 0.54              |
| 27:BD:143:PRO:O   | 27:BD:144:GLY:O    | 2.26                     | 0.54              |
| 27:BD:90:PHE:HB2  | 27:BD:92:VAL:HG23  | 1.90                     | 0.54              |
| 27:BD:99:GLU:CG   | 27:BD:100:LEU:N    | 2.69                     | 0.54              |
| 30:BG:86:LEU:HD11 | 30:BG:132:LEU:HD21 | 1.90                     | 0.54              |
| 38:BO:75:GLY:HA3  | 38:BO:106:LEU:HA   | 1.89                     | 0.54              |
| 39:BP:4:ILE:O     | 39:BP:6:GLN:N      | 2.41                     | 0.54              |
| 40:BQ:10:ARG:CZ   | 40:BQ:10:ARG:HB2   | 2.38                     | 0.54              |
| 24:BA:1252:G:C2   | 40:BQ:32:ARG:HG2   | 2.41                     | 0.54              |
| 24:BA:996:A:H4'   | 40:BQ:91:ARG:HG2   | 1.90                     | 0.54              |
| 41:BR:90:ARG:O    | 41:BR:91:GLN:CB    | 2.56                     | 0.54              |
| 55:CA:1004:A:C4   | 55:CA:1026:G:N7    | 2.76                     | 0.54              |
| 55:CA:1161:C:O2'  | 55:CA:1162:C:C6    | 2.61                     | 0.54              |
| 55:CA:197:A:N6    | 55:CA:221:C:H4'    | 2.22                     | 0.54              |
| 55:CA:252:U:O2'   | 55:CA:253:A:C8     | 2.47                     | 0.54              |
| 55:CA:274:A:H4'   | 55:CA:275:G:O5'    | 2.08                     | 0.54              |
| 55:CA:545:C:O2'   | 55:CA:549:C:OP1    | 2.22                     | 0.54              |
| 1:CB:208:ALA:HA   | 1:CB:211:LEU:CB    | 2.37                     | 0.54              |
| 3:CD:104:MET:SD   | 3:CD:179:GLY:HA3   | 2.48                     | 0.54              |
| 6:CG:19:SER:OG    | 6:CG:22:LEU:HB3    | 2.07                     | 0.54              |
| 8:CI:25:GLY:HA3   | 8:CI:58:GLU:N      | 2.22                     | 0.54              |
| 12:CM:49:GLU:HA   | 12:CM:49:GLU:OE1   | 2.07                     | 0.54              |
| 53:D3:28:LEU:HA   | 53:D3:32:LEU:HD21  | 1.88                     | 0.54              |
| 24:DA:1623:G:C6   | 24:DA:1624:U:C5    | 2.96                     | 0.54              |
| 24:DA:1731:G:H4'  | 24:DA:1732:C:OP1   | 2.08                     | 0.54              |
| 24:DA:529:A:C5    | 24:DA:2023:C:C4    | 2.95                     | 0.54              |
| 24:DA:2366:A:C2   | 24:DA:2367:G:H1'   | 2.43                     | 0.54              |
| 24:DA:851:C:H2'   | 24:DA:852:U:H6     | 1.73                     | 0.54              |
| 27:DD:39:ASP:CG   | 27:DD:40:LEU:H     | 2.11                     | 0.54              |
| 29:DF:32:LYS:HD2  | 29:DF:156:THR:HG21 | 1.89                     | 0.54              |
| 34:DK:87:LEU:HB2  | 34:DK:92:GLU:O     | 2.07                     | 0.54              |
| 24:DA:1011:G:OP1  | 40:DQ:76:SER:HB3   | 2.07                     | 0.54              |
| 41:DR:3:ALA:HB2   | 41:DR:101:ILE:HD13 | 1.90                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:DS:7:HIS:CE1   | 42:DS:10:ALA:HA    | 2.42                     | 0.54              |
| 44:DU:35:VAL:HG12 | 44:DU:36:GLU:N     | 2.22                     | 0.54              |
| 21:AA:1228:C:O2'  | 21:AA:1229:A:H8    | 1.90                     | 0.54              |
| 21:AA:282:A:H2'   | 21:AA:283:U:C6     | 2.43                     | 0.54              |
| 3:AD:204:SER:HB2  | 21:AA:8:A:H62      | 1.73                     | 0.54              |
| 4:AE:37:VAL:HG11  | 4:AE:113:VAL:CA    | 2.38                     | 0.54              |
| 8:AI:33:SER:HB3   | 8:AI:36:GLN:HG2    | 1.89                     | 0.54              |
| 9:AJ:36:VAL:HG22  | 9:AJ:76:ILE:HG23   | 1.89                     | 0.54              |
| 15:AP:79:ASN:O    | 15:AP:80:LYS:HB2   | 2.08                     | 0.54              |
| 19:AT:78:LEU:O    | 19:AT:82:ILE:HG23  | 2.07                     | 0.54              |
| 20:AU:9:GLU:HG3   | 20:AU:10:PRO:HD3   | 1.89                     | 0.54              |
| 24:BA:1394:U:C4   | 24:BA:1395:A:C6    | 2.96                     | 0.54              |
| 24:BA:1422:G:H2'  | 24:BA:1423:G:H8    | 1.73                     | 0.54              |
| 24:BA:2508:G:C4   | 24:BA:2509:G:C8    | 2.96                     | 0.54              |
| 24:BA:321:U:C6    | 28:BE:159:LEU:HD23 | 2.43                     | 0.54              |
| 24:BA:554:U:O4    | 24:BA:555:G:C6     | 2.61                     | 0.54              |
| 24:BA:621:A:H2'   | 24:BA:622:G:O4'    | 2.08                     | 0.54              |
| 24:BA:63:A:N3     | 24:BA:64:A:C8      | 2.76                     | 0.54              |
| 26:BC:105:ALA:O   | 26:BC:195:GLY:HA3  | 2.08                     | 0.54              |
| 28:BE:104:ALA:O   | 28:BE:108:ILE:CG2  | 2.56                     | 0.54              |
| 29:BF:131:VAL:CG2 | 29:BF:151:LEU:H    | 2.19                     | 0.54              |
| 30:BG:21:GLN:O    | 30:BG:36:LEU:HD13  | 2.08                     | 0.54              |
| 34:BK:108:ARG:HG3 | 34:BK:108:ARG:O    | 2.08                     | 0.54              |
| 37:BN:81:ASN:O    | 37:BN:85:PRO:HG3   | 2.08                     | 0.54              |
| 39:BP:50:ARG:O    | 39:BP:51:ASN:HB2   | 2.07                     | 0.54              |
| 15:CP:1:MET:HB2   | 55:CA:135:C:O2     | 2.07                     | 0.54              |
| 55:CA:28:A:C5     | 55:CA:29:U:C5      | 2.96                     | 0.54              |
| 55:CA:313:A:H2'   | 55:CA:314:C:C6     | 2.43                     | 0.54              |
| 55:CA:428:G:H1'   | 55:CA:430:A:N7     | 2.22                     | 0.54              |
| 55:CA:463:U:C4    | 55:CA:464:U:O4     | 2.61                     | 0.54              |
| 3:CD:194:ILE:HG13 | 3:CD:194:ILE:O     | 2.07                     | 0.54              |
| 4:CE:98:ALA:HB2   | 4:CE:123:LEU:CG    | 2.36                     | 0.54              |
| 24:DA:84:A:C4     | 24:DA:103:A:N6     | 2.76                     | 0.54              |
| 24:DA:1063:G:H2'  | 24:DA:1064:C:C5    | 2.42                     | 0.54              |
| 24:DA:1123:C:H2'  | 24:DA:1124:G:H8    | 1.73                     | 0.54              |
| 24:DA:1219:U:H2'  | 24:DA:1220:G:H8    | 1.73                     | 0.54              |
| 24:DA:123:G:H2'   | 24:DA:124:G:O4'    | 2.08                     | 0.54              |
| 24:DA:1548:A:H2'  | 24:DA:1549:A:H8    | 1.73                     | 0.54              |
| 24:DA:2586:U:H6   | 24:DA:2586:U:O5'   | 1.90                     | 0.54              |
| 24:DA:2786:U:O2'  | 24:DA:2787:C:H5'   | 2.08                     | 0.54              |
| 24:DA:320:A:H2'   | 28:DE:131:THR:OG1  | 2.07                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:DA:300:A:H1'    | 24:DA:333:G:N2    | 2.22                     | 0.54              |
| 24:DA:597:G:H2'    | 24:DA:598:U:O4'   | 2.08                     | 0.54              |
| 27:DD:121:THR:HG21 | 27:DD:127:PHE:CD1 | 2.42                     | 0.54              |
| 29:DF:107:VAL:N    | 29:DF:108:PRO:CD  | 2.71                     | 0.54              |
| 35:DL:93:ASN:CG    | 35:DL:94:THR:H    | 2.10                     | 0.54              |
| 36:DM:27:SER:N     | 36:DM:66:ARG:HH22 | 2.00                     | 0.54              |
| 39:DP:50:ARG:HA    | 39:DP:57:ALA:H    | 1.73                     | 0.54              |
| 44:DU:90:LYS:HE2   | 44:DU:92:VAL:HG12 | 1.89                     | 0.54              |
| 45:DV:56:PHE:C     | 45:DV:58:SER:H    | 2.12                     | 0.54              |
| 24:DA:857:G:H1'    | 46:DW:19:ARG:CZ   | 2.38                     | 0.54              |
| 47:DX:19:HIS:C     | 47:DX:21:LEU:H    | 2.11                     | 0.54              |
| 48:DY:31:GLN:C     | 48:DY:33:ALA:H    | 2.10                     | 0.54              |
| 21:AA:1208:C:H2'   | 21:AA:1209:C:O4'  | 2.08                     | 0.54              |
| 21:AA:260:G:O2'    | 21:AA:261:U:H5'   | 2.08                     | 0.54              |
| 21:AA:374:A:OP1    | 21:AA:452:A:N1    | 2.41                     | 0.54              |
| 21:AA:402:G:C6     | 21:AA:403:C:C4    | 2.95                     | 0.54              |
| 21:AA:607:A:H2'    | 21:AA:608:A:H8    | 1.72                     | 0.54              |
| 21:AA:903:G:C6     | 21:AA:904:U:C4    | 2.96                     | 0.54              |
| 21:AA:954:G:C6     | 21:AA:955:U:C4    | 2.96                     | 0.54              |
| 21:AA:976:G:N7     | 21:AA:1358:U:C2   | 2.76                     | 0.54              |
| 21:AA:98:A:H2'     | 21:AA:99:C:C6     | 2.43                     | 0.54              |
| 4:AE:95:MET:SD     | 4:AE:139:THR:HG22 | 2.47                     | 0.54              |
| 7:AH:91:LEU:HD21   | 7:AH:103:VAL:HG11 | 1.89                     | 0.54              |
| 24:BA:1178:C:H2'   | 24:BA:1179:G:N7   | 2.22                     | 0.54              |
| 24:BA:1849:G:H2'   | 24:BA:1850:G:H8   | 1.73                     | 0.54              |
| 24:BA:2332:C:H4'   | 24:BA:2336:A:C6   | 2.43                     | 0.54              |
| 24:BA:2727:A:H2'   | 24:BA:2728:U:C6   | 2.43                     | 0.54              |
| 24:BA:2733:A:O5'   | 24:BA:2733:A:C8   | 2.54                     | 0.54              |
| 24:BA:401:A:C2     | 24:BA:402:A:C4    | 2.96                     | 0.54              |
| 24:BA:821:A:H2'    | 24:BA:946:C:H5''  | 1.89                     | 0.54              |
| 25:BB:20:G:C2      | 25:BB:64:G:N3     | 2.76                     | 0.54              |
| 25:BB:45:A:H2'     | 25:BB:46:A:H8     | 1.73                     | 0.54              |
| 28:BE:60:TRP:CZ2   | 28:BE:70:SER:HB3  | 2.43                     | 0.54              |
| 30:BG:115:GLN:CD   | 30:BG:115:GLN:H   | 2.11                     | 0.54              |
| 34:BK:8:LEU:HD23   | 34:BK:8:LEU:N     | 2.23                     | 0.54              |
| 36:BM:65:ILE:HG12  | 36:BM:103:TYR:CD2 | 2.42                     | 0.54              |
| 39:BP:50:ARG:CG    | 39:BP:57:ALA:N    | 2.71                     | 0.54              |
| 39:BP:83:ILE:HD13  | 39:BP:83:ILE:C    | 2.28                     | 0.54              |
| 42:BS:24:ILE:HG22  | 42:BS:71:VAL:HG21 | 1.91                     | 0.54              |
| 55:CA:1327:C:H2'   | 55:CA:1328:C:C6   | 2.42                     | 0.54              |
| 55:CA:1430:A:N6    | 55:CA:1431:A:C2   | 2.76                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:CA:1431:A:C6    | 55:CA:1432:G:N1    | 2.76                     | 0.54              |
| 55:CA:198:G:HO2'   | 55:CA:199:A:H8     | 1.56                     | 0.54              |
| 55:CA:410:G:H2'    | 55:CA:429:U:C5     | 2.43                     | 0.54              |
| 4:CE:22:LYS:HB3    | 4:CE:29:ILE:CG2    | 2.38                     | 0.54              |
| 6:CG:139:ASP:O     | 6:CG:142:ARG:HB2   | 2.09                     | 0.54              |
| 7:CH:124:ILE:HG22  | 7:CH:125:ILE:H     | 1.73                     | 0.54              |
| 8:CI:4:GLN:HB3     | 8:CI:21:LYS:HD3    | 1.90                     | 0.54              |
| 11:CL:97:VAL:HG23  | 11:CL:100:ALA:HB3  | 1.90                     | 0.54              |
| 13:CN:20:PHE:HE1   | 13:CN:54:SER:CB    | 2.20                     | 0.54              |
| 14:CO:8:ALA:O      | 14:CO:11:VAL:HB    | 2.08                     | 0.54              |
| 18:CS:45:GLY:H     | 18:CS:61:VAL:HB    | 1.72                     | 0.54              |
| 20:CU:16:ARG:HG3   | 20:CU:19:LYS:CG    | 2.33                     | 0.54              |
| 22:CX:40:C:H2'     | 22:CX:41:C:C6      | 2.41                     | 0.54              |
| 24:DA:1059:G:C5    | 24:DA:1060:U:C2    | 2.96                     | 0.54              |
| 24:DA:1355:G:C6    | 24:DA:1377:G:N2    | 2.76                     | 0.54              |
| 24:DA:1535:A:N1    | 24:DA:1537:G:N7    | 2.56                     | 0.54              |
| 24:DA:1782:U:O2'   | 24:DA:1783:A:C5'   | 2.55                     | 0.54              |
| 24:DA:225:C:H2'    | 24:DA:226:A:C8     | 2.43                     | 0.54              |
| 24:DA:2300:C:H2'   | 24:DA:2301:C:H6    | 1.72                     | 0.54              |
| 24:DA:2612:C:O2    | 50:D0:1:ALA:HB2    | 2.08                     | 0.54              |
| 24:DA:547:A:H3'    | 24:DA:548:G:C5'    | 2.36                     | 0.54              |
| 26:DC:70:LYS:HD3   | 26:DC:101:ARG:HH12 | 1.72                     | 0.54              |
| 24:DA:2724:U:P     | 27:DD:116:LYS:HZ3  | 2.31                     | 0.54              |
| 27:DD:117:GLY:O    | 27:DD:119:ALA:N    | 2.41                     | 0.54              |
| 24:DA:2060:A:H2'   | 28:DE:63:LYS:NZ    | 2.23                     | 0.54              |
| 30:DG:94:ARG:CZ    | 30:DG:105:SER:HB2  | 2.38                     | 0.54              |
| 33:DJ:103:ILE:HD12 | 33:DJ:103:ILE:O    | 2.08                     | 0.54              |
| 37:DN:110:MET:HE2  | 37:DN:110:MET:HA   | 1.89                     | 0.54              |
| 39:DP:22:GLY:HA3   | 39:DP:91:VAL:CG2   | 2.38                     | 0.54              |
| 39:DP:28:LYS:HB3   | 39:DP:39:LEU:HD23  | 1.90                     | 0.54              |
| 40:DQ:4:LYS:HZ1    | 40:DQ:6:GLY:HA3    | 1.65                     | 0.54              |
| 40:DQ:78:PHE:CE1   | 40:DQ:82:LEU:HD11  | 2.43                     | 0.54              |
| 24:DA:2331:G:O2'   | 46:DW:40:ARG:HB3   | 2.08                     | 0.54              |
| 21:AA:1386:G:C2    | 21:AA:1387:G:C5    | 2.96                     | 0.53              |
| 21:AA:1409:C:H5'   | 24:BA:1916:A:C2    | 2.43                     | 0.53              |
| 21:AA:201:G:N3     | 21:AA:202:G:H1'    | 2.23                     | 0.53              |
| 21:AA:372:C:H4'    | 21:AA:373:A:OP1    | 2.07                     | 0.53              |
| 1:AB:110:ILE:HD11  | 1:AB:147:LEU:HD22  | 1.90                     | 0.53              |
| 8:AI:17:ARG:O      | 8:AI:64:ILE:HG23   | 2.08                     | 0.53              |
| 13:AN:51:PRO:O     | 13:AN:52:ARG:HB2   | 2.08                     | 0.53              |
| 22:AV:39:U:H2'     | 22:AV:40:C:C6      | 2.42                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:1007:C:H5'' | 33:BJ:37:ARG:NH2   | 2.24                     | 0.53              |
| 24:BA:1142:A:C8   | 24:BA:1144:A:N6    | 2.76                     | 0.53              |
| 24:BA:1659:G:C6   | 24:BA:1660:G:N7    | 2.76                     | 0.53              |
| 24:BA:1820:U:O2   | 26:BC:200:MET:N    | 2.40                     | 0.53              |
| 24:BA:2308:G:O2'  | 24:BA:2310:C:C5    | 2.51                     | 0.53              |
| 24:BA:2776:A:O2'  | 24:BA:2777:G:OP2   | 2.20                     | 0.53              |
| 24:BA:361:G:HO2'  | 24:BA:362:A:C5'    | 2.20                     | 0.53              |
| 24:BA:860:U:O2'   | 24:BA:861:A:C5'    | 2.52                     | 0.53              |
| 24:BA:675:A:H4'   | 28:BE:62:GLN:HE22  | 1.72                     | 0.53              |
| 29:BF:40:GLY:HA2  | 29:BF:84:ILE:HD11  | 1.89                     | 0.53              |
| 30:BG:86:LEU:N    | 30:BG:86:LEU:HD12  | 2.22                     | 0.53              |
| 31:BH:81:ALA:HB2  | 31:BH:147:VAL:HG23 | 1.89                     | 0.53              |
| 32:BI:72:THR:HB   | 32:BI:112:LYS:NZ   | 2.23                     | 0.53              |
| 35:BL:94:THR:HG22 | 35:BL:95:LEU:H     | 1.73                     | 0.53              |
| 38:BO:79:ALA:HB2  | 38:BO:110:ALA:HA   | 1.90                     | 0.53              |
| 38:BO:7:ARG:HD2   | 38:BO:97:PHE:CE1   | 2.43                     | 0.53              |
| 41:BR:46:GLU:HG2  | 41:BR:47:VAL:N     | 2.23                     | 0.53              |
| 43:BT:48:GLN:HB2  | 43:BT:49:LYS:HE3   | 1.89                     | 0.53              |
| 44:BU:100:GLU:O   | 44:BU:101:THR:HB   | 2.07                     | 0.53              |
| 45:BV:72:VAL:HG21 | 45:BV:91:PHE:HB3   | 1.90                     | 0.53              |
| 46:BW:52:CYS:HA   | 46:BW:57:THR:O     | 2.08                     | 0.53              |
| 55:CA:1173:U:H2'  | 55:CA:1174:G:H8    | 1.73                     | 0.53              |
| 55:CA:1392:G:C6   | 55:CA:1393:U:C4    | 2.95                     | 0.53              |
| 55:CA:1417:G:H2'  | 55:CA:1482:G:H22   | 1.74                     | 0.53              |
| 55:CA:1460:C:C4   | 55:CA:1461:G:C5    | 2.96                     | 0.53              |
| 55:CA:425:G:O2'   | 55:CA:426:U:H5'    | 2.08                     | 0.53              |
| 55:CA:75:G:C2     | 55:CA:96:U:N3      | 2.76                     | 0.53              |
| 1:CB:103:TRP:CD1  | 1:CB:107:ARG:HB3   | 2.43                     | 0.53              |
| 5:CF:11:HIS:CD2   | 5:CF:13:ASP:H      | 2.25                     | 0.53              |
| 24:DA:1079:C:O2'  | 24:DA:1080:A:C8    | 2.57                     | 0.53              |
| 24:DA:1450:G:N2   | 24:DA:1462:C:C2    | 2.76                     | 0.53              |
| 24:DA:1666:G:H4'  | 34:DK:6:THR:HG23   | 1.90                     | 0.53              |
| 24:DA:191:A:N6    | 24:DA:203:A:H2'    | 2.23                     | 0.53              |
| 24:DA:2423:U:H5'' | 24:DA:2424:C:OP1   | 2.07                     | 0.53              |
| 24:DA:197:A:N7    | 24:DA:2430:A:C5    | 2.76                     | 0.53              |
| 24:DA:2590:A:H5'' | 26:DC:237:ARG:HG3  | 1.90                     | 0.53              |
| 24:DA:475:C:O2'   | 24:DA:476:G:H5'    | 2.08                     | 0.53              |
| 24:DA:804:A:C2'   | 24:DA:806:C:C4     | 2.91                     | 0.53              |
| 56:DB:112:G:H2'   | 56:DB:113:C:O4'    | 2.09                     | 0.53              |
| 26:DC:95:TYR:C    | 26:DC:97:ASP:H     | 2.09                     | 0.53              |
| 31:DH:66:ASN:HD22 | 31:DH:137:GLU:HB3  | 1.73                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DL:110:VAL:O   | 35:DL:111:ILE:HG12 | 2.08                     | 0.53              |
| 37:DN:73:ASN:HA   | 37:DN:76:VAL:HG22  | 1.90                     | 0.53              |
| 40:DQ:10:ARG:HB2  | 40:DQ:10:ARG:CZ    | 2.38                     | 0.53              |
| 44:DU:86:PHE:HB2  | 44:DU:92:VAL:HG22  | 1.89                     | 0.53              |
| 48:DY:4:LYS:HB2   | 48:DY:4:LYS:NZ     | 2.22                     | 0.53              |
| 21:AA:1227:A:C2'  | 21:AA:1228:C:H5''  | 2.38                     | 0.53              |
| 21:AA:1348:U:C2'  | 21:AA:1349:A:H8    | 2.21                     | 0.53              |
| 21:AA:794:A:O2'   | 21:AA:795:C:C5'    | 2.56                     | 0.53              |
| 21:AA:872:A:C4    | 21:AA:874:G:C8     | 2.97                     | 0.53              |
| 1:AB:26:MET:CE    | 1:AB:192:PRO:HG3   | 2.38                     | 0.53              |
| 3:AD:157:ALA:O    | 3:AD:161:ALA:HB2   | 2.07                     | 0.53              |
| 5:AF:42:TRP:HB2   | 5:AF:59:TYR:HB2    | 1.91                     | 0.53              |
| 4:AE:156:ARG:HA   | 7:AH:63:LYS:CE     | 2.38                     | 0.53              |
| 10:AK:116:PRO:HB3 | 21:AA:676:A:H1'    | 1.90                     | 0.53              |
| 12:AM:40:GLU:HG3  | 12:AM:41:ASP:N     | 2.23                     | 0.53              |
| 10:AK:124:LYS:HE3 | 20:AU:34:ARG:NE    | 2.23                     | 0.53              |
| 24:BA:1477:A:N6   | 24:BA:1514:G:H1'   | 2.23                     | 0.53              |
| 24:BA:1677:A:N6   | 24:BA:1678:A:C6    | 2.76                     | 0.53              |
| 24:BA:1799:G:OP1  | 26:BC:257:ARG:HG2  | 2.08                     | 0.53              |
| 24:BA:1943:U:H4'  | 24:BA:1944:U:O5'   | 2.08                     | 0.53              |
| 24:BA:1964:G:C2   | 24:BA:1967:C:C5    | 2.96                     | 0.53              |
| 24:BA:2226:C:H2'  | 24:BA:2227:A:C8    | 2.43                     | 0.53              |
| 24:BA:2383:G:C4   | 24:BA:2384:U:H5    | 2.26                     | 0.53              |
| 24:BA:2407:A:H2'  | 24:BA:2408:U:C5    | 2.43                     | 0.53              |
| 24:BA:2540:C:C2'  | 24:BA:2541:A:H5'   | 2.38                     | 0.53              |
| 24:BA:2545:G:C6   | 24:BA:2546:U:N3    | 2.76                     | 0.53              |
| 24:BA:528:A:H8    | 24:BA:528:A:C3'    | 2.21                     | 0.53              |
| 24:BA:659:G:H4'   | 28:BE:95:LYS:HD3   | 1.88                     | 0.53              |
| 24:BA:785:G:H2'   | 24:BA:786:C:H6     | 1.73                     | 0.53              |
| 24:BA:9:G:N1      | 24:BA:2629:U:C6    | 2.76                     | 0.53              |
| 26:BC:147:PRO:HD3 | 26:BC:187:CYS:SG   | 2.49                     | 0.53              |
| 26:BC:90:ILE:HG21 | 26:BC:102:TYR:CD1  | 2.43                     | 0.53              |
| 29:BF:134:GLN:NE2 | 29:BF:150:GLY:H    | 2.04                     | 0.53              |
| 32:BI:32:VAL:HG13 | 32:BI:66:PHE:CE2   | 2.43                     | 0.53              |
| 35:BL:91:ASP:HB2  | 35:BL:94:THR:HB    | 1.90                     | 0.53              |
| 40:BQ:82:LEU:HD23 | 40:BQ:112:ALA:HB2  | 1.90                     | 0.53              |
| 41:BR:42:ALA:HA   | 41:BR:46:GLU:CB    | 2.31                     | 0.53              |
| 55:CA:1306:A:N6   | 55:CA:1331:G:H1'   | 2.22                     | 0.53              |
| 55:CA:1446:A:N6   | 55:CA:1447:A:C6    | 2.76                     | 0.53              |
| 55:CA:1495:U:O2   | 24:DA:1919:A:H2    | 1.91                     | 0.53              |
| 55:CA:650:G:C6    | 55:CA:651:C:C4     | 2.97                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:818:G:C2'   | 55:CA:819:A:H5''  | 2.39                     | 0.53              |
| 55:CA:858:G:N7    | 59:CA:1824:HOH:O  | 2.33                     | 0.53              |
| 55:CA:913:A:HO2'  | 55:CA:914:A:H5''  | 1.69                     | 0.53              |
| 3:CD:57:LYS:HG3   | 3:CD:58:GLN:N     | 2.22                     | 0.53              |
| 6:CG:45:ALA:O     | 6:CG:120:ALA:HB1  | 2.09                     | 0.53              |
| 9:CJ:50:THR:HA    | 9:CJ:63:ASP:O     | 2.08                     | 0.53              |
| 51:D1:3:GLY:C     | 51:D1:5:ARG:H     | 2.12                     | 0.53              |
| 53:D3:54:LEU:O    | 53:D3:58:ILE:HG13 | 2.08                     | 0.53              |
| 24:DA:1061:U:C6   | 32:DI:9:LYS:HD3   | 2.43                     | 0.53              |
| 24:DA:1056:G:H1'  | 24:DA:1103:A:C6   | 2.43                     | 0.53              |
| 24:DA:1275:A:C6   | 24:DA:1296:G:H4'  | 2.44                     | 0.53              |
| 24:DA:1352:U:C6   | 24:DA:1377:G:C6   | 2.96                     | 0.53              |
| 24:DA:1668:A:H4'  | 24:DA:1669:A:O5'  | 2.08                     | 0.53              |
| 24:DA:2052:A:C2   | 24:DA:2053:G:C8   | 2.97                     | 0.53              |
| 24:DA:2520:C:C2   | 24:DA:2521:C:C5   | 2.97                     | 0.53              |
| 24:DA:298:G:OP1   | 44:DU:83:GLY:HA2  | 2.08                     | 0.53              |
| 24:DA:422:A:C6    | 24:DA:423:A:N6    | 2.77                     | 0.53              |
| 24:DA:468:G:H5''  | 28:DE:55:SER:HB2  | 1.90                     | 0.53              |
| 24:DA:528:A:H2    | 24:DA:2043:C:O5'  | 1.91                     | 0.53              |
| 24:DA:955:U:OP1   | 36:DM:13:HIS:HA   | 2.07                     | 0.53              |
| 26:DC:30:ALA:HB3  | 26:DC:31:PRO:HD3  | 1.90                     | 0.53              |
| 29:DF:91:ARG:HA   | 29:DF:95:MET:SD   | 2.48                     | 0.53              |
| 33:DJ:57:LEU:HG   | 33:DJ:128:ASN:H   | 1.73                     | 0.53              |
| 34:DK:73:ASP:OD1  | 34:DK:73:ASP:N    | 2.39                     | 0.53              |
| 39:DP:22:GLY:HA3  | 39:DP:91:VAL:HG21 | 1.90                     | 0.53              |
| 39:DP:92:ARG:HG2  | 39:DP:92:ARG:O    | 2.07                     | 0.53              |
| 43:DT:5:GLU:HA    | 43:DT:8:LEU:HD12  | 1.90                     | 0.53              |
| 45:DV:57:TYR:HD2  | 45:DV:74:ALA:CB   | 2.21                     | 0.53              |
| 24:DA:1364:G:N7   | 47:DX:1:SER:HB2   | 2.24                     | 0.53              |
| 21:AA:1084:G:C5   | 21:AA:1085:U:C4   | 2.96                     | 0.53              |
| 21:AA:688:G:O6    | 21:AA:700:G:C6    | 2.61                     | 0.53              |
| 21:AA:834:U:H2'   | 21:AA:835:U:C6    | 2.43                     | 0.53              |
| 1:AB:108:GLN:HA   | 1:AB:111:LYS:CB   | 2.37                     | 0.53              |
| 1:AB:36:LYS:HA    | 1:AB:36:LYS:HE3   | 1.90                     | 0.53              |
| 1:AB:59:ILE:HD12  | 1:AB:60:ALA:N     | 2.23                     | 0.53              |
| 2:AC:143:LEU:HD22 | 2:AC:143:LEU:H    | 1.71                     | 0.53              |
| 4:AE:111:ARG:O    | 4:AE:111:ARG:HG2  | 2.07                     | 0.53              |
| 6:AG:121:ASN:H    | 6:AG:121:ASN:HD22 | 1.56                     | 0.53              |
| 7:AH:34:ALA:HB1   | 7:AH:109:VAL:HB   | 1.90                     | 0.53              |
| 11:AL:17:LYS:HD2  | 11:AL:17:LYS:O    | 2.08                     | 0.53              |
| 12:AM:67:ASP:O    | 12:AM:70:ARG:CG   | 2.55                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:AV:29:G:H2'    | 22:AV:30:G:H8      | 1.73                     | 0.53              |
| 24:BA:1346:G:H2'  | 24:BA:1347:A:H8    | 1.73                     | 0.53              |
| 24:BA:1677:A:C6   | 24:BA:1678:A:C5    | 2.97                     | 0.53              |
| 24:BA:2365:G:H2'  | 24:BA:2366:A:C8    | 2.44                     | 0.53              |
| 24:BA:2378:A:H8   | 24:BA:2378:A:O5'   | 1.91                     | 0.53              |
| 24:BA:243:U:HO2'  | 24:BA:244:A:H5'    | 1.72                     | 0.53              |
| 24:BA:2555:U:C5   | 24:BA:2556:C:C6    | 2.97                     | 0.53              |
| 24:BA:2813:A:H2   | 24:BA:2887:A:H62   | 1.55                     | 0.53              |
| 24:BA:785:G:H2'   | 24:BA:786:C:C6     | 2.43                     | 0.53              |
| 24:BA:790:U:O2'   | 24:BA:791:C:C5'    | 2.56                     | 0.53              |
| 28:BE:46:GLN:HG2  | 28:BE:87:ALA:H     | 1.73                     | 0.53              |
| 32:BI:32:VAL:HG22 | 32:BI:66:PHE:CG    | 2.43                     | 0.53              |
| 35:BL:78:ARG:HB2  | 35:BL:80:SER:OG    | 2.09                     | 0.53              |
| 24:BA:1248:G:O2'  | 40:BQ:2:ARG:HA     | 2.07                     | 0.53              |
| 40:BQ:57:ARG:NH2  | 40:BQ:92:LYS:CE    | 2.71                     | 0.53              |
| 41:BR:12:HIS:CE1  | 41:BR:22:LEU:CD2   | 2.91                     | 0.53              |
| 40:BQ:94:LEU:CD1  | 41:BR:4:VAL:HG11   | 2.36                     | 0.53              |
| 42:BS:97:LEU:CD2  | 42:BS:97:LEU:N     | 2.70                     | 0.53              |
| 43:BT:32:LEU:O    | 43:BT:83:ALA:HB2   | 2.08                     | 0.53              |
| 43:BT:43:ILE:CD1  | 43:BT:58:VAL:HG21  | 2.38                     | 0.53              |
| 55:CA:577:G:N2    | 55:CA:578:C:O2     | 2.41                     | 0.53              |
| 55:CA:754:C:H5''  | 55:CA:754:C:O2     | 2.09                     | 0.53              |
| 1:CB:25:LYS:HD2   | 1:CB:25:LYS:N      | 2.23                     | 0.53              |
| 8:CI:30:ASN:O     | 8:CI:32:ARG:HG2    | 2.08                     | 0.53              |
| 8:CI:45:MET:HA    | 8:CI:48:ARG:HG2    | 1.89                     | 0.53              |
| 13:CN:80:ARG:HG2  | 13:CN:81:ILE:N     | 2.23                     | 0.53              |
| 22:CX:31:A:C2'    | 22:CX:32:U:H5'     | 2.39                     | 0.53              |
| 24:DA:1098:A:H2'  | 24:DA:1099:G:O4'   | 2.08                     | 0.53              |
| 24:DA:1420:A:C2   | 24:DA:2211:A:N7    | 2.76                     | 0.53              |
| 24:DA:1439:A:N7   | 24:DA:1440:U:C2    | 2.76                     | 0.53              |
| 24:DA:2225:A:H4'  | 24:DA:2226:C:C6    | 2.43                     | 0.53              |
| 24:DA:2311:A:H3'  | 24:DA:2312:U:C6    | 2.42                     | 0.53              |
| 24:DA:962:G:H4'   | 24:DA:2496:C:O2'   | 2.08                     | 0.53              |
| 24:DA:2630:G:O2'  | 24:DA:2631:G:H8    | 1.92                     | 0.53              |
| 24:DA:2756:U:H4'  | 24:DA:2757:A:O5'   | 2.08                     | 0.53              |
| 56:DB:17:C:O2'    | 56:DB:18:G:C5'     | 2.57                     | 0.53              |
| 32:DI:96:LYS:HE2  | 32:DI:138:VAL:HG11 | 1.90                     | 0.53              |
| 46:DW:18:LYS:HD3  | 46:DW:19:ARG:H     | 1.72                     | 0.53              |
| 49:DZ:51:SER:C    | 49:DZ:53:MET:H     | 2.10                     | 0.53              |
| 21:AA:1177:G:H2'  | 21:AA:1178:G:O4'   | 2.08                     | 0.53              |
| 21:AA:1316:G:N2   | 21:AA:1318:A:H3'   | 2.24                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:228:A:H2'   | 21:AA:229:U:C6    | 2.43                     | 0.53              |
| 21:AA:240:G:H4'   | 21:AA:240:G:OP2   | 2.09                     | 0.53              |
| 21:AA:262:A:H2'   | 21:AA:263:A:C8    | 2.43                     | 0.53              |
| 1:AB:107:ARG:NH2  | 1:AB:108:GLN:HE22 | 2.04                     | 0.53              |
| 2:AC:156:LEU:N    | 2:AC:156:LEU:HD12 | 2.24                     | 0.53              |
| 8:AI:105:ARG:HE   | 21:AA:1117:A:H4'  | 1.73                     | 0.53              |
| 11:AL:34:THR:HB   | 11:AL:35:ARG:HG2  | 1.91                     | 0.53              |
| 13:AN:29:ILE:HG23 | 13:AN:34:ASN:OD1  | 2.09                     | 0.53              |
| 2:AC:5:HIS:HB3    | 13:AN:88:MET:HE3  | 1.90                     | 0.53              |
| 19:AT:79:THR:O    | 19:AT:82:ILE:HG13 | 2.08                     | 0.53              |
| 50:B0:39:ARG:HB2  | 50:B0:39:ARG:NH1  | 2.23                     | 0.53              |
| 50:B0:42:ILE:HD12 | 50:B0:48:TYR:HB2  | 1.90                     | 0.53              |
| 24:BA:1081:U:H2'  | 24:BA:1081:U:O2   | 2.07                     | 0.53              |
| 24:BA:1483:G:C2   | 24:BA:1484:U:C2   | 2.96                     | 0.53              |
| 24:BA:1714:U:H6   | 24:BA:1714:U:H5'' | 1.73                     | 0.53              |
| 24:BA:1744:A:H3'  | 24:BA:1745:A:C8   | 2.43                     | 0.53              |
| 24:BA:1899:A:O2'  | 24:BA:1900:A:H5'' | 2.09                     | 0.53              |
| 24:BA:1770:G:C5   | 24:BA:1983:G:C6   | 2.97                     | 0.53              |
| 24:BA:2014:A:H2'  | 24:BA:2015:A:C8   | 2.43                     | 0.53              |
| 24:BA:2532:G:C5   | 24:BA:2533:U:C6   | 2.97                     | 0.53              |
| 24:BA:2588:G:H2'  | 24:BA:2589:A:O4'  | 2.08                     | 0.53              |
| 27:BD:45:TYR:HD1  | 27:BD:45:TYR:N    | 2.04                     | 0.53              |
| 30:BG:35:THR:O    | 30:BG:36:LEU:HD22 | 2.09                     | 0.53              |
| 32:BI:56:VAL:HG23 | 32:BI:69:VAL:O    | 2.08                     | 0.53              |
| 33:BJ:3:THR:HB    | 33:BJ:44:TYR:OH   | 2.08                     | 0.53              |
| 33:BJ:56:VAL:CG1  | 33:BJ:57:LEU:H    | 2.20                     | 0.53              |
| 34:BK:10:VAL:HB   | 34:BK:16:ALA:HB1  | 1.91                     | 0.53              |
| 36:BM:25:ASP:OD2  | 36:BM:25:ASP:N    | 2.42                     | 0.53              |
| 42:BS:25:ARG:HE   | 42:BS:73:LYS:HZ1  | 1.53                     | 0.53              |
| 24:BA:2013:A:C2   | 42:BS:88:ARG:NH1  | 2.76                     | 0.53              |
| 44:BU:73:ASN:C    | 44:BU:75:ALA:H    | 2.12                     | 0.53              |
| 47:BX:52:ALA:O    | 47:BX:53:LYS:HB3  | 2.08                     | 0.53              |
| 55:CA:1032:G:N2   | 55:CA:1033:G:C5   | 2.77                     | 0.53              |
| 55:CA:1139:G:H4'  | 55:CA:1140:C:O5'  | 2.09                     | 0.53              |
| 55:CA:575:G:C6    | 55:CA:821:G:C5    | 2.96                     | 0.53              |
| 55:CA:597:G:O2'   | 55:CA:598:U:H5'   | 2.08                     | 0.53              |
| 55:CA:654:G:C6    | 55:CA:753:A:C5    | 2.96                     | 0.53              |
| 2:CC:109:GLU:HG2  | 2:CC:139:ASN:HB2  | 1.89                     | 0.53              |
| 6:CG:115:MET:HE3  | 6:CG:119:LEU:HB3  | 1.91                     | 0.53              |
| 6:CG:14:ASP:HB3   | 6:CG:19:SER:N     | 2.24                     | 0.53              |
| 4:CE:156:ARG:NH1  | 7:CH:43:GLY:HA3   | 2.23                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:CL:84:GLY:H    | 11:CL:94:TYR:HA   | 1.73                     | 0.53              |
| 12:CM:75:SER:O    | 12:CM:79:LEU:HG   | 2.08                     | 0.53              |
| 13:CN:33:VAL:HB   | 55:CA:1272:G:H5'  | 1.90                     | 0.53              |
| 24:DA:1338:G:O2'  | 43:DT:18:GLU:HG3  | 2.09                     | 0.53              |
| 24:DA:1416:G:C6   | 24:DA:1417:C:C4   | 2.96                     | 0.53              |
| 24:DA:1522:A:H1'  | 24:DA:1524:G:C4   | 2.43                     | 0.53              |
| 24:DA:1649:G:O6   | 24:DA:2009:A:N6   | 2.41                     | 0.53              |
| 24:DA:1827:U:H2'  | 24:DA:1828:G:O4'  | 2.08                     | 0.53              |
| 24:DA:2077:A:C5   | 24:DA:2435:A:C5   | 2.96                     | 0.53              |
| 24:DA:2312:U:H2'  | 24:DA:2312:U:O2   | 2.09                     | 0.53              |
| 24:DA:401:A:H2'   | 24:DA:402:A:C8    | 2.44                     | 0.53              |
| 24:DA:437:U:H2'   | 24:DA:438:G:C8    | 2.43                     | 0.53              |
| 24:DA:547:A:C2'   | 24:DA:548:G:H5'   | 2.38                     | 0.53              |
| 24:DA:571:U:C5    | 24:DA:575:A:C6    | 2.97                     | 0.53              |
| 24:DA:669:G:H2'   | 24:DA:669:G:N3    | 2.22                     | 0.53              |
| 24:DA:674:G:H4'   | 28:DE:69:ARG:HB3  | 1.91                     | 0.53              |
| 24:DA:695:G:N3    | 24:DA:768:G:C2    | 2.77                     | 0.53              |
| 24:DA:781:A:H5''  | 24:DA:782:A:OP1   | 2.08                     | 0.53              |
| 24:DA:90:U:H3'    | 24:DA:91:A:H5''   | 1.91                     | 0.53              |
| 29:DF:131:VAL:C   | 29:DF:133:GLU:H   | 2.12                     | 0.53              |
| 24:DA:632:A:H5''  | 35:DL:68:SER:OG   | 2.09                     | 0.53              |
| 24:DA:2720:U:H5'' | 39:DP:52:ARG:NH2  | 2.23                     | 0.53              |
| 24:DA:1248:G:H2'  | 40:DQ:1:ALA:O     | 2.08                     | 0.53              |
| 41:DR:61:ALA:HB1  | 41:DR:96:VAL:HB   | 1.90                     | 0.53              |
| 21:AA:1171:A:H2'  | 21:AA:1172:C:C6   | 2.44                     | 0.53              |
| 21:AA:1305:G:N2   | 21:AA:1331:G:H2'  | 2.24                     | 0.53              |
| 21:AA:1305:G:H21  | 21:AA:1332:A:H2   | 1.56                     | 0.53              |
| 21:AA:142:G:C4    | 21:AA:143:A:C8    | 2.97                     | 0.53              |
| 21:AA:1513:A:H2'  | 21:AA:1514:G:C8   | 2.42                     | 0.53              |
| 21:AA:20:U:H2'    | 21:AA:21:G:O4'    | 2.08                     | 0.53              |
| 21:AA:266:G:HO2'  | 21:AA:267:C:P     | 2.31                     | 0.53              |
| 21:AA:524:G:C6    | 21:AA:525:C:N4    | 2.76                     | 0.53              |
| 21:AA:532:A:O2'   | 21:AA:533:A:OP1   | 2.26                     | 0.53              |
| 21:AA:692:U:H2'   | 21:AA:694:A:OP2   | 2.07                     | 0.53              |
| 21:AA:983:A:O2'   | 21:AA:984:C:H5'   | 2.07                     | 0.53              |
| 3:AD:160:LEU:H    | 3:AD:160:LEU:HD13 | 1.73                     | 0.53              |
| 6:AG:22:LEU:HD23  | 6:AG:22:LEU:O     | 2.08                     | 0.53              |
| 12:AM:13:HIS:ND1  | 12:AM:41:ASP:HB2  | 2.24                     | 0.53              |
| 13:AN:19:TYR:O    | 13:AN:22:LYS:HB3  | 2.08                     | 0.53              |
| 14:AO:9:LYS:NZ    | 14:AO:9:LYS:HB3   | 2.24                     | 0.53              |
| 20:AU:40:PRO:HA   | 20:AU:43:GLU:HB2  | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:1062:G:C6   | 24:BA:1063:G:C6   | 2.96                     | 0.53              |
| 24:BA:1873:G:H2'  | 24:BA:1874:C:C6   | 2.43                     | 0.53              |
| 24:BA:1967:C:O2'  | 24:BA:1968:G:H5'  | 2.08                     | 0.53              |
| 24:BA:2523:G:O2'  | 24:BA:2524:G:H5'  | 2.08                     | 0.53              |
| 24:BA:587:C:H5''  | 24:BA:588:U:H5'   | 1.91                     | 0.53              |
| 26:BC:184:GLU:O   | 26:BC:186:ASP:N   | 2.39                     | 0.53              |
| 26:BC:195:GLY:O   | 26:BC:196:ASN:HB3 | 2.09                     | 0.53              |
| 27:BD:113:SER:HB2 | 27:BD:114:LYS:HE3 | 1.89                     | 0.53              |
| 28:BE:150:THR:CG2 | 28:BE:153:LEU:HA  | 2.38                     | 0.53              |
| 28:BE:27:LEU:O    | 28:BE:31:VAL:HG23 | 2.08                     | 0.53              |
| 28:BE:7:ASP:O     | 28:BE:9:GLN:N     | 2.42                     | 0.53              |
| 29:BF:30:VAL:HG12 | 29:BF:96:TRP:CH2  | 2.43                     | 0.53              |
| 35:BL:18:ARG:O    | 35:BL:19:LEU:HB3  | 2.07                     | 0.53              |
| 38:BO:75:GLY:HA3  | 38:BO:109:ALA:HB3 | 1.90                     | 0.53              |
| 38:BO:88:LYS:O    | 38:BO:89:ASP:HB2  | 2.08                     | 0.53              |
| 43:BT:8:LEU:HD13  | 43:BT:46:ALA:HA   | 1.91                     | 0.53              |
| 43:BT:9:LYS:HG3   | 43:BT:9:LYS:O     | 2.07                     | 0.53              |
| 44:BU:3:LYS:O     | 44:BU:82:VAL:HG21 | 2.08                     | 0.53              |
| 45:BV:72:VAL:HG12 | 45:BV:93:ARG:HA   | 1.89                     | 0.53              |
| 46:BW:33:GLY:O    | 46:BW:34:SER:HB3  | 2.08                     | 0.53              |
| 55:CA:1134:G:C2   | 55:CA:1141:C:N3   | 2.76                     | 0.53              |
| 18:CS:72:GLU:HA   | 55:CA:1320:C:O2'  | 2.08                     | 0.53              |
| 55:CA:557:G:C6    | 55:CA:558:G:C6    | 2.97                     | 0.53              |
| 55:CA:612:C:N3    | 55:CA:629:A:C2    | 2.76                     | 0.53              |
| 55:CA:652:U:H1'   | 55:CA:653:U:H5    | 1.72                     | 0.53              |
| 2:CC:129:PHE:CE1  | 2:CC:156:LEU:HB3  | 2.44                     | 0.53              |
| 2:CC:86:LEU:O     | 2:CC:90:VAL:HG13  | 2.08                     | 0.53              |
| 15:CP:12:LYS:HD2  | 55:CA:393:A:OP2   | 2.08                     | 0.53              |
| 53:D3:22:LYS:H    | 53:D3:48:MET:CB   | 2.20                     | 0.53              |
| 24:DA:1057:A:C8   | 24:DA:1086:A:H2'  | 2.43                     | 0.53              |
| 24:DA:1853:A:N1   | 24:DA:2087:G:H1'  | 2.23                     | 0.53              |
| 24:DA:957:C:C2    | 24:DA:2459:A:O4'  | 2.62                     | 0.53              |
| 24:DA:1783:A:H5'' | 24:DA:2608:G:H4'  | 1.91                     | 0.53              |
| 24:DA:284:U:O2'   | 24:DA:285:G:H5'   | 2.08                     | 0.53              |
| 24:DA:377:G:C6    | 24:DA:378:C:C4    | 2.96                     | 0.53              |
| 24:DA:437:U:H2'   | 24:DA:438:G:H8    | 1.74                     | 0.53              |
| 24:DA:686:U:HO2'  | 24:DA:788:A:H2    | 1.56                     | 0.53              |
| 24:DA:818:G:C2'   | 24:DA:819:A:H5''  | 2.38                     | 0.53              |
| 56:DB:13:G:H21    | 56:DB:69:G:H21    | 1.55                     | 0.53              |
| 56:DB:75:G:H2'    | 56:DB:76:G:H5'    | 1.90                     | 0.53              |
| 27:DD:55:LYS:HB3  | 27:DD:75:ALA:HB1  | 1.89                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:DD:94:GLN:HG2  | 27:DD:94:GLN:O    | 2.08                     | 0.53              |
| 31:DH:50:ARG:HA   | 31:DH:53:GLU:CB   | 2.39                     | 0.53              |
| 31:DH:58:LEU:HG   | 31:DH:62:LEU:HD11 | 1.90                     | 0.53              |
| 32:DI:21:PRO:N    | 32:DI:22:PRO:HD2  | 2.24                     | 0.53              |
| 38:DO:31:THR:HG23 | 38:DO:34:HIS:C    | 2.28                     | 0.53              |
| 40:DQ:57:ARG:CZ   | 40:DQ:92:LYS:HE2  | 2.39                     | 0.53              |
| 40:DQ:90:ASP:O    | 40:DQ:94:LEU:HB2  | 2.08                     | 0.53              |
| 43:DT:9:LYS:O     | 43:DT:9:LYS:HG2   | 2.08                     | 0.53              |
| 44:DU:43:LYS:HE3  | 44:DU:45:GLN:CD   | 2.29                     | 0.53              |
| 24:DA:1808:A:N7   | 47:DX:27:ARG:NH1  | 2.57                     | 0.53              |
| 21:AA:1090:U:H3   | 21:AA:1095:U:H3   | 1.54                     | 0.53              |
| 8:AI:67:LYS:HE2   | 21:AA:1148:U:O2'  | 2.09                     | 0.53              |
| 21:AA:1169:A:H2'  | 21:AA:1170:A:C8   | 2.44                     | 0.53              |
| 12:AM:94:LEU:HD11 | 21:AA:1226:C:H5'  | 1.90                     | 0.53              |
| 21:AA:1287:A:H2'  | 21:AA:1288:A:C8   | 2.44                     | 0.53              |
| 21:AA:1423:G:O2'  | 21:AA:1424:U:H5'  | 2.09                     | 0.53              |
| 1:AB:70:GLY:HA2   | 1:AB:163:ILE:HG22 | 1.91                     | 0.53              |
| 2:AC:156:LEU:H    | 2:AC:156:LEU:HD12 | 1.73                     | 0.53              |
| 6:AG:148:LYS:C    | 6:AG:150:PHE:H    | 2.12                     | 0.53              |
| 8:AI:8:THR:H      | 8:AI:84:ARG:HH12  | 1.54                     | 0.53              |
| 11:AL:19:ASN:C    | 11:AL:21:PRO:HD3  | 2.29                     | 0.53              |
| 11:AL:65:TYR:CE1  | 11:AL:67:GLY:HA2  | 2.43                     | 0.53              |
| 19:AT:56:ILE:O    | 19:AT:60:GLN:HG2  | 2.09                     | 0.53              |
| 24:BA:1062:G:C4   | 24:BA:1088:A:N7   | 2.77                     | 0.53              |
| 24:BA:1071:G:C5   | 24:BA:1089:A:N1   | 2.76                     | 0.53              |
| 24:BA:1121:C:H2'  | 24:BA:1122:G:O4'  | 2.08                     | 0.53              |
| 24:BA:1403:A:H2'  | 24:BA:1404:C:H6   | 1.73                     | 0.53              |
| 24:BA:1422:G:C2   | 24:BA:1423:G:C8   | 2.97                     | 0.53              |
| 24:BA:1813:G:N3   | 26:BC:49:THR:CG2  | 2.71                     | 0.53              |
| 24:BA:1858:A:H2'  | 24:BA:1859:U:C6   | 2.43                     | 0.53              |
| 24:BA:2004:G:H2'  | 24:BA:2005:A:H5'  | 1.89                     | 0.53              |
| 24:BA:2078:C:H2'  | 24:BA:2079:U:O4'  | 2.08                     | 0.53              |
| 24:BA:2185:U:H2'  | 24:BA:2186:G:H8   | 1.72                     | 0.53              |
| 24:BA:2298:A:H2'  | 24:BA:2299:U:O4'  | 2.09                     | 0.53              |
| 24:BA:2443:C:O2'  | 24:BA:2444:G:H5'  | 2.07                     | 0.53              |
| 24:BA:2713:U:H3'  | 24:BA:2714:G:H5'' | 1.91                     | 0.53              |
| 24:BA:2847:U:H2'  | 24:BA:2848:G:H5'  | 1.91                     | 0.53              |
| 24:BA:455:C:N4    | 24:BA:473:G:H5'   | 2.23                     | 0.53              |
| 24:BA:17:G:C6     | 24:BA:524:G:C6    | 2.96                     | 0.53              |
| 24:BA:730:A:O2'   | 24:BA:731:C:H5'   | 2.08                     | 0.53              |
| 24:BA:855:G:C2    | 46:BW:23:LYS:HG2  | 2.44                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BC:146:LYS:O   | 26:BC:147:PRO:C    | 2.45                     | 0.53              |
| 30:BG:61:TRP:O    | 30:BG:62:ALA:C     | 2.46                     | 0.53              |
| 31:BH:67:ALA:C    | 31:BH:69:ALA:H     | 2.12                     | 0.53              |
| 35:BL:92:LEU:HA   | 35:BL:125:LEU:HD21 | 1.91                     | 0.53              |
| 37:BN:117:ASP:OD2 | 37:BN:118:ARG:N    | 2.42                     | 0.53              |
| 42:BS:37:THR:HG22 | 42:BS:37:THR:O     | 2.09                     | 0.53              |
| 43:BT:40:LYS:CA   | 43:BT:43:ILE:HG23  | 2.39                     | 0.53              |
| 46:BW:23:LYS:HZ1  | 46:BW:24:ARG:HG3   | 1.72                     | 0.53              |
| 55:CA:1118:U:H1'  | 55:CA:1179:A:C4    | 2.44                     | 0.53              |
| 55:CA:501:C:H1'   | 55:CA:549:C:H1'    | 1.90                     | 0.53              |
| 55:CA:560:A:C8    | 55:CA:566:G:N3     | 2.77                     | 0.53              |
| 55:CA:695:A:H2'   | 55:CA:696:A:O4'    | 2.08                     | 0.53              |
| 55:CA:962:C:N3    | 55:CA:974:A:N6     | 2.57                     | 0.53              |
| 3:CD:109:THR:HG22 | 3:CD:111:ALA:N     | 2.20                     | 0.53              |
| 11:CL:111:GLN:HB3 | 55:CA:538:G:OP2    | 2.09                     | 0.53              |
| 12:CM:15:VAL:O    | 12:CM:19:THR:HG23  | 2.09                     | 0.53              |
| 12:CM:1:ALA:H3    | 12:CM:2:ARG:HH11   | 1.56                     | 0.53              |
| 13:CN:53:ASP:HA   | 13:CN:58:ARG:HD3   | 1.91                     | 0.53              |
| 19:CT:34:VAL:HG22 | 19:CT:49:ALA:CB    | 2.38                     | 0.53              |
| 50:D0:4:GLN:HG2   | 50:D0:4:GLN:O      | 2.09                     | 0.53              |
| 51:D1:8:ILE:HD12  | 51:D1:52:LYS:HG3   | 1.88                     | 0.53              |
| 24:DA:1001:A:H2'  | 24:DA:1002:G:O4'   | 2.09                     | 0.53              |
| 24:DA:579:G:C2    | 24:DA:1262:A:C4    | 2.97                     | 0.53              |
| 24:DA:1266:G:N7   | 42:DS:16:LYS:HE3   | 2.24                     | 0.53              |
| 24:DA:1324:G:O2'  | 24:DA:1616:A:C5    | 2.59                     | 0.53              |
| 24:DA:1359:A:C2   | 24:DA:1360:G:H1'   | 2.44                     | 0.53              |
| 24:DA:1376:C:H5'' | 59:DA:3414:HOH:O   | 2.08                     | 0.53              |
| 24:DA:1608:A:C5   | 24:DA:1611:C:C4    | 2.96                     | 0.53              |
| 24:DA:2370:G:C6   | 24:DA:2371:G:C6    | 2.97                     | 0.53              |
| 24:DA:2418:A:C2   | 24:DA:2419:U:C2    | 2.97                     | 0.53              |
| 24:DA:2758:A:O2'  | 24:DA:2759:G:H5'   | 2.09                     | 0.53              |
| 24:DA:554:U:H2'   | 24:DA:555:G:O4'    | 2.09                     | 0.53              |
| 24:DA:705:A:N6    | 24:DA:726:G:H1'    | 2.23                     | 0.53              |
| 56:DB:61:G:H2'    | 56:DB:62:C:O4'     | 2.09                     | 0.53              |
| 24:DA:1567:G:H5'' | 26:DC:84:PRO:HB3   | 1.90                     | 0.53              |
| 30:DG:149:ALA:O   | 30:DG:151:ARG:N    | 2.42                     | 0.53              |
| 35:DL:3:LEU:C     | 35:DL:3:LEU:HD12   | 2.29                     | 0.53              |
| 44:DU:34:ILE:HG12 | 44:DU:62:ALA:O     | 2.09                     | 0.53              |
| 44:DU:44:HIS:CD2  | 44:DU:57:ILE:HG21  | 2.44                     | 0.53              |
| 44:DU:73:ASN:HB3  | 44:DU:95:PHE:HE2   | 1.73                     | 0.53              |
| 21:AA:386:C:H2'   | 21:AA:387:U:H5'    | 1.91                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:575:G:C8    | 21:AA:881:G:N2     | 2.76                     | 0.53              |
| 21:AA:704:A:H2'   | 21:AA:705:G:C8     | 2.43                     | 0.53              |
| 3:AD:71:PHE:HE1   | 3:AD:199:ILE:HD11  | 1.74                     | 0.53              |
| 5:AF:54:LEU:HD22  | 5:AF:55:HIS:N      | 2.23                     | 0.53              |
| 5:AF:90:MET:HB3   | 17:AR:60:ARG:HH21  | 1.74                     | 0.53              |
| 15:AP:20:VAL:HG23 | 15:AP:34:GLU:O     | 2.08                     | 0.53              |
| 52:B2:34:ARG:NH1  | 52:B2:39:ARG:HG2   | 2.24                     | 0.53              |
| 24:BA:1174:U:O2   | 24:BA:1174:U:H5''  | 2.08                     | 0.53              |
| 24:BA:839:U:H1'   | 24:BA:1191:G:H1'   | 1.90                     | 0.53              |
| 24:BA:1497:U:H5'' | 24:BA:1498:C:OP2   | 2.08                     | 0.53              |
| 24:BA:1682:G:H2'  | 24:BA:1683:U:C6    | 2.44                     | 0.53              |
| 24:BA:264:C:H2'   | 24:BA:265:A:H5''   | 1.89                     | 0.53              |
| 24:BA:355:U:H2'   | 24:BA:356:G:C8     | 2.44                     | 0.53              |
| 24:BA:374:A:C2    | 24:BA:401:A:C4     | 2.96                     | 0.53              |
| 24:BA:463:G:C6    | 24:BA:467:G:C6     | 2.96                     | 0.53              |
| 24:BA:871:U:H2'   | 24:BA:872:U:C6     | 2.44                     | 0.53              |
| 27:BD:110:THR:N   | 27:BD:202:ILE:O    | 2.34                     | 0.53              |
| 29:BF:151:LEU:C   | 29:BF:151:LEU:HD12 | 2.29                     | 0.53              |
| 39:BP:56:SER:C    | 39:BP:75:THR:HG23  | 2.29                     | 0.53              |
| 43:BT:29:THR:CB   | 43:BT:86:THR:HG22  | 2.35                     | 0.53              |
| 55:CA:1219:A:C5   | 55:CA:1220:G:N7    | 2.76                     | 0.53              |
| 55:CA:1245:C:O2'  | 55:CA:1246:A:C5'   | 2.56                     | 0.53              |
| 55:CA:1282:C:O2'  | 55:CA:1283:U:C6    | 2.57                     | 0.53              |
| 55:CA:49:U:O4     | 55:CA:362:G:N2     | 2.42                     | 0.53              |
| 55:CA:685:G:O2'   | 55:CA:686:U:H5'    | 2.09                     | 0.53              |
| 2:CC:6:PRO:O      | 2:CC:9:ILE:HG22    | 2.09                     | 0.53              |
| 24:DA:1181:U:H2'  | 24:DA:1182:G:H8    | 1.72                     | 0.53              |
| 24:DA:1276:A:H4'  | 24:DA:1276:A:OP1   | 2.08                     | 0.53              |
| 24:DA:1338:G:H5'' | 43:DT:17:SER:HB3   | 1.89                     | 0.53              |
| 24:DA:1428:C:O2'  | 24:DA:1429:G:H5'   | 2.09                     | 0.53              |
| 24:DA:1439:A:C8   | 24:DA:1440:U:C6    | 2.97                     | 0.53              |
| 24:DA:1578:U:O2'  | 24:DA:1579:A:H5'   | 2.09                     | 0.53              |
| 24:DA:2262:U:H1'  | 24:DA:2328:A:H1'   | 1.91                     | 0.53              |
| 24:DA:2348:U:O2'  | 24:DA:2349:G:O4'   | 2.22                     | 0.53              |
| 24:DA:2542:A:H4'  | 24:DA:2543:G:C5'   | 2.37                     | 0.53              |
| 24:DA:2556:C:H2'  | 24:DA:2557:G:O4'   | 2.08                     | 0.53              |
| 24:DA:2591:C:H2'  | 24:DA:2592:G:C8    | 2.44                     | 0.53              |
| 24:DA:2636:C:H4'  | 27:DD:81:GLU:OE2   | 2.08                     | 0.53              |
| 24:DA:739:A:O2'   | 24:DA:740:C:C5     | 2.61                     | 0.53              |
| 26:DC:43:ASN:ND2  | 26:DC:44:ASN:N     | 2.55                     | 0.53              |
| 34:DK:17:ARG:HD3  | 34:DK:18:ARG:HG3   | 1.90                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DL:73:ILE:O     | 35:DL:105:ILE:HG23 | 2.08                     | 0.53              |
| 36:DM:73:ILE:HG21  | 36:DM:91:TYR:CZ    | 2.43                     | 0.53              |
| 21:AA:1331:G:C2'   | 21:AA:1332:A:OP2   | 2.57                     | 0.53              |
| 21:AA:181:A:N6     | 21:AA:195:A:OP2    | 2.42                     | 0.53              |
| 10:AK:63:GLN:HG3   | 10:AK:98:ALA:CB    | 2.39                     | 0.53              |
| 13:AN:86:ALA:HA    | 13:AN:89:ARG:HH21  | 1.73                     | 0.53              |
| 16:AQ:59:GLU:HG2   | 16:AQ:60:ILE:N     | 2.23                     | 0.53              |
| 24:BA:1142:A:C5    | 24:BA:1144:A:C5    | 2.96                     | 0.53              |
| 24:BA:1202:G:C6    | 24:BA:1203:U:N3    | 2.76                     | 0.53              |
| 24:BA:1224:U:C4    | 24:BA:1225:G:C6    | 2.97                     | 0.53              |
| 24:BA:1333:G:C2    | 24:BA:1334:G:C8    | 2.96                     | 0.53              |
| 24:BA:1850:G:C6    | 24:BA:1851:U:C4    | 2.97                     | 0.53              |
| 24:BA:2070:A:C2    | 24:BA:2442:C:C2    | 2.96                     | 0.53              |
| 24:BA:2147:A:H3'   | 24:BA:2148:G:H5'   | 1.90                     | 0.53              |
| 24:BA:2268:A:H8    | 24:BA:2268:A:O5'   | 1.91                     | 0.53              |
| 24:BA:2297:A:C5    | 24:BA:2320:U:N3    | 2.77                     | 0.53              |
| 24:BA:2683:C:H4'   | 27:BD:13:ARG:HH22  | 1.73                     | 0.53              |
| 24:BA:371:A:N6     | 24:BA:401:A:H3'    | 2.22                     | 0.53              |
| 24:BA:459:U:O2'    | 24:BA:460:A:C5'    | 2.44                     | 0.53              |
| 25:BB:73:A:C4      | 25:BB:104:A:C2     | 2.96                     | 0.53              |
| 28:BE:119:ILE:O    | 28:BE:119:ILE:HG12 | 2.07                     | 0.53              |
| 28:BE:148:ILE:HD13 | 28:BE:187:VAL:CG2  | 2.38                     | 0.53              |
| 33:BJ:44:TYR:O     | 33:BJ:45:THR:CB    | 2.56                     | 0.53              |
| 38:BO:34:HIS:CD2   | 38:BO:53:THR:O     | 2.61                     | 0.53              |
| 47:BX:14:GLY:O     | 47:BX:26:ARG:N     | 2.39                     | 0.53              |
| 55:CA:1441:A:H2'   | 55:CA:1442:G:C8    | 2.44                     | 0.53              |
| 55:CA:429:U:C1'    | 55:CA:430:A:H5''   | 2.39                     | 0.53              |
| 55:CA:429:U:H4'    | 55:CA:430:A:O5'    | 2.09                     | 0.53              |
| 11:CL:114:SER:OG   | 55:CA:501:C:O3'    | 2.27                     | 0.53              |
| 3:CD:20:LEU:O      | 3:CD:21:LYS:C      | 2.46                     | 0.53              |
| 9:CJ:38:GLY:O      | 9:CJ:40:ILE:HD12   | 2.09                     | 0.53              |
| 9:CJ:40:ILE:HG12   | 55:CA:1125:U:C5    | 2.43                     | 0.53              |
| 24:DA:1035:U:H2'   | 24:DA:1036:G:H8    | 1.73                     | 0.53              |
| 24:DA:1090:A:C2'   | 24:DA:1091:G:H5''  | 2.39                     | 0.53              |
| 24:DA:1135:C:N4    | 24:DA:1139:G:C6    | 2.76                     | 0.53              |
| 24:DA:1511:G:O2'   | 24:DA:1512:C:O4'   | 2.27                     | 0.53              |
| 24:DA:164:C:H2'    | 24:DA:165:A:O4'    | 2.09                     | 0.53              |
| 24:DA:201:C:C5     | 24:DA:202:U:C5     | 2.97                     | 0.53              |
| 24:DA:2536:G:C6    | 24:DA:2537:U:C4    | 2.97                     | 0.53              |
| 24:DA:444:C:O2'    | 24:DA:445:C:C5'    | 2.56                     | 0.53              |
| 24:DA:615:U:H5''   | 24:DA:616:A:C8     | 2.43                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:616:A:O2'    | 24:DA:617:G:C5'    | 2.56                     | 0.53              |
| 24:DA:70:G:H5'     | 24:DA:112:U:O2     | 2.08                     | 0.53              |
| 24:DA:976:G:H2'    | 24:DA:977:G:H8     | 1.73                     | 0.53              |
| 28:DE:146:VAL:O    | 28:DE:167:VAL:HA   | 2.09                     | 0.53              |
| 34:DK:10:VAL:HG13  | 34:DK:12:ASP:OD1   | 2.09                     | 0.53              |
| 40:DQ:18:LYS:HD2   | 40:DQ:18:LYS:O     | 2.09                     | 0.53              |
| 41:DR:2:TYR:HE1    | 41:DR:13:ARG:HD2   | 1.73                     | 0.53              |
| 42:DS:32:ALA:O     | 42:DS:33:LEU:HB2   | 2.09                     | 0.53              |
| 45:DV:72:VAL:HA    | 45:DV:92:VAL:O     | 2.09                     | 0.53              |
| 49:DZ:6:ILE:HD12   | 49:DZ:47:ILE:HD11  | 1.90                     | 0.53              |
| 21:AA:1074:G:N1    | 21:AA:1102:A:C6    | 2.77                     | 0.53              |
| 21:AA:1095:U:C5'   | 21:AA:1109:C:O2    | 2.56                     | 0.53              |
| 21:AA:1120:C:H2'   | 21:AA:1121:U:H6    | 1.74                     | 0.53              |
| 21:AA:243:A:N3     | 21:AA:245:U:H2'    | 2.23                     | 0.53              |
| 21:AA:532:A:HO2'   | 21:AA:533:A:P      | 2.32                     | 0.53              |
| 21:AA:638:U:H2'    | 21:AA:639:G:O4'    | 2.09                     | 0.53              |
| 21:AA:88:U:O2      | 21:AA:89:U:C6      | 2.62                     | 0.53              |
| 21:AA:94:G:H5''    | 21:AA:95:C:C6      | 2.44                     | 0.53              |
| 1:AB:143:LEU:HD12  | 1:AB:147:LEU:CD1   | 2.38                     | 0.53              |
| 1:AB:65:LYS:HG2    | 1:AB:153:MET:SD    | 2.49                     | 0.53              |
| 1:AB:67:LEU:HD21   | 1:AB:91:VAL:CG2    | 2.39                     | 0.53              |
| 2:AC:1:GLY:O       | 21:AA:1061:G:OP2   | 2.27                     | 0.53              |
| 2:AC:79:LYS:N      | 2:AC:79:LYS:HE3    | 2.24                     | 0.53              |
| 4:AE:115:GLU:HG2   | 4:AE:120:HIS:NE2   | 2.24                     | 0.53              |
| 5:AF:3:HIS:ND1     | 5:AF:65:GLU:HB2    | 2.24                     | 0.53              |
| 6:AG:23:ALA:O      | 6:AG:26:VAL:HG22   | 2.08                     | 0.53              |
| 10:AK:86:LYS:HG3   | 10:AK:114:PRO:HD3  | 1.90                     | 0.53              |
| 50:B0:29:VAL:HG13  | 50:B0:34:GLY:O     | 2.08                     | 0.53              |
| 24:BA:1032:A:H1'   | 54:B4:23:ILE:HD13  | 1.91                     | 0.53              |
| 24:BA:1506:U:H2'   | 24:BA:1507:C:C6    | 2.43                     | 0.53              |
| 24:BA:2209:G:C2    | 24:BA:2216:G:C2    | 2.97                     | 0.53              |
| 24:BA:2514:U:H2'   | 24:BA:2515:C:C6    | 2.44                     | 0.53              |
| 24:BA:2527:C:C5    | 24:BA:2528:U:C5    | 2.96                     | 0.53              |
| 24:BA:216:A:N7     | 24:BA:432:A:C5     | 2.77                     | 0.53              |
| 24:BA:528:A:C8     | 24:BA:528:A:H3'    | 2.42                     | 0.53              |
| 24:BA:747:U:C5     | 24:BA:2613:U:C5    | 2.96                     | 0.53              |
| 24:BA:958:U:C2     | 25:BB:89:U:O2'     | 2.62                     | 0.53              |
| 26:BC:90:ILE:HG21  | 26:BC:102:TYR:CE1  | 2.44                     | 0.53              |
| 26:BC:254:LYS:O    | 26:BC:256:THR:N    | 2.40                     | 0.53              |
| 28:BE:112:LEU:HD13 | 28:BE:186:VAL:HG11 | 1.90                     | 0.53              |
| 29:BF:114:ARG:HD2  | 29:BF:114:ARG:N    | 2.20                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:BP:67:GLU:HG3  | 39:BP:68:GLY:N     | 2.20                     | 0.53              |
| 39:BP:3:ILE:O     | 39:BP:7:LEU:HB2    | 2.09                     | 0.53              |
| 45:BV:4:ILE:O     | 45:BV:63:ILE:HA    | 2.09                     | 0.53              |
| 48:BY:45:GLN:O    | 48:BY:46:VAL:CB    | 2.51                     | 0.53              |
| 55:CA:1347:G:H22  | 55:CA:1373:G:H2'   | 1.73                     | 0.53              |
| 55:CA:517:G:N2    | 55:CA:533:A:OP2    | 2.42                     | 0.53              |
| 55:CA:551:U:N3    | 55:CA:552:U:C4     | 2.76                     | 0.53              |
| 55:CA:995:C:N3    | 55:CA:1046:A:O2'   | 2.42                     | 0.53              |
| 1:CB:146:SER:HB2  | 1:CB:147:LEU:HD12  | 1.91                     | 0.53              |
| 1:CB:159:ALA:HB1  | 1:CB:183:PHE:HE1   | 1.73                     | 0.53              |
| 7:CH:33:VAL:HG22  | 7:CH:58:LEU:CD1    | 2.39                     | 0.53              |
| 12:CM:75:SER:HB2  | 12:CM:79:LEU:HG    | 1.90                     | 0.53              |
| 17:CR:61:ALA:HB1  | 17:CR:67:LEU:HG    | 1.91                     | 0.53              |
| 52:D2:19:ARG:HH21 | 52:D2:19:ARG:CB    | 2.20                     | 0.53              |
| 24:DA:1153:C:H2'  | 24:DA:1154:G:C8    | 2.44                     | 0.53              |
| 24:DA:1286:A:H1'  | 24:DA:1288:G:N2    | 2.24                     | 0.53              |
| 24:DA:138:U:H2'   | 24:DA:140:C:H1'    | 1.89                     | 0.53              |
| 24:DA:1945:G:O2'  | 24:DA:1946:U:H5'   | 2.09                     | 0.53              |
| 24:DA:2143:C:H3'  | 24:DA:2144:G:C8    | 2.43                     | 0.53              |
| 24:DA:2660:A:H2   | 24:DA:2661:G:N7    | 2.06                     | 0.53              |
| 24:DA:540:C:H2'   | 24:DA:541:A:C8     | 2.44                     | 0.53              |
| 24:DA:856:G:C1'   | 46:DW:23:LYS:HB3   | 2.38                     | 0.53              |
| 27:DD:124:ARG:NH1 | 27:DD:125:TRP:CE2  | 2.77                     | 0.53              |
| 28:DE:73:ILE:O    | 28:DE:73:ILE:HG13  | 2.09                     | 0.53              |
| 30:DG:28:LYS:H    | 30:DG:79:THR:HG22  | 1.73                     | 0.53              |
| 33:DJ:36:LEU:HD21 | 33:DJ:122:LEU:HD13 | 1.91                     | 0.53              |
| 37:DN:78:LYS:O    | 37:DN:82:GLU:HB3   | 2.08                     | 0.53              |
| 34:DK:77:ILE:HG23 | 39:DP:71:ARG:HD2   | 1.91                     | 0.53              |
| 41:DR:49:ILE:HB   | 41:DR:51:VAL:O     | 2.09                     | 0.53              |
| 44:DU:85:ARG:HE   | 44:DU:85:ARG:HA    | 1.73                     | 0.53              |
| 45:DV:61:LEU:O    | 45:DV:72:VAL:HG22  | 2.09                     | 0.53              |
| 48:DY:4:LYS:HZ3   | 48:DY:4:LYS:HB2    | 1.74                     | 0.53              |
| 21:AA:1239:A:H5'  | 21:AA:1240:U:OP1   | 2.09                     | 0.53              |
| 21:AA:1261:A:C2   | 21:AA:1275:A:C6    | 2.96                     | 0.53              |
| 21:AA:497:G:HO2'  | 21:AA:498:A:H8     | 1.43                     | 0.53              |
| 21:AA:627:G:H2'   | 21:AA:628:G:O4'    | 2.09                     | 0.53              |
| 21:AA:817:C:C5    | 21:AA:819:A:H1'    | 2.44                     | 0.53              |
| 9:AJ:59:LYS:HE3   | 21:AA:972:C:P      | 2.49                     | 0.53              |
| 1:AB:142:LYS:HZ1  | 21:AA:1098:C:P     | 2.32                     | 0.53              |
| 1:AB:46:VAL:HA    | 1:AB:49:PHE:CE2    | 2.43                     | 0.53              |
| 3:AD:71:PHE:CE1   | 3:AD:199:ILE:HD11  | 2.44                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:AH:77:VAL:HG12   | 7:AH:78:SER:N     | 2.24                     | 0.53              |
| 13:AN:4:SER:HB2    | 21:AA:1216:A:H5'' | 1.91                     | 0.53              |
| 20:AU:39:LYS:H     | 20:AU:40:PRO:HD2  | 1.73                     | 0.53              |
| 51:B1:31:GLU:O     | 51:B1:31:GLU:HG2  | 2.09                     | 0.53              |
| 24:BA:1421:G:C2    | 24:BA:1422:G:C8   | 2.97                     | 0.53              |
| 24:BA:2103:C:C2'   | 24:BA:2104:C:H5'  | 2.38                     | 0.53              |
| 24:BA:2305:U:C2'   | 24:BA:2306:C:O4'  | 2.55                     | 0.53              |
| 24:BA:2854:G:H2'   | 24:BA:2855:C:C6   | 2.43                     | 0.53              |
| 24:BA:376:G:O2'    | 24:BA:377:G:H5'   | 2.09                     | 0.53              |
| 24:BA:910:A:H2'    | 24:BA:911:A:C8    | 2.44                     | 0.53              |
| 25:BB:30:C:H2'     | 25:BB:30:C:O2     | 2.08                     | 0.53              |
| 28:BE:12:LEU:O     | 28:BE:13:THR:HB   | 2.09                     | 0.53              |
| 28:BE:153:LEU:HD12 | 28:BE:153:LEU:C   | 2.29                     | 0.53              |
| 29:BF:7:TYR:O      | 29:BF:12:VAL:HG12 | 2.09                     | 0.53              |
| 30:BG:156:TYR:O    | 30:BG:157:LYS:HG3 | 2.09                     | 0.53              |
| 31:BH:43:ASN:HD22  | 31:BH:43:ASN:N    | 2.07                     | 0.53              |
| 34:BK:20:MET:O     | 34:BK:42:THR:HG22 | 2.08                     | 0.53              |
| 35:BL:93:ASN:O     | 35:BL:94:THR:HG22 | 2.08                     | 0.53              |
| 43:BT:39:THR:CG2   | 43:BT:39:THR:O    | 2.57                     | 0.53              |
| 48:BY:9:LYS:HB3    | 48:BY:12:GLU:HB2  | 1.90                     | 0.53              |
| 55:CA:1156:G:HO2'  | 55:CA:1180:A:H61  | 1.57                     | 0.53              |
| 55:CA:441:A:H61    | 55:CA:493:A:H62   | 1.57                     | 0.53              |
| 55:CA:596:A:HO2'   | 55:CA:597:G:H8    | 1.55                     | 0.53              |
| 55:CA:891:U:O2'    | 55:CA:892:A:C5'   | 2.57                     | 0.53              |
| 2:CC:181:ILE:HG23  | 2:CC:201:ILE:O    | 2.09                     | 0.53              |
| 4:CE:29:ILE:CG2    | 4:CE:30:PHE:N     | 2.70                     | 0.53              |
| 4:CE:45:VAL:HG12   | 4:CE:73:VAL:HG21  | 1.91                     | 0.53              |
| 6:CG:115:MET:SD    | 6:CG:118:ARG:HB2  | 2.49                     | 0.53              |
| 7:CH:65:PHE:CE2    | 7:CH:66:GLN:HG2   | 2.44                     | 0.53              |
| 8:CI:24:ASN:HD22   | 8:CI:26:LYS:CG    | 2.22                     | 0.53              |
| 10:CK:63:GLN:HG3   | 10:CK:64:VAL:N    | 2.23                     | 0.53              |
| 12:CM:89:ARG:NE    | 12:CM:94:LEU:HB2  | 2.24                     | 0.53              |
| 17:CR:47:ARG:HD2   | 17:CR:50:TYR:CD2  | 2.44                     | 0.53              |
| 18:CS:55:GLN:CD    | 18:CS:56:HIS:H    | 2.12                     | 0.53              |
| 24:DA:2286:G:N7    | 51:D1:33:LEU:HD23 | 2.24                     | 0.53              |
| 24:DA:99:U:O3'     | 24:DA:100:U:H3'   | 2.07                     | 0.53              |
| 24:DA:1274:A:C6    | 24:DA:1302:A:C2   | 2.97                     | 0.53              |
| 24:DA:1621:U:H5''  | 24:DA:1622:G:OP1  | 2.09                     | 0.53              |
| 24:DA:1789:A:H2'   | 24:DA:1790:C:C6   | 2.44                     | 0.53              |
| 24:DA:1992:G:N2    | 24:DA:1995:U:C5   | 2.77                     | 0.53              |
| 24:DA:20:C:O2'     | 24:DA:21:A:H5'    | 2.08                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:2314:A:H2'  | 24:DA:2315:G:H8    | 1.72                     | 0.53              |
| 24:DA:288:U:H2'   | 24:DA:289:G:C8     | 2.44                     | 0.53              |
| 24:DA:656:G:O2'   | 24:DA:657:U:C5'    | 2.57                     | 0.53              |
| 27:DD:99:GLU:HG3  | 27:DD:100:LEU:N    | 2.24                     | 0.53              |
| 31:DH:132:PHE:HB3 | 31:DH:140:ALA:CB   | 2.38                     | 0.53              |
| 31:DH:22:LYS:HB3  | 31:DH:22:LYS:NZ    | 2.24                     | 0.53              |
| 31:DH:32:PRO:HA   | 47:DX:38:TRP:HD1   | 1.74                     | 0.53              |
| 33:DJ:92:MET:CE   | 33:DJ:92:MET:HA    | 2.39                     | 0.53              |
| 36:DM:41:LEU:O    | 36:DM:93:VAL:HG23  | 2.08                     | 0.53              |
| 37:DN:72:ASP:O    | 37:DN:75:ILE:HG13  | 2.09                     | 0.53              |
| 37:DN:92:GLY:H    | 37:DN:94:TYR:HE1   | 1.54                     | 0.53              |
| 41:DR:24:LYS:HA   | 41:DR:94:THR:HG23  | 1.91                     | 0.53              |
| 44:DU:43:LYS:HE3  | 44:DU:45:GLN:CG    | 2.39                     | 0.53              |
| 21:AA:1138:G:C2'  | 21:AA:1138:G:N3    | 2.68                     | 0.52              |
| 21:AA:1356:G:N2   | 21:AA:1357:A:C2    | 2.76                     | 0.52              |
| 21:AA:505:G:H2'   | 21:AA:506:G:H8     | 1.73                     | 0.52              |
| 21:AA:587:G:C2    | 21:AA:755:G:C6     | 2.96                     | 0.52              |
| 21:AA:690:G:H2'   | 21:AA:691:G:O4'    | 2.08                     | 0.52              |
| 21:AA:938:A:N1    | 21:AA:939:G:C5     | 2.77                     | 0.52              |
| 1:AB:41:ASN:HD22  | 1:AB:42:LEU:N      | 2.05                     | 0.52              |
| 4:AE:37:VAL:HG11  | 4:AE:113:VAL:CB    | 2.39                     | 0.52              |
| 6:AG:78:ARG:NH2   | 6:AG:81:GLY:HA2    | 2.23                     | 0.52              |
| 6:AG:83:THR:HG22  | 6:AG:85:GLN:H      | 1.73                     | 0.52              |
| 10:AK:66:ALA:HB1  | 10:AK:99:LEU:CD1   | 2.36                     | 0.52              |
| 24:BA:1522:A:O2'  | 24:BA:1523:U:OP2   | 2.27                     | 0.52              |
| 24:BA:1964:G:C6   | 24:BA:1967:C:N4    | 2.77                     | 0.52              |
| 24:BA:235:U:H2'   | 24:BA:236:C:H6     | 1.73                     | 0.52              |
| 24:BA:2420:C:OP1  | 53:B3:33:THR:HB    | 2.08                     | 0.52              |
| 24:BA:435:C:O2'   | 24:BA:436:C:C5'    | 2.57                     | 0.52              |
| 24:BA:811:U:O2'   | 24:BA:1250:G:H2'   | 2.09                     | 0.52              |
| 27:BD:149:ASN:OD1 | 27:BD:150:GLN:N    | 2.42                     | 0.52              |
| 27:BD:16:THR:HG22 | 27:BD:20:VAL:O     | 2.10                     | 0.52              |
| 29:BF:129:MET:SD  | 29:BF:153:ILE:HD11 | 2.49                     | 0.52              |
| 33:BJ:67:ASN:O    | 33:BJ:69:ARG:N     | 2.42                     | 0.52              |
| 36:BM:126:ILE:O   | 36:BM:128:THR:HG23 | 2.08                     | 0.52              |
| 36:BM:93:VAL:HG22 | 36:BM:94:ALA:N     | 2.24                     | 0.52              |
| 24:BA:1156:A:C8   | 40:BQ:50:ARG:HG2   | 2.45                     | 0.52              |
| 44:BU:25:LYS:O    | 44:BU:26:ASN:HB3   | 2.08                     | 0.52              |
| 55:CA:1215:G:N3   | 55:CA:1216:A:C8    | 2.77                     | 0.52              |
| 55:CA:1441:A:H62  | 55:CA:1462:C:H1'   | 1.74                     | 0.52              |
| 55:CA:322:C:O2    | 55:CA:332:G:N2     | 2.42                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:358:U:H2'   | 55:CA:359:G:C8    | 2.43                     | 0.52              |
| 2:CC:135:ARG:HA   | 2:CC:138:GLN:OE1  | 2.09                     | 0.52              |
| 3:CD:151:GLN:O    | 3:CD:154:VAL:HG12 | 2.09                     | 0.52              |
| 2:CC:22:PHE:HD1   | 9:CJ:13:PHE:CD1   | 2.27                     | 0.52              |
| 17:CR:46:THR:HG23 | 17:CR:51:GLN:HB2  | 1.92                     | 0.52              |
| 12:CM:82:LEU:HB2  | 18:CS:73:PHE:HE2  | 1.75                     | 0.52              |
| 10:CK:124:LYS:O   | 20:CU:33:ARG:NE   | 2.41                     | 0.52              |
| 24:DA:1178:C:C2   | 24:DA:1179:G:C8   | 2.98                     | 0.52              |
| 24:DA:1277:G:H2'  | 24:DA:1278:C:C6   | 2.43                     | 0.52              |
| 24:DA:1327:A:H2'  | 24:DA:1328:A:C8   | 2.44                     | 0.52              |
| 24:DA:1439:A:N6   | 24:DA:1440:U:O2   | 2.42                     | 0.52              |
| 24:DA:1512:C:H2'  | 24:DA:1513:U:O4'  | 2.09                     | 0.52              |
| 24:DA:1537:G:H2'  | 24:DA:1538:G:C4'  | 2.21                     | 0.52              |
| 24:DA:2056:G:H2'  | 24:DA:2056:G:N3   | 2.24                     | 0.52              |
| 24:DA:2084:C:H2'  | 24:DA:2085:U:C6   | 2.44                     | 0.52              |
| 24:DA:2193:G:H2'  | 24:DA:2194:U:C6   | 2.44                     | 0.52              |
| 24:DA:2313:C:O2'  | 24:DA:2314:A:C5'  | 2.43                     | 0.52              |
| 24:DA:2387:U:H1'  | 46:DW:38:ARG:NH1  | 2.23                     | 0.52              |
| 24:DA:2734:A:H61  | 24:DA:2770:G:H1'  | 1.72                     | 0.52              |
| 24:DA:344:A:H2'   | 24:DA:345:A:C8    | 2.44                     | 0.52              |
| 24:DA:687:C:O2'   | 24:DA:688:U:H5'   | 2.09                     | 0.52              |
| 26:DC:43:ASN:CG   | 26:DC:44:ASN:H    | 2.12                     | 0.52              |
| 29:DF:73:VAL:O    | 29:DF:73:VAL:HG12 | 2.08                     | 0.52              |
| 30:DG:74:MET:O    | 30:DG:78:VAL:HG13 | 2.09                     | 0.52              |
| 35:DL:29:LYS:HG2  | 35:DL:30:THR:HG23 | 1.90                     | 0.52              |
| 37:DN:51:LEU:HA   | 37:DN:54:LEU:CD2  | 2.40                     | 0.52              |
| 38:DO:56:LYS:HD3  | 38:DO:56:LYS:O    | 2.09                     | 0.52              |
| 40:DQ:6:GLY:C     | 40:DQ:8:ILE:H     | 2.12                     | 0.52              |
| 24:DA:381:G:H5'   | 47:DX:15:ASN:HD22 | 1.73                     | 0.52              |
| 48:DY:17:GLU:HG2  | 48:DY:50:VAL:HG13 | 1.91                     | 0.52              |
| 21:AA:1026:G:C6   | 21:AA:1027:C:N4   | 2.77                     | 0.52              |
| 21:AA:1088:G:N1   | 21:AA:1089:G:C5   | 2.77                     | 0.52              |
| 21:AA:1136:C:H5'' | 21:AA:1137:C:OP2  | 2.10                     | 0.52              |
| 21:AA:1160:G:C6   | 21:AA:1181:G:O6   | 2.63                     | 0.52              |
| 21:AA:1418:A:N7   | 21:AA:1419:G:H1'  | 2.25                     | 0.52              |
| 21:AA:243:A:C2    | 21:AA:245:U:H2'   | 2.44                     | 0.52              |
| 21:AA:429:U:H1'   | 21:AA:430:A:H5''  | 1.91                     | 0.52              |
| 21:AA:439:U:C2'   | 21:AA:440:C:H5'   | 2.39                     | 0.52              |
| 21:AA:845:A:C8    | 21:AA:846:G:H4'   | 2.43                     | 0.52              |
| 4:AE:34:ALA:O     | 4:AE:49:TYR:CG    | 2.62                     | 0.52              |
| 8:AI:107:ALA:O    | 8:AI:109:GLN:HG2  | 2.10                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:AI:98:ARG:NH2   | 21:AA:1179:A:H5''  | 2.24                     | 0.52              |
| 12:AM:100:ARG:NH2 | 21:AA:951:G:OP2    | 2.42                     | 0.52              |
| 24:BA:1333:G:H2'  | 24:BA:1334:G:C8    | 2.39                     | 0.52              |
| 24:BA:142:A:O2'   | 24:BA:143:C:O4'    | 2.19                     | 0.52              |
| 24:BA:1450:G:H2'  | 24:BA:1451:C:C6    | 2.44                     | 0.52              |
| 24:BA:1665:A:C2'  | 24:BA:1666:G:H5'   | 2.39                     | 0.52              |
| 24:BA:1885:A:O2'  | 24:BA:1886:U:H5'   | 2.09                     | 0.52              |
| 24:BA:2834:G:O6   | 24:BA:2879:A:H2'   | 2.09                     | 0.52              |
| 27:BD:120:GLY:HA2 | 27:BD:162:ALA:HB1  | 1.91                     | 0.52              |
| 27:BD:35:THR:OG1  | 27:BD:49:GLN:HG2   | 2.09                     | 0.52              |
| 27:BD:97:SER:O    | 27:BD:99:GLU:HG2   | 2.09                     | 0.52              |
| 24:BA:615:U:C4    | 28:BE:35:TYR:CE1   | 2.97                     | 0.52              |
| 35:BL:101:ILE:CG2 | 35:BL:102:GLY:N    | 2.73                     | 0.52              |
| 35:BL:55:MET:HE2  | 35:BL:56:PRO:HD3   | 1.91                     | 0.52              |
| 43:BT:80:TRP:HE3  | 43:BT:81:LYS:O     | 1.93                     | 0.52              |
| 55:CA:1241:G:O2'  | 55:CA:1242:G:O5'   | 2.27                     | 0.52              |
| 55:CA:143:A:N3    | 55:CA:143:A:H2'    | 2.23                     | 0.52              |
| 55:CA:560:A:C8    | 55:CA:566:G:C2     | 2.97                     | 0.52              |
| 55:CA:82:G:H2'    | 55:CA:83:C:C4'     | 2.25                     | 0.52              |
| 1:CB:104:LYS:N    | 1:CB:104:LYS:HD2   | 2.13                     | 0.52              |
| 1:CB:174:GLU:O    | 1:CB:178:LEU:HB2   | 2.09                     | 0.52              |
| 2:CC:129:PHE:O    | 2:CC:132:ALA:HB3   | 2.08                     | 0.52              |
| 3:CD:72:ARG:HD2   | 3:CD:203:TYR:CD1   | 2.44                     | 0.52              |
| 5:CF:3:HIS:ND1    | 5:CF:92:THR:HG23   | 2.24                     | 0.52              |
| 7:CH:44:PHE:O     | 7:CH:70:VAL:HG11   | 2.09                     | 0.52              |
| 11:CL:80:LEU:HB2  | 11:CL:101:LEU:HD23 | 1.91                     | 0.52              |
| 16:CQ:26:ARG:O    | 16:CQ:38:LYS:HA    | 2.09                     | 0.52              |
| 24:DA:1071:G:O4'  | 24:DA:1088:A:O2'   | 2.28                     | 0.52              |
| 24:DA:1358:G:O6   | 24:DA:1371:G:C8    | 2.63                     | 0.52              |
| 24:DA:1439:A:N3   | 24:DA:1552:A:C6    | 2.77                     | 0.52              |
| 24:DA:1508:A:C4'  | 24:DA:1509:A:OP1   | 2.53                     | 0.52              |
| 24:DA:1759:A:O2'  | 24:DA:1760:C:H5'   | 2.08                     | 0.52              |
| 24:DA:284:U:H2'   | 24:DA:285:G:H8     | 1.74                     | 0.52              |
| 24:DA:296:U:H5''  | 44:DU:91:LYS:NZ    | 2.23                     | 0.52              |
| 24:DA:352:A:H2'   | 24:DA:353:C:H4'    | 1.90                     | 0.52              |
| 24:DA:36:G:H4'    | 24:DA:451:U:C2     | 2.45                     | 0.52              |
| 24:DA:615:U:H5''  | 24:DA:616:A:H8     | 1.74                     | 0.52              |
| 26:DC:75:ALA:HB1  | 26:DC:93:VAL:HG22  | 1.90                     | 0.52              |
| 29:DF:45:ASP:C    | 29:DF:47:LYS:H     | 2.12                     | 0.52              |
| 33:DJ:110:PRO:HG2 | 33:DJ:111:LYS:HG2  | 1.91                     | 0.52              |
| 33:DJ:123:LYS:HG2 | 33:DJ:132:HIS:NE2  | 2.24                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:DP:13:LYS:H     | 39:DP:13:LYS:HD2   | 1.74                     | 0.52              |
| 24:DA:2847:U:H3'   | 39:DP:94:ALA:HB2   | 1.89                     | 0.52              |
| 43:DT:8:LEU:HD22   | 43:DT:46:ALA:HA    | 1.90                     | 0.52              |
| 44:DU:47:PRO:HB3   | 44:DU:54:PRO:HG3   | 1.90                     | 0.52              |
| 21:AA:1090:U:O2'   | 21:AA:1091:U:H5'   | 2.09                     | 0.52              |
| 21:AA:1103:C:O2'   | 21:AA:1104:G:O4'   | 2.16                     | 0.52              |
| 9:AJ:15:HIS:CD2    | 21:AA:1152:A:H5'   | 2.44                     | 0.52              |
| 21:AA:488:C:H2'    | 21:AA:489:C:H6     | 1.74                     | 0.52              |
| 21:AA:792:A:C2     | 21:AA:794:A:C6     | 2.97                     | 0.52              |
| 1:AB:140:LEU:O     | 1:AB:143:LEU:HD23  | 2.09                     | 0.52              |
| 3:AD:187:ARG:HE    | 3:AD:196:GLU:CD    | 2.13                     | 0.52              |
| 6:AG:149:ALA:HA    | 10:AK:60:PHE:CB    | 2.40                     | 0.52              |
| 6:AG:35:LYS:O      | 6:AG:39:GLU:HG2    | 2.10                     | 0.52              |
| 10:AK:26:PHE:CE1   | 10:AK:88:PRO:HG2   | 2.44                     | 0.52              |
| 12:AM:39:ALA:HB3   | 12:AM:42:VAL:CG1   | 2.39                     | 0.52              |
| 50:B0:30:ASP:O     | 50:B0:33:SER:O     | 2.26                     | 0.52              |
| 24:BA:1011:G:O2'   | 24:BA:1013:C:H5''  | 2.10                     | 0.52              |
| 24:BA:1441:G:H2'   | 24:BA:1442:U:C6    | 2.45                     | 0.52              |
| 24:BA:1468:U:N3    | 24:BA:1522:A:C2    | 2.78                     | 0.52              |
| 24:BA:2216:G:C6    | 24:BA:2217:G:C6    | 2.97                     | 0.52              |
| 24:BA:2295:C:O2'   | 24:BA:2296:U:H5'   | 2.09                     | 0.52              |
| 24:BA:197:A:C6     | 24:BA:2430:A:C2    | 2.97                     | 0.52              |
| 24:BA:2553:G:N1    | 24:BA:2554:U:O2    | 2.42                     | 0.52              |
| 24:BA:2555:U:H2'   | 24:BA:2556:C:O4'   | 2.09                     | 0.52              |
| 24:BA:2860:A:C8    | 24:BA:2860:A:H3'   | 2.44                     | 0.52              |
| 24:BA:34:U:H4'     | 24:BA:35:G:OP2     | 2.10                     | 0.52              |
| 24:BA:449:A:C4'    | 40:BQ:2:ARG:NH1    | 2.73                     | 0.52              |
| 24:BA:498:G:N2     | 24:BA:499:U:C2     | 2.78                     | 0.52              |
| 24:BA:580:U:H2'    | 24:BA:581:C:C6     | 2.45                     | 0.52              |
| 24:BA:604:G:H2'    | 24:BA:605:G:C8     | 2.43                     | 0.52              |
| 24:BA:604:G:H2'    | 24:BA:605:G:H8     | 1.74                     | 0.52              |
| 24:BA:966:G:H2'    | 24:BA:967:U:O4'    | 2.09                     | 0.52              |
| 25:BB:109:A:H2'    | 25:BB:110:C:C6     | 2.44                     | 0.52              |
| 25:BB:55:U:O2'     | 25:BB:56:G:H5'     | 2.09                     | 0.52              |
| 26:BC:114:GLN:O    | 26:BC:115:ILE:HD13 | 2.09                     | 0.52              |
| 26:BC:170:TYR:CD2  | 26:BC:184:GLU:HA   | 2.43                     | 0.52              |
| 28:BE:175:ILE:HG23 | 28:BE:175:ILE:O    | 2.09                     | 0.52              |
| 32:BI:19:PRO:HG2   | 32:BI:23:VAL:CG2   | 2.38                     | 0.52              |
| 32:BI:78:LEU:HD13  | 32:BI:108:ILE:CG2  | 2.35                     | 0.52              |
| 24:BA:558:U:P      | 33:BJ:113:PRO:HB2  | 2.50                     | 0.52              |
| 37:BN:79:LEU:O     | 37:BN:80:PHE:CB    | 2.50                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:BS:43:ALA:O    | 42:BS:46:LEU:HB2  | 2.10                     | 0.52              |
| 48:BY:5:GLU:O     | 48:BY:8:GLU:HB2   | 2.10                     | 0.52              |
| 55:CA:1129:C:HO2' | 55:CA:1130:A:H8   | 1.48                     | 0.52              |
| 55:CA:1161:C:O2'  | 55:CA:1162:C:H6   | 1.93                     | 0.52              |
| 55:CA:33:A:O2'    | 55:CA:34:C:H5'    | 2.09                     | 0.52              |
| 55:CA:386:C:C2'   | 55:CA:387:U:H5'   | 2.40                     | 0.52              |
| 55:CA:388:G:HO2'  | 55:CA:389:A:P     | 2.33                     | 0.52              |
| 55:CA:369:G:OP2   | 55:CA:388:G:N2    | 2.41                     | 0.52              |
| 55:CA:438:U:C5    | 55:CA:494:G:C5    | 2.96                     | 0.52              |
| 15:CP:32:PHE:HZ   | 55:CA:608:A:H1'   | 1.75                     | 0.52              |
| 9:CJ:56:HIS:HE1   | 55:CA:973:G:N3    | 2.08                     | 0.52              |
| 3:CD:170:LEU:HA   | 3:CD:182:LYS:HB2  | 1.90                     | 0.52              |
| 4:CE:18:ASN:OD1   | 4:CE:33:THR:HG23  | 2.09                     | 0.52              |
| 8:CI:16:ALA:HA    | 8:CI:65:THR:O     | 2.08                     | 0.52              |
| 12:CM:8:ILE:N     | 12:CM:9:PRO:HD3   | 2.24                     | 0.52              |
| 22:CV:27:G:C8     | 22:CV:27:G:H5''   | 2.44                     | 0.52              |
| 52:D2:38:GLY:O    | 52:D2:42:LEU:HD13 | 2.08                     | 0.52              |
| 53:D3:31:ILE:HG21 | 53:D3:34:LYS:NZ   | 2.24                     | 0.52              |
| 24:DA:1022:G:N2   | 24:DA:1142:A:H2   | 2.07                     | 0.52              |
| 24:DA:1494:A:H3'  | 24:DA:1494:A:OP2  | 2.09                     | 0.52              |
| 24:DA:1428:C:C5   | 24:DA:1569:A:H5'  | 2.44                     | 0.52              |
| 24:DA:1638:C:O2   | 24:DA:2698:U:O2'  | 2.27                     | 0.52              |
| 24:DA:1654:A:O2'  | 24:DA:1655:A:O5'  | 2.28                     | 0.52              |
| 24:DA:1725:U:H2'  | 24:DA:1726:C:C6   | 2.43                     | 0.52              |
| 24:DA:1759:A:H2'  | 24:DA:1760:C:C5   | 2.44                     | 0.52              |
| 24:DA:2026:U:O2   | 24:DA:2038:G:N2   | 2.43                     | 0.52              |
| 24:DA:2079:U:H2'  | 24:DA:2080:A:H8   | 1.74                     | 0.52              |
| 24:DA:2472:G:H2'  | 24:DA:2475:C:H42  | 1.75                     | 0.52              |
| 24:DA:2533:U:H4'  | 24:DA:2664:G:H4'  | 1.91                     | 0.52              |
| 24:DA:679:C:O5'   | 24:DA:679:C:H6    | 1.92                     | 0.52              |
| 24:DA:86:G:HO2'   | 24:DA:87:U:H6     | 1.56                     | 0.52              |
| 24:DA:93:G:O2'    | 24:DA:94:A:O4'    | 2.23                     | 0.52              |
| 26:DC:94:LEU:HA   | 26:DC:100:ARG:HG2 | 1.92                     | 0.52              |
| 21:AA:1203:C:H2'  | 21:AA:1204:A:C8   | 2.43                     | 0.52              |
| 21:AA:66:A:O4'    | 21:AA:173:U:C4    | 2.63                     | 0.52              |
| 21:AA:784:A:N6    | 21:AA:799:G:C6    | 2.77                     | 0.52              |
| 21:AA:76:G:N1     | 21:AA:95:C:N4     | 2.57                     | 0.52              |
| 2:AC:180:ASP:HB3  | 2:AC:204:GLY:H    | 1.72                     | 0.52              |
| 3:AD:14:GLU:HG3   | 3:AD:18:LEU:HD11  | 1.91                     | 0.52              |
| 4:AE:55:VAL:N     | 4:AE:56:PRO:CD    | 2.71                     | 0.52              |
| 5:AF:85:ILE:O     | 5:AF:86:ARG:C     | 2.48                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:AL:113:ARG:NH2 | 21:AA:501:C:OP1   | 2.43                     | 0.52              |
| 14:AO:25:GLU:HG3  | 14:AO:69:LEU:HD11 | 1.91                     | 0.52              |
| 22:AX:36:A:H2'    | 22:AX:37:A:C8     | 2.44                     | 0.52              |
| 24:BA:1000:A:C6   | 24:BA:1001:A:C6   | 2.98                     | 0.52              |
| 24:BA:1141:U:H4'  | 24:BA:1142:A:O4'  | 2.09                     | 0.52              |
| 24:BA:1142:A:N7   | 24:BA:1144:A:C6   | 2.78                     | 0.52              |
| 24:BA:1171:G:C6   | 24:BA:1172:C:C4   | 2.97                     | 0.52              |
| 24:BA:121:G:O2'   | 24:BA:122:G:H8    | 1.92                     | 0.52              |
| 24:BA:1275:A:OP2  | 24:BA:1646:C:N4   | 2.42                     | 0.52              |
| 24:BA:1326:U:H2'  | 24:BA:1327:A:C8   | 2.44                     | 0.52              |
| 24:BA:1408:G:H2'  | 24:BA:1409:U:C6   | 2.42                     | 0.52              |
| 24:BA:1600:C:OP1  | 43:BT:81:LYS:NZ   | 2.42                     | 0.52              |
| 24:BA:1856:U:H3   | 24:BA:1886:U:H3   | 1.58                     | 0.52              |
| 24:BA:2180:U:H2'  | 24:BA:2181:U:C5   | 2.45                     | 0.52              |
| 24:BA:2291:U:N3   | 24:BA:2292:U:O4   | 2.43                     | 0.52              |
| 24:BA:2251:G:C8   | 24:BA:2450:A:H4'  | 2.44                     | 0.52              |
| 24:BA:9:G:C5      | 24:BA:2629:U:C5   | 2.97                     | 0.52              |
| 24:BA:2788:C:H2'  | 24:BA:2789:C:C6   | 2.44                     | 0.52              |
| 24:BA:308:G:H1'   | 24:BA:501:A:OP1   | 2.10                     | 0.52              |
| 24:BA:506:G:C5'   | 24:BA:509:C:H1'   | 2.40                     | 0.52              |
| 24:BA:922:C:HO2'  | 46:BW:25:PHE:HE2  | 1.56                     | 0.52              |
| 24:BA:986:C:C2'   | 24:BA:987:C:H5'   | 2.39                     | 0.52              |
| 27:BD:90:PHE:C    | 27:BD:92:VAL:H    | 2.12                     | 0.52              |
| 27:BD:9:VAL:HG13  | 27:BD:26:VAL:O    | 2.10                     | 0.52              |
| 41:BR:54:VAL:HG23 | 41:BR:55:ASP:OD1  | 2.10                     | 0.52              |
| 55:CA:1049:U:H4'  | 55:CA:1050:G:H5'  | 1.91                     | 0.52              |
| 55:CA:1117:A:C6   | 55:CA:1184:G:O6   | 2.62                     | 0.52              |
| 55:CA:509:A:C2    | 55:CA:510:A:N1    | 2.78                     | 0.52              |
| 55:CA:663:A:O2'   | 55:CA:664:G:H5'   | 2.09                     | 0.52              |
| 55:CA:763:G:H2'   | 55:CA:764:C:H6    | 1.73                     | 0.52              |
| 7:CH:85:TYR:CD2   | 7:CH:123:GLU:HB2  | 2.44                     | 0.52              |
| 14:CO:42:PHE:O    | 14:CO:46:LYS:HG2  | 2.09                     | 0.52              |
| 16:CQ:45:VAL:HG21 | 16:CQ:60:ILE:HG21 | 1.90                     | 0.52              |
| 5:CF:5:GLU:OE2    | 17:CR:23:LYS:HE2  | 2.10                     | 0.52              |
| 18:CS:35:ARG:NH2  | 55:CA:1221:G:H4'  | 2.24                     | 0.52              |
| 19:CT:66:ILE:HG13 | 19:CT:67:HIS:N    | 2.24                     | 0.52              |
| 22:CV:27:G:O2'    | 22:CV:28:G:H5'    | 2.10                     | 0.52              |
| 50:D0:37:HIS:HB2  | 50:D0:41:HIS:HE1  | 1.75                     | 0.52              |
| 24:DA:1127:A:N7   | 24:DA:2488:G:O2'  | 2.41                     | 0.52              |
| 24:DA:1154:G:OP1  | 40:DQ:57:ARG:HD2  | 2.09                     | 0.52              |
| 24:DA:1286:A:C5   | 24:DA:1289:C:C4   | 2.97                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:1430:G:H2'  | 24:DA:1431:A:C8    | 2.43                     | 0.52              |
| 24:DA:160:A:C6    | 24:DA:161:A:C6     | 2.97                     | 0.52              |
| 24:DA:1651:G:C6   | 24:DA:1652:A:C5    | 2.98                     | 0.52              |
| 24:DA:1673:G:O2'  | 24:DA:1674:G:H5'   | 2.09                     | 0.52              |
| 24:DA:1794:A:H2'  | 24:DA:1795:C:C6    | 2.45                     | 0.52              |
| 24:DA:200:U:O4    | 24:DA:248:G:C2     | 2.63                     | 0.52              |
| 24:DA:2048:G:C6   | 24:DA:2049:G:C5    | 2.98                     | 0.52              |
| 24:DA:2370:G:O6   | 24:DA:2371:G:C6    | 2.62                     | 0.52              |
| 24:DA:240:C:O5'   | 24:DA:240:C:H6     | 1.93                     | 0.52              |
| 24:DA:2563:U:H2'  | 24:DA:2565:A:OP2   | 2.10                     | 0.52              |
| 24:DA:2577:A:C2   | 50:D0:1:ALA:N      | 2.77                     | 0.52              |
| 24:DA:2591:C:H2'  | 24:DA:2592:G:H8    | 1.73                     | 0.52              |
| 24:DA:807:U:OP2   | 35:DL:36:LYS:HG2   | 2.10                     | 0.52              |
| 24:DA:910:A:C6    | 24:DA:911:A:C6     | 2.98                     | 0.52              |
| 30:DG:162:ARG:HG3 | 30:DG:166:GLU:HG3  | 1.91                     | 0.52              |
| 31:DH:116:ARG:O   | 31:DH:117:LEU:HG   | 2.09                     | 0.52              |
| 31:DH:96:THR:O    | 31:DH:97:ARG:HG3   | 2.09                     | 0.52              |
| 33:DJ:44:TYR:CD1  | 40:DQ:59:LEU:HD11  | 2.45                     | 0.52              |
| 35:DL:20:GLY:HA2  | 35:DL:28:GLY:HA2   | 1.90                     | 0.52              |
| 35:DL:81:ASP:O    | 35:DL:83:ALA:N     | 2.42                     | 0.52              |
| 37:DN:20:MET:C    | 37:DN:22:ARG:H     | 2.13                     | 0.52              |
| 46:DW:40:ARG:NH1  | 46:DW:40:ARG:CG    | 2.58                     | 0.52              |
| 21:AA:1101:A:H4'  | 21:AA:1102:A:C4'   | 2.38                     | 0.52              |
| 21:AA:1239:A:N1   | 21:AA:1297:G:H1'   | 2.24                     | 0.52              |
| 21:AA:1411:C:H2'  | 21:AA:1412:C:H5'   | 1.92                     | 0.52              |
| 21:AA:88:U:O2     | 21:AA:89:U:C5      | 2.63                     | 0.52              |
| 21:AA:993:G:H4'   | 21:AA:994:A:OP2    | 2.08                     | 0.52              |
| 8:AI:33:SER:HB3   | 8:AI:36:GLN:CG     | 2.40                     | 0.52              |
| 11:AL:27:PRO:HB2  | 11:AL:28:GLN:OE1   | 2.09                     | 0.52              |
| 19:AT:53:MET:O    | 19:AT:56:ILE:HG22  | 2.10                     | 0.52              |
| 24:BA:1026:G:H2'  | 24:BA:1027:A:N7    | 2.23                     | 0.52              |
| 24:BA:1048:A:C4   | 24:BA:1049:C:C5    | 2.97                     | 0.52              |
| 24:BA:1528:A:H2'  | 24:BA:1529:G:O4'   | 2.10                     | 0.52              |
| 24:BA:1857:G:O2'  | 24:BA:1858:A:P     | 2.68                     | 0.52              |
| 24:BA:1876:A:H2'  | 24:BA:1877:A:H8    | 1.74                     | 0.52              |
| 24:BA:2699:C:H2'  | 24:BA:2700:A:O4'   | 2.10                     | 0.52              |
| 24:BA:2856:A:N6   | 24:BA:2857:G:C6    | 2.78                     | 0.52              |
| 24:BA:858:G:H21   | 24:BA:2268:A:C2'   | 2.23                     | 0.52              |
| 25:BB:33:G:C2     | 25:BB:50:A:C2      | 2.98                     | 0.52              |
| 24:BA:1998:A:P    | 27:BD:141:ARG:HH22 | 2.32                     | 0.52              |
| 31:BH:66:ASN:C    | 31:BH:68:ARG:H     | 2.13                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:BJ:31:GLU:O    | 33:BJ:32:LEU:C     | 2.48                     | 0.52              |
| 33:BJ:88:THR:HG23 | 33:BJ:91:GLU:H     | 1.73                     | 0.52              |
| 38:BO:93:ASP:C    | 38:BO:95:SER:H     | 2.13                     | 0.52              |
| 40:BQ:63:ARG:HH12 | 40:BQ:96:ASP:HB2   | 1.74                     | 0.52              |
| 46:BW:40:ARG:H    | 46:BW:56:HIS:HB3   | 1.74                     | 0.52              |
| 55:CA:1134:G:C6   | 55:CA:1135:U:H1'   | 2.44                     | 0.52              |
| 55:CA:1173:U:H2'  | 55:CA:1174:G:C8    | 2.44                     | 0.52              |
| 55:CA:1408:A:C5   | 55:CA:1409:C:C5    | 2.97                     | 0.52              |
| 55:CA:16:A:C6     | 55:CA:17:U:C5      | 2.98                     | 0.52              |
| 55:CA:246:A:C4    | 55:CA:282:A:N6     | 2.78                     | 0.52              |
| 55:CA:352:C:H5''  | 55:CA:352:C:H6     | 1.73                     | 0.52              |
| 55:CA:642:A:HO2'  | 55:CA:643:C:H6     | 1.49                     | 0.52              |
| 55:CA:677:U:H3    | 55:CA:714:G:H22    | 1.57                     | 0.52              |
| 1:CB:164:ASP:OD2  | 1:CB:203:ASP:HB2   | 2.10                     | 0.52              |
| 4:CE:35:LEU:HD11  | 4:CE:136:VAL:HG11  | 1.91                     | 0.52              |
| 10:CK:51:PHE:HB3  | 10:CK:55:ARG:CB    | 2.39                     | 0.52              |
| 11:CL:31:GLY:HA3  | 11:CL:54:VAL:CG1   | 2.40                     | 0.52              |
| 14:CO:62:ARG:O    | 14:CO:66:LEU:HG    | 2.10                     | 0.52              |
| 16:CQ:39:ARG:HA   | 16:CQ:39:ARG:HH11  | 1.74                     | 0.52              |
| 54:D4:7:VAL:CG1   | 54:D4:8:LYS:H      | 2.23                     | 0.52              |
| 24:DA:171:U:H2'   | 24:DA:172:A:H8     | 1.74                     | 0.52              |
| 24:DA:1748:C:H2'  | 24:DA:1749:A:C8    | 2.43                     | 0.52              |
| 24:DA:1776:G:N2   | 24:DA:1789:A:C4    | 2.78                     | 0.52              |
| 24:DA:2459:A:H2'  | 24:DA:2460:U:C6    | 2.45                     | 0.52              |
| 24:DA:2585:U:O2'  | 24:DA:2586:U:C5'   | 2.57                     | 0.52              |
| 24:DA:2644:G:O2'  | 24:DA:2732:G:H1'   | 2.09                     | 0.52              |
| 24:DA:3:U:H2'     | 24:DA:4:U:H6       | 1.75                     | 0.52              |
| 24:DA:600:G:H2'   | 24:DA:601:C:O4'    | 2.10                     | 0.52              |
| 24:DA:866:A:C5    | 24:DA:914:G:N7     | 2.77                     | 0.52              |
| 56:DB:50:A:C2     | 56:DB:51:G:H1'     | 2.44                     | 0.52              |
| 56:DB:77:U:H2'    | 56:DB:78:A:H5'     | 1.91                     | 0.52              |
| 27:DD:46:ARG:HB3  | 27:DD:84:LEU:HD12  | 1.92                     | 0.52              |
| 29:DF:30:VAL:HA   | 29:DF:157:THR:HG22 | 1.91                     | 0.52              |
| 33:DJ:6:ALA:HB3   | 33:DJ:45:THR:HB    | 1.92                     | 0.52              |
| 34:DK:119:ALA:N   | 34:DK:120:PRO:HD2  | 2.25                     | 0.52              |
| 40:DQ:42:GLY:HA3  | 41:DR:75:VAL:HG21  | 1.91                     | 0.52              |
| 40:DQ:4:LYS:HZ2   | 40:DQ:6:GLY:CA     | 2.12                     | 0.52              |
| 42:DS:86:MET:CE   | 42:DS:87:PRO:HD2   | 2.39                     | 0.52              |
| 49:DZ:4:ILE:CD1   | 49:DZ:58:GLU:HA    | 2.40                     | 0.52              |
| 2:AC:168:ARG:CZ   | 21:AA:1106:G:O2'   | 2.57                     | 0.52              |
| 21:AA:1372:U:C4   | 21:AA:1373:G:C5    | 2.98                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 21:AA:1395:C:H5'   | 21:AA:1401:G:N2   | 2.20                     | 0.52              |
| 21:AA:209:U:H5'    | 21:AA:210:C:OP2   | 2.09                     | 0.52              |
| 21:AA:72:A:O2'     | 21:AA:73:C:O4'    | 2.17                     | 0.52              |
| 21:AA:920:U:H2'    | 21:AA:921:U:C6    | 2.45                     | 0.52              |
| 2:AC:107:LYS:HB2   | 2:AC:107:LYS:NZ   | 2.25                     | 0.52              |
| 2:AC:78:LYS:HG2    | 2:AC:78:LYS:O     | 2.07                     | 0.52              |
| 20:AU:3:ILE:HA     | 20:AU:19:LYS:HE3  | 1.91                     | 0.52              |
| 24:BA:1252:G:N3    | 40:BQ:32:ARG:HG2  | 2.25                     | 0.52              |
| 24:BA:1464:G:H2'   | 24:BA:1465:G:H8   | 1.75                     | 0.52              |
| 24:BA:1537:G:H2'   | 24:BA:1538:G:O4'  | 2.10                     | 0.52              |
| 24:BA:1549:A:C6    | 24:BA:1550:C:C4   | 2.97                     | 0.52              |
| 24:BA:2269:G:O2'   | 46:BW:18:LYS:HG2  | 2.09                     | 0.52              |
| 24:BA:278:A:H2'    | 24:BA:278:A:N3    | 2.25                     | 0.52              |
| 24:BA:2048:G:H4'   | 24:BA:2823:A:C2   | 2.44                     | 0.52              |
| 24:BA:2856:A:C6    | 24:BA:2857:G:C5   | 2.97                     | 0.52              |
| 24:BA:431:U:C2'    | 24:BA:432:A:H5'   | 2.40                     | 0.52              |
| 27:BD:98:VAL:O     | 27:BD:99:GLU:C    | 2.47                     | 0.52              |
| 29:BF:134:GLN:HE21 | 29:BF:134:GLN:H   | 1.57                     | 0.52              |
| 30:BG:93:TYR:O     | 30:BG:94:ARG:O    | 2.27                     | 0.52              |
| 36:BM:28:PHE:HB3   | 36:BM:64:TRP:CE2  | 2.44                     | 0.52              |
| 36:BM:66:ARG:HB2   | 36:BM:101:VAL:O   | 2.10                     | 0.52              |
| 38:BO:70:ALA:O     | 38:BO:73:ALA:HB3  | 2.10                     | 0.52              |
| 39:BP:19:PHE:CE2   | 39:BP:83:ILE:HD12 | 2.44                     | 0.52              |
| 41:BR:39:LEU:HA    | 41:BR:49:ILE:CG2  | 2.40                     | 0.52              |
| 49:BZ:13:ILE:HG22  | 49:BZ:14:GLY:N    | 2.24                     | 0.52              |
| 55:CA:1168:U:H2'   | 55:CA:1168:U:O2   | 2.09                     | 0.52              |
| 55:CA:1316:G:OP2   | 55:CA:1316:G:H8   | 1.93                     | 0.52              |
| 55:CA:1520:C:H2'   | 55:CA:1521:C:C6   | 2.45                     | 0.52              |
| 55:CA:154:U:C2'    | 55:CA:155:A:H5'   | 2.39                     | 0.52              |
| 55:CA:373:A:N3     | 55:CA:374:A:C8    | 2.78                     | 0.52              |
| 55:CA:388:G:O2'    | 55:CA:389:A:OP2   | 2.25                     | 0.52              |
| 55:CA:961:U:C4     | 55:CA:983:A:C6    | 2.97                     | 0.52              |
| 55:CA:978:A:C5     | 55:CA:1318:A:C6   | 2.97                     | 0.52              |
| 8:CI:21:LYS:O      | 8:CI:60:LEU:HB2   | 2.09                     | 0.52              |
| 11:CL:43:LYS:CB    | 11:CL:44:PRO:HD2  | 2.07                     | 0.52              |
| 20:CU:40:PRO:HA    | 20:CU:43:GLU:HB2  | 1.90                     | 0.52              |
| 54:D4:3:VAL:O      | 54:D4:4:ARG:CB    | 2.57                     | 0.52              |
| 24:DA:1427:A:H4'   | 24:DA:1428:C:O5'  | 2.10                     | 0.52              |
| 24:DA:1478:G:C6    | 24:DA:1514:G:C2   | 2.97                     | 0.52              |
| 24:DA:197:A:C5     | 24:DA:2430:A:C4   | 2.98                     | 0.52              |
| 24:DA:2287:A:HO2'  | 24:DA:2288:A:P    | 2.31                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:2423:U:H1'  | 24:DA:2425:A:N7    | 2.23                     | 0.52              |
| 24:DA:2759:G:H2'  | 24:DA:2760:C:O4'   | 2.10                     | 0.52              |
| 24:DA:604:G:C2    | 24:DA:605:G:C5     | 2.98                     | 0.52              |
| 24:DA:81:G:H2'    | 24:DA:82:U:O4'     | 2.10                     | 0.52              |
| 24:DA:850:U:O2'   | 49:DZ:22:THR:HG22  | 2.09                     | 0.52              |
| 28:DE:170:ARG:CZ  | 28:DE:176:ASP:OD2  | 2.57                     | 0.52              |
| 29:DF:36:ASN:O    | 29:DF:37:MET:HB3   | 2.09                     | 0.52              |
| 33:DJ:23:LYS:HB3  | 33:DJ:28:LEU:HD13  | 1.90                     | 0.52              |
| 36:DM:1:MET:O     | 36:DM:2:LEU:O      | 2.27                     | 0.52              |
| 37:DN:72:ASP:O    | 37:DN:76:VAL:HG13  | 2.10                     | 0.52              |
| 39:DP:26:GLU:OE1  | 39:DP:28:LYS:HE2   | 2.10                     | 0.52              |
| 45:DV:30:ILE:HB   | 45:DV:38:LEU:HB3   | 1.91                     | 0.52              |
| 13:AN:48:GLN:CG   | 21:AA:1317:C:H4'   | 2.40                     | 0.52              |
| 21:AA:1418:A:C3'  | 21:AA:1418:A:C8    | 2.93                     | 0.52              |
| 21:AA:594:U:H1'   | 21:AA:646:G:N2     | 2.24                     | 0.52              |
| 21:AA:587:G:N2    | 21:AA:755:G:C4     | 2.77                     | 0.52              |
| 21:AA:838:G:H2'   | 21:AA:839:C:C6     | 2.45                     | 0.52              |
| 3:AD:10:LEU:HD22  | 3:AD:62:ARG:HG3    | 1.92                     | 0.52              |
| 4:AE:32:PHE:CD2   | 4:AE:53:ARG:O      | 2.62                     | 0.52              |
| 5:AF:55:HIS:O     | 5:AF:56:LYS:HB2    | 2.09                     | 0.52              |
| 10:AK:117:HIS:CD2 | 21:AA:675:A:H1'    | 2.45                     | 0.52              |
| 15:AP:46:LYS:NZ   | 15:AP:48:GLU:H     | 2.07                     | 0.52              |
| 19:AT:60:GLN:HA   | 19:AT:63:LYS:HB2   | 1.91                     | 0.52              |
| 24:BA:1510:G:HO2' | 24:BA:1511:G:H8    | 1.54                     | 0.52              |
| 24:BA:1579:A:O2'  | 24:BA:1580:A:H5'   | 2.10                     | 0.52              |
| 24:BA:1693:U:O4   | 24:BA:1977:A:C5    | 2.63                     | 0.52              |
| 24:BA:1824:G:C6   | 24:BA:1825:U:C4    | 2.98                     | 0.52              |
| 24:BA:231:A:N6    | 24:BA:232:G:C2     | 2.77                     | 0.52              |
| 24:BA:2400:G:C6   | 24:BA:2401:U:C4    | 2.97                     | 0.52              |
| 24:BA:2816:G:N2   | 24:BA:2831:G:C4    | 2.77                     | 0.52              |
| 24:BA:623:C:O5'   | 24:BA:623:C:H6     | 1.93                     | 0.52              |
| 25:BB:51:G:N2     | 25:BB:53:A:H62     | 2.06                     | 0.52              |
| 31:BH:32:PRO:O    | 31:BH:33:GLN:HB2   | 2.08                     | 0.52              |
| 24:BA:1064:C:H5'  | 32:BI:88:GLY:CA    | 2.40                     | 0.52              |
| 38:BO:2:ASP:O     | 38:BO:3:LYS:HB3    | 2.10                     | 0.52              |
| 38:BO:7:ARG:CD    | 38:BO:97:PHE:CE1   | 2.92                     | 0.52              |
| 40:BQ:71:ASN:CB   | 40:BQ:109:VAL:HG11 | 2.38                     | 0.52              |
| 42:BS:24:ILE:O    | 42:BS:25:ARG:C     | 2.47                     | 0.52              |
| 43:BT:68:LYS:O    | 43:BT:69:ARG:O     | 2.28                     | 0.52              |
| 43:BT:64:LYS:HA   | 43:BT:79:ASP:OD1   | 2.09                     | 0.52              |
| 55:CA:1061:G:N7   | 55:CA:1062:U:C5    | 2.77                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:CA:1350:A:C2    | 55:CA:1351:U:C2    | 2.97                     | 0.52              |
| 55:CA:811:C:O2'    | 55:CA:901:A:N1     | 2.43                     | 0.52              |
| 1:CB:80:LYS:HG3    | 1:CB:81:ASP:H      | 1.75                     | 0.52              |
| 3:CD:101:VAL:HG13  | 3:CD:106:PHE:HB2   | 1.92                     | 0.52              |
| 4:CE:132:PRO:O     | 4:CE:136:VAL:HG12  | 2.10                     | 0.52              |
| 7:CH:1:SER:C       | 7:CH:3:GLN:H       | 2.11                     | 0.52              |
| 14:CO:34:GLN:HE22  | 14:CO:38:LEU:HD13  | 1.75                     | 0.52              |
| 53:D3:15:LYS:HG2   | 53:D3:16:THR:H     | 1.74                     | 0.52              |
| 53:D3:33:THR:HG23  | 53:D3:34:LYS:N     | 2.25                     | 0.52              |
| 54:D4:37:GLN:HG2   | 54:D4:38:GLY:N     | 2.25                     | 0.52              |
| 24:DA:1923:U:C2    | 24:DA:1924:C:C5    | 2.97                     | 0.52              |
| 24:DA:2149:U:O2'   | 24:DA:2150:C:H5'   | 2.10                     | 0.52              |
| 24:DA:2480:C:H2'   | 24:DA:2481:G:H5'   | 1.92                     | 0.52              |
| 24:DA:2811:G:C2    | 24:DA:2812:G:C4    | 2.98                     | 0.52              |
| 24:DA:422:A:O2'    | 24:DA:423:A:H5'    | 2.10                     | 0.52              |
| 24:DA:538:A:H61    | 24:DA:555:G:C2'    | 2.23                     | 0.52              |
| 24:DA:753:A:C2     | 24:DA:754:U:C2     | 2.98                     | 0.52              |
| 56:DB:60:C:H2'     | 56:DB:61:G:H8      | 1.73                     | 0.52              |
| 26:DC:189:ALA:O    | 26:DC:190:THR:CB   | 2.56                     | 0.52              |
| 30:DG:167:VAL:HG23 | 30:DG:168:VAL:N    | 2.24                     | 0.52              |
| 33:DJ:55:ILE:HG13  | 33:DJ:55:ILE:O     | 2.09                     | 0.52              |
| 36:DM:66:ARG:CZ    | 36:DM:101:VAL:HG11 | 2.39                     | 0.52              |
| 38:DO:24:THR:OG1   | 38:DO:90:VAL:HG11  | 2.09                     | 0.52              |
| 39:DP:24:THR:HA    | 39:DP:44:GLY:O     | 2.10                     | 0.52              |
| 40:DQ:4:LYS:HE3    | 40:DQ:7:VAL:H      | 1.74                     | 0.52              |
| 44:DU:33:VAL:O     | 44:DU:34:ILE:HG13  | 2.09                     | 0.52              |
| 47:DX:76:LYS:HG3   | 47:DX:77:TYR:N     | 2.25                     | 0.52              |
| 21:AA:1173:U:H2'   | 21:AA:1174:G:H8    | 1.73                     | 0.52              |
| 21:AA:190:A:O5'    | 21:AA:190:A:H8     | 1.93                     | 0.52              |
| 21:AA:539:A:H2'    | 21:AA:540:G:C8     | 2.44                     | 0.52              |
| 3:AD:60:VAL:O      | 3:AD:61:ARG:C      | 2.48                     | 0.52              |
| 6:AG:110:ARG:HG2   | 6:AG:111:GLY:H     | 1.74                     | 0.52              |
| 9:AJ:32:THR:HG23   | 9:AJ:33:GLY:H      | 1.75                     | 0.52              |
| 24:BA:1014:A:C4    | 24:BA:1149:G:N2    | 2.78                     | 0.52              |
| 24:BA:1010:A:N3    | 24:BA:1153:C:H1'   | 2.25                     | 0.52              |
| 24:BA:1385:A:N3    | 24:BA:1386:C:C5    | 2.78                     | 0.52              |
| 24:BA:1805:A:C5    | 24:BA:1806:C:C5    | 2.96                     | 0.52              |
| 24:BA:1941:C:H2'   | 24:BA:1942:C:C6    | 2.45                     | 0.52              |
| 24:BA:1956:U:H2'   | 24:BA:1957:C:C6    | 2.40                     | 0.52              |
| 24:BA:2550:G:C6    | 24:BA:2551:C:C4    | 2.97                     | 0.52              |
| 24:BA:2662:A:H2'   | 24:BA:2663:G:O4'   | 2.08                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:518:G:H2'   | 24:BA:519:U:C6    | 2.45                     | 0.52              |
| 24:BA:570:G:O2'   | 24:BA:571:U:H5'   | 2.09                     | 0.52              |
| 24:BA:855:G:N3    | 46:BW:23:LYS:CD   | 2.72                     | 0.52              |
| 24:BA:866:A:O2'   | 24:BA:867:C:C5'   | 2.57                     | 0.52              |
| 25:BB:37:C:C4     | 25:BB:38:C:C4     | 2.98                     | 0.52              |
| 25:BB:49:C:OP1    | 38:BO:101:GLY:HA3 | 2.09                     | 0.52              |
| 26:BC:245:THR:O   | 26:BC:247:TRP:N   | 2.42                     | 0.52              |
| 28:BE:24:ASN:C    | 28:BE:24:ASN:HD22 | 2.13                     | 0.52              |
| 29:BF:45:ASP:CB   | 29:BF:48:LEU:HB2  | 2.39                     | 0.52              |
| 32:BI:135:MET:HG2 | 32:BI:137:LEU:HG  | 1.91                     | 0.52              |
| 40:BQ:15:LYS:O    | 40:BQ:19:GLN:HG3  | 2.09                     | 0.52              |
| 40:BQ:91:ARG:CD   | 41:BR:11:GLN:H    | 2.22                     | 0.52              |
| 42:BS:20:VAL:HA   | 42:BS:23:LEU:HD12 | 1.92                     | 0.52              |
| 44:BU:25:LYS:HG2  | 44:BU:36:GLU:HB3  | 1.91                     | 0.52              |
| 44:BU:73:ASN:O    | 44:BU:75:ALA:N    | 2.42                     | 0.52              |
| 55:CA:1064:G:H1'  | 55:CA:1066:C:C5   | 2.44                     | 0.52              |
| 55:CA:937:A:N6    | 55:CA:1345:U:O4   | 2.42                     | 0.52              |
| 55:CA:1387:G:C5   | 55:CA:1388:C:C5   | 2.97                     | 0.52              |
| 55:CA:198:G:O6    | 55:CA:220:G:C4    | 2.62                     | 0.52              |
| 55:CA:219:U:H2'   | 55:CA:220:G:C8    | 2.43                     | 0.52              |
| 55:CA:236:A:H2'   | 55:CA:237:G:C8    | 2.45                     | 0.52              |
| 55:CA:301:G:H2'   | 55:CA:302:G:C8    | 2.41                     | 0.52              |
| 55:CA:734:G:C2    | 55:CA:735:C:C2    | 2.98                     | 0.52              |
| 10:CK:126:ARG:NH2 | 55:CA:796:C:H4'   | 2.24                     | 0.52              |
| 1:CB:26:MET:C     | 1:CB:28:PRO:HD2   | 2.30                     | 0.52              |
| 2:CC:88:LYS:O     | 2:CC:92:ASP:HB2   | 2.09                     | 0.52              |
| 6:CG:119:LEU:HG   | 6:CG:123:LEU:HD23 | 1.91                     | 0.52              |
| 6:CG:29:LEU:HD21  | 6:CG:41:ILE:HD12  | 1.92                     | 0.52              |
| 7:CH:54:THR:HG23  | 7:CH:55:LYS:HD3   | 1.90                     | 0.52              |
| 10:CK:78:ILE:N    | 10:CK:78:ILE:HD13 | 2.24                     | 0.52              |
| 18:CS:35:ARG:HG3  | 18:CS:35:ARG:O    | 2.09                     | 0.52              |
| 22:CV:27:G:C5'    | 22:CV:27:G:H8     | 2.23                     | 0.52              |
| 24:DA:1020:A:H1'  | 24:DA:1021:A:N6   | 2.24                     | 0.52              |
| 24:DA:1028:A:N6   | 24:DA:1125:G:H2'  | 2.24                     | 0.52              |
| 24:DA:1158:C:O2'  | 24:DA:1159:U:O4'  | 2.28                     | 0.52              |
| 24:DA:48:G:C6     | 24:DA:178:G:O6    | 2.62                     | 0.52              |
| 24:DA:177:G:H5''  | 24:DA:178:G:OP2   | 2.10                     | 0.52              |
| 24:DA:1866:A:H2'  | 24:DA:1867:G:O4'  | 2.09                     | 0.52              |
| 24:DA:2264:C:C2   | 24:DA:2277:G:C2   | 2.97                     | 0.52              |
| 24:DA:2711:A:N6   | 24:DA:2714:G:C5   | 2.77                     | 0.52              |
| 24:DA:2752:C:O2'  | 24:DA:2753:A:O4'  | 2.26                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:2752:C:H2'  | 24:DA:2753:A:C8    | 2.45                     | 0.52              |
| 24:DA:323:C:H6    | 28:DE:165:HIS:CE1  | 2.28                     | 0.52              |
| 24:DA:352:A:C4    | 24:DA:353:C:H1'    | 2.44                     | 0.52              |
| 24:DA:989:G:H4'   | 24:DA:990:A:OP1    | 2.09                     | 0.52              |
| 56:DB:62:C:H2'    | 56:DB:63:C:O4'     | 2.09                     | 0.52              |
| 26:DC:147:PRO:CD  | 26:DC:184:GLU:HG3  | 2.37                     | 0.52              |
| 28:DE:111:GLU:HB2 | 28:DE:114:ARG:HH21 | 1.75                     | 0.52              |
| 28:DE:79:ARG:O    | 28:DE:80:SER:C     | 2.48                     | 0.52              |
| 32:DI:57:VAL:O    | 32:DI:58:ILE:HG13  | 2.10                     | 0.52              |
| 33:DJ:3:THR:CG2   | 40:DQ:60:TRP:HE1   | 2.22                     | 0.52              |
| 41:DR:68:ARG:CZ   | 41:DR:90:ARG:HG2   | 2.40                     | 0.52              |
| 43:DT:38:ALA:HB1  | 43:DT:81:LYS:HZ3   | 1.75                     | 0.52              |
| 47:DX:31:ASN:HD22 | 47:DX:31:ASN:N     | 2.04                     | 0.52              |
| 21:AA:1348:U:H2'  | 21:AA:1349:A:H8    | 1.75                     | 0.52              |
| 21:AA:1452:C:H2'  | 21:AA:1452:C:OP2   | 2.10                     | 0.52              |
| 21:AA:183:C:O2'   | 21:AA:184:G:C5'    | 2.49                     | 0.52              |
| 21:AA:341:C:O2'   | 21:AA:342:C:H5'    | 2.09                     | 0.52              |
| 1:AB:212:TYR:HA   | 1:AB:215:ALA:CB    | 2.40                     | 0.52              |
| 1:AB:26:MET:HE3   | 1:AB:192:PRO:HG3   | 1.92                     | 0.52              |
| 3:AD:84:ASN:O     | 3:AD:87:GLU:HG2    | 2.09                     | 0.52              |
| 11:AL:72:ASN:OD1  | 11:AL:104:SER:HB3  | 2.10                     | 0.52              |
| 11:AL:71:HIS:HB2  | 11:AL:73:LEU:HD23  | 1.92                     | 0.52              |
| 18:AS:51:HIS:HB2  | 18:AS:56:HIS:CD2   | 2.44                     | 0.52              |
| 22:AX:40:C:H2'    | 22:AX:41:C:C6      | 2.45                     | 0.52              |
| 24:BA:1062:G:N7   | 24:BA:1088:A:H8    | 2.07                     | 0.52              |
| 24:BA:1008:A:N6   | 24:BA:1136:G:C6    | 2.78                     | 0.52              |
| 24:BA:1368:G:H2'  | 24:BA:1369:G:C8    | 2.35                     | 0.52              |
| 24:BA:1421:G:C2   | 24:BA:1422:G:N7    | 2.77                     | 0.52              |
| 24:BA:1847:A:C8   | 24:BA:1848:A:N7    | 2.66                     | 0.52              |
| 24:BA:233:A:O2'   | 24:BA:234:U:H5'    | 2.10                     | 0.52              |
| 24:BA:2383:G:H2'  | 24:BA:2384:U:C6    | 2.45                     | 0.52              |
| 24:BA:2392:A:N3   | 24:BA:2392:A:H2'   | 2.25                     | 0.52              |
| 24:BA:2478:A:OP2  | 54:B4:2:LYS:NZ     | 2.43                     | 0.52              |
| 24:BA:2857:G:N2   | 24:BA:2859:G:H3'   | 2.24                     | 0.52              |
| 24:BA:431:U:O2'   | 24:BA:432:A:H5'    | 2.09                     | 0.52              |
| 24:BA:42:A:C2     | 24:BA:438:G:C6     | 2.97                     | 0.52              |
| 24:BA:455:C:N4    | 24:BA:472:A:H2'    | 2.25                     | 0.52              |
| 24:BA:541:A:C2    | 24:BA:553:G:C4     | 2.97                     | 0.52              |
| 24:BA:616:A:H2'   | 24:BA:617:G:H8     | 1.74                     | 0.52              |
| 24:BA:799:G:C6    | 24:BA:800:A:C6     | 2.97                     | 0.52              |
| 24:BA:538:A:O2'   | 33:BJ:8:PRO:HD2    | 2.10                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BP:105:LYS:HA   | 39:BP:108:ARG:CD   | 2.39                     | 0.52              |
| 39:BP:92:ARG:O     | 39:BP:93:LYS:HB2   | 2.10                     | 0.52              |
| 44:BU:97:SER:O     | 44:BU:98:ASN:CB    | 2.54                     | 0.52              |
| 45:BV:14:LYS:O     | 45:BV:15:GLY:C     | 2.48                     | 0.52              |
| 46:BW:17:ALA:HB1   | 46:BW:36:ILE:HA    | 1.91                     | 0.52              |
| 55:CA:1001:C:H2'   | 55:CA:1002:G:O4'   | 2.10                     | 0.52              |
| 55:CA:1127:G:O2'   | 55:CA:1128:C:C5'   | 2.58                     | 0.52              |
| 55:CA:1279:G:C8    | 55:CA:1282:C:N3    | 2.77                     | 0.52              |
| 55:CA:616:G:C2     | 55:CA:625:U:O2     | 2.62                     | 0.52              |
| 55:CA:860:A:N6     | 55:CA:861:G:C2     | 2.77                     | 0.52              |
| 4:CE:81:GLN:CD     | 4:CE:149:PRO:HD3   | 2.31                     | 0.52              |
| 5:CF:18:VAL:O      | 5:CF:22:ILE:N      | 2.41                     | 0.52              |
| 24:DA:1439:A:H5''  | 24:DA:1440:U:OP2   | 2.10                     | 0.52              |
| 24:DA:1517:G:H2'   | 24:DA:1518:C:C6    | 2.45                     | 0.52              |
| 24:DA:1552:A:H2    | 24:DA:1553:A:H8    | 1.57                     | 0.52              |
| 24:DA:1570:A:C6    | 24:DA:1571:A:N1    | 2.78                     | 0.52              |
| 24:DA:216:A:C2'    | 24:DA:217:A:C8     | 2.93                     | 0.52              |
| 24:DA:2297:A:HO2'  | 24:DA:2298:A:C5'   | 2.23                     | 0.52              |
| 24:DA:2720:U:C2    | 24:DA:2872:A:C5    | 2.98                     | 0.52              |
| 24:DA:33:C:HO2'    | 24:DA:34:U:H5'     | 1.73                     | 0.52              |
| 24:DA:476:G:C4     | 24:DA:478:A:OP2    | 2.63                     | 0.52              |
| 24:DA:680:C:O2     | 24:DA:681:G:C8     | 2.63                     | 0.52              |
| 24:DA:727:A:H2'    | 24:DA:728:G:C8     | 2.44                     | 0.52              |
| 27:DD:137:SER:HB3  | 27:DD:138:LEU:HD22 | 1.91                     | 0.52              |
| 29:DF:155:ILE:HD12 | 29:DF:155:ILE:H    | 1.75                     | 0.52              |
| 29:DF:42:ALA:CB    | 29:DF:49:LEU:HD21  | 2.39                     | 0.52              |
| 30:DG:7:PRO:O      | 30:DG:8:VAL:HB     | 2.10                     | 0.52              |
| 34:DK:11:ALA:O     | 34:DK:99:ILE:HG23  | 2.10                     | 0.52              |
| 37:DN:93:GLY:O     | 37:DN:116:VAL:HG21 | 2.10                     | 0.52              |
| 24:DA:2882:A:C5'   | 37:DN:96:ARG:HD3   | 2.40                     | 0.52              |
| 39:DP:56:SER:O     | 39:DP:75:THR:HG22  | 2.09                     | 0.52              |
| 40:DQ:71:ASN:ND2   | 40:DQ:106:THR:HA   | 2.24                     | 0.52              |
| 21:AA:1058:G:C6    | 21:AA:1059:C:N3    | 2.78                     | 0.52              |
| 4:AE:61:LYS:HD3    | 21:AA:1073:U:OP2   | 2.10                     | 0.52              |
| 21:AA:109:A:C6     | 21:AA:326:G:C6     | 2.97                     | 0.52              |
| 21:AA:1319:A:H2'   | 21:AA:1323:G:N7    | 2.25                     | 0.52              |
| 21:AA:1503:A:C8    | 21:AA:1531:A:O2'   | 2.57                     | 0.52              |
| 21:AA:299:G:H2'    | 21:AA:300:A:C8     | 2.45                     | 0.52              |
| 15:AP:13:LYS:NZ    | 21:AA:483:C:O2     | 2.37                     | 0.52              |
| 21:AA:548:G:O2'    | 21:AA:549:C:C5'    | 2.56                     | 0.52              |
| 21:AA:604:G:H2'    | 21:AA:605:U:O4'    | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:615:G:C4    | 21:AA:616:G:C8    | 2.97                     | 0.52              |
| 21:AA:244:U:C2    | 21:AA:894:G:N3    | 2.78                     | 0.52              |
| 1:AB:52:ALA:C     | 1:AB:54:ALA:H     | 2.14                     | 0.52              |
| 6:AG:119:LEU:O    | 6:AG:123:LEU:HB2  | 2.10                     | 0.52              |
| 6:AG:147:ASN:ND2  | 6:AG:147:ASN:N    | 2.48                     | 0.52              |
| 8:AI:11:ARG:CD    | 8:AI:106:ASP:HB2  | 2.40                     | 0.52              |
| 8:AI:90:ASP:OD2   | 8:AI:93:LEU:HG    | 2.10                     | 0.52              |
| 15:AP:67:ILE:HD11 | 15:AP:71:VAL:CG1  | 2.40                     | 0.52              |
| 15:AP:54:LEU:HD23 | 15:AP:80:LYS:HE3  | 1.91                     | 0.52              |
| 51:B1:7:LYS:HE3   | 53:B3:33:THR:CG2  | 2.40                     | 0.52              |
| 24:BA:2156:G:H2'  | 24:BA:2157:G:H21  | 1.75                     | 0.52              |
| 24:BA:2243:U:O2   | 24:BA:2434:A:C2   | 2.62                     | 0.52              |
| 24:BA:2567:G:H2'  | 24:BA:2568:U:C6   | 2.45                     | 0.52              |
| 24:BA:2816:G:C5   | 24:BA:2817:U:C5   | 2.98                     | 0.52              |
| 24:BA:2832:U:O2   | 24:BA:2834:G:C2   | 2.63                     | 0.52              |
| 26:BC:7:PRO:C     | 26:BC:9:SER:H     | 2.13                     | 0.52              |
| 27:BD:114:LYS:HZ3 | 27:BD:116:LYS:HE2 | 1.75                     | 0.52              |
| 28:BE:76:PRO:HA   | 28:BE:82:GLY:HA3  | 1.91                     | 0.52              |
| 33:BJ:12:LYS:O    | 33:BJ:13:ARG:HB2  | 2.10                     | 0.52              |
| 34:BK:43:ILE:HG13 | 34:BK:56:ASP:HB2  | 1.92                     | 0.52              |
| 34:BK:4:GLU:O     | 34:BK:5:GLN:HB2   | 2.09                     | 0.52              |
| 34:BK:91:SER:O    | 34:BK:92:GLU:C    | 2.48                     | 0.52              |
| 36:BM:64:TRP:CH2  | 36:BM:106:ASP:HB2 | 2.45                     | 0.52              |
| 38:BO:57:ALA:C    | 38:BO:59:ALA:H    | 2.12                     | 0.52              |
| 55:CA:1402:C:C2   | 55:CA:1403:C:C6   | 2.97                     | 0.52              |
| 55:CA:1488:G:N2   | 55:CA:1489:G:H1'  | 2.25                     | 0.52              |
| 55:CA:577:G:C6    | 55:CA:812:G:N2    | 2.78                     | 0.52              |
| 55:CA:662:U:H2'   | 55:CA:663:A:H8    | 1.76                     | 0.52              |
| 55:CA:677:U:H3    | 55:CA:714:G:N2    | 2.08                     | 0.52              |
| 1:CB:162:VAL:O    | 1:CB:184:ALA:HA   | 2.09                     | 0.52              |
| 20:AU:9:GLU:HB2   | 2:CC:48:LYS:HZ1   | 1.75                     | 0.52              |
| 4:CE:87:VAL:HG12  | 4:CE:92:ARG:HA    | 1.91                     | 0.52              |
| 6:CG:76:SER:HA    | 6:CG:85:GLN:HA    | 1.92                     | 0.52              |
| 7:CH:54:THR:HG23  | 7:CH:55:LYS:H     | 1.75                     | 0.52              |
| 8:CI:112:ARG:HG3  | 8:CI:112:ARG:O    | 2.09                     | 0.52              |
| 9:CJ:15:HIS:HA    | 9:CJ:18:ILE:CG2   | 2.38                     | 0.52              |
| 17:CR:55:ALA:O    | 17:CR:59:LYS:HG3  | 2.09                     | 0.52              |
| 24:DA:1296:G:N2   | 24:DA:1645:G:C5   | 2.78                     | 0.52              |
| 24:DA:1812:U:H1'  | 26:DC:43:ASN:HD21 | 1.75                     | 0.52              |
| 24:DA:1827:U:O4'  | 24:DA:1970:A:O2'  | 2.28                     | 0.52              |
| 24:DA:2064:C:H2'  | 24:DA:2065:C:C6   | 2.44                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:21:A:H2'     | 24:DA:22:C:H6      | 1.74                     | 0.52              |
| 24:DA:2349:G:N1    | 24:DA:2350:C:C2    | 2.77                     | 0.52              |
| 24:DA:2450:A:O2'   | 24:DA:2451:A:H5'   | 2.09                     | 0.52              |
| 24:DA:2592:G:C6    | 24:DA:2593:U:C4    | 2.98                     | 0.52              |
| 24:DA:2691:C:O2'   | 24:DA:2692:G:H5'   | 2.10                     | 0.52              |
| 24:DA:45:G:H2'     | 24:DA:215:G:C5     | 2.45                     | 0.52              |
| 24:DA:684:G:C2     | 24:DA:794:A:C2     | 2.98                     | 0.52              |
| 24:DA:697:G:C2     | 24:DA:766:U:O2     | 2.63                     | 0.52              |
| 24:DA:686:U:C6     | 24:DA:788:A:N1     | 2.77                     | 0.52              |
| 24:DA:985:C:N4     | 24:DA:986:C:N4     | 2.58                     | 0.52              |
| 26:DC:119:VAL:HG13 | 26:DC:133:ASN:ND2  | 2.21                     | 0.52              |
| 26:DC:179:GLU:HA   | 26:DC:269:ARG:O    | 2.10                     | 0.52              |
| 28:DE:23:PHE:HB2   | 28:DE:114:ARG:HH22 | 1.74                     | 0.52              |
| 28:DE:178:VAL:HG13 | 28:DE:179:SER:N    | 2.25                     | 0.52              |
| 35:DL:9:ALA:HB3    | 35:DL:12:SER:CB    | 2.40                     | 0.52              |
| 42:DS:17:VAL:HG21  | 42:DS:103:ILE:HD11 | 1.90                     | 0.52              |
| 42:DS:33:LEU:HA    | 42:DS:36:LEU:HD23  | 1.92                     | 0.52              |
| 46:DW:70:VAL:O     | 46:DW:70:VAL:HG22  | 2.08                     | 0.52              |
| 21:AA:46:G:C6      | 21:AA:366:A:C2     | 2.98                     | 0.51              |
| 21:AA:549:C:H2'    | 21:AA:550:G:C8     | 2.43                     | 0.51              |
| 1:AB:51:GLU:CG     | 1:AB:197:PHE:HE1   | 2.23                     | 0.51              |
| 3:AD:196:GLU:C     | 3:AD:198:LEU:N     | 2.63                     | 0.51              |
| 3:AD:196:GLU:O     | 3:AD:200:VAL:HG23  | 2.10                     | 0.51              |
| 12:AM:44:ILE:HG22  | 12:AM:44:ILE:O     | 2.08                     | 0.51              |
| 24:BA:1333:G:C2    | 24:BA:1334:G:N7    | 2.78                     | 0.51              |
| 24:BA:740:C:H1'    | 24:BA:1981:A:H1'   | 1.92                     | 0.51              |
| 24:BA:2585:U:O2'   | 24:BA:2586:U:C5'   | 2.58                     | 0.51              |
| 26:BC:75:ALA:HB1   | 26:BC:94:LEU:O     | 2.10                     | 0.51              |
| 27:BD:9:VAL:CG2    | 27:BD:10:GLY:N     | 2.72                     | 0.51              |
| 24:BA:38:A:O2'     | 28:BE:43:THR:HA    | 2.09                     | 0.51              |
| 30:BG:26:LYS:HA    | 30:BG:32:LEU:HA    | 1.91                     | 0.51              |
| 32:BI:16:MET:O     | 32:BI:19:PRO:HD3   | 2.09                     | 0.51              |
| 32:BI:24:GLY:O     | 32:BI:34:ILE:HD12  | 2.10                     | 0.51              |
| 32:BI:78:LEU:HD23  | 32:BI:81:LYS:HE3   | 1.92                     | 0.51              |
| 33:BJ:64:VAL:HG13  | 33:BJ:65:THR:N     | 2.24                     | 0.51              |
| 41:BR:1:MET:HB2    | 41:BR:43:ASN:HD21  | 1.75                     | 0.51              |
| 43:BT:40:LYS:HG2   | 43:BT:58:VAL:HG13  | 1.92                     | 0.51              |
| 24:BA:64:A:O2'     | 43:BT:70:HIS:HE1   | 1.93                     | 0.51              |
| 46:BW:39:GLN:O     | 46:BW:40:ARG:C     | 2.48                     | 0.51              |
| 55:CA:1058:G:H2'   | 55:CA:1059:C:O4'   | 2.10                     | 0.51              |
| 55:CA:1255:G:H21   | 55:CA:1259:C:H1'   | 1.74                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:1270:G:H2'  | 55:CA:1271:A:H8   | 1.75                     | 0.51              |
| 55:CA:243:A:H62   | 55:CA:281:G:H1'   | 1.75                     | 0.51              |
| 55:CA:774:G:C6    | 55:CA:775:G:N7    | 2.77                     | 0.51              |
| 8:CI:10:ARG:HG2   | 8:CI:105:ARG:HH21 | 1.75                     | 0.51              |
| 12:CM:45:SER:O    | 12:CM:47:LEU:N    | 2.43                     | 0.51              |
| 14:CO:88:ARG:HH21 | 24:DA:715:A:H4'   | 1.74                     | 0.51              |
| 55:CA:1230:C:O5'  | 22:CV:30:G:H5''   | 2.09                     | 0.51              |
| 24:DA:517:C:H5''  | 50:D0:12:ARG:HH12 | 1.75                     | 0.51              |
| 24:DA:1156:A:P    | 40:DQ:54:ARG:HE   | 2.33                     | 0.51              |
| 24:DA:1288:G:N3   | 24:DA:1288:G:H2'  | 2.25                     | 0.51              |
| 24:DA:1616:A:H4'  | 24:DA:1617:C:OP2  | 2.08                     | 0.51              |
| 24:DA:161:A:C6    | 24:DA:162:U:O4    | 2.62                     | 0.51              |
| 24:DA:1714:U:H3'  | 24:DA:1715:G:H5'  | 1.92                     | 0.51              |
| 24:DA:1809:A:C6   | 24:DA:1810:A:C6   | 2.98                     | 0.51              |
| 24:DA:1973:G:C5   | 24:DA:1974:C:C5   | 2.98                     | 0.51              |
| 24:DA:2311:A:H5'  | 24:DA:2312:U:C6   | 2.45                     | 0.51              |
| 24:DA:2337:G:OP1  | 24:DA:2385:C:OP2  | 2.28                     | 0.51              |
| 24:DA:2638:G:H1'  | 24:DA:2778:A:N6   | 2.25                     | 0.51              |
| 24:DA:428:A:O2'   | 24:DA:429:A:H5'   | 2.10                     | 0.51              |
| 24:DA:263:G:H4'   | 24:DA:430:A:O4'   | 2.09                     | 0.51              |
| 24:DA:673:C:C5'   | 28:DE:76:PRO:HD2  | 2.41                     | 0.51              |
| 26:DC:130:PRO:N   | 26:DC:188:ARG:HG3 | 2.25                     | 0.51              |
| 24:DA:1826:G:OP2  | 26:DC:220:ARG:HB3 | 2.09                     | 0.51              |
| 29:DF:11:VAL:HG22 | 29:DF:171:ALA:HA  | 1.91                     | 0.51              |
| 29:DF:136:ILE:CG2 | 29:DF:142:TYR:CG  | 2.93                     | 0.51              |
| 29:DF:65:LEU:HD11 | 29:DF:87:LYS:HZ2  | 1.74                     | 0.51              |
| 31:DH:68:ARG:HD3  | 31:DH:71:LYS:HB2  | 1.92                     | 0.51              |
| 33:DJ:30:THR:CG2  | 33:DJ:31:GLU:N    | 2.73                     | 0.51              |
| 34:DK:2:ILE:HD11  | 34:DK:65:THR:HG22 | 1.92                     | 0.51              |
| 37:DN:75:ILE:HD12 | 37:DN:79:LEU:HD12 | 1.93                     | 0.51              |
| 56:DB:48:U:H5'    | 38:DO:30:ARG:NE   | 2.26                     | 0.51              |
| 43:DT:34:VAL:O    | 43:DT:34:VAL:HG12 | 2.09                     | 0.51              |
| 45:DV:42:LEU:HD13 | 45:DV:47:VAL:HG21 | 1.92                     | 0.51              |
| 21:AA:1478:U:H2'  | 21:AA:1479:C:C6   | 2.45                     | 0.51              |
| 19:AT:75:LYS:HG3  | 21:AA:186:C:H4'   | 1.91                     | 0.51              |
| 21:AA:289:G:C6    | 21:AA:290:C:N4    | 2.78                     | 0.51              |
| 21:AA:31:G:N2     | 21:AA:46:G:H5''   | 2.23                     | 0.51              |
| 21:AA:438:U:C5    | 21:AA:494:G:N7    | 2.78                     | 0.51              |
| 21:AA:874:G:O2'   | 21:AA:875:U:C5'   | 2.57                     | 0.51              |
| 1:AB:130:LYS:HZ2  | 1:AB:130:LYS:HA   | 1.76                     | 0.51              |
| 7:AH:104:SER:HB2  | 7:AH:125:ILE:HD11 | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:AH:85:TYR:HD2   | 7:AH:123:GLU:HB2  | 1.74                     | 0.51              |
| 10:AK:13:LYS:O    | 10:AK:14:GLN:CB   | 2.58                     | 0.51              |
| 14:AO:18:ALA:O    | 14:AO:19:ASN:HB2  | 2.09                     | 0.51              |
| 24:BA:1045:C:C2   | 24:BA:1047:G:N2   | 2.78                     | 0.51              |
| 24:BA:1223:G:C5   | 24:BA:1225:G:OP2  | 2.64                     | 0.51              |
| 24:BA:1346:G:C2   | 24:BA:1601:G:C4   | 2.98                     | 0.51              |
| 24:BA:1487:U:C2   | 24:BA:1503:A:C2   | 2.97                     | 0.51              |
| 24:BA:1730:C:H1'  | 24:BA:1731:G:C2   | 2.45                     | 0.51              |
| 24:BA:414:C:H1'   | 24:BA:1864:U:O2'  | 2.10                     | 0.51              |
| 24:BA:2031:A:C6   | 24:BA:2498:C:H1'  | 2.46                     | 0.51              |
| 24:BA:2782:G:N2   | 24:BA:2783:U:C2   | 2.78                     | 0.51              |
| 24:BA:278:A:H3'   | 24:BA:278:A:OP2   | 2.10                     | 0.51              |
| 24:BA:451:U:C2    | 24:BA:453:A:N7    | 2.78                     | 0.51              |
| 24:BA:536:G:H2'   | 24:BA:537:G:H5'   | 1.92                     | 0.51              |
| 27:BD:40:LEU:HD12 | 27:BD:40:LEU:H    | 1.74                     | 0.51              |
| 28:BE:132:LYS:O   | 28:BE:135:ALA:HB3 | 2.09                     | 0.51              |
| 30:BG:35:THR:C    | 30:BG:36:LEU:HD22 | 2.30                     | 0.51              |
| 31:BH:29:PHE:O    | 31:BH:33:GLN:HB3  | 2.10                     | 0.51              |
| 34:BK:1:MET:HE2   | 34:BK:32:TYR:CE1  | 2.45                     | 0.51              |
| 39:BP:74:GLN:O    | 39:BP:77:SER:HB3  | 2.10                     | 0.51              |
| 40:BQ:51:GLN:HE21 | 40:BQ:55:GLN:HE21 | 1.56                     | 0.51              |
| 44:BU:17:ASP:O    | 44:BU:18:LYS:C    | 2.49                     | 0.51              |
| 45:BV:51:GLN:CD   | 45:BV:51:GLN:C    | 2.69                     | 0.51              |
| 45:BV:83:LYS:O    | 45:BV:85:LYS:N    | 2.41                     | 0.51              |
| 46:BW:22:VAL:O    | 46:BW:25:PHE:HB2  | 2.11                     | 0.51              |
| 55:CA:1140:C:O2'  | 55:CA:1141:C:C6   | 2.61                     | 0.51              |
| 55:CA:1229:A:O2'  | 55:CA:1230:C:O4'  | 2.26                     | 0.51              |
| 55:CA:1258:G:C2   | 55:CA:1278:G:N2   | 2.78                     | 0.51              |
| 55:CA:1256:A:C4   | 55:CA:1278:G:C5   | 2.99                     | 0.51              |
| 55:CA:1321:U:H2'  | 55:CA:1322:C:C4   | 2.45                     | 0.51              |
| 55:CA:1387:G:H2'  | 55:CA:1388:C:H6   | 1.74                     | 0.51              |
| 55:CA:528:C:H5'   | 55:CA:535:A:N6    | 2.25                     | 0.51              |
| 55:CA:733:G:O2'   | 55:CA:734:G:H5''  | 2.10                     | 0.51              |
| 2:CC:187:GLU:O    | 2:CC:188:ALA:HB2  | 2.09                     | 0.51              |
| 3:CD:29:THR:HG22  | 3:CD:30:LYS:HD3   | 1.92                     | 0.51              |
| 3:CD:40:HIS:O     | 3:CD:43:ARG:HB2   | 2.10                     | 0.51              |
| 5:CF:3:HIS:O      | 5:CF:4:TYR:CG     | 2.64                     | 0.51              |
| 10:CK:81:LEU:HD13 | 10:CK:81:LEU:N    | 2.25                     | 0.51              |
| 10:CK:57:SER:HA   | 10:CK:90:PRO:HG3  | 1.91                     | 0.51              |
| 53:D3:18:LYS:HG3  | 53:D3:19:GLY:N    | 2.25                     | 0.51              |
| 24:DA:120:U:C2    | 24:DA:149:A:C6    | 2.98                     | 0.51              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 24:DA:1629:U:H2' | 24:DA:1630:A:O4'   | 2.10                     | 0.51              |
| 24:DA:1722:A:O5' | 24:DA:1722:A:H8    | 1.93                     | 0.51              |
| 24:DA:1900:A:C2  | 24:DA:1970:A:C5    | 2.97                     | 0.51              |
| 24:DA:1953:A:C6  | 24:DA:2550:G:O4'   | 2.63                     | 0.51              |
| 24:DA:2086:U:H2' | 24:DA:2087:G:O4'   | 2.10                     | 0.51              |
| 24:DA:2140:G:C6  | 24:DA:2152:G:C6    | 2.98                     | 0.51              |
| 24:DA:2283:C:C4  | 24:DA:2389:G:C5    | 2.99                     | 0.51              |
| 24:DA:2284:A:H1' | 24:DA:2325:G:C2    | 2.45                     | 0.51              |
| 24:DA:2294:G:P   | 38:DO:94:ARG:HH11  | 2.34                     | 0.51              |
| 24:DA:2409:G:H2' | 24:DA:2410:G:O4'   | 2.10                     | 0.51              |
| 24:DA:2615:U:N3  | 50:D0:3:GLN:HA     | 2.24                     | 0.51              |
| 24:DA:2636:C:H2' | 24:DA:2637:U:H6    | 1.75                     | 0.51              |
| 24:DA:2769:U:H2' | 24:DA:2770:G:C8    | 2.44                     | 0.51              |
| 24:DA:788:A:O2'  | 52:D2:4:THR:HB     | 2.09                     | 0.51              |
| 24:DA:815:C:OP2  | 41:DR:85:LYS:HE2   | 2.09                     | 0.51              |
| 56:DB:75:G:O2'   | 56:DB:76:G:H5'     | 2.11                     | 0.51              |
| 29:DF:28:PRO:CB  | 29:DF:168:LEU:HD21 | 2.39                     | 0.51              |
| 29:DF:3:LEU:HG   | 29:DF:100:GLU:CD   | 2.31                     | 0.51              |
| 31:DH:80:ILE:HB  | 31:DH:101:ASP:HB3  | 1.90                     | 0.51              |
| 38:DO:71:ALA:CB  | 38:DO:102:ARG:HB3  | 2.39                     | 0.51              |
| 21:AA:110:C:H2'  | 21:AA:111:G:C8     | 2.46                     | 0.51              |
| 21:AA:1164:G:C6  | 21:AA:1165:U:C4    | 2.98                     | 0.51              |
| 21:AA:509:A:H2'  | 21:AA:510:A:C8     | 2.46                     | 0.51              |
| 1:AB:131:LYS:O   | 1:AB:135:MET:HB2   | 2.10                     | 0.51              |
| 4:AE:83:PRO:CD   | 4:AE:97:PRO:HD3    | 2.39                     | 0.51              |
| 5:AF:79:ARG:CA   | 5:AF:79:ARG:HE     | 2.23                     | 0.51              |
| 7:AH:14:ARG:HB2  | 7:AH:74:ILE:CG2    | 2.41                     | 0.51              |
| 14:AO:25:GLU:OE2 | 14:AO:76:ARG:CZ    | 2.58                     | 0.51              |
| 19:AT:53:MET:CE  | 19:AT:57:VAL:HG21  | 2.40                     | 0.51              |
| 24:BA:1062:G:C8  | 24:BA:1088:A:H8    | 2.27                     | 0.51              |
| 24:BA:111:A:C2   | 24:BA:112:U:C2     | 2.97                     | 0.51              |
| 24:BA:1268:A:C2  | 24:BA:2013:A:C4    | 2.99                     | 0.51              |
| 24:BA:1369:G:C2  | 24:BA:1370:C:C2    | 2.99                     | 0.51              |
| 24:BA:1510:G:O2' | 24:BA:1511:G:H8    | 1.93                     | 0.51              |
| 24:BA:2195:U:H2' | 24:BA:2196:C:C6    | 2.43                     | 0.51              |
| 24:BA:2489:U:O2  | 24:BA:2491:U:C4    | 2.63                     | 0.51              |
| 24:BA:405:U:H3'  | 24:BA:406:G:H5'    | 1.92                     | 0.51              |
| 24:BA:28:A:N6    | 24:BA:512:G:H1'    | 2.25                     | 0.51              |
| 26:BC:104:LEU:O  | 26:BC:105:ALA:CB   | 2.54                     | 0.51              |
| 24:BA:2578:G:N7  | 27:BD:145:SER:HB2  | 2.25                     | 0.51              |
| 27:BD:163:GLY:O  | 27:BD:164:GLN:C    | 2.48                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BD:54:ALA:N     | 27:BD:76:GLY:HA2  | 2.26                     | 0.51              |
| 31:BH:125:THR:HG23 | 31:BH:126:GLY:H   | 1.76                     | 0.51              |
| 31:BH:147:VAL:HG12 | 31:BH:149:GLU:HG3 | 1.90                     | 0.51              |
| 43:BT:15:HIS:O     | 43:BT:17:SER:N    | 2.43                     | 0.51              |
| 43:BT:70:HIS:HB2   | 43:BT:73:ARG:O    | 2.10                     | 0.51              |
| 55:CA:1008:U:C4    | 55:CA:1009:U:C4   | 2.99                     | 0.51              |
| 55:CA:1261:A:H2'   | 55:CA:1262:C:O4'  | 2.10                     | 0.51              |
| 55:CA:181:A:H5''   | 55:CA:182:A:OP1   | 2.10                     | 0.51              |
| 55:CA:279:A:H5'    | 55:CA:281:G:H5'   | 1.92                     | 0.51              |
| 2:CC:71:ARG:HH12   | 2:CC:74:ILE:HB    | 1.75                     | 0.51              |
| 3:CD:66:VAL:CG1    | 3:CD:70:GLN:HB3   | 2.41                     | 0.51              |
| 5:CF:43:GLY:HA2    | 5:CF:58:HIS:CE1   | 2.45                     | 0.51              |
| 5:CF:99:ALA:O      | 5:CF:100:SER:HB2  | 2.10                     | 0.51              |
| 11:CL:31:GLY:HA2   | 11:CL:56:LEU:HA   | 1.91                     | 0.51              |
| 15:CP:54:LEU:HG    | 15:CP:55:ASP:N    | 2.22                     | 0.51              |
| 24:DA:2418:A:OP1   | 53:D3:44:ARG:HD3  | 2.10                     | 0.51              |
| 54:D4:22:VAL:O     | 54:D4:24:ARG:HG3  | 2.11                     | 0.51              |
| 24:DA:1252:G:O2'   | 24:DA:1253:A:H5'' | 2.11                     | 0.51              |
| 24:DA:1313:U:H2'   | 24:DA:1313:U:O2   | 2.08                     | 0.51              |
| 24:DA:1598:A:H2'   | 24:DA:1599:U:H6   | 1.75                     | 0.51              |
| 24:DA:160:A:C2     | 24:DA:161:A:C4    | 2.99                     | 0.51              |
| 24:DA:1775:U:C2'   | 24:DA:1776:G:O5'  | 2.58                     | 0.51              |
| 24:DA:1933:G:H22   | 24:DA:1968:G:H1'  | 1.74                     | 0.51              |
| 24:DA:2389:G:C5'   | 24:DA:2390:U:H5'  | 2.39                     | 0.51              |
| 24:DA:2840:C:OP1   | 37:DN:50:PRO:HA   | 2.11                     | 0.51              |
| 24:DA:2860:A:C8    | 24:DA:2860:A:O5'  | 2.62                     | 0.51              |
| 24:DA:581:C:H2'    | 24:DA:582:A:C8    | 2.45                     | 0.51              |
| 24:DA:845:A:H2     | 24:DA:934:U:O2    | 1.92                     | 0.51              |
| 56:DB:50:A:OP2     | 38:DO:67:ASN:HA   | 2.11                     | 0.51              |
| 29:DF:107:VAL:O    | 29:DF:109:ARG:N   | 2.44                     | 0.51              |
| 32:DI:12:VAL:HG12  | 32:DI:13:ALA:N    | 2.24                     | 0.51              |
| 34:DK:39:ILE:HD11  | 34:DK:62:VAL:CG2  | 2.41                     | 0.51              |
| 35:DL:94:THR:O     | 35:DL:98:ALA:N    | 2.44                     | 0.51              |
| 38:DO:25:ARG:HB3   | 38:DO:93:ASP:HB2  | 1.92                     | 0.51              |
| 39:DP:113:LEU:HD23 | 39:DP:113:LEU:C   | 2.30                     | 0.51              |
| 41:DR:43:ASN:ND2   | 41:DR:44:GLY:H    | 2.08                     | 0.51              |
| 43:DT:40:LYS:HA    | 43:DT:43:ILE:HG22 | 1.92                     | 0.51              |
| 44:DU:34:ILE:HG12  | 44:DU:63:ALA:HA   | 1.92                     | 0.51              |
| 47:DX:39:VAL:HG22  | 47:DX:44:ARG:O    | 2.09                     | 0.51              |
| 48:DY:49:ASP:HA    | 48:DY:52:ARG:HD2  | 1.92                     | 0.51              |
| 21:AA:1067:A:H1'   | 21:AA:1068:G:H8   | 1.68                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:1492:A:C2   | 21:AA:1493:A:C2   | 2.98                     | 0.51              |
| 21:AA:15:G:C5     | 21:AA:1396:A:C2   | 2.98                     | 0.51              |
| 1:AB:55:GLU:OE2   | 1:AB:58:LYS:HD2   | 2.10                     | 0.51              |
| 3:AD:57:LYS:HG2   | 3:AD:202:LEU:HD23 | 1.93                     | 0.51              |
| 6:AG:136:LYS:O    | 6:AG:139:ASP:HB2  | 2.10                     | 0.51              |
| 7:AH:10:LEU:HB3   | 7:AH:74:ILE:HG13  | 1.93                     | 0.51              |
| 10:AK:91:GLY:O    | 10:AK:95:THR:HB   | 2.09                     | 0.51              |
| 15:AP:35:ARG:HH21 | 15:AP:51:ARG:NH1  | 2.09                     | 0.51              |
| 50:B0:46:GLY:O    | 50:B0:53:VAL:HG22 | 2.10                     | 0.51              |
| 24:BA:195:A:N7    | 59:BA:3767:HOH:O  | 2.33                     | 0.51              |
| 24:BA:2577:A:O4'  | 24:BA:2612:C:N4   | 2.44                     | 0.51              |
| 24:BA:2765:A:H2'  | 24:BA:2765:A:N3   | 2.26                     | 0.51              |
| 24:BA:2787:C:C2'  | 24:BA:2788:C:H5'  | 2.41                     | 0.51              |
| 24:BA:2:G:C6      | 24:BA:3:U:C4      | 2.99                     | 0.51              |
| 24:BA:532:A:N3    | 24:BA:532:A:H2'   | 2.24                     | 0.51              |
| 24:BA:84:A:C2     | 24:BA:103:A:C6    | 2.99                     | 0.51              |
| 26:BC:105:ALA:O   | 26:BC:106:PRO:O   | 2.29                     | 0.51              |
| 27:BD:106:LYS:HB3 | 27:BD:206:ALA:CB  | 2.28                     | 0.51              |
| 35:BL:55:MET:HG3  | 35:BL:59:ARG:HB2  | 1.92                     | 0.51              |
| 37:BN:20:MET:HG3  | 37:BN:21:PHE:N    | 2.21                     | 0.51              |
| 45:BV:19:ARG:O    | 45:BV:22:ALA:HB3  | 2.10                     | 0.51              |
| 47:BX:10:ARG:HB2  | 47:BX:11:PRO:CD   | 2.40                     | 0.51              |
| 55:CA:1275:A:H2'  | 55:CA:1276:G:C8   | 2.45                     | 0.51              |
| 55:CA:1348:U:H2'  | 55:CA:1349:A:C8   | 2.37                     | 0.51              |
| 55:CA:1508:A:O2'  | 55:CA:1509:C:C5'  | 2.58                     | 0.51              |
| 55:CA:503:C:H2'   | 55:CA:504:C:C6    | 2.43                     | 0.51              |
| 55:CA:549:C:H2'   | 55:CA:550:G:C8    | 2.45                     | 0.51              |
| 55:CA:642:A:O2'   | 55:CA:643:C:H6    | 1.92                     | 0.51              |
| 1:CB:99:MET:O     | 1:CB:103:TRP:HB2  | 2.09                     | 0.51              |
| 1:CB:80:LYS:HD3   | 1:CB:90:PHE:CZ    | 2.46                     | 0.51              |
| 2:CC:129:PHE:CZ   | 2:CC:156:LEU:HB3  | 2.45                     | 0.51              |
| 5:CF:53:LYS:O     | 5:CF:53:LYS:HD3   | 2.10                     | 0.51              |
| 5:CF:57:ALA:HB3   | 5:CF:59:TYR:HE1   | 1.75                     | 0.51              |
| 8:CI:118:ARG:NH2  | 8:CI:122:ARG:HE   | 2.08                     | 0.51              |
| 9:CJ:5:ARG:NH1    | 9:CJ:7:ARG:HH12   | 2.09                     | 0.51              |
| 11:CL:6:LEU:HD13  | 16:CQ:33:TYR:CE2  | 2.44                     | 0.51              |
| 12:CM:36:ALA:HB3  | 12:CM:55:LEU:HD11 | 1.93                     | 0.51              |
| 24:DA:1180:U:N3   | 24:DA:1181:U:C2   | 2.79                     | 0.51              |
| 24:DA:1210:G:H4'  | 24:DA:1211:C:OP2  | 2.10                     | 0.51              |
| 24:DA:1439:A:H3'  | 24:DA:1439:A:C8   | 2.46                     | 0.51              |
| 24:DA:1522:A:H1'  | 24:DA:1524:G:C6   | 2.45                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:1529:G:H2'   | 24:DA:1530:G:O4'   | 2.09                     | 0.51              |
| 24:DA:154:U:H2'    | 24:DA:155:A:O4'    | 2.11                     | 0.51              |
| 24:DA:1760:C:O2'   | 24:DA:1761:C:H5'   | 2.10                     | 0.51              |
| 24:DA:191:A:H2'    | 24:DA:192:C:C6     | 2.46                     | 0.51              |
| 24:DA:2074:U:N3    | 24:DA:2075:U:C4    | 2.78                     | 0.51              |
| 24:DA:2135:A:C2    | 24:DA:2136:G:H1'   | 2.46                     | 0.51              |
| 24:DA:2306:C:OP2   | 24:DA:2307:G:H3'   | 2.09                     | 0.51              |
| 24:DA:2511:U:C6    | 24:DA:2511:U:H3'   | 2.45                     | 0.51              |
| 24:DA:2611:C:HO2'  | 24:DA:2612:C:H6    | 1.58                     | 0.51              |
| 24:DA:2700:A:C2    | 24:DA:2708:G:C2    | 2.98                     | 0.51              |
| 24:DA:529:A:C8     | 24:DA:2042:A:N1    | 2.79                     | 0.51              |
| 24:DA:845:A:N6     | 24:DA:932:U:N3     | 2.59                     | 0.51              |
| 26:DC:16:VAL:H     | 26:DC:203:VAL:HG12 | 1.76                     | 0.51              |
| 27:DD:113:SER:OG   | 27:DD:114:LYS:N    | 2.44                     | 0.51              |
| 27:DD:3:GLY:O      | 27:DD:4:LEU:HD13   | 2.10                     | 0.51              |
| 28:DE:149:ILE:HG12 | 28:DE:149:ILE:O    | 2.11                     | 0.51              |
| 29:DF:110:ILE:CD1  | 29:DF:110:ILE:H    | 2.21                     | 0.51              |
| 29:DF:113:PHE:O    | 29:DF:114:ARG:CB   | 2.59                     | 0.51              |
| 33:DJ:95:ARG:O     | 33:DJ:96:ARG:C     | 2.48                     | 0.51              |
| 35:DL:47:ARG:CG    | 35:DL:47:ARG:HH21  | 2.18                     | 0.51              |
| 43:DT:29:THR:HA    | 43:DT:87:LEU:HB2   | 1.93                     | 0.51              |
| 21:AA:1101:A:H4'   | 21:AA:1102:A:O4'   | 2.10                     | 0.51              |
| 21:AA:342:C:O2'    | 21:AA:343:U:H5'    | 2.11                     | 0.51              |
| 21:AA:923:A:H2'    | 21:AA:924:C:H6     | 1.75                     | 0.51              |
| 1:AB:127:LYS:HG3   | 1:AB:128:LEU:H     | 1.74                     | 0.51              |
| 1:AB:128:LEU:HD12  | 1:AB:132:GLU:HB2   | 1.93                     | 0.51              |
| 1:AB:17:HIS:HD2    | 1:AB:204:ASP:OD2   | 1.93                     | 0.51              |
| 2:AC:113:LYS:HD3   | 2:AC:184:ASN:ND2   | 2.26                     | 0.51              |
| 2:AC:113:LYS:HB2   | 2:AC:184:ASN:OD1   | 2.11                     | 0.51              |
| 3:AD:12:ARG:HG2    | 3:AD:33:ILE:HD12   | 1.92                     | 0.51              |
| 7:AH:54:THR:HG23   | 7:AH:55:LYS:HG3    | 1.91                     | 0.51              |
| 14:AO:5:GLU:O      | 14:AO:9:LYS:HG3    | 2.10                     | 0.51              |
| 51:B1:42:VAL:CG1   | 51:B1:42:VAL:O     | 2.58                     | 0.51              |
| 52:B2:43:THR:O     | 52:B2:44:VAL:CG2   | 2.58                     | 0.51              |
| 24:BA:1019:U:O4    | 24:BA:1020:A:N6    | 2.43                     | 0.51              |
| 24:BA:1028:A:N6    | 24:BA:1125:G:H2'   | 2.25                     | 0.51              |
| 24:BA:1468:U:N3    | 24:BA:1522:A:H2    | 2.08                     | 0.51              |
| 24:BA:1630:A:H2'   | 24:BA:1631:G:H5'   | 1.93                     | 0.51              |
| 24:BA:1675:C:O2'   | 24:BA:1676:A:H5'   | 2.10                     | 0.51              |
| 24:BA:1734:G:H2'   | 24:BA:1735:A:C8    | 2.46                     | 0.51              |
| 24:BA:182:A:C6     | 24:BA:183:C:C4     | 2.98                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:1989:G:O2'  | 24:BA:1990:C:H5'   | 2.10                     | 0.51              |
| 24:BA:2690:U:HO2' | 24:BA:2872:A:H1'   | 1.76                     | 0.51              |
| 24:BA:2870:C:C2'  | 24:BA:2871:U:H5'   | 2.41                     | 0.51              |
| 24:BA:856:G:H2'   | 24:BA:857:G:C8     | 2.46                     | 0.51              |
| 26:BC:94:LEU:HB2  | 26:BC:100:ARG:HD3  | 1.92                     | 0.51              |
| 29:BF:39:VAL:HG11 | 29:BF:42:ALA:HB2   | 1.93                     | 0.51              |
| 31:BH:48:GLU:CA   | 31:BH:51:ARG:HG3   | 2.40                     | 0.51              |
| 55:CA:1447:A:O3'  | 55:CA:1448:C:H6    | 1.94                     | 0.51              |
| 55:CA:321:A:N7    | 55:CA:328:C:C2     | 2.78                     | 0.51              |
| 2:CC:63:ILE:HG12  | 2:CC:65:VAL:HG23   | 1.90                     | 0.51              |
| 2:CC:75:VAL:O     | 2:CC:82:ASP:HB2    | 2.11                     | 0.51              |
| 7:CH:93:LYS:N     | 7:CH:93:LYS:HD3    | 2.25                     | 0.51              |
| 9:CJ:72:ARG:O     | 9:CJ:73:LEU:HD23   | 2.11                     | 0.51              |
| 13:CN:11:LYS:O    | 13:CN:14:ALA:HB3   | 2.11                     | 0.51              |
| 13:CN:87:ALA:HB2  | 13:CN:92:ILE:HD12  | 1.92                     | 0.51              |
| 16:CQ:61:ARG:HD3  | 16:CQ:75:VAL:HG11  | 1.92                     | 0.51              |
| 24:DA:1024:G:C6   | 24:DA:1025:G:C6    | 2.99                     | 0.51              |
| 24:DA:1680:U:O4   | 24:DA:1681:G:C2    | 2.64                     | 0.51              |
| 24:DA:1821:A:O2'  | 24:DA:1822:C:O5'   | 2.27                     | 0.51              |
| 24:DA:2079:U:C2   | 24:DA:2080:A:C8    | 2.98                     | 0.51              |
| 24:DA:2259:U:HO2' | 24:DA:2260:C:H6    | 0.71                     | 0.51              |
| 24:DA:2337:G:N3   | 24:DA:2337:G:C2'   | 2.73                     | 0.51              |
| 24:DA:2646:C:H2'  | 24:DA:2647:U:O4'   | 2.11                     | 0.51              |
| 24:DA:2667:C:O2'  | 30:DG:110:HIS:CE1  | 2.63                     | 0.51              |
| 24:DA:374:A:H2'   | 24:DA:375:G:H8     | 1.71                     | 0.51              |
| 24:DA:508:A:H3'   | 24:DA:509:C:C5'    | 2.40                     | 0.51              |
| 29:DF:60:SER:C    | 29:DF:62:GLN:H     | 2.14                     | 0.51              |
| 31:DH:24:GLY:O    | 31:DH:25:TYR:C     | 2.48                     | 0.51              |
| 33:DJ:94:ALA:O    | 33:DJ:95:ARG:CB    | 2.58                     | 0.51              |
| 34:DK:108:ARG:HB2 | 34:DK:116:ILE:HD13 | 1.92                     | 0.51              |
| 34:DK:99:ILE:HD12 | 34:DK:118:LEU:HB2  | 1.92                     | 0.51              |
| 24:DA:1278:C:O2'  | 37:DN:27:SER:HB3   | 2.11                     | 0.51              |
| 41:DR:98:ILE:HG22 | 41:DR:98:ILE:O     | 2.10                     | 0.51              |
| 21:AA:1380:U:H5'  | 21:AA:1381:U:OP1   | 2.10                     | 0.51              |
| 21:AA:205:A:N6    | 21:AA:214:C:H1'    | 2.26                     | 0.51              |
| 21:AA:502:A:H2'   | 21:AA:503:C:O4'    | 2.10                     | 0.51              |
| 21:AA:567:G:O2'   | 21:AA:568:G:O5'    | 2.28                     | 0.51              |
| 21:AA:791:G:C5    | 21:AA:792:A:N7     | 2.79                     | 0.51              |
| 1:AB:39:ILE:HG22  | 1:AB:40:ILE:H      | 1.74                     | 0.51              |
| 2:AC:63:ILE:HG12  | 2:AC:65:VAL:HG23   | 1.93                     | 0.51              |
| 4:AE:19:ARG:CA    | 4:AE:31:SER:O      | 2.50                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:AG:52:ARG:NH2   | 6:AG:121:ASN:HA   | 2.25                     | 0.51              |
| 22:AV:29:G:H2'    | 22:AV:30:G:C8     | 2.46                     | 0.51              |
| 52:B2:43:THR:O    | 52:B2:44:VAL:HG23 | 2.11                     | 0.51              |
| 53:B3:57:VAL:O    | 53:B3:60:CYS:HB2  | 2.11                     | 0.51              |
| 24:BA:1026:G:C2'  | 24:BA:1027:A:C8   | 2.89                     | 0.51              |
| 24:BA:1157:G:H2'  | 24:BA:1158:C:H6   | 1.74                     | 0.51              |
| 24:BA:1213:A:O2'  | 24:BA:1214:A:H5'  | 2.11                     | 0.51              |
| 24:BA:1275:A:H4'  | 24:BA:1276:A:OP1  | 2.09                     | 0.51              |
| 24:BA:14:A:C6     | 24:BA:526:A:C2    | 2.98                     | 0.51              |
| 24:BA:151:C:C2    | 24:BA:176:A:C2    | 2.99                     | 0.51              |
| 24:BA:1815:A:C5   | 24:BA:1817:G:C6   | 2.99                     | 0.51              |
| 24:BA:1973:G:H2'  | 24:BA:1974:C:O4'  | 2.11                     | 0.51              |
| 24:BA:2247:A:H2'  | 24:BA:2248:C:H6   | 1.76                     | 0.51              |
| 24:BA:2409:G:H2'  | 24:BA:2410:G:O4'  | 2.10                     | 0.51              |
| 24:BA:2555:U:C6   | 24:BA:2556:C:C6   | 2.98                     | 0.51              |
| 24:BA:2821:A:H2'  | 24:BA:2822:G:O4'  | 2.09                     | 0.51              |
| 24:BA:533:G:H8    | 24:BA:533:G:H5''  | 1.75                     | 0.51              |
| 24:BA:60:G:C8     | 24:BA:62:U:C6     | 2.98                     | 0.51              |
| 30:BG:27:GLY:O    | 30:BG:28:LYS:C    | 2.48                     | 0.51              |
| 36:BM:117:PHE:HD2 | 36:BM:130:PHE:CE1 | 2.29                     | 0.51              |
| 41:BR:62:GLU:O    | 41:BR:64:VAL:HG23 | 2.09                     | 0.51              |
| 42:BS:1:MET:HA    | 42:BS:1:MET:CE    | 2.40                     | 0.51              |
| 43:BT:32:LEU:HD23 | 43:BT:83:ALA:HB3  | 1.92                     | 0.51              |
| 43:BT:83:ALA:O    | 43:BT:84:TYR:O    | 2.28                     | 0.51              |
| 48:BY:20:ASN:O    | 48:BY:21:LEU:C    | 2.49                     | 0.51              |
| 48:BY:9:LYS:HB3   | 48:BY:12:GLU:HG3  | 1.93                     | 0.51              |
| 55:CA:1062:U:H2'  | 55:CA:1063:C:C6   | 2.45                     | 0.51              |
| 55:CA:1086:U:H6   | 55:CA:1086:U:O5'  | 1.93                     | 0.51              |
| 55:CA:1332:A:H2'  | 55:CA:1333:A:H5'  | 1.91                     | 0.51              |
| 55:CA:412:A:H4'   | 55:CA:413:G:OP1   | 2.10                     | 0.51              |
| 1:CB:59:ILE:HA    | 1:CB:62:ARG:HG3   | 1.93                     | 0.51              |
| 2:CC:46:LEU:HD22  | 2:CC:75:VAL:HG22  | 1.93                     | 0.51              |
| 3:CD:56:GLU:HG2   | 3:CD:198:LEU:HD12 | 1.93                     | 0.51              |
| 6:CG:84:TYR:HB3   | 6:CG:86:VAL:HG23  | 1.92                     | 0.51              |
| 10:CK:127:ARG:HB3 | 55:CA:796:C:OP1   | 2.11                     | 0.51              |
| 20:CU:3:ILE:HG22  | 20:CU:19:LYS:HZ1  | 1.75                     | 0.51              |
| 24:DA:126:A:O5'   | 52:D2:19:ARG:HG3  | 2.10                     | 0.51              |
| 24:DA:511:U:C5'   | 24:DA:1235:G:H4'  | 2.40                     | 0.51              |
| 24:DA:1438:U:C4   | 24:DA:1552:A:N1   | 2.78                     | 0.51              |
| 24:DA:1562:U:C4   | 24:DA:1563:U:C4   | 2.98                     | 0.51              |
| 24:DA:1698:A:H4'  | 24:DA:1699:G:O5'  | 2.09                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:1969:A:H2'  | 24:DA:1972:G:H21   | 1.75                     | 0.51              |
| 24:DA:2026:U:H2'  | 24:DA:2027:G:O4'   | 2.11                     | 0.51              |
| 24:DA:2052:A:N6   | 24:DA:2618:G:C2    | 2.78                     | 0.51              |
| 24:DA:225:C:O2'   | 24:DA:226:A:C5'    | 2.58                     | 0.51              |
| 24:DA:2351:G:O6   | 53:D3:42:HIS:HE1   | 1.93                     | 0.51              |
| 24:DA:252:G:H2'   | 24:DA:253:C:C6     | 2.45                     | 0.51              |
| 24:DA:2725:A:H2'  | 24:DA:2727:A:N7    | 2.25                     | 0.51              |
| 24:DA:2884:U:H2'  | 24:DA:2885:G:C8    | 2.46                     | 0.51              |
| 24:DA:247:G:C4'   | 24:DA:386:G:C5     | 2.89                     | 0.51              |
| 24:DA:392:U:O2'   | 24:DA:393:C:O4'    | 2.28                     | 0.51              |
| 24:DA:533:G:C2    | 24:DA:534:U:C2     | 2.99                     | 0.51              |
| 24:DA:843:G:H2'   | 24:DA:844:A:C8     | 2.44                     | 0.51              |
| 26:DC:184:GLU:HB2 | 26:DC:187:CYS:SG   | 2.51                     | 0.51              |
| 26:DC:67:LYS:CG   | 26:DC:150:GLY:HA2  | 2.41                     | 0.51              |
| 28:DE:147:LEU:HB3 | 28:DE:186:VAL:HG23 | 1.92                     | 0.51              |
| 29:DF:147:ARG:HG2 | 29:DF:149:ARG:HH12 | 1.75                     | 0.51              |
| 31:DH:147:VAL:O   | 31:DH:148:ALA:HB3  | 2.11                     | 0.51              |
| 33:DJ:27:ARG:O    | 33:DJ:30:THR:HG22  | 2.10                     | 0.51              |
| 24:DA:1667:G:P    | 34:DK:6:THR:HA     | 2.50                     | 0.51              |
| 37:DN:90:ARG:HH21 | 37:DN:116:VAL:HG11 | 1.74                     | 0.51              |
| 24:DA:1251:C:H6   | 40:DQ:5:ARG:NH1    | 2.09                     | 0.51              |
| 40:DQ:63:ARG:HH12 | 40:DQ:99:VAL:CG2   | 2.24                     | 0.51              |
| 43:DT:67:VAL:O    | 43:DT:68:LYS:HG3   | 2.10                     | 0.51              |
| 44:DU:39:ASN:OD1  | 44:DU:64:ILE:HB    | 2.10                     | 0.51              |
| 47:DX:31:ASN:HB2  | 47:DX:33:HIS:HE1   | 1.75                     | 0.51              |
| 21:AA:103:U:C2    | 21:AA:104:G:C8     | 2.99                     | 0.51              |
| 21:AA:1213:A:C8   | 21:AA:1215:G:C5    | 2.99                     | 0.51              |
| 21:AA:1258:G:HO2' | 21:AA:1259:C:H6    | 1.59                     | 0.51              |
| 21:AA:1275:A:H2'  | 21:AA:1276:G:O4'   | 2.10                     | 0.51              |
| 21:AA:1423:G:H2'  | 21:AA:1424:U:C6    | 2.46                     | 0.51              |
| 21:AA:339:C:H2'   | 21:AA:340:U:C6     | 2.45                     | 0.51              |
| 21:AA:341:C:C2    | 21:AA:349:A:C2     | 2.99                     | 0.51              |
| 21:AA:31:G:H22    | 21:AA:47:C:H5''    | 1.75                     | 0.51              |
| 21:AA:967:C:C4    | 21:AA:968:A:C5     | 2.98                     | 0.51              |
| 21:AA:974:A:H4'   | 21:AA:975:A:H5'    | 1.93                     | 0.51              |
| 1:AB:159:ALA:HB1  | 1:AB:183:PHE:CE2   | 2.44                     | 0.51              |
| 3:AD:109:THR:HG23 | 3:AD:112:GLU:N     | 2.14                     | 0.51              |
| 3:AD:115:GLN:HG2  | 3:AD:153:ARG:HH12  | 1.76                     | 0.51              |
| 6:AG:12:LEU:HB3   | 6:AG:13:PRO:HD2    | 1.91                     | 0.51              |
| 8:AI:27:ILE:HG22  | 8:AI:29:ILE:H      | 1.76                     | 0.51              |
| 9:AJ:14:ASP:HB3   | 9:AJ:17:LEU:HB3    | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:AP:41:PRO:O    | 15:AP:42:ILE:HD13 | 2.10                     | 0.51              |
| 24:BA:1277:G:C6   | 24:BA:1278:C:C4   | 2.99                     | 0.51              |
| 24:BA:1333:G:H8   | 24:BA:1333:G:H5'  | 1.76                     | 0.51              |
| 24:BA:1494:A:C2   | 24:BA:1495:A:C4   | 2.99                     | 0.51              |
| 24:BA:167:A:C5    | 24:BA:168:G:C8    | 2.99                     | 0.51              |
| 24:BA:1759:A:C8   | 24:BA:2696:U:H1'  | 2.46                     | 0.51              |
| 24:BA:191:A:H2'   | 24:BA:192:C:C6    | 2.46                     | 0.51              |
| 24:BA:2019:A:H4'  | 40:BQ:33:VAL:HG21 | 1.93                     | 0.51              |
| 24:BA:2690:U:O2'  | 24:BA:2872:A:H1'  | 2.10                     | 0.51              |
| 24:BA:508:A:C6    | 42:BS:9:HIS:CE1   | 2.99                     | 0.51              |
| 24:BA:28:A:C8     | 24:BA:513:A:C6    | 2.99                     | 0.51              |
| 24:BA:522:A:C4    | 24:BA:523:C:C5    | 2.99                     | 0.51              |
| 24:BA:740:C:H6    | 24:BA:740:C:O5'   | 1.93                     | 0.51              |
| 24:BA:60:G:C4     | 24:BA:74:A:C2     | 2.98                     | 0.51              |
| 25:BB:58:A:O2'    | 25:BB:59:A:H5'    | 2.11                     | 0.51              |
| 26:BC:229:HIS:CD2 | 26:BC:246:PRO:HA  | 2.46                     | 0.51              |
| 27:BD:35:THR:CG2  | 27:BD:51:THR:HG22 | 2.40                     | 0.51              |
| 29:BF:19:PHE:O    | 29:BF:20:ASN:C    | 2.49                     | 0.51              |
| 30:BG:53:PRO:HD3  | 30:BG:61:TRP:CD2  | 2.45                     | 0.51              |
| 24:BA:2720:U:OP1  | 39:BP:52:ARG:NH2  | 2.43                     | 0.51              |
| 40:BQ:97:ILE:HD11 | 40:BQ:105:PHE:N   | 2.25                     | 0.51              |
| 42:BS:53:SER:O    | 42:BS:56:ALA:HB3  | 2.11                     | 0.51              |
| 44:BU:31:GLY:O    | 44:BU:66:VAL:HG12 | 2.11                     | 0.51              |
| 55:CA:1014:A:H2   | 55:CA:1219:A:H1'  | 1.76                     | 0.51              |
| 55:CA:283:U:O2'   | 55:CA:284:C:H5'   | 2.11                     | 0.51              |
| 55:CA:424:G:O2'   | 55:CA:425:G:H5'   | 2.09                     | 0.51              |
| 55:CA:522:C:O4'   | 55:CA:536:C:H4'   | 2.10                     | 0.51              |
| 55:CA:534:U:O2'   | 55:CA:535:A:C5'   | 2.59                     | 0.51              |
| 55:CA:585:G:N3    | 55:CA:879:C:H4'   | 2.25                     | 0.51              |
| 55:CA:635:A:C6    | 55:CA:636:U:C4    | 2.99                     | 0.51              |
| 14:CO:20:ASP:HB2  | 55:CA:750:C:H4'   | 1.93                     | 0.51              |
| 5:CF:98:GLU:O     | 5:CF:99:ALA:HB3   | 2.10                     | 0.51              |
| 6:CG:14:ASP:HB3   | 6:CG:19:SER:H     | 1.75                     | 0.51              |
| 9:CJ:26:VAL:HG13  | 9:CJ:30:LYS:HB3   | 1.92                     | 0.51              |
| 12:CM:78:ARG:HH11 | 12:CM:78:ARG:HG2  | 1.75                     | 0.51              |
| 14:CO:69:LEU:HD13 | 14:CO:77:TYR:HB2  | 1.92                     | 0.51              |
| 24:DA:135:U:H2'   | 24:DA:136:G:C8    | 2.45                     | 0.51              |
| 24:DA:1558:C:C2   | 24:DA:1560:G:C6   | 2.99                     | 0.51              |
| 24:DA:1576:U:H2'  | 24:DA:1577:C:C6   | 2.46                     | 0.51              |
| 24:DA:1678:A:H2'  | 24:DA:1679:A:O4'  | 2.11                     | 0.51              |
| 24:DA:1686:C:N3   | 24:DA:1703:G:C2   | 2.78                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:1744:A:H3'  | 24:DA:1745:A:C8   | 2.46                     | 0.51              |
| 24:DA:2107:G:H2'  | 24:DA:2108:A:C8   | 2.46                     | 0.51              |
| 24:DA:2499:C:O2'  | 24:DA:2500:U:O4'  | 2.24                     | 0.51              |
| 24:DA:2769:U:H2'  | 24:DA:2770:G:H8   | 1.76                     | 0.51              |
| 24:DA:2782:G:N2   | 24:DA:2783:U:C2   | 2.79                     | 0.51              |
| 24:DA:35:G:C2'    | 24:DA:36:G:O5'    | 2.58                     | 0.51              |
| 24:DA:504:A:C2    | 24:DA:1234:U:H4'  | 2.45                     | 0.51              |
| 24:DA:527:C:C2    | 24:DA:2779:U:H2'  | 2.46                     | 0.51              |
| 24:DA:54:G:H2'    | 24:DA:55:G:O4'    | 2.11                     | 0.51              |
| 24:DA:571:U:C6    | 24:DA:575:A:N6    | 2.79                     | 0.51              |
| 24:DA:680:C:C2    | 24:DA:681:G:C8    | 2.99                     | 0.51              |
| 24:DA:779:U:O2'   | 24:DA:780:G:H5'   | 2.10                     | 0.51              |
| 56:DB:21:G:H2'    | 56:DB:22:U:O4'    | 2.11                     | 0.51              |
| 32:DI:52:LEU:HD12 | 32:DI:53:PRO:HD2  | 1.92                     | 0.51              |
| 46:DW:17:ALA:HB1  | 46:DW:36:ILE:HA   | 1.91                     | 0.51              |
| 46:DW:44:PHE:HB3  | 46:DW:78:PHE:CD1  | 2.46                     | 0.51              |
| 49:DZ:51:SER:HA   | 49:DZ:54:VAL:HG22 | 1.93                     | 0.51              |
| 20:AU:38:GLU:HB2  | 21:AA:1526:G:OP2  | 2.11                     | 0.51              |
| 21:AA:82:G:H2'    | 21:AA:83:C:O4'    | 2.09                     | 0.51              |
| 3:AD:8:LEU:HD21   | 3:AD:21:LYS:HB2   | 1.92                     | 0.51              |
| 4:AE:56:PRO:C     | 4:AE:58:ALA:H     | 2.14                     | 0.51              |
| 5:AF:44:ARG:HG3   | 5:AF:58:HIS:ND1   | 2.26                     | 0.51              |
| 5:AF:43:GLY:HA2   | 5:AF:58:HIS:NE2   | 2.26                     | 0.51              |
| 5:AF:90:MET:CG    | 17:AR:60:ARG:HH21 | 2.23                     | 0.51              |
| 7:AH:45:ILE:HB    | 7:AH:61:THR:O     | 2.10                     | 0.51              |
| 8:AI:51:LEU:HB3   | 8:AI:56:MET:HG3   | 1.92                     | 0.51              |
| 12:AM:67:ASP:C    | 12:AM:70:ARG:HB3  | 2.30                     | 0.51              |
| 14:AO:26:VAL:O    | 14:AO:30:LEU:HG   | 2.11                     | 0.51              |
| 19:AT:60:GLN:C    | 19:AT:66:ILE:HG22 | 2.31                     | 0.51              |
| 24:BA:1113:U:H2'  | 24:BA:1114:C:H6   | 1.75                     | 0.51              |
| 24:BA:1702:G:H2'  | 24:BA:1703:G:O4'  | 2.11                     | 0.51              |
| 24:BA:1866:A:H2'  | 24:BA:1867:G:O4'  | 2.11                     | 0.51              |
| 24:BA:2020:A:H2   | 24:BA:2022:U:O4'  | 1.93                     | 0.51              |
| 24:BA:677:A:O2'   | 24:BA:2071:A:H5'  | 2.11                     | 0.51              |
| 24:BA:2472:G:C2'  | 24:BA:2475:C:H42  | 2.20                     | 0.51              |
| 24:BA:2860:A:H3'  | 24:BA:2860:A:H8   | 1.76                     | 0.51              |
| 24:BA:28:A:H2'    | 24:BA:29:U:C6     | 2.46                     | 0.51              |
| 24:BA:628:G:H4'   | 24:BA:651:G:O2'   | 2.11                     | 0.51              |
| 24:BA:855:G:N3    | 46:BW:23:LYS:CG   | 2.73                     | 0.51              |
| 27:BD:9:VAL:CG2   | 27:BD:26:VAL:HB   | 2.35                     | 0.51              |
| 30:BG:54:ARG:HG3  | 30:BG:57:TYR:CD1  | 2.46                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:BK:63:VAL:HG12 | 34:BK:64:ARG:HG3  | 1.92                     | 0.51              |
| 35:BL:93:ASN:HD22 | 35:BL:94:THR:H    | 1.54                     | 0.51              |
| 37:BN:2:ARG:HA    | 37:BN:5:LYS:HD2   | 1.93                     | 0.51              |
| 37:BN:69:ARG:O    | 37:BN:70:THR:OG1  | 2.23                     | 0.51              |
| 39:BP:102:ARG:HD3 | 39:BP:106:ALA:O   | 2.11                     | 0.51              |
| 39:BP:25:VAL:HG11 | 39:BP:46:VAL:CG2  | 2.40                     | 0.51              |
| 43:BT:29:THR:CA   | 43:BT:86:THR:HA   | 2.39                     | 0.51              |
| 45:BV:10:LYS:H    | 45:BV:10:LYS:CD   | 2.20                     | 0.51              |
| 46:BW:25:PHE:O    | 46:BW:26:GLY:C    | 2.49                     | 0.51              |
| 55:CA:1140:C:H2'  | 55:CA:1141:C:H5   | 1.75                     | 0.51              |
| 55:CA:1333:A:H2'  | 55:CA:1334:G:O4'  | 2.11                     | 0.51              |
| 55:CA:1412:C:H2'  | 55:CA:1413:A:H8   | 1.76                     | 0.51              |
| 55:CA:1514:G:H2'  | 55:CA:1515:G:C8   | 2.44                     | 0.51              |
| 55:CA:38:G:C2     | 55:CA:397:A:C2    | 2.98                     | 0.51              |
| 55:CA:861:G:C6    | 55:CA:862:C:C4    | 2.98                     | 0.51              |
| 1:CB:157:PRO:O    | 1:CB:180:ILE:HD12 | 2.10                     | 0.51              |
| 4:CE:22:LYS:HD2   | 55:CA:1081:A:C5'  | 2.38                     | 0.51              |
| 6:CG:115:MET:HE1  | 6:CG:119:LEU:HB3  | 1.93                     | 0.51              |
| 9:CJ:21:ALA:O     | 9:CJ:25:ILE:HG13  | 2.11                     | 0.51              |
| 11:CL:28:GLN:HG3  | 11:CL:80:LEU:HD21 | 1.92                     | 0.51              |
| 50:D0:32:THR:HG21 | 50:D0:47:TYR:CE2  | 2.46                     | 0.51              |
| 24:DA:1560:G:H2'  | 24:DA:1561:C:C6   | 2.46                     | 0.51              |
| 24:DA:1707:G:C8   | 24:DA:1756:G:C5   | 2.99                     | 0.51              |
| 24:DA:1812:U:H2'  | 24:DA:1813:G:H8   | 1.75                     | 0.51              |
| 24:DA:1901:A:OP2  | 26:DC:252:LYS:HE3 | 2.11                     | 0.51              |
| 24:DA:2015:A:C2   | 50:D0:2:VAL:CG1   | 2.91                     | 0.51              |
| 24:DA:2142:A:H2'  | 24:DA:2143:C:H4'  | 1.91                     | 0.51              |
| 24:DA:2741:A:H2'  | 24:DA:2742:G:O4'  | 2.10                     | 0.51              |
| 24:DA:522:A:H2'   | 24:DA:523:C:C6    | 2.45                     | 0.51              |
| 24:DA:628:G:C6    | 24:DA:636:G:C2    | 2.99                     | 0.51              |
| 24:DA:860:U:O2'   | 24:DA:861:A:H8    | 1.94                     | 0.51              |
| 26:DC:212:TRP:C   | 26:DC:212:TRP:CD1 | 2.84                     | 0.51              |
| 27:DD:16:THR:HG23 | 27:DD:19:GLY:H    | 1.76                     | 0.51              |
| 29:DF:52:ALA:HA   | 29:DF:55:ASP:HB2  | 1.91                     | 0.51              |
| 33:DJ:43:GLU:O    | 33:DJ:45:THR:N    | 2.43                     | 0.51              |
| 35:DL:90:VAL:HB   | 35:DL:122:VAL:HA  | 1.93                     | 0.51              |
| 42:DS:87:PRO:HG2  | 42:DS:87:PRO:O    | 2.10                     | 0.51              |
| 44:DU:94:PHE:O    | 44:DU:95:PHE:C    | 2.48                     | 0.51              |
| 47:DX:6:VAL:HG13  | 47:DX:7:THR:H     | 1.75                     | 0.51              |
| 21:AA:1324:A:H2'  | 21:AA:1325:C:O4'  | 2.10                     | 0.51              |
| 21:AA:146:G:N2    | 21:AA:177:G:C8    | 2.79                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:389:A:O2'    | 21:AA:390:U:H5'    | 2.10                     | 0.51              |
| 21:AA:579:A:H5'    | 21:AA:728:A:H1'    | 1.93                     | 0.51              |
| 21:AA:632:U:OP1    | 21:AA:633:G:C8     | 2.64                     | 0.51              |
| 21:AA:869:G:H4'    | 21:AA:872:A:O4'    | 2.11                     | 0.51              |
| 4:AE:80:LEU:HD12   | 4:AE:146:MET:SD    | 2.51                     | 0.51              |
| 5:AF:19:PRO:O      | 5:AF:22:ILE:HB     | 2.11                     | 0.51              |
| 5:AF:52:ASN:O      | 5:AF:53:LYS:HB3    | 2.11                     | 0.51              |
| 9:AJ:35:GLN:HA     | 9:AJ:35:GLN:NE2    | 2.21                     | 0.51              |
| 2:AC:17:TRP:HZ2    | 13:AN:95:LEU:O     | 1.93                     | 0.51              |
| 19:AT:4:LYS:CE     | 19:AT:5:SER:HB3    | 2.40                     | 0.51              |
| 20:AU:35:GLU:O     | 20:AU:36:PHE:C     | 2.49                     | 0.51              |
| 24:BA:1576:U:H2'   | 24:BA:1577:C:C6    | 2.45                     | 0.51              |
| 24:BA:176:A:C6     | 24:BA:177:G:N7     | 2.79                     | 0.51              |
| 24:BA:194:G:N7     | 59:BA:3767:HOH:O   | 2.34                     | 0.51              |
| 24:BA:2305:U:C4'   | 29:BF:130:GLY:HA3  | 2.41                     | 0.51              |
| 24:BA:2516:A:H2'   | 24:BA:2517:C:O4'   | 2.11                     | 0.51              |
| 24:BA:482:A:N6     | 24:BA:506:G:H1'    | 2.26                     | 0.51              |
| 24:BA:931:U:O2'    | 24:BA:932:U:P      | 2.69                     | 0.51              |
| 26:BC:261:ARG:HG2  | 26:BC:261:ARG:O    | 2.11                     | 0.51              |
| 27:BD:143:PRO:HD2  | 27:BD:144:GLY:H    | 1.74                     | 0.51              |
| 28:BE:147:LEU:HB3  | 28:BE:186:VAL:HG23 | 1.93                     | 0.51              |
| 28:BE:7:ASP:CG     | 28:BE:8:ALA:H      | 2.14                     | 0.51              |
| 30:BG:153:PRO:HA   | 30:BG:159:LYS:O    | 2.11                     | 0.51              |
| 31:BH:41:LYS:O     | 31:BH:44:ILE:HG12  | 2.11                     | 0.51              |
| 35:BL:100:ILE:HD12 | 35:BL:100:ILE:C    | 2.31                     | 0.51              |
| 39:BP:37:LYS:CD    | 39:BP:37:LYS:N     | 2.74                     | 0.51              |
| 55:CA:1192:C:C5    | 55:CA:1193:G:C8    | 2.98                     | 0.51              |
| 55:CA:1435:G:C5    | 55:CA:1436:U:C4    | 2.99                     | 0.51              |
| 55:CA:183:C:O2'    | 55:CA:184:G:C5'    | 2.49                     | 0.51              |
| 55:CA:500:G:HO2'   | 55:CA:501:C:H5'    | 1.73                     | 0.51              |
| 55:CA:511:C:C2     | 55:CA:512:U:C5     | 2.99                     | 0.51              |
| 55:CA:560:A:N7     | 55:CA:566:G:C4     | 2.79                     | 0.51              |
| 1:CB:103:TRP:O     | 1:CB:103:TRP:CD1   | 2.64                     | 0.51              |
| 1:CB:187:ASP:O     | 1:CB:189:ASN:N     | 2.43                     | 0.51              |
| 5:CF:2:ARG:HD2     | 5:CF:92:THR:OG1    | 2.10                     | 0.51              |
| 6:CG:90:VAL:HG23   | 6:CG:95:ARG:HG2    | 1.93                     | 0.51              |
| 10:CK:51:PHE:HB3   | 10:CK:55:ARG:HB2   | 1.92                     | 0.51              |
| 11:CL:39:THR:O     | 11:CL:48:LEU:HA    | 2.11                     | 0.51              |
| 13:CN:51:PRO:HG2   | 13:CN:54:SER:OG    | 2.11                     | 0.51              |
| 16:CQ:77:VAL:HG12  | 16:CQ:78:VAL:N     | 2.25                     | 0.51              |
| 54:D4:9:LYS:O      | 54:D4:9:LYS:HD3    | 2.11                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:1338:G:O2'  | 24:DA:1339:G:H5'   | 2.11                     | 0.51              |
| 24:DA:1417:C:H4'  | 24:DA:1587:G:N2    | 2.26                     | 0.51              |
| 24:DA:1498:C:O2'  | 24:DA:1499:C:C5'   | 2.59                     | 0.51              |
| 24:DA:120:U:H1'   | 24:DA:149:A:C8     | 2.46                     | 0.51              |
| 24:DA:1716:U:O2'  | 24:DA:1717:A:C5'   | 2.59                     | 0.51              |
| 24:DA:1775:U:H2'  | 24:DA:1776:G:O5'   | 2.11                     | 0.51              |
| 24:DA:2314:A:H2'  | 24:DA:2315:G:C8    | 2.45                     | 0.51              |
| 24:DA:2417:C:H2'  | 24:DA:2418:A:C8    | 2.45                     | 0.51              |
| 24:DA:2626:C:C2'  | 24:DA:2627:G:H5'   | 2.40                     | 0.51              |
| 24:DA:28:A:C6     | 24:DA:29:U:C2      | 2.99                     | 0.51              |
| 24:DA:311:A:HO2'  | 24:DA:332:A:H5'    | 1.75                     | 0.51              |
| 24:DA:223:A:N6    | 24:DA:422:A:C5     | 2.78                     | 0.51              |
| 24:DA:745:G:O2'   | 24:DA:748:G:H1'    | 2.11                     | 0.51              |
| 24:DA:910:A:N6    | 24:DA:911:A:N1     | 2.59                     | 0.51              |
| 24:DA:975:A:O2'   | 24:DA:976:G:C5'    | 2.58                     | 0.51              |
| 29:DF:59:ILE:HG23 | 29:DF:137:PHE:HE1  | 1.74                     | 0.51              |
| 30:DG:120:ILE:O   | 30:DG:120:ILE:HG23 | 2.09                     | 0.51              |
| 32:DI:83:ALA:HB2  | 32:DI:99:LYS:O     | 2.10                     | 0.51              |
| 37:DN:103:ARG:HD3 | 37:DN:110:MET:SD   | 2.51                     | 0.51              |
| 39:DP:87:ARG:HG2  | 39:DP:88:ARG:H     | 1.75                     | 0.51              |
| 42:DS:80:PRO:HD2  | 42:DS:100:THR:OG1  | 2.11                     | 0.51              |
| 49:DZ:13:ILE:HG22 | 49:DZ:14:GLY:N     | 2.26                     | 0.51              |
| 21:AA:1007:U:C2'  | 21:AA:1008:U:H5''  | 2.38                     | 0.51              |
| 21:AA:71:A:C6     | 21:AA:100:G:N7     | 2.79                     | 0.51              |
| 21:AA:1140:C:O2'  | 21:AA:1141:C:H6    | 1.93                     | 0.51              |
| 21:AA:1444:U:H2'  | 21:AA:1445:U:C6    | 2.45                     | 0.51              |
| 21:AA:174:A:O2'   | 21:AA:175:C:H5'    | 2.11                     | 0.51              |
| 21:AA:204:G:H1'   | 21:AA:465:A:C2     | 2.46                     | 0.51              |
| 21:AA:857:C:N4    | 21:AA:858:G:C6     | 2.79                     | 0.51              |
| 21:AA:899:C:H2'   | 21:AA:900:A:O4'    | 2.11                     | 0.51              |
| 21:AA:914:A:O2'   | 21:AA:915:A:C5'    | 2.59                     | 0.51              |
| 8:AI:121:ARG:HG3  | 21:AA:1348:U:H4'   | 1.92                     | 0.51              |
| 6:AG:149:ALA:HB2  | 10:AK:55:ARG:HH21  | 1.76                     | 0.51              |
| 20:AU:9:GLU:CG    | 20:AU:10:PRO:HD3   | 2.41                     | 0.51              |
| 24:BA:1135:C:N4   | 24:BA:1139:G:C6    | 2.79                     | 0.51              |
| 24:BA:1315:C:C2   | 24:BA:1338:G:C2    | 2.99                     | 0.51              |
| 24:BA:1469:A:H2'  | 24:BA:1470:A:H8    | 1.69                     | 0.51              |
| 24:BA:962:G:H21   | 24:BA:2250:G:H1    | 1.59                     | 0.51              |
| 24:BA:2385:C:H2'  | 24:BA:2386:A:C8    | 2.46                     | 0.51              |
| 24:BA:281:C:H2'   | 24:BA:282:A:C8     | 2.45                     | 0.51              |
| 24:BA:638:G:C5    | 24:BA:651:G:C2     | 2.99                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:726:G:O2'   | 24:BA:727:A:H8    | 1.93                     | 0.51              |
| 24:BA:1819:A:H3'  | 26:BC:176:ARG:HG2 | 1.92                     | 0.51              |
| 24:BA:1972:G:OP2  | 26:BC:237:ARG:NH1 | 2.44                     | 0.51              |
| 28:BE:79:ARG:O    | 28:BE:80:SER:C    | 2.49                     | 0.51              |
| 30:BG:97:VAL:HA   | 30:BG:102:ILE:HA  | 1.92                     | 0.51              |
| 30:BG:115:GLN:CD  | 30:BG:115:GLN:N   | 2.65                     | 0.51              |
| 34:BK:88:ASN:ND2  | 34:BK:90:ASN:H    | 2.09                     | 0.51              |
| 35:BL:66:PHE:O    | 35:BL:66:PHE:CG   | 2.64                     | 0.51              |
| 35:BL:94:THR:CG2  | 35:BL:95:LEU:N    | 2.74                     | 0.51              |
| 38:BO:4:LYS:O     | 38:BO:8:ILE:HG13  | 2.11                     | 0.51              |
| 42:BS:29:VAL:HB   | 42:BS:69:LEU:O    | 2.09                     | 0.51              |
| 43:BT:61:LEU:C    | 43:BT:61:LEU:HD12 | 2.31                     | 0.51              |
| 46:BW:19:ARG:NH1  | 46:BW:22:VAL:HG11 | 2.26                     | 0.51              |
| 55:CA:1336:C:H1'  | 55:CA:1337:G:N1   | 2.25                     | 0.51              |
| 55:CA:456:A:H2'   | 55:CA:457:G:H8    | 1.76                     | 0.51              |
| 55:CA:83:C:H2'    | 55:CA:83:C:O2     | 2.11                     | 0.51              |
| 55:CA:857:C:H2'   | 55:CA:858:G:O4'   | 2.11                     | 0.51              |
| 2:CC:39:ARG:CG    | 2:CC:54:ILE:HD13  | 2.41                     | 0.51              |
| 6:CG:78:ARG:HH21  | 55:CA:1382:C:H4'  | 1.75                     | 0.51              |
| 8:CI:35:GLU:HA    | 8:CI:39:GLY:CA    | 2.41                     | 0.51              |
| 12:CM:71:GLU:O    | 12:CM:74:MET:HB3  | 2.11                     | 0.51              |
| 14:CO:52:ARG:O    | 14:CO:55:LEU:HB3  | 2.11                     | 0.51              |
| 16:CQ:29:LYS:HE2  | 16:CQ:36:PHE:CZ   | 2.45                     | 0.51              |
| 18:CS:20:LYS:HZ3  | 18:CS:27:LYS:HD3  | 1.74                     | 0.51              |
| 24:DA:1069:A:O2'  | 24:DA:1071:G:H5'' | 2.11                     | 0.51              |
| 24:DA:1206:G:H2'  | 24:DA:1207:C:C6   | 2.46                     | 0.51              |
| 24:DA:1399:C:HO2' | 24:DA:1400:U:H6   | 1.53                     | 0.51              |
| 24:DA:1669:A:C8   | 34:DK:5:GLN:HG3   | 2.46                     | 0.51              |
| 24:DA:15:G:O2'    | 24:DA:16:C:H5'    | 2.10                     | 0.51              |
| 24:DA:1828:G:O2'  | 24:DA:1829:A:H5'  | 2.11                     | 0.51              |
| 24:DA:2331:G:N1   | 24:DA:2385:C:N4   | 2.58                     | 0.51              |
| 24:DA:2748:A:C2   | 24:DA:2757:A:C5   | 2.99                     | 0.51              |
| 24:DA:410:G:N1    | 24:DA:2407:A:N6   | 2.59                     | 0.51              |
| 24:DA:587:C:H5''  | 24:DA:588:U:H5'   | 1.93                     | 0.51              |
| 24:DA:755:U:HO2'  | 24:DA:756:A:H8    | 1.58                     | 0.51              |
| 24:DA:855:G:H21   | 46:DW:23:LYS:NZ   | 2.07                     | 0.51              |
| 24:DA:981:A:H2    | 24:DA:2027:G:N3   | 2.09                     | 0.51              |
| 24:DA:1826:G:H5'' | 26:DC:239:PHE:HE2 | 1.76                     | 0.51              |
| 38:DO:88:LYS:O    | 38:DO:89:ASP:HB3  | 2.11                     | 0.51              |
| 38:DO:99:TYR:CD1  | 38:DO:99:TYR:O    | 2.64                     | 0.51              |
| 24:DA:995:C:H5''  | 40:DQ:53:LYS:HG2  | 1.92                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:DQ:64:ILE:HD12  | 40:DQ:95:ALA:CB   | 2.40                     | 0.51              |
| 41:DR:55:ASP:CG    | 41:DR:56:GLY:H    | 2.13                     | 0.51              |
| 47:DX:29:LEU:HB2   | 47:DX:30:PRO:HD2  | 1.91                     | 0.51              |
| 24:DA:397:U:OP2    | 47:DX:9:LYS:HE2   | 2.11                     | 0.51              |
| 21:AA:1277:C:HO2'  | 21:AA:1279:G:H8   | 1.58                     | 0.50              |
| 21:AA:1234:C:C4'   | 21:AA:1364:U:H1'  | 2.41                     | 0.50              |
| 21:AA:463:U:C4     | 21:AA:464:U:C4    | 2.99                     | 0.50              |
| 21:AA:505:G:H2'    | 21:AA:506:G:C8    | 2.46                     | 0.50              |
| 21:AA:525:C:H2'    | 21:AA:526:C:C6    | 2.46                     | 0.50              |
| 21:AA:688:G:H2'    | 21:AA:689:C:H6    | 1.76                     | 0.50              |
| 21:AA:702:A:O2'    | 21:AA:703:G:P     | 2.69                     | 0.50              |
| 21:AA:960:U:C2     | 21:AA:1225:A:C5   | 2.98                     | 0.50              |
| 2:AC:156:LEU:C     | 2:AC:158:GLY:H    | 2.14                     | 0.50              |
| 10:AK:21:HIS:CD2   | 10:AK:34:THR:CG2  | 2.94                     | 0.50              |
| 13:AN:60:ARG:O     | 13:AN:61:ASN:CB   | 2.57                     | 0.50              |
| 16:AQ:22:VAL:O     | 16:AQ:42:LYS:HA   | 2.12                     | 0.50              |
| 24:BA:1098:A:H3'   | 24:BA:1099:G:C8   | 2.46                     | 0.50              |
| 24:BA:1108:U:H2'   | 24:BA:1109:C:O4'  | 2.10                     | 0.50              |
| 24:BA:1482:G:H1'   | 24:BA:1509:A:H61  | 1.76                     | 0.50              |
| 21:AA:702:A:N6     | 24:BA:1846:G:O2'  | 2.44                     | 0.50              |
| 24:BA:1954:G:O2'   | 24:BA:1955:U:OP2  | 2.29                     | 0.50              |
| 24:BA:2140:G:C6    | 24:BA:2152:G:N1   | 2.79                     | 0.50              |
| 24:BA:2199:A:H3'   | 24:BA:2200:C:H6   | 1.76                     | 0.50              |
| 24:BA:683:U:H2'    | 24:BA:684:G:O5'   | 2.11                     | 0.50              |
| 24:BA:923:G:H5'    | 46:BW:25:PHE:HZ   | 1.75                     | 0.50              |
| 25:BB:33:G:C2'     | 25:BB:34:A:H5'    | 2.41                     | 0.50              |
| 27:BD:64:GLU:O     | 27:BD:68:PHE:CD1  | 2.64                     | 0.50              |
| 29:BF:131:VAL:HG21 | 29:BF:151:LEU:HG  | 1.92                     | 0.50              |
| 32:BI:126:ARG:HA   | 32:BI:129:GLU:CD  | 2.32                     | 0.50              |
| 34:BK:107:LEU:C    | 34:BK:109:SER:H   | 2.15                     | 0.50              |
| 35:BL:89:VAL:HA    | 35:BL:121:THR:O   | 2.11                     | 0.50              |
| 41:BR:74:ILE:N     | 41:BR:74:ILE:HD12 | 2.26                     | 0.50              |
| 42:BS:74:ILE:HD12  | 42:BS:104:THR:O   | 2.10                     | 0.50              |
| 55:CA:1183:U:O2'   | 55:CA:1184:G:OP1  | 2.26                     | 0.50              |
| 55:CA:1528:U:O2'   | 55:CA:1529:G:H3'  | 2.11                     | 0.50              |
| 55:CA:181:A:H1'    | 55:CA:182:A:N1    | 2.26                     | 0.50              |
| 55:CA:268:U:H2'    | 55:CA:269:C:H6    | 1.71                     | 0.50              |
| 55:CA:317:U:H2'    | 55:CA:318:G:C8    | 2.41                     | 0.50              |
| 1:CB:125:PHE:HA    | 1:CB:136:ARG:HH22 | 1.76                     | 0.50              |
| 1:CB:185:ILE:HA    | 1:CB:199:ILE:O    | 2.11                     | 0.50              |
| 7:CH:104:SER:OG    | 7:CH:109:VAL:HG22 | 2.11                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:CN:62:ARG:NH2   | 13:CN:69:PRO:HD3   | 2.26                     | 0.50              |
| 20:CU:16:ARG:HE    | 20:CU:16:ARG:HA    | 1.75                     | 0.50              |
| 24:DA:1019:U:HO2'  | 24:DA:1021:A:H2    | 1.49                     | 0.50              |
| 24:DA:118:A:OP2    | 24:DA:119:A:H5''   | 2.11                     | 0.50              |
| 24:DA:1191:G:N2    | 24:DA:1192:G:C4    | 2.79                     | 0.50              |
| 24:DA:1269:A:H2'   | 24:DA:1270:C:C6    | 2.46                     | 0.50              |
| 24:DA:1435:G:N2    | 24:DA:1558:C:N4    | 2.59                     | 0.50              |
| 24:DA:1662:U:C2'   | 24:DA:1663:G:H5''  | 2.34                     | 0.50              |
| 24:DA:1853:A:N6    | 24:DA:1888:G:O2'   | 2.45                     | 0.50              |
| 24:DA:2750:A:O2'   | 24:DA:2752:C:N4    | 2.42                     | 0.50              |
| 24:DA:2864:G:C5    | 24:DA:2865:U:C4    | 2.99                     | 0.50              |
| 24:DA:312:G:H2'    | 24:DA:313:G:C8     | 2.45                     | 0.50              |
| 24:DA:467:G:H2'    | 24:DA:468:G:H8     | 1.75                     | 0.50              |
| 24:DA:594:U:H2'    | 24:DA:595:C:H6     | 1.72                     | 0.50              |
| 24:DA:648:G:H2'    | 24:DA:649:G:H8     | 1.76                     | 0.50              |
| 24:DA:941:A:H2'    | 24:DA:942:G:C8     | 2.46                     | 0.50              |
| 26:DC:169:ALA:O    | 26:DC:185:ALA:HB3  | 2.11                     | 0.50              |
| 26:DC:52:HIS:HD2   | 26:DC:217:PRO:O    | 1.93                     | 0.50              |
| 30:DG:112:VAL:HG13 | 30:DG:150:TYR:CE1  | 2.44                     | 0.50              |
| 32:DI:98:GLY:HA2   | 32:DI:137:LEU:HD23 | 1.93                     | 0.50              |
| 33:DJ:127:GLY:O    | 33:DJ:129:GLU:HG3  | 2.10                     | 0.50              |
| 35:DL:77:ILE:HG12  | 35:DL:101:ILE:HD11 | 1.93                     | 0.50              |
| 36:DM:19:GLY:N     | 36:DM:38:ARG:NH2   | 2.56                     | 0.50              |
| 37:DN:31:HIS:O     | 37:DN:33:ILE:HG13  | 2.11                     | 0.50              |
| 37:DN:54:LEU:HD11  | 37:DN:66:ALA:HB2   | 1.93                     | 0.50              |
| 41:DR:5:PHE:HA     | 41:DR:39:LEU:HD23  | 1.93                     | 0.50              |
| 21:AA:329:A:N7     | 21:AA:332:G:C6     | 2.79                     | 0.50              |
| 21:AA:423:G:O2'    | 21:AA:424:G:C4'    | 2.59                     | 0.50              |
| 21:AA:451:A:N6     | 21:AA:481:G:C4     | 2.79                     | 0.50              |
| 21:AA:82:G:N1      | 21:AA:88:U:H1'     | 2.26                     | 0.50              |
| 21:AA:70:U:C2      | 21:AA:94:G:C5      | 2.99                     | 0.50              |
| 1:AB:60:ALA:C      | 1:AB:223:GLY:HA3   | 2.31                     | 0.50              |
| 2:AC:113:LYS:HD3   | 2:AC:184:ASN:CG    | 2.31                     | 0.50              |
| 5:AF:6:ILE:HB      | 5:AF:62:MET:HB2    | 1.93                     | 0.50              |
| 5:AF:7:VAL:O       | 5:AF:7:VAL:HG22    | 2.11                     | 0.50              |
| 8:AI:55:ASP:CG     | 8:AI:56:MET:N      | 2.64                     | 0.50              |
| 16:AQ:6:THR:C      | 16:AQ:7:LEU:HD12   | 2.30                     | 0.50              |
| 24:BA:1592:C:O2'   | 24:BA:1593:A:H5'   | 2.11                     | 0.50              |
| 24:BA:1809:A:O2'   | 24:BA:1810:A:C5'   | 2.59                     | 0.50              |
| 24:BA:528:A:C2     | 24:BA:2043:C:H4'   | 2.46                     | 0.50              |
| 24:BA:2408:U:C2'   | 24:BA:2409:G:H5'   | 2.41                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:2472:G:C8    | 24:BA:2475:C:N4    | 2.79                     | 0.50              |
| 24:BA:2631:G:C4    | 24:BA:2632:A:C8    | 2.99                     | 0.50              |
| 24:BA:2656:U:C4    | 24:BA:2664:G:N2    | 2.79                     | 0.50              |
| 24:BA:2756:U:C1'   | 24:BA:2757:A:H5''  | 2.38                     | 0.50              |
| 24:BA:2789:C:N4    | 24:BA:2893:A:C2    | 2.79                     | 0.50              |
| 24:BA:932:U:H4'    | 24:BA:933:A:O5'    | 2.11                     | 0.50              |
| 30:BG:8:VAL:CG1    | 30:BG:9:VAL:N      | 2.74                     | 0.50              |
| 36:BM:66:ARG:HG3   | 36:BM:101:VAL:HG13 | 1.93                     | 0.50              |
| 38:BO:40:ILE:HG12  | 38:BO:47:VAL:HG12  | 1.93                     | 0.50              |
| 42:BS:107:VAL:HG12 | 42:BS:107:VAL:O    | 2.11                     | 0.50              |
| 45:BV:43:ASP:OD1   | 45:BV:43:ASP:C     | 2.50                     | 0.50              |
| 48:BY:7:ARG:H      | 48:BY:60:LYS:NZ    | 2.08                     | 0.50              |
| 55:CA:1011:C:H2'   | 55:CA:1012:A:C8    | 2.45                     | 0.50              |
| 55:CA:1089:G:C2    | 55:CA:1090:U:H1'   | 2.46                     | 0.50              |
| 55:CA:1299:A:C2'   | 55:CA:1299:A:N3    | 2.71                     | 0.50              |
| 55:CA:389:A:H2'    | 55:CA:389:A:N3     | 2.26                     | 0.50              |
| 55:CA:875:U:HO2'   | 55:CA:876:C:P      | 2.33                     | 0.50              |
| 3:CD:7:LYS:HB3     | 3:CD:20:LEU:HD13   | 1.93                     | 0.50              |
| 4:CE:55:VAL:O      | 4:CE:59:ILE:HG22   | 2.11                     | 0.50              |
| 6:CG:105:GLU:O     | 6:CG:109:LYS:HD3   | 2.11                     | 0.50              |
| 6:CG:92:PRO:HA     | 6:CG:95:ARG:HB2    | 1.92                     | 0.50              |
| 7:CH:63:LYS:HB2    | 7:CH:70:VAL:HG11   | 1.94                     | 0.50              |
| 16:CQ:13:SER:O     | 16:CQ:20:ILE:HB    | 2.11                     | 0.50              |
| 18:CS:9:PHE:CZ     | 55:CA:1318:A:H4'   | 2.45                     | 0.50              |
| 24:DA:1182:G:H2'   | 24:DA:1183:U:O4'   | 2.11                     | 0.50              |
| 24:DA:1572:A:H2'   | 24:DA:1573:G:C8    | 2.45                     | 0.50              |
| 24:DA:1998:A:C5    | 24:DA:1999:C:C5    | 2.99                     | 0.50              |
| 24:DA:2271:G:H2'   | 24:DA:2272:U:C6    | 2.47                     | 0.50              |
| 24:DA:260:G:C6     | 24:DA:261:G:N7     | 2.79                     | 0.50              |
| 24:DA:289:G:C2     | 24:DA:352:A:C2     | 2.99                     | 0.50              |
| 24:DA:301:G:C6     | 24:DA:317:G:C6     | 2.99                     | 0.50              |
| 24:DA:637:A:N6     | 24:DA:652:U:H4'    | 2.26                     | 0.50              |
| 24:DA:90:U:H3'     | 24:DA:91:A:C5'     | 2.41                     | 0.50              |
| 24:DA:93:G:N2      | 24:DA:94:A:H1'     | 2.26                     | 0.50              |
| 56:DB:66:A:OP2     | 56:DB:108:A:N6     | 2.44                     | 0.50              |
| 56:DB:77:U:C2'     | 56:DB:78:A:H5'     | 2.41                     | 0.50              |
| 27:DD:135:GLY:O    | 27:DD:136:ASN:O    | 2.29                     | 0.50              |
| 27:DD:148:GLN:CG   | 27:DD:152:PRO:HG2  | 2.41                     | 0.50              |
| 29:DF:111:ARG:HG3  | 29:DF:135:ILE:HG12 | 1.93                     | 0.50              |
| 39:DP:9:GLN:HB3    | 39:DP:12:MET:HE2   | 1.93                     | 0.50              |
| 39:DP:50:ARG:CB    | 39:DP:56:SER:HB3   | 2.37                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:DQ:4:LYS:NZ    | 40:DQ:6:GLY:CA    | 2.65                     | 0.50              |
| 42:DS:17:VAL:HG11 | 42:DS:103:ILE:CG1 | 2.38                     | 0.50              |
| 45:DV:2:PHE:CD1   | 45:DV:50:MET:HE3  | 2.46                     | 0.50              |
| 47:DX:10:ARG:O    | 47:DX:12:VAL:HG13 | 2.11                     | 0.50              |
| 47:DX:69:GLU:HA   | 47:DX:72:ALA:HB3  | 1.92                     | 0.50              |
| 21:AA:1243:C:O2'  | 21:AA:1244:G:H5'  | 2.12                     | 0.50              |
| 21:AA:1253:G:N1   | 21:AA:1285:A:N6   | 2.59                     | 0.50              |
| 21:AA:1338:G:N2   | 21:AA:1339:A:C4   | 2.79                     | 0.50              |
| 21:AA:942:G:C2    | 21:AA:1342:C:C2   | 2.99                     | 0.50              |
| 21:AA:316:C:N4    | 21:AA:351:G:C2    | 2.80                     | 0.50              |
| 21:AA:428:G:C1'   | 21:AA:430:A:N7    | 2.74                     | 0.50              |
| 21:AA:908:A:H2'   | 21:AA:909:A:H8    | 1.75                     | 0.50              |
| 21:AA:961:U:N3    | 21:AA:983:A:C6    | 2.79                     | 0.50              |
| 21:AA:967:C:C4    | 21:AA:968:A:C6    | 2.99                     | 0.50              |
| 21:AA:97:G:H2'    | 21:AA:98:A:O4'    | 2.12                     | 0.50              |
| 1:AB:113:LEU:HD22 | 1:AB:143:LEU:CG   | 2.32                     | 0.50              |
| 3:AD:40:HIS:O     | 3:AD:43:ARG:HB2   | 2.12                     | 0.50              |
| 12:AM:70:ARG:HG2  | 12:AM:71:GLU:HA   | 1.92                     | 0.50              |
| 15:AP:19:VAL:HG13 | 15:AP:37:GLY:C    | 2.31                     | 0.50              |
| 18:AS:18:VAL:O    | 18:AS:22:VAL:HG23 | 2.11                     | 0.50              |
| 19:AT:53:MET:HE1  | 19:AT:57:VAL:HG21 | 1.93                     | 0.50              |
| 20:AU:16:ARG:NH1  | 20:AU:19:LYS:HG3  | 2.27                     | 0.50              |
| 20:AU:52:VAL:HG22 | 20:AU:53:LYS:HG2  | 1.93                     | 0.50              |
| 22:AX:30:G:H2'    | 22:AX:31:A:C8     | 2.34                     | 0.50              |
| 24:BA:1176:U:C4   | 24:BA:1177:G:C6   | 2.99                     | 0.50              |
| 24:BA:1437:C:H2'  | 24:BA:1438:U:C6   | 2.45                     | 0.50              |
| 24:BA:1343:G:O4'  | 24:BA:1597:A:H2'  | 2.10                     | 0.50              |
| 24:BA:1839:G:C4   | 24:BA:1927:A:C8   | 2.99                     | 0.50              |
| 24:BA:2552:U:O2   | 24:BA:2554:U:C5'  | 2.59                     | 0.50              |
| 24:BA:2652:C:C4   | 24:BA:2653:U:C4   | 2.99                     | 0.50              |
| 24:BA:401:A:H2'   | 24:BA:402:A:H8    | 1.76                     | 0.50              |
| 24:BA:536:G:C2'   | 24:BA:537:G:H5'   | 2.41                     | 0.50              |
| 24:BA:685:A:H2'   | 24:BA:773:U:O4    | 2.12                     | 0.50              |
| 24:BA:854:C:C2'   | 24:BA:855:G:H5'   | 2.41                     | 0.50              |
| 24:BA:90:U:C6     | 24:BA:91:A:C8     | 2.99                     | 0.50              |
| 25:BB:28:C:C2'    | 25:BB:29:A:H5'    | 2.41                     | 0.50              |
| 27:BD:48:ILE:HG23 | 27:BD:84:LEU:HD21 | 1.93                     | 0.50              |
| 33:BJ:54:ILE:O    | 33:BJ:54:ILE:HG13 | 2.12                     | 0.50              |
| 34:BK:64:ARG:HH12 | 34:BK:101:GLY:HA3 | 1.76                     | 0.50              |
| 36:BM:136:MET:HE2 | 45:BV:57:TYR:CD2  | 2.45                     | 0.50              |
| 36:BM:97:GLN:CD   | 36:BM:97:GLN:N    | 2.65                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:BT:39:THR:HB   | 43:BT:42:GLU:CB   | 2.35                     | 0.50              |
| 46:BW:24:ARG:HD2  | 46:BW:25:PHE:H    | 1.73                     | 0.50              |
| 48:BY:21:LEU:O    | 48:BY:22:LEU:O    | 2.28                     | 0.50              |
| 49:BZ:29:ARG:CG   | 49:BZ:29:ARG:NH2  | 2.69                     | 0.50              |
| 55:CA:247:G:N2    | 55:CA:248:C:C2    | 2.79                     | 0.50              |
| 55:CA:429:U:O4'   | 55:CA:430:A:H5''  | 2.11                     | 0.50              |
| 55:CA:659:U:H2'   | 55:CA:660:C:H6    | 1.75                     | 0.50              |
| 55:CA:730:G:H2'   | 55:CA:766:A:H5'   | 1.92                     | 0.50              |
| 7:CH:11:THR:HG21  | 55:CA:876:C:H1'   | 1.92                     | 0.50              |
| 55:CA:960:U:O2'   | 55:CA:1223:C:H5'  | 2.12                     | 0.50              |
| 1:CB:27:LYS:N     | 1:CB:28:PRO:HD2   | 2.25                     | 0.50              |
| 3:CD:156:ALA:O    | 3:CD:160:LEU:HD23 | 2.12                     | 0.50              |
| 4:CE:44:ARG:HG2   | 4:CE:72:ASN:HA    | 1.93                     | 0.50              |
| 9:CJ:76:ILE:HG22  | 9:CJ:77:VAL:N     | 2.26                     | 0.50              |
| 11:CL:109:ARG:C   | 11:CL:110:LYS:HD2 | 2.31                     | 0.50              |
| 11:CL:2:THR:CB    | 11:CL:5:GLN:HB2   | 2.35                     | 0.50              |
| 15:CP:20:VAL:HG21 | 15:CP:32:PHE:CB   | 2.34                     | 0.50              |
| 17:CR:35:SER:HA   | 17:CR:71:ASP:OD1  | 2.11                     | 0.50              |
| 18:CS:42:ASN:HB2  | 18:CS:43:MET:CE   | 2.38                     | 0.50              |
| 20:CU:40:PRO:HA   | 20:CU:43:GLU:HB3  | 1.91                     | 0.50              |
| 24:DA:143:C:H3'   | 24:DA:144:A:C8    | 2.46                     | 0.50              |
| 24:DA:158:U:H1'   | 24:DA:169:G:N2    | 2.26                     | 0.50              |
| 24:DA:1754:A:H2'  | 24:DA:1755:A:C8   | 2.47                     | 0.50              |
| 24:DA:182:A:H2'   | 24:DA:183:C:C6    | 2.47                     | 0.50              |
| 24:DA:1847:A:O2'  | 24:DA:1848:A:H8   | 1.89                     | 0.50              |
| 24:DA:1982:U:H2'  | 24:DA:1983:G:H8   | 1.76                     | 0.50              |
| 24:DA:2550:G:C6   | 24:DA:2551:C:C4   | 2.99                     | 0.50              |
| 24:DA:2653:U:N3   | 24:DA:2654:A:C6   | 2.79                     | 0.50              |
| 24:DA:2674:G:C5   | 24:DA:2675:A:N7   | 2.79                     | 0.50              |
| 24:DA:298:G:O5'   | 24:DA:298:G:H8    | 1.94                     | 0.50              |
| 24:DA:301:G:O2'   | 24:DA:302:C:P     | 2.70                     | 0.50              |
| 24:DA:338:G:H2'   | 24:DA:339:U:H5'   | 1.93                     | 0.50              |
| 24:DA:279:A:C2    | 24:DA:362:A:H4'   | 2.47                     | 0.50              |
| 24:DA:766:U:O2'   | 24:DA:767:U:O4'   | 2.28                     | 0.50              |
| 24:DA:848:C:H2'   | 24:DA:849:A:H8    | 1.75                     | 0.50              |
| 56:DB:18:G:H2'    | 56:DB:19:C:O4'    | 2.10                     | 0.50              |
| 26:DC:15:VAL:HG13 | 26:DC:204:LEU:O   | 2.11                     | 0.50              |
| 26:DC:260:LYS:HA  | 26:DC:263:ASP:CG  | 2.32                     | 0.50              |
| 29:DF:43:ILE:HD13 | 29:DF:82:TYR:CE2  | 2.46                     | 0.50              |
| 30:DG:103:ASN:HA  | 30:DG:112:VAL:HB  | 1.93                     | 0.50              |
| 30:DG:87:GLN:HA   | 30:DG:129:GLU:HA  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:DQ:65:ASN:HA   | 40:DQ:75:TYR:HB2   | 1.93                     | 0.50              |
| 16:AQ:65:PRO:HD2  | 21:AA:264:C:O2'    | 2.12                     | 0.50              |
| 21:AA:318:G:C2    | 21:AA:336:A:C2     | 3.00                     | 0.50              |
| 21:AA:414:A:C2    | 21:AA:415:A:C4     | 2.98                     | 0.50              |
| 21:AA:595:A:N6    | 21:AA:641:U:C6     | 2.80                     | 0.50              |
| 1:AB:63:LYS:HZ1   | 1:AB:87:ASP:HB3    | 1.75                     | 0.50              |
| 2:AC:159:ALA:C    | 2:AC:161:ILE:H     | 2.14                     | 0.50              |
| 2:AC:57:GLU:OE2   | 2:AC:64:ARG:HB3    | 2.12                     | 0.50              |
| 11:AL:24:GLU:HB2  | 11:AL:29:LYS:HD2   | 1.93                     | 0.50              |
| 13:AN:13:VAL:HA   | 13:AN:59:GLN:NE2   | 2.26                     | 0.50              |
| 12:AM:92:ARG:NH1  | 18:AS:79:TYR:CZ    | 2.79                     | 0.50              |
| 24:BA:814:C:C2    | 24:BA:1194:A:C2    | 2.99                     | 0.50              |
| 24:BA:1386:C:H2'  | 24:BA:1387:A:C8    | 2.47                     | 0.50              |
| 24:BA:1385:A:C5   | 24:BA:1403:A:C6    | 2.99                     | 0.50              |
| 24:BA:2020:A:C6   | 24:BA:2022:U:C2    | 2.99                     | 0.50              |
| 24:BA:2309:A:H2'  | 24:BA:2310:C:C6    | 2.46                     | 0.50              |
| 24:BA:28:A:C5     | 24:BA:513:A:N7     | 2.79                     | 0.50              |
| 24:BA:669:G:N3    | 24:BA:669:G:C2'    | 2.71                     | 0.50              |
| 24:BA:957:C:O2'   | 24:BA:959:A:O5'    | 2.28                     | 0.50              |
| 24:BA:980:A:C6    | 24:BA:981:A:N1     | 2.80                     | 0.50              |
| 26:BC:255:LYS:C   | 26:BC:256:THR:HG23 | 2.32                     | 0.50              |
| 29:BF:45:ASP:HB2  | 29:BF:48:LEU:HB2   | 1.92                     | 0.50              |
| 30:BG:44:HIS:HA   | 30:BG:49:LEU:HD23  | 1.94                     | 0.50              |
| 32:BI:58:ILE:HG22 | 32:BI:60:VAL:HG23  | 1.92                     | 0.50              |
| 35:BL:131:ALA:O   | 35:BL:135:ILE:HD12 | 2.11                     | 0.50              |
| 42:BS:25:ARG:HE   | 42:BS:73:LYS:HZ3   | 1.57                     | 0.50              |
| 49:BZ:16:LEU:O    | 49:BZ:19:HIS:HB2   | 2.11                     | 0.50              |
| 55:CA:1148:U:H2'  | 55:CA:1149:C:O4'   | 2.12                     | 0.50              |
| 55:CA:173:U:H1'   | 55:CA:197:A:C2     | 2.46                     | 0.50              |
| 55:CA:206:C:H3'   | 55:CA:206:C:C6     | 2.47                     | 0.50              |
| 55:CA:397:A:H8    | 55:CA:548:G:OP2    | 1.95                     | 0.50              |
| 7:CH:88:LYS:HG2   | 55:CA:600:A:H5''   | 1.93                     | 0.50              |
| 55:CA:866:C:N3    | 55:CA:867:G:H1'    | 2.26                     | 0.50              |
| 2:CC:171:ARG:HH21 | 2:CC:173:PRO:HG3   | 1.76                     | 0.50              |
| 6:CG:12:LEU:O     | 6:CG:12:LEU:HD13   | 2.11                     | 0.50              |
| 16:CQ:27:PHE:CD1  | 16:CQ:36:PHE:HB3   | 2.47                     | 0.50              |
| 20:CU:19:LYS:C    | 20:CU:21:SER:H     | 2.13                     | 0.50              |
| 20:CU:35:GLU:HG3  | 20:CU:36:PHE:N     | 2.25                     | 0.50              |
| 24:DA:1047:G:C2   | 24:DA:1110:G:C5    | 3.00                     | 0.50              |
| 24:DA:1203:U:C4   | 24:DA:1204:A:C6    | 3.00                     | 0.50              |
| 24:DA:1206:G:N2   | 24:DA:1207:C:C2    | 2.80                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:DA:146:A:C2     | 24:DA:147:C:C2    | 3.00                     | 0.50              |
| 24:DA:1587:G:H21   | 24:DA:1588:G:H1'  | 1.77                     | 0.50              |
| 24:DA:573:U:H3     | 24:DA:2030:A:H3'  | 1.76                     | 0.50              |
| 24:DA:21:A:H2'     | 24:DA:22:C:C6     | 2.47                     | 0.50              |
| 24:DA:246:C:H4'    | 24:DA:385:C:O2'   | 2.10                     | 0.50              |
| 24:DA:2800:A:H2'   | 24:DA:2801:G:O4'  | 2.12                     | 0.50              |
| 24:DA:228:C:O2     | 24:DA:418:C:H4'   | 2.11                     | 0.50              |
| 24:DA:43:G:C2      | 24:DA:437:U:C2    | 2.99                     | 0.50              |
| 24:DA:489:G:C6     | 24:DA:491:G:C6    | 2.99                     | 0.50              |
| 24:DA:28:A:O2'     | 24:DA:583:G:H5'   | 2.11                     | 0.50              |
| 24:DA:636:G:H5'    | 24:DA:639:U:OP1   | 2.11                     | 0.50              |
| 24:DA:664:G:H4'    | 24:DA:941:A:OP1   | 2.11                     | 0.50              |
| 24:DA:961:C:C5     | 24:DA:2031:A:C2   | 2.99                     | 0.50              |
| 24:DA:960:A:H2'    | 24:DA:962:G:H5'   | 1.93                     | 0.50              |
| 26:DC:194:VAL:HG13 | 26:DC:194:VAL:O   | 2.11                     | 0.50              |
| 29:DF:135:ILE:O    | 29:DF:137:PHE:N   | 2.37                     | 0.50              |
| 31:DH:96:THR:O     | 31:DH:97:ARG:CG   | 2.60                     | 0.50              |
| 34:DK:64:ARG:HD2   | 34:DK:102:PRO:O   | 2.11                     | 0.50              |
| 36:DM:17:ASN:OD1   | 36:DM:95:LEU:HB3  | 2.11                     | 0.50              |
| 37:DN:103:ARG:HG3  | 37:DN:104:ALA:N   | 2.27                     | 0.50              |
| 37:DN:67:PHE:HE2   | 37:DN:73:ASN:ND2  | 2.08                     | 0.50              |
| 42:DS:39:THR:O     | 42:DS:40:ASN:HB3  | 2.11                     | 0.50              |
| 21:AA:120:A:C5     | 21:AA:122:G:C6    | 3.00                     | 0.50              |
| 21:AA:1385:G:H2'   | 21:AA:1386:G:O4'  | 2.10                     | 0.50              |
| 21:AA:276:G:O2'    | 21:AA:277:C:H5'   | 2.12                     | 0.50              |
| 21:AA:409:U:C4     | 21:AA:410:G:C5    | 3.00                     | 0.50              |
| 21:AA:434:U:H2'    | 21:AA:435:A:O4'   | 2.12                     | 0.50              |
| 21:AA:590:U:C2     | 21:AA:650:G:C2    | 3.00                     | 0.50              |
| 21:AA:885:G:C2     | 21:AA:886:G:C5    | 2.99                     | 0.50              |
| 2:AC:10:ARG:O      | 2:AC:13:ILE:N     | 2.45                     | 0.50              |
| 3:AD:125:ASN:HA    | 3:AD:141:VAL:HG23 | 1.94                     | 0.50              |
| 3:AD:191:SER:OG    | 3:AD:192:ALA:N    | 2.42                     | 0.50              |
| 3:AD:29:THR:HG22   | 3:AD:30:LYS:H     | 1.76                     | 0.50              |
| 6:AG:37:THR:O      | 6:AG:41:ILE:HG13  | 2.12                     | 0.50              |
| 7:AH:17:GLN:HB3    | 7:AH:69:ALA:CB    | 2.41                     | 0.50              |
| 18:AS:42:ASN:C     | 18:AS:42:ASN:HD22 | 2.14                     | 0.50              |
| 52:B2:1:MET:CE     | 52:B2:2:LYS:HB3   | 2.42                     | 0.50              |
| 54:B4:1:MET:HE2    | 54:B4:34:LYS:HG2  | 1.93                     | 0.50              |
| 54:B4:7:VAL:HG23   | 54:B4:8:LYS:N     | 2.26                     | 0.50              |
| 24:BA:1019:U:H2'   | 24:BA:1020:A:C8   | 2.46                     | 0.50              |
| 24:BA:1090:A:N6    | 24:BA:1102:C:N3   | 2.59                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:993:G:C6     | 24:BA:1162:G:C6    | 2.99                     | 0.50              |
| 24:BA:1753:G:OP1   | 39:BP:92:ARG:HD3   | 2.11                     | 0.50              |
| 24:BA:1821:A:H2'   | 24:BA:1822:C:C6    | 2.47                     | 0.50              |
| 24:BA:2663:G:C2'   | 24:BA:2664:G:O5'   | 2.60                     | 0.50              |
| 24:BA:2648:G:N2    | 24:BA:2673:G:H1'   | 2.27                     | 0.50              |
| 24:BA:396:G:H8     | 24:BA:396:G:O5'    | 1.93                     | 0.50              |
| 24:BA:538:A:C2     | 24:BA:556:A:C4     | 3.00                     | 0.50              |
| 24:BA:822:G:C5     | 24:BA:836:G:C2     | 3.00                     | 0.50              |
| 24:BA:912:C:H2'    | 24:BA:913:U:H6     | 1.76                     | 0.50              |
| 24:BA:996:A:C2     | 24:BA:997:G:C8     | 3.00                     | 0.50              |
| 30:BG:126:THR:HG22 | 30:BG:127:GLN:N    | 2.24                     | 0.50              |
| 30:BG:84:LYS:HG2   | 30:BG:85:LYS:N     | 2.26                     | 0.50              |
| 34:BK:114:LYS:O    | 34:BK:118:LEU:HD13 | 2.11                     | 0.50              |
| 34:BK:17:ARG:HB3   | 34:BK:45:GLU:HB3   | 1.93                     | 0.50              |
| 36:BM:14:LYS:O     | 36:BM:15:GLY:C     | 2.50                     | 0.50              |
| 38:BO:33:ARG:HG2   | 38:BO:34:HIS:CE1   | 2.47                     | 0.50              |
| 42:BS:25:ARG:NE    | 42:BS:73:LYS:HZ1   | 2.09                     | 0.50              |
| 44:BU:4:ILE:HD12   | 44:BU:69:VAL:HG23  | 1.94                     | 0.50              |
| 55:CA:1206:G:C6    | 55:CA:1207:G:C5    | 3.00                     | 0.50              |
| 55:CA:295:C:H2'    | 55:CA:296:U:C6     | 2.47                     | 0.50              |
| 55:CA:687:A:C2     | 55:CA:704:A:C5     | 2.99                     | 0.50              |
| 55:CA:724:G:N3     | 55:CA:725:G:C8     | 2.79                     | 0.50              |
| 55:CA:914:A:C2'    | 55:CA:915:A:H8     | 2.25                     | 0.50              |
| 2:CC:18:ASN:HA     | 2:CC:55:VAL:HG12   | 1.92                     | 0.50              |
| 2:CC:52:SER:C      | 2:CC:113:LYS:HD3   | 2.31                     | 0.50              |
| 3:CD:24:VAL:O      | 3:CD:25:ARG:C      | 2.48                     | 0.50              |
| 7:CH:33:VAL:C      | 7:CH:35:ILE:H      | 2.14                     | 0.50              |
| 11:CL:31:GLY:HA3   | 11:CL:54:VAL:HG11  | 1.94                     | 0.50              |
| 24:DA:1794:A:H2'   | 24:DA:1795:C:H6    | 1.76                     | 0.50              |
| 24:DA:1835:G:C2    | 24:DA:1836:C:C2    | 3.00                     | 0.50              |
| 24:DA:1935:G:C2    | 24:DA:1962:C:C2    | 3.00                     | 0.50              |
| 24:DA:1999:C:H5''  | 24:DA:2723:C:O2'   | 2.12                     | 0.50              |
| 24:DA:2009:A:N1    | 24:DA:2010:G:C5    | 2.79                     | 0.50              |
| 24:DA:2267:A:N6    | 24:DA:2271:G:C6    | 2.79                     | 0.50              |
| 24:DA:2469:A:C2    | 24:DA:2470:G:H1'   | 2.47                     | 0.50              |
| 24:DA:2515:C:O2    | 24:DA:2570:G:C2    | 2.65                     | 0.50              |
| 24:DA:315:G:H2'    | 24:DA:316:C:O4'    | 2.11                     | 0.50              |
| 24:DA:325:G:HO2'   | 24:DA:326:G:C5'    | 2.25                     | 0.50              |
| 24:DA:38:A:C5      | 24:DA:39:G:C8      | 2.99                     | 0.50              |
| 24:DA:507:A:H5''   | 24:DA:509:C:O4'    | 2.12                     | 0.50              |
| 24:DA:510:C:H2'    | 24:DA:511:U:H6     | 1.69                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:656:G:C5     | 24:DA:657:U:C4     | 2.99                     | 0.50              |
| 24:DA:710:U:H2'    | 24:DA:711:G:C8     | 2.47                     | 0.50              |
| 24:DA:775:G:H22    | 24:DA:794:A:H5'    | 1.73                     | 0.50              |
| 24:DA:800:A:H4'    | 24:DA:801:G:O5'    | 2.11                     | 0.50              |
| 24:DA:837:C:C2'    | 24:DA:838:C:H5'    | 2.41                     | 0.50              |
| 26:DC:156:SER:O    | 26:DC:194:VAL:HG11 | 2.11                     | 0.50              |
| 28:DE:112:LEU:HD12 | 28:DE:118:LEU:HD13 | 1.93                     | 0.50              |
| 29:DF:101:ARG:HH11 | 29:DF:138:PRO:CB   | 2.25                     | 0.50              |
| 34:DK:10:VAL:HG13  | 34:DK:12:ASP:H     | 1.77                     | 0.50              |
| 36:DM:112:LEU:O    | 36:DM:112:LEU:HD13 | 2.12                     | 0.50              |
| 42:DS:88:ARG:HH21  | 42:DS:88:ARG:CG    | 2.23                     | 0.50              |
| 43:DT:38:ALA:HB1   | 43:DT:81:LYS:HZ2   | 1.75                     | 0.50              |
| 21:AA:1043:G:H2'   | 21:AA:1044:A:C8    | 2.44                     | 0.50              |
| 21:AA:1075:U:C2    | 21:AA:1076:U:C5    | 3.00                     | 0.50              |
| 21:AA:1151:A:C6    | 21:AA:1152:A:N6    | 2.79                     | 0.50              |
| 21:AA:1227:A:C3'   | 21:AA:1228:C:H5''  | 2.42                     | 0.50              |
| 21:AA:15:G:C8      | 21:AA:1396:A:N3    | 2.80                     | 0.50              |
| 21:AA:1442:G:N2    | 21:AA:1461:G:H1'   | 2.26                     | 0.50              |
| 21:AA:1524:C:H2'   | 21:AA:1525:G:C8    | 2.47                     | 0.50              |
| 21:AA:35:G:H2'     | 21:AA:36:C:C6      | 2.47                     | 0.50              |
| 21:AA:428:G:O4'    | 21:AA:430:A:C8     | 2.65                     | 0.50              |
| 21:AA:575:G:H4'    | 21:AA:576:C:H5'    | 1.90                     | 0.50              |
| 21:AA:21:G:H1'     | 21:AA:915:A:N6     | 2.26                     | 0.50              |
| 12:AM:5:GLY:HA3    | 12:AM:65:GLU:HG3   | 1.94                     | 0.50              |
| 17:AR:58:ILE:O     | 17:AR:59:LYS:C     | 2.48                     | 0.50              |
| 19:AT:57:VAL:HG12  | 19:AT:71:ALA:CB    | 2.41                     | 0.50              |
| 54:B4:36:ARG:CG    | 54:B4:37:GLN:N     | 2.71                     | 0.50              |
| 24:BA:1062:G:N9    | 24:BA:1088:A:N7    | 2.60                     | 0.50              |
| 24:BA:1317:G:C2    | 24:BA:1336:A:C2    | 3.00                     | 0.50              |
| 24:BA:143:C:O5'    | 24:BA:143:C:H6     | 1.93                     | 0.50              |
| 24:BA:1561:C:H2'   | 24:BA:1562:U:C6    | 2.47                     | 0.50              |
| 24:BA:1973:G:C4    | 24:BA:1974:C:C6    | 3.00                     | 0.50              |
| 24:BA:2204:G:C5    | 24:BA:2221:G:C2    | 3.00                     | 0.50              |
| 24:BA:646:U:H5''   | 24:BA:646:U:H6     | 1.77                     | 0.50              |
| 30:BG:61:TRP:O     | 30:BG:65:GLY:N     | 2.32                     | 0.50              |
| 33:BJ:114:LEU:O    | 33:BJ:114:LEU:HD23 | 2.11                     | 0.50              |
| 36:BM:78:LEU:C     | 36:BM:80:VAL:N     | 2.64                     | 0.50              |
| 37:BN:71:ARG:HH21  | 37:BN:71:ARG:HG2   | 1.75                     | 0.50              |
| 44:BU:36:GLU:O     | 44:BU:38:ILE:HG12  | 2.11                     | 0.50              |
| 46:BW:41:GLY:HA2   | 46:BW:44:PHE:CZ    | 2.46                     | 0.50              |
| 55:CA:1031:C:C5'   | 55:CA:1032:G:H5''  | 2.23                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 55:CA:1363:A:C5  | 55:CA:1365:G:C6   | 3.00                     | 0.50              |
| 55:CA:1438:G:N2  | 55:CA:1464:U:H1'  | 2.26                     | 0.50              |
| 55:CA:203:G:HO2' | 55:CA:204:G:H8    | 1.58                     | 0.50              |
| 55:CA:444:G:C6   | 55:CA:445:G:N7    | 2.80                     | 0.50              |
| 55:CA:704:A:C4   | 55:CA:705:G:C8    | 3.00                     | 0.50              |
| 1:CB:199:ILE:O   | 1:CB:199:ILE:HG13 | 2.11                     | 0.50              |
| 3:CD:102:TYR:HD2 | 3:CD:103:ARG:HG2  | 1.76                     | 0.50              |
| 5:CF:10:VAL:O    | 5:CF:57:ALA:HA    | 2.12                     | 0.50              |
| 11:CL:85:ARG:HG2 | 11:CL:86:VAL:N    | 2.26                     | 0.50              |
| 16:CQ:21:VAL:HA  | 16:CQ:43:LEU:O    | 2.11                     | 0.50              |
| 50:D0:37:HIS:CG  | 50:D0:43:THR:HG22 | 2.47                     | 0.50              |
| 24:DA:100:U:O2'  | 24:DA:101:A:P     | 2.69                     | 0.50              |
| 24:DA:1168:G:C2  | 24:DA:1182:G:C2   | 3.00                     | 0.50              |
| 24:DA:1558:C:H1' | 24:DA:1560:G:C8   | 2.46                     | 0.50              |
| 24:DA:1622:G:C2  | 24:DA:1623:G:C8   | 2.99                     | 0.50              |
| 24:DA:1683:U:O2' | 24:DA:1684:G:O5'  | 2.29                     | 0.50              |
| 24:DA:1814:G:C6  | 24:DA:1815:A:C6   | 3.00                     | 0.50              |
| 24:DA:2189:U:H2' | 24:DA:2190:G:C5'  | 2.38                     | 0.50              |
| 24:DA:2239:G:O2' | 24:DA:2240:U:C6   | 2.62                     | 0.50              |
| 24:DA:2472:G:H1' | 24:DA:2478:A:H61  | 1.76                     | 0.50              |
| 24:DA:2809:A:OP2 | 24:DA:2890:G:N1   | 2.41                     | 0.50              |
| 24:DA:2818:U:H2' | 24:DA:2819:G:C8   | 2.46                     | 0.50              |
| 24:DA:422:A:C6   | 24:DA:423:A:C6    | 2.99                     | 0.50              |
| 24:DA:36:G:N2    | 24:DA:445:C:C2    | 2.79                     | 0.50              |
| 24:DA:475:C:N3   | 24:DA:479:A:N7    | 2.59                     | 0.50              |
| 24:DA:656:G:H8   | 24:DA:656:G:O5'   | 1.95                     | 0.50              |
| 24:DA:992:C:H4'  | 41:DR:74:ILE:HD13 | 1.94                     | 0.50              |
| 32:DI:86:LYS:O   | 32:DI:87:SER:HB2  | 2.11                     | 0.50              |
| 34:DK:1:MET:HG3  | 34:DK:1:MET:O     | 2.12                     | 0.50              |
| 42:DS:22:ASP:HA  | 42:DS:25:ARG:HH12 | 1.76                     | 0.50              |
| 21:AA:244:U:H4'  | 21:AA:245:U:H5'   | 1.93                     | 0.50              |
| 21:AA:554:A:O2'  | 21:AA:555:U:H5'   | 2.12                     | 0.50              |
| 21:AA:582:C:H2'  | 21:AA:583:A:O4'   | 2.12                     | 0.50              |
| 21:AA:623:C:O5'  | 21:AA:623:C:H6    | 1.95                     | 0.50              |
| 21:AA:713:G:H2'  | 21:AA:714:G:C8    | 2.47                     | 0.50              |
| 21:AA:914:A:HO2' | 21:AA:915:A:H8    | 1.59                     | 0.50              |
| 21:AA:96:U:O2'   | 21:AA:97:G:C8     | 2.48                     | 0.50              |
| 3:AD:23:GLY:O    | 3:AD:160:LEU:HG   | 2.12                     | 0.50              |
| 5:AF:78:PHE:HD1  | 5:AF:87:SER:HG    | 1.60                     | 0.50              |
| 7:AH:102:VAL:HB  | 7:AH:126:CYS:SG   | 2.52                     | 0.50              |
| 19:AT:29:THR:HA  | 19:AT:32:LYS:CG   | 2.42                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:AU:52:VAL:O    | 20:AU:53:LYS:HD2   | 2.12                     | 0.50              |
| 53:B3:21:PHE:HB2  | 53:B3:49:VAL:CG1   | 2.41                     | 0.50              |
| 24:BA:1085:A:H3'  | 24:BA:1086:A:H2    | 1.75                     | 0.50              |
| 24:BA:1253:A:H4'  | 24:BA:1254:A:OP2   | 2.11                     | 0.50              |
| 24:BA:1277:G:H4'  | 37:BN:20:MET:HE2   | 1.94                     | 0.50              |
| 24:BA:1476:U:O2'  | 24:BA:1477:A:H5'   | 2.12                     | 0.50              |
| 24:BA:1820:U:O2'  | 26:BC:157:ALA:O    | 2.28                     | 0.50              |
| 24:BA:1942:C:C4   | 24:BA:1943:U:C5    | 2.98                     | 0.50              |
| 24:BA:2037:A:H2'  | 24:BA:2038:G:C8    | 2.46                     | 0.50              |
| 24:BA:244:A:H2'   | 24:BA:245:G:O4'    | 2.12                     | 0.50              |
| 24:BA:2456:C:C5   | 24:BA:2457:U:C5    | 3.00                     | 0.50              |
| 24:BA:28:A:H2'    | 24:BA:29:U:H6      | 1.77                     | 0.50              |
| 24:BA:480:A:H3'   | 24:BA:481:G:H5''   | 1.94                     | 0.50              |
| 24:BA:633:A:C8    | 24:BA:633:A:O5'    | 2.57                     | 0.50              |
| 24:BA:63:A:C2     | 24:BA:64:A:C5      | 3.00                     | 0.50              |
| 24:BA:735:A:H3'   | 24:BA:736:C:H6     | 1.75                     | 0.50              |
| 24:BA:809:G:C2'   | 24:BA:810:U:O5'    | 2.59                     | 0.50              |
| 24:BA:920:A:C5    | 24:BA:921:C:C5     | 2.99                     | 0.50              |
| 26:BC:242:HIS:O   | 26:BC:244:VAL:HG13 | 2.11                     | 0.50              |
| 26:BC:83:ASP:HB2  | 26:BC:90:ILE:HG12  | 1.94                     | 0.50              |
| 28:BE:151:GLY:HA2 | 28:BE:192:ALA:HB2  | 1.94                     | 0.50              |
| 28:BE:42:GLY:O    | 28:BE:43:THR:O     | 2.30                     | 0.50              |
| 29:BF:37:MET:CE   | 29:BF:150:GLY:O    | 2.60                     | 0.50              |
| 29:BF:99:PHE:O    | 29:BF:102:LEU:HB3  | 2.10                     | 0.50              |
| 34:BK:18:ARG:HB2  | 34:BK:45:GLU:CG    | 2.42                     | 0.50              |
| 35:BL:65:GLY:O    | 35:BL:66:PHE:CB    | 2.58                     | 0.50              |
| 40:BQ:42:GLY:HA3  | 41:BR:75:VAL:HG21  | 1.93                     | 0.50              |
| 41:BR:97:LYS:O    | 41:BR:98:ILE:HB    | 2.10                     | 0.50              |
| 42:BS:74:ILE:HG23 | 42:BS:74:ILE:O     | 2.12                     | 0.50              |
| 47:BX:58:ILE:HD11 | 47:BX:66:VAL:HG11  | 1.94                     | 0.50              |
| 48:BY:12:GLU:O    | 48:BY:15:ASN:HB2   | 2.12                     | 0.50              |
| 48:BY:17:GLU:HG3  | 48:BY:18:LEU:N     | 2.25                     | 0.50              |
| 55:CA:71:A:C6     | 55:CA:100:G:C5     | 3.00                     | 0.50              |
| 55:CA:1133:G:H2'  | 55:CA:1134:G:H8    | 1.76                     | 0.50              |
| 55:CA:1250:A:C5   | 55:CA:1287:A:N7    | 2.79                     | 0.50              |
| 55:CA:134:G:H2'   | 55:CA:135:C:O4'    | 2.12                     | 0.50              |
| 55:CA:1394:A:C6   | 55:CA:1501:C:H4'   | 2.46                     | 0.50              |
| 55:CA:779:C:H2'   | 55:CA:780:A:O4'    | 2.12                     | 0.50              |
| 1:CB:151:LYS:HG3  | 1:CB:152:ASP:N     | 2.26                     | 0.50              |
| 1:CB:54:ALA:HA    | 1:CB:57:ASN:HB3    | 1.94                     | 0.50              |
| 2:CC:54:ILE:HG12  | 2:CC:54:ILE:O      | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CD:23:GLY:O     | 3:CD:24:VAL:O     | 2.29                     | 0.50              |
| 4:CE:155:LYS:HD3  | 7:CH:70:VAL:HG23  | 1.94                     | 0.50              |
| 8:CI:27:ILE:CD1   | 8:CI:62:LEU:HG    | 2.42                     | 0.50              |
| 22:CX:38:A:H2'    | 22:CX:39:U:C6     | 2.47                     | 0.50              |
| 24:DA:1055:G:C2'  | 24:DA:1056:G:H5'  | 2.42                     | 0.50              |
| 24:DA:1285:A:H2'  | 24:DA:1286:A:H5'' | 1.93                     | 0.50              |
| 24:DA:1312:U:C2   | 24:DA:1603:A:C6   | 3.00                     | 0.50              |
| 24:DA:1475:G:O2'  | 24:DA:1476:U:C6   | 2.63                     | 0.50              |
| 24:DA:801:G:C8    | 28:DE:49:ARG:HG3  | 2.47                     | 0.50              |
| 24:DA:870:U:H2'   | 24:DA:871:U:H5'   | 1.93                     | 0.50              |
| 56:DB:76:G:H2'    | 56:DB:77:U:C6     | 2.46                     | 0.50              |
| 31:DH:102:ALA:C   | 31:DH:104:THR:H   | 2.14                     | 0.50              |
| 24:DA:558:U:OP1   | 33:DJ:113:PRO:HD2 | 2.12                     | 0.50              |
| 37:DN:97:ILE:HG13 | 37:DN:98:LEU:N    | 2.27                     | 0.50              |
| 48:DY:30:MET:SD   | 48:DY:30:MET:O    | 2.70                     | 0.50              |
| 49:DZ:4:ILE:HG21  | 49:DZ:56:VAL:HG13 | 1.93                     | 0.50              |
| 21:AA:1098:C:H2'  | 21:AA:1099:G:H8   | 1.76                     | 0.50              |
| 21:AA:351:G:H4'   | 21:AA:352:C:OP1   | 2.12                     | 0.50              |
| 21:AA:474:G:C6    | 21:AA:475:C:C4    | 3.00                     | 0.50              |
| 1:AB:107:ARG:NE   | 1:AB:108:GLN:HE22 | 2.08                     | 0.50              |
| 4:AE:36:THR:CG2   | 4:AE:59:ILE:HD12  | 2.41                     | 0.50              |
| 5:AF:43:GLY:HA2   | 5:AF:58:HIS:CE1   | 2.45                     | 0.50              |
| 9:AJ:10:LEU:HB2   | 9:AJ:72:ARG:HB2   | 1.92                     | 0.50              |
| 10:AK:31:VAL:O    | 10:AK:43:TRP:HA   | 2.11                     | 0.50              |
| 5:AF:47:LEU:HD22  | 17:AR:65:SER:HB3  | 1.93                     | 0.50              |
| 20:AU:24:LYS:HG2  | 20:AU:25:ALA:N    | 2.26                     | 0.50              |
| 24:BA:1144:A:H2'  | 24:BA:1145:C:C6   | 2.46                     | 0.50              |
| 24:BA:1327:A:H2'  | 24:BA:1328:A:C5'  | 2.37                     | 0.50              |
| 24:BA:1844:C:O2'  | 24:BA:1845:G:H5'  | 2.11                     | 0.50              |
| 24:BA:2352:A:C5   | 46:BW:30:VAL:HG11 | 2.46                     | 0.50              |
| 24:BA:2472:G:O6   | 24:BA:2476:A:H4'  | 2.12                     | 0.50              |
| 24:BA:2654:A:N1   | 24:BA:2665:A:H5'' | 2.27                     | 0.50              |
| 24:BA:276:U:O2'   | 24:BA:277:G:O5'   | 2.30                     | 0.50              |
| 24:BA:327:G:H2'   | 24:BA:328:U:C6    | 2.47                     | 0.50              |
| 24:BA:381:G:N2    | 24:BA:382:A:H1'   | 2.27                     | 0.50              |
| 24:BA:639:U:H2'   | 24:BA:640:C:C5    | 2.43                     | 0.50              |
| 24:BA:789:A:H5''  | 59:BA:3765:HOH:O  | 2.12                     | 0.50              |
| 24:BA:821:A:N7    | 24:BA:946:C:C2    | 2.80                     | 0.50              |
| 24:BA:858:G:C2    | 24:BA:2268:A:C4   | 2.99                     | 0.50              |
| 24:BA:866:A:N7    | 24:BA:914:G:C6    | 2.80                     | 0.50              |
| 24:BA:974:G:N1    | 24:BA:1186:G:C6   | 2.80                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BD:103:ASP:O   | 27:BD:104:VAL:O    | 2.30                     | 0.50              |
| 29:BF:46:LYS:H    | 29:BF:46:LYS:CD    | 2.25                     | 0.50              |
| 35:BL:23:ILE:O    | 35:BL:24:GLY:C     | 2.50                     | 0.50              |
| 36:BM:46:ILE:HD12 | 36:BM:47:GLU:N     | 2.27                     | 0.50              |
| 24:BA:2275:C:HO2' | 36:BM:84:LYS:HA    | 1.77                     | 0.50              |
| 37:BN:66:ALA:O    | 37:BN:70:THR:OG1   | 2.30                     | 0.50              |
| 49:BZ:29:ARG:HG3  | 49:BZ:29:ARG:NH2   | 2.14                     | 0.50              |
| 55:CA:1288:A:N1   | 55:CA:1371:G:H1'   | 2.26                     | 0.50              |
| 55:CA:46:G:H2'    | 55:CA:366:A:N7     | 2.27                     | 0.50              |
| 55:CA:763:G:N3    | 55:CA:764:C:C6     | 2.80                     | 0.50              |
| 55:CA:91:U:O2'    | 55:CA:92:U:O4'     | 2.12                     | 0.50              |
| 1:CB:122:ASP:C    | 1:CB:124:THR:H     | 2.14                     | 0.50              |
| 3:CD:24:VAL:HG23  | 3:CD:25:ARG:N      | 2.26                     | 0.50              |
| 9:CJ:11:LYS:HE2   | 9:CJ:97:ASP:OD1    | 2.11                     | 0.50              |
| 11:CL:3:VAL:HG23  | 11:CL:4:ASN:H      | 1.76                     | 0.50              |
| 14:CO:60:SER:O    | 14:CO:64:LYS:HG3   | 2.11                     | 0.50              |
| 15:CP:40:ASN:ND2  | 15:CP:42:ILE:HB    | 2.26                     | 0.50              |
| 20:CU:26:GLY:O    | 20:CU:30:GLU:HG3   | 2.12                     | 0.50              |
| 53:D3:18:LYS:CG   | 53:D3:19:GLY:N     | 2.75                     | 0.50              |
| 24:DA:1494:A:H3'  | 24:DA:1494:A:P     | 2.52                     | 0.50              |
| 24:DA:155:A:C2'   | 24:DA:156:A:H5'    | 2.42                     | 0.50              |
| 24:DA:1565:C:O2'  | 24:DA:1566:A:C8    | 2.57                     | 0.50              |
| 24:DA:1613:G:N1   | 24:DA:1617:C:C2    | 2.80                     | 0.50              |
| 24:DA:1613:G:C2   | 24:DA:1617:C:C2    | 2.99                     | 0.50              |
| 24:DA:1912:A:H62  | 24:DA:1918:A:H1'   | 1.74                     | 0.50              |
| 24:DA:2285:C:O4'  | 24:DA:2288:A:C2    | 2.65                     | 0.50              |
| 24:DA:2402:U:H6   | 24:DA:2402:U:H5'   | 1.76                     | 0.50              |
| 24:DA:2630:G:C5   | 24:DA:2894:G:C6    | 3.00                     | 0.50              |
| 24:DA:2686:G:C6   | 24:DA:2687:U:C4    | 2.99                     | 0.50              |
| 24:DA:352:A:C6    | 24:DA:353:C:C2     | 3.00                     | 0.50              |
| 24:DA:419:U:H5''  | 59:DA:3234:HOH:O   | 2.09                     | 0.50              |
| 24:DA:699:A:H2'   | 24:DA:700:G:O4'    | 2.12                     | 0.50              |
| 26:DC:66:PHE:HD2  | 26:DC:142:ASN:HD21 | 1.58                     | 0.50              |
| 26:DC:264:LYS:HG3 | 26:DC:265:PHE:CD2  | 2.47                     | 0.50              |
| 28:DE:158:PHE:HA  | 28:DE:169:VAL:HG11 | 1.93                     | 0.50              |
| 29:DF:34:THR:O    | 29:DF:35:LEU:HB2   | 2.10                     | 0.50              |
| 30:DG:104:LEU:H   | 30:DG:112:VAL:HG23 | 1.77                     | 0.50              |
| 30:DG:139:VAL:HA  | 30:DG:142:GLN:HB3  | 1.93                     | 0.50              |
| 31:DH:84:ALA:N    | 31:DH:148:ALA:HA   | 2.26                     | 0.50              |
| 33:DJ:56:VAL:HG11 | 33:DJ:101:ILE:HG21 | 1.92                     | 0.50              |
| 33:DJ:43:GLU:CG   | 33:DJ:43:GLU:O     | 2.59                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DL:3:LEU:O     | 35:DL:4:ASN:C      | 2.49                     | 0.50              |
| 36:DM:2:LEU:O     | 36:DM:69:PRO:HG2   | 2.11                     | 0.50              |
| 39:DP:28:LYS:NZ   | 39:DP:28:LYS:H     | 2.10                     | 0.50              |
| 40:DQ:91:ARG:NH2  | 40:DQ:93:ILE:HD13  | 2.27                     | 0.50              |
| 42:DS:21:ALA:O    | 42:DS:74:ILE:HD13  | 2.12                     | 0.50              |
| 48:DY:57:LEU:O    | 48:DY:57:LEU:HD13  | 2.12                     | 0.50              |
| 21:AA:132:C:O2'   | 21:AA:133:U:O4'    | 2.22                     | 0.50              |
| 7:AH:12:ARG:NH2   | 21:AA:826:C:H5'    | 2.27                     | 0.50              |
| 21:AA:885:G:N2    | 21:AA:886:G:C5     | 2.80                     | 0.50              |
| 21:AA:898:G:N2    | 21:AA:901:A:OP2    | 2.39                     | 0.50              |
| 2:AC:129:PHE:CE2  | 2:AC:156:LEU:HD23  | 2.47                     | 0.50              |
| 8:AI:17:ARG:NH2   | 21:AA:1129:C:H5''  | 2.27                     | 0.50              |
| 9:AJ:52:LEU:CD2   | 9:AJ:59:LYS:HA     | 2.40                     | 0.50              |
| 16:AQ:66:LEU:HB2  | 16:AQ:70:LYS:HE2   | 1.93                     | 0.50              |
| 16:AQ:8:GLN:OE1   | 16:AQ:8:GLN:HA     | 2.12                     | 0.50              |
| 19:AT:53:MET:O    | 19:AT:57:VAL:HG23  | 2.12                     | 0.50              |
| 24:BA:1190:G:H5'' | 35:BL:32:GLY:HA2   | 1.93                     | 0.50              |
| 24:BA:1205:A:N1   | 28:BE:165:HIS:HB2  | 2.27                     | 0.50              |
| 24:BA:1333:G:H5'  | 24:BA:1333:G:C8    | 2.46                     | 0.50              |
| 24:BA:1808:A:N1   | 47:BX:27:ARG:HD2   | 2.27                     | 0.50              |
| 24:BA:1829:A:N3   | 26:BC:14:HIS:HE1   | 2.09                     | 0.50              |
| 24:BA:2004:G:C2'  | 24:BA:2005:A:H5'   | 2.42                     | 0.50              |
| 24:BA:2058:A:H5'' | 24:BA:2059:A:P     | 2.52                     | 0.50              |
| 24:BA:2572:A:C8   | 27:BD:150:GLN:HB3  | 2.47                     | 0.50              |
| 24:BA:2816:G:C6   | 24:BA:2817:U:C4    | 3.00                     | 0.50              |
| 24:BA:545:U:H3'   | 24:BA:545:U:C6     | 2.47                     | 0.50              |
| 24:BA:687:C:C4    | 24:BA:688:U:C4     | 3.00                     | 0.50              |
| 24:BA:769:U:H2'   | 24:BA:770:G:H8     | 1.77                     | 0.50              |
| 24:BA:799:G:H2'   | 24:BA:800:A:C8     | 2.46                     | 0.50              |
| 24:BA:883:G:C2    | 24:BA:894:U:O2     | 2.65                     | 0.50              |
| 25:BB:90:C:OP1    | 36:BM:16:ARG:HB3   | 2.12                     | 0.50              |
| 29:BF:110:ILE:O   | 29:BF:111:ARG:O    | 2.29                     | 0.50              |
| 30:BG:86:LEU:CD1  | 30:BG:132:LEU:HD21 | 2.42                     | 0.50              |
| 32:BI:9:LYS:HB2   | 32:BI:55:PRO:HB2   | 1.93                     | 0.50              |
| 32:BI:60:VAL:HG22 | 32:BI:66:PHE:HB2   | 1.93                     | 0.50              |
| 24:BA:954:G:OP2   | 36:BM:16:ARG:NH2   | 2.42                     | 0.50              |
| 38:BO:67:ASN:O    | 38:BO:68:LYS:C     | 2.49                     | 0.50              |
| 40:BQ:13:HIS:CD2  | 40:BQ:31:TYR:CG    | 2.99                     | 0.50              |
| 48:BY:26:PHE:CE1  | 48:BY:30:MET:HG3   | 2.47                     | 0.50              |
| 55:CA:1157:A:H1'  | 55:CA:1181:G:H22   | 1.76                     | 0.50              |
| 55:CA:1250:A:H2'  | 55:CA:1251:A:O4'   | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:1239:A:N7   | 55:CA:1298:U:N3   | 2.60                     | 0.50              |
| 55:CA:1349:A:H2'  | 55:CA:1350:A:O4'  | 2.11                     | 0.50              |
| 55:CA:1387:G:C6   | 55:CA:1388:C:N4   | 2.79                     | 0.50              |
| 55:CA:13:U:O2'    | 55:CA:14:U:OP1    | 2.30                     | 0.50              |
| 55:CA:1508:A:O2'  | 55:CA:1509:C:H5'  | 2.12                     | 0.50              |
| 16:CQ:70:LYS:CD   | 55:CA:254:G:H5''  | 2.42                     | 0.50              |
| 55:CA:304:U:H2'   | 55:CA:305:G:C8    | 2.47                     | 0.50              |
| 55:CA:647:C:H2'   | 55:CA:648:A:C8    | 2.46                     | 0.50              |
| 55:CA:13:U:O2     | 55:CA:914:A:H2'   | 2.11                     | 0.50              |
| 2:CC:91:ALA:HB2   | 2:CC:98:ALA:HB3   | 1.92                     | 0.50              |
| 4:CE:95:MET:CE    | 4:CE:143:LEU:HD21 | 2.42                     | 0.50              |
| 4:CE:57:ALA:HA    | 4:CE:60:GLN:HB3   | 1.94                     | 0.50              |
| 7:CH:15:ASN:ND2   | 55:CA:875:U:O2    | 2.45                     | 0.50              |
| 9:CJ:15:HIS:ND1   | 9:CJ:70:HIS:CD2   | 2.80                     | 0.50              |
| 10:CK:117:HIS:O   | 10:CK:118:ASN:HB2 | 2.12                     | 0.50              |
| 12:CM:52:ILE:C    | 12:CM:54:THR:H    | 2.15                     | 0.50              |
| 50:D0:12:ARG:HG3  | 50:D0:15:ARG:NH1  | 2.19                     | 0.50              |
| 24:DA:1124:G:H1'  | 54:D4:38:GLY:OXT  | 2.12                     | 0.50              |
| 24:DA:105:C:H2'   | 24:DA:106:C:H6    | 1.76                     | 0.50              |
| 24:DA:1338:G:H4'  | 43:DT:18:GLU:CD   | 2.32                     | 0.50              |
| 24:DA:1381:G:H2'  | 24:DA:1381:G:N3   | 2.27                     | 0.50              |
| 24:DA:14:A:H3'    | 24:DA:15:G:H5''   | 1.94                     | 0.50              |
| 24:DA:1653:G:H5'' | 24:DA:1654:A:OP1  | 2.12                     | 0.50              |
| 24:DA:1789:A:OP2  | 26:DC:220:ARG:NH1 | 2.45                     | 0.50              |
| 24:DA:2363:G:OP1  | 53:D3:39:ARG:HD2  | 2.12                     | 0.50              |
| 24:DA:540:C:H2'   | 24:DA:541:A:H8    | 1.76                     | 0.50              |
| 24:DA:754:U:O2'   | 24:DA:755:U:C5'   | 2.60                     | 0.50              |
| 56:DB:65:U:H2'    | 56:DB:108:A:N6    | 2.26                     | 0.50              |
| 27:DD:118:PHE:CG  | 27:DD:119:ALA:N   | 2.80                     | 0.50              |
| 27:DD:125:TRP:CD1 | 27:DD:160:LYS:HB3 | 2.46                     | 0.50              |
| 28:DE:139:LYS:NZ  | 28:DE:139:LYS:HB2 | 2.27                     | 0.50              |
| 29:DF:36:ASN:O    | 29:DF:37:MET:CB   | 2.59                     | 0.50              |
| 32:DI:8:VAL:C     | 32:DI:9:LYS:CG    | 2.80                     | 0.50              |
| 33:DJ:20:ALA:HA   | 33:DJ:23:LYS:CG   | 2.42                     | 0.50              |
| 34:DK:107:LEU:C   | 34:DK:109:SER:H   | 2.15                     | 0.50              |
| 34:DK:111:LYS:N   | 34:DK:111:LYS:HE3 | 2.14                     | 0.50              |
| 38:DO:51:ALA:HB3  | 38:DO:78:VAL:CG2  | 2.42                     | 0.50              |
| 40:DQ:59:LEU:O    | 40:DQ:63:ARG:HD3  | 2.12                     | 0.50              |
| 24:DA:855:G:O2'   | 46:DW:23:LYS:HD3  | 2.12                     | 0.50              |
| 49:DZ:37:ARG:HA   | 49:DZ:37:ARG:NE   | 2.27                     | 0.50              |
| 21:AA:1071:C:C2   | 21:AA:1105:A:C2   | 3.00                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 21:AA:1234:C:C1'   | 21:AA:1364:U:H6   | 2.20                     | 0.49              |
| 21:AA:503:C:O2     | 21:AA:510:A:H2    | 1.95                     | 0.49              |
| 21:AA:602:A:H2'    | 21:AA:603:U:H6    | 1.76                     | 0.49              |
| 21:AA:872:A:C5     | 21:AA:874:G:C8    | 3.00                     | 0.49              |
| 21:AA:86:G:N2      | 21:AA:87:C:N4     | 2.60                     | 0.49              |
| 1:AB:83:ALA:HB1    | 1:AB:89:PHE:O     | 2.12                     | 0.49              |
| 6:AG:76:SER:HA     | 6:AG:85:GLN:HB3   | 1.94                     | 0.49              |
| 10:AK:39:ASN:O     | 10:AK:40:ALA:HB3  | 2.11                     | 0.49              |
| 24:BA:1438:U:O2'   | 24:BA:1439:A:H5'  | 2.12                     | 0.49              |
| 24:BA:1525:A:H2'   | 24:BA:1526:C:O4'  | 2.12                     | 0.49              |
| 24:BA:1569:A:N1    | 24:BA:1570:A:C2   | 2.80                     | 0.49              |
| 24:BA:1724:G:C5    | 24:BA:1725:U:C4   | 2.99                     | 0.49              |
| 24:BA:1813:G:N3    | 26:BC:49:THR:HG21 | 2.27                     | 0.49              |
| 24:BA:2365:G:H4'   | 46:BW:59:PHE:CE2  | 2.46                     | 0.49              |
| 24:BA:792:A:C6     | 24:BA:2440:C:C6   | 3.00                     | 0.49              |
| 24:BA:2531:A:H5'   | 30:BG:156:TYR:CE2 | 2.46                     | 0.49              |
| 24:BA:33:C:H2'     | 24:BA:446:G:N2    | 2.27                     | 0.49              |
| 24:BA:623:C:O2'    | 24:BA:624:C:H5'   | 2.11                     | 0.49              |
| 24:BA:919:U:H5''   | 24:BA:919:U:C6    | 2.44                     | 0.49              |
| 24:BA:954:G:C5     | 24:BA:955:U:C6    | 2.99                     | 0.49              |
| 26:BC:245:THR:HG23 | 26:BC:249:VAL:O   | 2.11                     | 0.49              |
| 27:BD:57:ALA:O     | 27:BD:60:VAL:HG12 | 2.12                     | 0.49              |
| 29:BF:46:LYS:HD2   | 29:BF:46:LYS:N    | 2.27                     | 0.49              |
| 36:BM:33:LEU:CD2   | 36:BM:128:THR:HB  | 2.41                     | 0.49              |
| 36:BM:46:ILE:CG1   | 36:BM:47:GLU:N    | 2.74                     | 0.49              |
| 24:BA:1653:G:H3'   | 37:BN:2:ARG:HG3   | 1.94                     | 0.49              |
| 47:BX:20:ALA:HB3   | 47:BX:22:ASN:ND2  | 2.27                     | 0.49              |
| 55:CA:132:C:O2'    | 55:CA:133:U:O5'   | 2.30                     | 0.49              |
| 55:CA:484:G:H4'    | 55:CA:485:U:H5'   | 1.94                     | 0.49              |
| 55:CA:90:C:O2'     | 55:CA:91:U:C6     | 2.64                     | 0.49              |
| 1:CB:45:THR:HG23   | 1:CB:200:PRO:HD2  | 1.94                     | 0.49              |
| 3:CD:187:ARG:NH1   | 3:CD:196:GLU:OE1  | 2.45                     | 0.49              |
| 3:CD:98:ASP:CG     | 3:CD:114:ARG:HH21 | 2.14                     | 0.49              |
| 4:CE:38:VAL:HG23   | 4:CE:66:ALA:HB1   | 1.94                     | 0.49              |
| 6:CG:30:MET:O      | 6:CG:31:VAL:CB    | 2.60                     | 0.49              |
| 6:CG:88:VAL:HG22   | 6:CG:89:GLU:N     | 2.25                     | 0.49              |
| 6:CG:94:ARG:C      | 6:CG:96:ASN:N     | 2.65                     | 0.49              |
| 8:CI:6:TYR:CE2     | 8:CI:17:ARG:HA    | 2.41                     | 0.49              |
| 9:CJ:7:ARG:HD3     | 9:CJ:102:LEU:HD23 | 1.93                     | 0.49              |
| 10:CK:27:ASN:O     | 10:CK:28:ASN:HB2  | 2.12                     | 0.49              |
| 12:CM:112:ARG:O    | 55:CA:1228:C:H5'' | 2.12                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:CM:5:GLY:O     | 12:CM:6:ILE:HG13   | 2.12                     | 0.49              |
| 14:CO:16:ARG:HB2  | 14:CO:23:SER:CB    | 2.36                     | 0.49              |
| 55:CA:1400:C:C5   | 22:CV:34:G:N7      | 2.80                     | 0.49              |
| 24:DA:1342:A:C4   | 24:DA:1345:C:N4    | 2.80                     | 0.49              |
| 24:DA:1885:A:C6   | 24:DA:1886:U:C2    | 3.00                     | 0.49              |
| 24:DA:2572:A:C8   | 27:DD:149:ASN:ND2  | 2.74                     | 0.49              |
| 24:DA:2607:G:H2'  | 24:DA:2608:G:O4'   | 2.11                     | 0.49              |
| 24:DA:2900:A:C6   | 24:DA:2901:C:C4    | 2.99                     | 0.49              |
| 24:DA:295:G:H2'   | 24:DA:295:G:N3     | 2.27                     | 0.49              |
| 24:DA:324:A:H2'   | 24:DA:325:G:C8     | 2.48                     | 0.49              |
| 56:DB:11:C:C5     | 56:DB:12:C:H5      | 2.27                     | 0.49              |
| 26:DC:94:LEU:HD13 | 26:DC:100:ARG:HD3  | 1.92                     | 0.49              |
| 27:DD:28:GLU:HA   | 27:DD:185:ASN:O    | 2.11                     | 0.49              |
| 24:DA:468:G:H5''  | 28:DE:55:SER:CB    | 2.42                     | 0.49              |
| 35:DL:40:SER:O    | 35:DL:41:ARG:O     | 2.30                     | 0.49              |
| 41:DR:37:GLU:HB2  | 41:DR:53:PHE:CG    | 2.47                     | 0.49              |
| 42:DS:96:ILE:HG12 | 42:DS:96:ILE:O     | 2.11                     | 0.49              |
| 44:DU:9:GLU:OE1   | 44:DU:23:LYS:HA    | 2.12                     | 0.49              |
| 47:DX:4:CYS:HA    | 47:DX:32:LEU:HD11  | 1.94                     | 0.49              |
| 47:DX:69:GLU:O    | 47:DX:71:ARG:N     | 2.45                     | 0.49              |
| 21:AA:1074:G:C6   | 21:AA:1102:A:N6    | 2.81                     | 0.49              |
| 21:AA:1338:G:C2   | 21:AA:1339:A:C5    | 3.00                     | 0.49              |
| 21:AA:14:U:C6     | 21:AA:16:A:OP2     | 2.65                     | 0.49              |
| 16:AQ:41:THR:HG23 | 21:AA:237:G:OP1    | 2.12                     | 0.49              |
| 21:AA:754:C:HO2'  | 21:AA:755:G:P      | 2.34                     | 0.49              |
| 21:AA:926:G:C6    | 21:AA:1505:G:O6    | 2.64                     | 0.49              |
| 1:AB:143:LEU:H    | 1:AB:143:LEU:HD23  | 1.77                     | 0.49              |
| 2:AC:130:ARG:O    | 2:AC:133:MET:HB2   | 2.12                     | 0.49              |
| 4:AE:76:ASN:HD22  | 4:AE:81:GLN:CG     | 2.26                     | 0.49              |
| 8:AI:11:ARG:HA    | 8:AI:105:ARG:NH1   | 2.27                     | 0.49              |
| 8:AI:21:LYS:HG2   | 8:AI:22:PRO:HD2    | 1.94                     | 0.49              |
| 9:AJ:56:HIS:O     | 9:AJ:57:VAL:HG12   | 2.12                     | 0.49              |
| 10:AK:115:ILE:O   | 10:AK:115:ILE:HG22 | 2.10                     | 0.49              |
| 16:AQ:32:ILE:HG22 | 16:AQ:33:TYR:CG    | 2.47                     | 0.49              |
| 21:AA:1054:C:C4   | 22:AX:34:G:C1'     | 2.95                     | 0.49              |
| 24:BA:1287:A:OP2  | 37:BN:103:ARG:CG   | 2.59                     | 0.49              |
| 24:BA:1322:A:C5   | 24:BA:1323:C:C5    | 3.00                     | 0.49              |
| 24:BA:1403:A:C5   | 24:BA:1404:C:C5    | 3.00                     | 0.49              |
| 24:BA:2093:G:C6   | 24:BA:2225:A:N7    | 2.80                     | 0.49              |
| 24:BA:2135:A:O2'  | 24:BA:2136:G:O4'   | 2.27                     | 0.49              |
| 24:BA:2612:C:O2   | 24:BA:2612:C:H2'   | 2.11                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:2674:G:H2'  | 24:BA:2675:A:H8    | 1.77                     | 0.49              |
| 24:BA:298:G:H8    | 24:BA:298:G:O5'    | 1.96                     | 0.49              |
| 24:BA:319:G:C4    | 24:BA:333:G:N2     | 2.80                     | 0.49              |
| 24:BA:329:G:O4'   | 24:BA:477:A:H1'    | 2.12                     | 0.49              |
| 24:BA:747:U:N3    | 24:BA:2613:U:C4    | 2.80                     | 0.49              |
| 24:BA:733:G:C8    | 24:BA:761:A:N6     | 2.80                     | 0.49              |
| 24:BA:825:A:C6    | 24:BA:833:A:N1     | 2.80                     | 0.49              |
| 25:BB:15:A:H1'    | 25:BB:109:A:C8     | 2.47                     | 0.49              |
| 29:BF:27:VAL:O    | 29:BF:27:VAL:HG13  | 2.11                     | 0.49              |
| 31:BH:32:PRO:HB3  | 47:BX:38:TRP:CB    | 2.38                     | 0.49              |
| 33:BJ:18:VAL:HG22 | 33:BJ:140:LEU:HD12 | 1.95                     | 0.49              |
| 34:BK:105:ARG:NE  | 34:BK:106:GLU:OE2  | 2.45                     | 0.49              |
| 41:BR:54:VAL:HG22 | 41:BR:54:VAL:O     | 2.11                     | 0.49              |
| 45:BV:10:LYS:N    | 45:BV:10:LYS:HD3   | 2.21                     | 0.49              |
| 47:BX:51:SER:O    | 47:BX:54:GLY:N     | 2.45                     | 0.49              |
| 55:CA:1102:A:C4   | 55:CA:1103:C:C5    | 3.00                     | 0.49              |
| 55:CA:1213:A:N7   | 55:CA:1215:G:C5    | 2.80                     | 0.49              |
| 55:CA:1256:A:C2   | 55:CA:1278:G:C4    | 3.00                     | 0.49              |
| 55:CA:1413:A:C6   | 55:CA:1414:U:C4    | 3.00                     | 0.49              |
| 55:CA:193:C:H2'   | 55:CA:194:C:C5     | 2.47                     | 0.49              |
| 55:CA:469:C:H2'   | 55:CA:470:C:O4'    | 2.12                     | 0.49              |
| 1:CB:74:ALA:O     | 1:CB:206:ILE:HD11  | 2.11                     | 0.49              |
| 2:CC:122:GLN:HB2  | 2:CC:127:VAL:CG2   | 2.42                     | 0.49              |
| 2:CC:134:LYS:HD3  | 2:CC:135:ARG:N     | 2.27                     | 0.49              |
| 2:CC:39:ARG:HG3   | 2:CC:54:ILE:HD13   | 1.94                     | 0.49              |
| 3:CD:33:ILE:O     | 3:CD:35:GLN:HG2    | 2.12                     | 0.49              |
| 9:CJ:101:SER:O    | 9:CJ:102:LEU:HB2   | 2.12                     | 0.49              |
| 11:CL:81:ILE:HD11 | 11:CL:94:TYR:HB2   | 1.93                     | 0.49              |
| 11:CL:80:LEU:HB3  | 11:CL:97:VAL:CG2   | 2.42                     | 0.49              |
| 15:CP:66:THR:HG22 | 15:CP:67:ILE:H     | 1.74                     | 0.49              |
| 51:D1:51:ALA:O    | 51:D1:52:LYS:CB    | 2.60                     | 0.49              |
| 24:DA:2184:A:C2   | 24:DA:2185:U:C2    | 3.00                     | 0.49              |
| 24:DA:2648:G:H2'  | 24:DA:2649:C:O4'   | 2.12                     | 0.49              |
| 24:DA:2848:G:N3   | 24:DA:2849:U:H5    | 2.10                     | 0.49              |
| 24:DA:860:U:O2'   | 24:DA:861:A:C5'    | 2.60                     | 0.49              |
| 24:DA:1819:A:H5'' | 26:DC:159:THR:HG21 | 1.94                     | 0.49              |
| 26:DC:231:HIS:O   | 26:DC:232:GLY:C    | 2.50                     | 0.49              |
| 26:DC:79:ARG:HG3  | 26:DC:92:LEU:HB2   | 1.93                     | 0.49              |
| 27:DD:208:LYS:O   | 27:DD:209:ALA:HB2  | 2.10                     | 0.49              |
| 27:DD:88:GLU:O    | 27:DD:89:GLU:HG3   | 2.12                     | 0.49              |
| 28:DE:46:GLN:HB3  | 28:DE:86:ALA:CB    | 2.39                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:DE:55:SER:OG   | 28:DE:56:GLY:N     | 2.45                     | 0.49              |
| 29:DF:59:ILE:HD13 | 29:DF:137:PHE:HZ   | 1.77                     | 0.49              |
| 31:DH:96:THR:HA   | 31:DH:113:SER:OG   | 2.12                     | 0.49              |
| 33:DJ:44:TYR:O    | 33:DJ:45:THR:CB    | 2.60                     | 0.49              |
| 33:DJ:73:VAL:HG23 | 33:DJ:74:TYR:N     | 2.27                     | 0.49              |
| 33:DJ:92:MET:HE2  | 33:DJ:95:ARG:HD2   | 1.94                     | 0.49              |
| 36:DM:49:ALA:O    | 36:DM:120:ALA:HB1  | 2.12                     | 0.49              |
| 45:DV:69:GLU:C    | 45:DV:70:ILE:HD13  | 2.32                     | 0.49              |
| 21:AA:1053:G:HO2' | 21:AA:1054:C:P     | 2.34                     | 0.49              |
| 21:AA:111:G:O6    | 21:AA:330:C:N4     | 2.45                     | 0.49              |
| 19:AT:59:ARG:NH2  | 21:AA:178:C:OP2    | 2.35                     | 0.49              |
| 21:AA:677:U:H2'   | 21:AA:678:U:C6     | 2.47                     | 0.49              |
| 21:AA:778:G:H2'   | 21:AA:779:C:H6     | 1.76                     | 0.49              |
| 21:AA:577:G:C4'   | 21:AA:816:A:H2'    | 2.42                     | 0.49              |
| 21:AA:828:U:C5    | 21:AA:829:G:C8     | 2.99                     | 0.49              |
| 21:AA:872:A:C8    | 21:AA:874:G:C8     | 3.00                     | 0.49              |
| 21:AA:985:C:H2'   | 21:AA:986:U:C6     | 2.47                     | 0.49              |
| 1:AB:163:ILE:HG23 | 1:AB:164:ASP:N     | 2.22                     | 0.49              |
| 1:AB:51:GLU:HG2   | 1:AB:197:PHE:CE1   | 2.47                     | 0.49              |
| 3:AD:197:HIS:O    | 3:AD:201:GLU:HB2   | 2.13                     | 0.49              |
| 4:AE:130:THR:O    | 4:AE:131:ASN:C     | 2.50                     | 0.49              |
| 4:AE:83:PRO:HB3   | 4:AE:97:PRO:CD     | 2.38                     | 0.49              |
| 13:AN:84:ARG:HA   | 13:AN:87:ALA:HB3   | 1.94                     | 0.49              |
| 53:B3:44:ARG:N    | 53:B3:45:PRO:HD2   | 2.27                     | 0.49              |
| 54:B4:9:LYS:HB3   | 54:B4:14:CYS:HB2   | 1.94                     | 0.49              |
| 24:BA:1067:A:H3'  | 24:BA:1068:G:C8    | 2.47                     | 0.49              |
| 24:BA:2036:C:O2'  | 24:BA:2037:A:H5'   | 2.12                     | 0.49              |
| 24:BA:2512:C:H2'  | 24:BA:2513:A:O4'   | 2.11                     | 0.49              |
| 24:BA:2557:G:O2'  | 24:BA:2558:C:H5'   | 2.13                     | 0.49              |
| 25:BB:38:C:O2'    | 25:BB:39:A:H5'     | 2.12                     | 0.49              |
| 36:BM:13:HIS:O    | 36:BM:14:LYS:CB    | 2.53                     | 0.49              |
| 37:BN:32:GLU:CB   | 37:BN:115:LEU:HD12 | 2.42                     | 0.49              |
| 39:BP:51:ASN:O    | 39:BP:52:ARG:HD3   | 2.12                     | 0.49              |
| 43:BT:11:LEU:HG   | 43:BT:46:ALA:HB1   | 1.93                     | 0.49              |
| 4:CE:51:LYS:HE3   | 55:CA:1081:A:N7    | 2.27                     | 0.49              |
| 55:CA:1241:G:O2'  | 55:CA:1242:G:C8    | 2.41                     | 0.49              |
| 55:CA:1452:C:H4'  | 55:CA:1453:G:C5'   | 2.43                     | 0.49              |
| 55:CA:423:G:N3    | 55:CA:423:G:H2'    | 2.28                     | 0.49              |
| 55:CA:427:U:C4    | 55:CA:428:G:C6     | 3.00                     | 0.49              |
| 55:CA:767:A:C6    | 55:CA:768:A:C5     | 3.00                     | 0.49              |
| 55:CA:770:C:O2'   | 55:CA:771:G:H5'    | 2.12                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:CK:126:ARG:NH2 | 55:CA:796:C:O2'    | 2.45                     | 0.49              |
| 55:CA:849:G:N2    | 55:CA:850:U:H1'    | 2.27                     | 0.49              |
| 55:CA:936:C:H2'   | 55:CA:937:A:H8     | 1.77                     | 0.49              |
| 55:CA:966:G:N2    | 55:CA:967:C:C2     | 2.81                     | 0.49              |
| 1:CB:133:ALA:HA   | 1:CB:137:THR:CG2   | 2.42                     | 0.49              |
| 1:CB:212:TYR:HA   | 1:CB:215:ALA:CB    | 2.43                     | 0.49              |
| 1:CB:67:LEU:HA    | 1:CB:89:PHE:O      | 2.12                     | 0.49              |
| 2:CC:63:ILE:HG12  | 2:CC:65:VAL:CG2    | 2.42                     | 0.49              |
| 3:CD:170:LEU:HB3  | 3:CD:182:LYS:H     | 1.76                     | 0.49              |
| 5:CF:39:LEU:HD12  | 5:CF:40:GLU:N      | 2.28                     | 0.49              |
| 7:CH:33:VAL:HG22  | 7:CH:58:LEU:HD11   | 1.95                     | 0.49              |
| 9:CJ:5:ARG:HH22   | 9:CJ:7:ARG:HH22    | 1.59                     | 0.49              |
| 24:DA:1223:G:H21  | 24:DA:1225:G:H3'   | 1.76                     | 0.49              |
| 24:DA:1782:U:HO2' | 24:DA:1783:A:C5'   | 2.25                     | 0.49              |
| 24:DA:2230:G:H1'  | 47:DX:31:ASN:HB3   | 1.95                     | 0.49              |
| 24:DA:2427:C:H5'' | 24:DA:2429:G:H5'   | 1.94                     | 0.49              |
| 24:DA:2455:G:N1   | 24:DA:2498:C:N4    | 2.60                     | 0.49              |
| 24:DA:2492:U:H2'  | 24:DA:2493:U:C6    | 2.46                     | 0.49              |
| 24:DA:2516:A:C4   | 24:DA:2569:G:N2    | 2.80                     | 0.49              |
| 24:DA:2722:G:H2'  | 24:DA:2723:C:C6    | 2.47                     | 0.49              |
| 24:DA:2745:C:C4   | 24:DA:2746:U:O4    | 2.66                     | 0.49              |
| 24:DA:41:C:H2'    | 24:DA:42:A:H8      | 1.75                     | 0.49              |
| 24:DA:6:A:H2'     | 24:DA:7:G:C8       | 2.44                     | 0.49              |
| 24:DA:751:A:H5'   | 42:DS:90:LYS:HA    | 1.93                     | 0.49              |
| 24:DA:856:G:O4'   | 46:DW:23:LYS:HB3   | 2.11                     | 0.49              |
| 24:DA:910:A:C2    | 36:DM:13:HIS:CE1   | 2.99                     | 0.49              |
| 56:DB:52:A:N6     | 38:DO:33:ARG:HB2   | 2.27                     | 0.49              |
| 29:DF:102:LEU:HB3 | 29:DF:103:ILE:HD12 | 1.94                     | 0.49              |
| 30:DG:148:ARG:HB2 | 30:DG:152:ARG:HH21 | 1.77                     | 0.49              |
| 35:DL:95:LEU:HB3  | 35:DL:100:ILE:HG23 | 1.93                     | 0.49              |
| 38:DO:98:GLN:HB3  | 38:DO:100:HIS:HB3  | 1.95                     | 0.49              |
| 38:DO:39:VAL:HB   | 38:DO:49:VAL:H     | 1.77                     | 0.49              |
| 41:DR:66:HIS:CD2  | 41:DR:94:THR:HG22  | 2.47                     | 0.49              |
| 44:DU:22:GLY:HA3  | 44:DU:36:GLU:HB3   | 1.94                     | 0.49              |
| 45:DV:29:ILE:HD13 | 45:DV:31:TYR:CD2   | 2.45                     | 0.49              |
| 45:DV:30:ILE:HD12 | 45:DV:38:LEU:HD23  | 1.94                     | 0.49              |
| 49:DZ:51:SER:HA   | 49:DZ:54:VAL:CG2   | 2.43                     | 0.49              |
| 21:AA:1094:G:O2'  | 21:AA:1095:U:OP2   | 2.26                     | 0.49              |
| 21:AA:1103:C:C2'  | 21:AA:1104:G:O5'   | 2.61                     | 0.49              |
| 21:AA:1223:C:H5'' | 21:AA:1224:U:H5''  | 1.94                     | 0.49              |
| 21:AA:1364:U:O2   | 21:AA:1364:U:H2'   | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:191:G:C6    | 21:AA:192:A:C5    | 3.01                     | 0.49              |
| 21:AA:418:C:N4    | 59:AA:1716:HOH:O  | 2.45                     | 0.49              |
| 21:AA:497:G:N2    | 21:AA:498:A:C6    | 2.81                     | 0.49              |
| 21:AA:57:G:C6     | 21:AA:58:C:N3     | 2.80                     | 0.49              |
| 21:AA:652:U:O4    | 21:AA:752:G:H2'   | 2.11                     | 0.49              |
| 21:AA:803:G:C6    | 21:AA:804:U:C4    | 3.01                     | 0.49              |
| 21:AA:853:C:O2'   | 21:AA:854:U:H5'   | 2.12                     | 0.49              |
| 1:AB:124:THR:O    | 1:AB:125:PHE:HB3  | 2.12                     | 0.49              |
| 1:AB:50:ASN:OD1   | 1:AB:51:GLU:N     | 2.45                     | 0.49              |
| 3:AD:115:GLN:CD   | 3:AD:119:HIS:HE1  | 2.15                     | 0.49              |
| 4:AE:19:ARG:HD2   | 4:AE:30:PHE:CB    | 2.42                     | 0.49              |
| 8:AI:3:ASN:CG     | 8:AI:4:GLN:N      | 2.65                     | 0.49              |
| 10:AK:62:ALA:CB   | 10:AK:91:GLY:HA3  | 2.43                     | 0.49              |
| 14:AO:44:GLU:HG3  | 14:AO:45:HIS:ND1  | 2.26                     | 0.49              |
| 16:AQ:12:VAL:CG1  | 16:AQ:13:SER:N    | 2.70                     | 0.49              |
| 54:B4:30:GLU:HB3  | 54:B4:33:HIS:ND1  | 2.28                     | 0.49              |
| 24:BA:1079:C:C2   | 24:BA:1080:A:C8   | 3.00                     | 0.49              |
| 24:BA:1083:U:C6   | 24:BA:1085:A:OP2  | 2.65                     | 0.49              |
| 24:BA:1132:U:H3'  | 24:BA:1133:A:H5'' | 1.94                     | 0.49              |
| 24:BA:1273:U:HO2' | 24:BA:1274:A:P    | 2.35                     | 0.49              |
| 24:BA:1561:C:H2'  | 24:BA:1562:U:H6   | 1.77                     | 0.49              |
| 24:BA:1429:G:O4'  | 24:BA:1568:G:H1'  | 2.13                     | 0.49              |
| 24:BA:1669:A:C2'  | 24:BA:1669:A:N3   | 2.74                     | 0.49              |
| 24:BA:2468:A:O2'  | 24:BA:2469:A:OP2  | 2.28                     | 0.49              |
| 24:BA:2540:C:H2'  | 24:BA:2541:A:H5'  | 1.93                     | 0.49              |
| 24:BA:270:A:C2    | 24:BA:370:G:C6    | 3.01                     | 0.49              |
| 24:BA:396:G:H1'   | 47:BX:28:PHE:HB3  | 1.93                     | 0.49              |
| 24:BA:455:C:N3    | 24:BA:472:A:H2'   | 2.27                     | 0.49              |
| 27:BD:189:VAL:C   | 27:BD:191:GLY:H   | 2.16                     | 0.49              |
| 30:BG:37:ASN:HB3  | 30:BG:40:VAL:HG13 | 1.95                     | 0.49              |
| 31:BH:95:GLY:C    | 31:BH:97:ARG:H    | 2.15                     | 0.49              |
| 33:BJ:70:THR:HG22 | 33:BJ:90:GLU:CD   | 2.33                     | 0.49              |
| 33:BJ:95:ARG:O    | 33:BJ:95:ARG:HG3  | 2.11                     | 0.49              |
| 37:BN:103:ARG:HB2 | 37:BN:110:MET:HE2 | 1.93                     | 0.49              |
| 45:BV:80:HIS:CD2  | 45:BV:83:LYS:CB   | 2.95                     | 0.49              |
| 46:BW:22:VAL:O    | 46:BW:23:LYS:O    | 2.30                     | 0.49              |
| 47:BX:40:GLU:O    | 47:BX:43:LYS:HD2  | 2.12                     | 0.49              |
| 55:CA:1004:A:H2'  | 55:CA:1005:A:O4'  | 2.11                     | 0.49              |
| 55:CA:1095:U:H5'  | 55:CA:1109:C:O2   | 2.12                     | 0.49              |
| 55:CA:1322:C:H2'  | 55:CA:1322:C:O2   | 2.11                     | 0.49              |
| 55:CA:239:U:O5'   | 55:CA:240:G:OP2   | 2.31                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:CA:265:G:H2'    | 55:CA:266:G:H5'    | 1.94                     | 0.49              |
| 55:CA:369:G:OP2    | 55:CA:388:G:N1     | 2.45                     | 0.49              |
| 55:CA:41:G:C2      | 55:CA:402:G:C2     | 3.01                     | 0.49              |
| 55:CA:96:U:O2'     | 55:CA:97:G:H5'     | 2.12                     | 0.49              |
| 3:CD:11:SER:HA     | 3:CD:18:LEU:HG     | 1.94                     | 0.49              |
| 6:CG:94:ARG:O      | 6:CG:98:LEU:HB2    | 2.12                     | 0.49              |
| 10:CK:125:LYS:O    | 10:CK:126:ARG:O    | 2.30                     | 0.49              |
| 15:CP:68:SER:HB3   | 15:CP:71:VAL:CG1   | 2.42                     | 0.49              |
| 17:CR:32:ILE:CA    | 17:CR:39:VAL:HG23  | 2.42                     | 0.49              |
| 24:DA:1019:U:O2'   | 24:DA:1021:A:C2    | 2.59                     | 0.49              |
| 24:DA:1264:A:N7    | 24:DA:1265:A:C5    | 2.81                     | 0.49              |
| 24:DA:1329:U:O2'   | 24:DA:1330:C:OP1   | 2.29                     | 0.49              |
| 24:DA:1331:G:HO2'  | 24:DA:1332:G:C5'   | 2.25                     | 0.49              |
| 24:DA:1399:C:O2'   | 24:DA:1400:U:C5'   | 2.56                     | 0.49              |
| 24:DA:1416:G:C6    | 24:DA:1417:C:N4    | 2.81                     | 0.49              |
| 24:DA:197:A:C8     | 24:DA:2430:A:C5    | 3.00                     | 0.49              |
| 24:DA:2443:C:O2'   | 24:DA:2444:G:H5'   | 2.12                     | 0.49              |
| 24:DA:251:A:HO2'   | 24:DA:252:G:P      | 2.35                     | 0.49              |
| 24:DA:2893:A:H4'   | 24:DA:2894:G:O5'   | 2.11                     | 0.49              |
| 24:DA:309:A:H1'    | 24:DA:329:G:C4     | 2.47                     | 0.49              |
| 24:DA:319:G:C6     | 24:DA:333:G:C6     | 3.00                     | 0.49              |
| 24:DA:354:A:H2'    | 24:DA:355:U:O4'    | 2.13                     | 0.49              |
| 24:DA:581:C:C2     | 24:DA:582:A:C8     | 3.00                     | 0.49              |
| 24:DA:725:G:N1     | 24:DA:726:G:N2     | 2.61                     | 0.49              |
| 56:DB:39:A:H2'     | 56:DB:40:U:C6      | 2.47                     | 0.49              |
| 26:DC:174:ARG:HA   | 26:DC:180:MET:HG2  | 1.93                     | 0.49              |
| 27:DD:148:GLN:HG2  | 27:DD:149:ASN:H    | 1.77                     | 0.49              |
| 29:DF:136:ILE:HD13 | 29:DF:145:VAL:CG1  | 2.39                     | 0.49              |
| 29:DF:147:ARG:HD3  | 29:DF:149:ARG:HH22 | 1.76                     | 0.49              |
| 30:DG:112:VAL:CG1  | 30:DG:114:HIS:HB3  | 2.42                     | 0.49              |
| 31:DH:49:ALA:O     | 31:DH:53:GLU:HB2   | 2.12                     | 0.49              |
| 32:DI:109:ALA:HB1  | 32:DI:125:THR:HG22 | 1.93                     | 0.49              |
| 35:DL:88:GLY:O     | 35:DL:89:VAL:HG12  | 2.11                     | 0.49              |
| 36:DM:103:TYR:O    | 36:DM:104:GLU:HG3  | 2.13                     | 0.49              |
| 37:DN:5:LYS:O      | 59:DN:202:HOH:O    | 2.20                     | 0.49              |
| 37:DN:83:LEU:O     | 37:DN:87:PHE:HB2   | 2.13                     | 0.49              |
| 42:DS:6:LYS:HZ1    | 42:DS:104:THR:HG23 | 1.76                     | 0.49              |
| 42:DS:66:ILE:HD13  | 42:DS:66:ILE:N     | 2.26                     | 0.49              |
| 46:DW:77:LYS:O     | 46:DW:78:PHE:HB2   | 2.11                     | 0.49              |
| 48:DY:18:LEU:HD13  | 48:DY:22:LEU:HD13  | 1.95                     | 0.49              |
| 24:DA:851:C:H4'    | 49:DZ:46:MET:HA    | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:1033:G:N3   | 21:AA:1033:G:H2'  | 2.27                     | 0.49              |
| 21:AA:1099:G:H2'  | 21:AA:1099:G:N3   | 2.28                     | 0.49              |
| 21:AA:1261:A:H2'  | 21:AA:1262:C:O4'  | 2.13                     | 0.49              |
| 21:AA:134:G:H2'   | 21:AA:135:C:C6    | 2.47                     | 0.49              |
| 21:AA:243:A:H4'   | 21:AA:244:U:H5'   | 1.94                     | 0.49              |
| 21:AA:266:G:H1'   | 21:AA:268:U:H5    | 1.76                     | 0.49              |
| 21:AA:294:U:H2'   | 21:AA:295:C:H6    | 1.77                     | 0.49              |
| 21:AA:451:A:N6    | 21:AA:481:G:O4'   | 2.46                     | 0.49              |
| 21:AA:508:U:O2'   | 21:AA:509:A:C8    | 2.66                     | 0.49              |
| 14:AO:22:GLY:HA3  | 21:AA:750:C:O2    | 2.12                     | 0.49              |
| 21:AA:575:G:N1    | 21:AA:821:G:C8    | 2.80                     | 0.49              |
| 21:AA:81:A:O2'    | 21:AA:89:U:O2     | 2.31                     | 0.49              |
| 21:AA:898:G:N2    | 21:AA:900:A:H3'   | 2.28                     | 0.49              |
| 1:AB:48:MET:C     | 1:AB:50:ASN:H     | 2.14                     | 0.49              |
| 3:AD:33:ILE:O     | 3:AD:34:GLU:HB3   | 2.13                     | 0.49              |
| 4:AE:120:HIS:O    | 4:AE:121:ASN:CB   | 2.60                     | 0.49              |
| 12:AM:109:LYS:HZ3 | 21:AA:1227:A:H5'  | 1.77                     | 0.49              |
| 12:AM:40:GLU:HG3  | 12:AM:41:ASP:H    | 1.78                     | 0.49              |
| 51:B1:24:LYS:HE3  | 51:B1:26:LYS:HA   | 1.93                     | 0.49              |
| 24:BA:1239:G:H5'' | 59:BA:3711:HOH:O  | 2.12                     | 0.49              |
| 24:BA:1255:U:C5   | 28:BE:67:ARG:O    | 2.66                     | 0.49              |
| 24:BA:1371:G:O2'  | 24:BA:1372:U:H5'  | 2.12                     | 0.49              |
| 24:BA:1392:A:C6   | 24:BA:1393:A:N6   | 2.81                     | 0.49              |
| 24:BA:1522:A:O2'  | 24:BA:1523:U:P    | 2.70                     | 0.49              |
| 24:BA:1805:A:C4   | 24:BA:1806:C:C5   | 3.01                     | 0.49              |
| 24:BA:2287:A:O2'  | 24:BA:2288:A:H3'  | 2.13                     | 0.49              |
| 24:BA:2312:U:C2'  | 24:BA:2313:C:H5'  | 2.41                     | 0.49              |
| 24:BA:2578:G:N2   | 24:BA:2579:C:C2   | 2.81                     | 0.49              |
| 24:BA:2603:G:O2'  | 24:BA:2604:U:H5'  | 2.12                     | 0.49              |
| 24:BA:2712:C:O2'  | 24:BA:2713:U:H5'  | 2.12                     | 0.49              |
| 24:BA:696:G:C4    | 24:BA:697:G:C8    | 2.99                     | 0.49              |
| 24:BA:919:U:C2    | 24:BA:920:A:N7    | 2.80                     | 0.49              |
| 24:BA:971:G:C2'   | 24:BA:972:A:H5'   | 2.42                     | 0.49              |
| 25:BB:24:G:H1'    | 25:BB:27:C:N4     | 2.28                     | 0.49              |
| 25:BB:42:C:O2'    | 25:BB:43:C:C5'    | 2.61                     | 0.49              |
| 26:BC:151:GLY:C   | 26:BC:152:GLN:HG3 | 2.32                     | 0.49              |
| 24:BA:2636:C:O2'  | 27:BD:45:TYR:CZ   | 2.65                     | 0.49              |
| 28:BE:134:LEU:CD2 | 28:BE:161:ALA:HB2 | 2.43                     | 0.49              |
| 34:BK:2:ILE:HG23  | 34:BK:6:THR:HG21  | 1.94                     | 0.49              |
| 35:BL:77:ILE:HD11 | 35:BL:108:ALA:HB1 | 1.93                     | 0.49              |
| 36:BM:34:LYS:HD3  | 36:BM:99:GLY:HA2  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:BP:13:LYS:HG3  | 39:BP:76:HIS:ND1  | 2.28                     | 0.49              |
| 24:BA:580:U:O3'   | 40:BQ:30:VAL:HG13 | 2.13                     | 0.49              |
| 42:BS:19:LEU:O    | 50:B0:21:LEU:HD12 | 2.13                     | 0.49              |
| 46:BW:41:GLY:O    | 46:BW:42:THR:C    | 2.51                     | 0.49              |
| 55:CA:117:G:O2'   | 55:CA:118:U:H5'   | 2.13                     | 0.49              |
| 55:CA:1217:C:H2'  | 55:CA:1218:C:H6   | 1.77                     | 0.49              |
| 55:CA:1393:U:O4'  | 55:CA:1502:A:H5'' | 2.12                     | 0.49              |
| 55:CA:1498:U:H6   | 55:CA:1498:U:OP2  | 1.95                     | 0.49              |
| 55:CA:51:A:C4'    | 55:CA:52:C:OP2    | 2.59                     | 0.49              |
| 55:CA:765:G:C6    | 55:CA:812:G:C5    | 3.00                     | 0.49              |
| 55:CA:765:G:O6    | 55:CA:811:C:H5    | 1.95                     | 0.49              |
| 2:CC:2:GLN:OE1    | 55:CA:1193:G:O6   | 2.30                     | 0.49              |
| 4:CE:151:MET:O    | 4:CE:155:LYS:HG3  | 2.12                     | 0.49              |
| 6:CG:2:ARG:HA     | 55:CA:1380:U:H5   | 1.77                     | 0.49              |
| 8:CI:54:VAL:HG23  | 8:CI:59:LYS:NZ    | 2.27                     | 0.49              |
| 11:CL:54:VAL:O    | 11:CL:61:GLU:HA   | 2.12                     | 0.49              |
| 18:CS:35:ARG:NH1  | 18:CS:76:THR:HG22 | 2.28                     | 0.49              |
| 18:CS:43:MET:HE3  | 18:CS:43:MET:H    | 1.76                     | 0.49              |
| 22:CV:35:A:C2     | 22:CV:36:A:C8     | 3.00                     | 0.49              |
| 24:DA:1087:G:H2'  | 24:DA:1089:A:C8   | 2.48                     | 0.49              |
| 24:DA:136:G:O5'   | 24:DA:136:G:H8    | 1.96                     | 0.49              |
| 24:DA:1299:G:O6   | 24:DA:1639:C:H5'' | 2.12                     | 0.49              |
| 24:DA:182:A:H2'   | 24:DA:183:C:H6    | 1.77                     | 0.49              |
| 24:DA:1982:U:H6   | 24:DA:1982:U:C5'  | 2.25                     | 0.49              |
| 24:DA:2015:A:C4   | 50:D0:2:VAL:HG11  | 2.48                     | 0.49              |
| 24:DA:204:A:C8    | 24:DA:206:U:C4    | 3.00                     | 0.49              |
| 24:DA:2263:C:H4'  | 24:DA:2329:U:H4'  | 1.95                     | 0.49              |
| 24:DA:249:C:P     | 24:DA:2394:C:HO2' | 2.35                     | 0.49              |
| 24:DA:2436:G:C2   | 24:DA:2437:G:C8   | 3.01                     | 0.49              |
| 24:DA:2445:G:O2'  | 24:DA:2446:G:H5'  | 2.13                     | 0.49              |
| 24:DA:2630:G:O2'  | 24:DA:2631:G:O5'  | 2.30                     | 0.49              |
| 24:DA:590:A:OP1   | 28:DE:90:GLN:NE2  | 2.43                     | 0.49              |
| 29:DF:49:LEU:N    | 29:DF:49:LEU:HD22 | 2.24                     | 0.49              |
| 30:DG:85:LYS:HD3  | 30:DG:164:ALA:HB3 | 1.94                     | 0.49              |
| 32:DI:52:LEU:O    | 32:DI:54:ILE:HD12 | 2.12                     | 0.49              |
| 33:DJ:45:THR:HG23 | 33:DJ:45:THR:O    | 2.12                     | 0.49              |
| 24:DA:671:C:C5    | 35:DL:33:ARG:NH2  | 2.80                     | 0.49              |
| 35:DL:48:ARG:HG3  | 35:DL:48:ARG:NH1  | 2.27                     | 0.49              |
| 37:DN:100:CYS:O   | 50:D0:41:HIS:HD2  | 1.95                     | 0.49              |
| 37:DN:5:LYS:O     | 37:DN:6:SER:HB2   | 2.13                     | 0.49              |
| 38:DO:111:ARG:HA  | 38:DO:115:LEU:O   | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:DO:26:LEU:HD23 | 38:DO:92:PHE:HE1  | 1.76                     | 0.49              |
| 40:DQ:87:VAL:HG12 | 40:DQ:88:GLU:H    | 1.77                     | 0.49              |
| 43:DT:7:LEU:O     | 43:DT:7:LEU:HD23  | 2.12                     | 0.49              |
| 24:DA:2200:C:OP1  | 47:DX:35:HIS:HA   | 2.12                     | 0.49              |
| 21:AA:428:G:N3    | 21:AA:430:A:N6    | 2.60                     | 0.49              |
| 21:AA:734:G:C6    | 21:AA:735:C:N4    | 2.81                     | 0.49              |
| 2:AC:133:MET:O    | 2:AC:136:ALA:HB3  | 2.12                     | 0.49              |
| 4:AE:33:THR:HB    | 4:AE:49:TYR:CE1   | 2.46                     | 0.49              |
| 7:AH:31:LEU:O     | 7:AH:35:ILE:HG13  | 2.13                     | 0.49              |
| 15:AP:41:PRO:C    | 15:AP:42:ILE:HD13 | 2.33                     | 0.49              |
| 20:AU:36:PHE:HD1  | 20:AU:39:LYS:CB   | 2.25                     | 0.49              |
| 50:B0:53:VAL:O    | 50:B0:54:ILE:O    | 2.30                     | 0.49              |
| 24:BA:1083:U:C5   | 24:BA:1085:A:OP2  | 2.65                     | 0.49              |
| 24:BA:1326:U:H2'  | 24:BA:1327:A:H8   | 1.77                     | 0.49              |
| 24:BA:189:G:H2'   | 24:BA:205:G:N2    | 2.28                     | 0.49              |
| 24:BA:2056:G:C8   | 24:BA:2056:G:H5'  | 2.47                     | 0.49              |
| 24:BA:2199:A:C5'  | 24:BA:2200:C:H5   | 2.25                     | 0.49              |
| 24:BA:858:G:C2    | 24:BA:2268:A:H2'  | 2.46                     | 0.49              |
| 24:BA:494:G:O2'   | 24:BA:495:G:H5'   | 2.12                     | 0.49              |
| 24:BA:704:G:C2'   | 24:BA:726:G:N2    | 2.75                     | 0.49              |
| 27:BD:101:PHE:CD1 | 27:BD:101:PHE:N   | 2.81                     | 0.49              |
| 28:BE:119:ILE:O   | 28:BE:187:VAL:O   | 2.30                     | 0.49              |
| 28:BE:48:THR:O    | 28:BE:50:ALA:N    | 2.46                     | 0.49              |
| 34:BK:77:ILE:HG13 | 39:BP:71:ARG:HG3  | 1.94                     | 0.49              |
| 36:BM:46:ILE:HG13 | 36:BM:47:GLU:N    | 2.26                     | 0.49              |
| 38:BO:3:LYS:HG3   | 38:BO:4:LYS:N     | 2.28                     | 0.49              |
| 40:BQ:85:ALA:HA   | 40:BQ:115:ALA:CB  | 2.43                     | 0.49              |
| 41:BR:39:LEU:O    | 41:BR:40:MET:HB2  | 2.13                     | 0.49              |
| 41:BR:64:VAL:O    | 41:BR:65:ALA:HB3  | 2.13                     | 0.49              |
| 45:BV:40:ILE:CG2  | 45:BV:41:GLU:N    | 2.76                     | 0.49              |
| 55:CA:1114:C:H2'  | 55:CA:1115:U:H6   | 1.78                     | 0.49              |
| 55:CA:1219:A:H2'  | 55:CA:1220:G:H8   | 1.76                     | 0.49              |
| 8:CI:69:GLY:O     | 55:CA:1250:A:H4'  | 2.11                     | 0.49              |
| 55:CA:1408:A:N1   | 55:CA:1494:G:C6   | 2.80                     | 0.49              |
| 1:CB:9:LEU:O      | 1:CB:10:LYS:HB2   | 2.11                     | 0.49              |
| 2:CC:120:THR:HG23 | 2:CC:187:GLU:O    | 2.12                     | 0.49              |
| 5:CF:5:GLU:O      | 5:CF:90:MET:HG2   | 2.11                     | 0.49              |
| 6:CG:4:ARG:HG3    | 6:CG:6:ILE:HG22   | 1.92                     | 0.49              |
| 9:CJ:37:ARG:HB3   | 9:CJ:75:ASP:HB3   | 1.94                     | 0.49              |
| 11:CL:65:TYR:HD1  | 11:CL:66:ILE:H    | 1.59                     | 0.49              |
| 12:CM:1:ALA:N     | 12:CM:2:ARG:HH11  | 2.10                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:CJ:52:LEU:HB2   | 13:CN:80:ARG:CD    | 2.42                     | 0.49              |
| 16:CQ:77:VAL:HG12 | 16:CQ:78:VAL:H     | 1.77                     | 0.49              |
| 20:CU:31:VAL:O    | 20:CU:33:ARG:N     | 2.43                     | 0.49              |
| 22:CV:30:G:O2'    | 22:CV:31:A:H5'     | 2.13                     | 0.49              |
| 24:DA:1071:G:O6   | 24:DA:1091:G:N7    | 2.45                     | 0.49              |
| 24:DA:1264:A:C6   | 24:DA:1265:A:N6    | 2.80                     | 0.49              |
| 24:DA:1338:G:N3   | 24:DA:1393:A:H2    | 2.10                     | 0.49              |
| 24:DA:1521:G:C6   | 24:DA:1522:A:C6    | 3.01                     | 0.49              |
| 24:DA:1840:G:H2'  | 24:DA:1841:U:C6    | 2.48                     | 0.49              |
| 24:DA:2373:G:C6   | 24:DA:2374:C:C4    | 3.01                     | 0.49              |
| 24:DA:2378:A:H2'  | 38:DO:21:LEU:HD13  | 1.95                     | 0.49              |
| 24:DA:241:A:O2'   | 24:DA:242:G:O5'    | 2.26                     | 0.49              |
| 24:DA:35:G:O2'    | 24:DA:36:G:O5'     | 2.30                     | 0.49              |
| 24:DA:464:U:H2'   | 24:DA:465:G:C8     | 2.48                     | 0.49              |
| 56:DB:75:G:H1     | 56:DB:102:G:H22    | 1.55                     | 0.49              |
| 24:DA:784:G:C6    | 26:DC:227:VAL:HG21 | 2.48                     | 0.49              |
| 29:DF:46:LYS:HD3  | 29:DF:50:ASP:HB2   | 1.95                     | 0.49              |
| 29:DF:74:ALA:HB1  | 29:DF:76:PHE:HD2   | 1.74                     | 0.49              |
| 36:DM:68:PHE:CG   | 36:DM:69:PRO:HD2   | 2.47                     | 0.49              |
| 39:DP:22:GLY:H    | 39:DP:46:VAL:HB    | 1.78                     | 0.49              |
| 44:DU:39:ASN:HD21 | 44:DU:64:ILE:HG22  | 1.77                     | 0.49              |
| 47:DX:26:ARG:HG3  | 47:DX:27:ARG:N     | 2.27                     | 0.49              |
| 21:AA:1185:G:C6   | 21:AA:1186:G:N7    | 2.80                     | 0.49              |
| 21:AA:1358:U:H2'  | 21:AA:1359:C:O4'   | 2.11                     | 0.49              |
| 21:AA:31:G:N2     | 21:AA:47:C:H5''    | 2.27                     | 0.49              |
| 21:AA:662:U:H2'   | 21:AA:663:A:C8     | 2.47                     | 0.49              |
| 21:AA:792:A:N3    | 21:AA:794:A:C6     | 2.79                     | 0.49              |
| 21:AA:794:A:H2'   | 21:AA:795:C:C5     | 2.47                     | 0.49              |
| 1:AB:132:GLU:HG3  | 1:AB:132:GLU:O     | 2.13                     | 0.49              |
| 1:AB:40:ILE:HG21  | 1:AB:201:GLY:N     | 2.27                     | 0.49              |
| 2:AC:49:ALA:HB1   | 2:AC:75:VAL:HG22   | 1.94                     | 0.49              |
| 8:AI:128:LYS:CD   | 8:AI:129:ARG:N     | 2.74                     | 0.49              |
| 8:AI:128:LYS:HD2  | 8:AI:129:ARG:N     | 2.28                     | 0.49              |
| 11:AL:115:LYS:O   | 11:AL:116:TYR:HB2  | 2.13                     | 0.49              |
| 13:AN:16:ALA:HB2  | 13:AN:55:SER:H     | 1.78                     | 0.49              |
| 15:AP:21:VAL:O    | 15:AP:33:ILE:N     | 2.45                     | 0.49              |
| 51:B1:3:GLY:O     | 51:B1:5:ARG:N      | 2.46                     | 0.49              |
| 24:BA:1071:G:C5   | 24:BA:1089:A:C6    | 3.00                     | 0.49              |
| 24:BA:1105:U:H2'  | 24:BA:1106:G:C8    | 2.46                     | 0.49              |
| 24:BA:1456:G:O2'  | 24:BA:1457:U:H5'   | 2.13                     | 0.49              |
| 24:BA:1435:G:C2   | 24:BA:1558:C:N4    | 2.81                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:1568:G:H4'  | 26:BC:58:LYS:HB3   | 1.94                     | 0.49              |
| 21:AA:1409:C:H5'  | 24:BA:1916:A:N1    | 2.27                     | 0.49              |
| 24:BA:562:U:C4    | 24:BA:2036:C:O4'   | 2.66                     | 0.49              |
| 24:BA:2339:C:H2'  | 24:BA:2340:A:C8    | 2.47                     | 0.49              |
| 24:BA:2571:U:C4   | 24:BA:2574:G:C8    | 3.01                     | 0.49              |
| 24:BA:2606:C:O2   | 24:BA:2606:C:H2'   | 2.13                     | 0.49              |
| 24:BA:2868:A:C2   | 24:BA:2869:G:C4    | 3.01                     | 0.49              |
| 24:BA:455:C:C4    | 24:BA:472:A:H2'    | 2.48                     | 0.49              |
| 24:BA:555:G:O2'   | 24:BA:556:A:OP2    | 2.28                     | 0.49              |
| 25:BB:57:A:O2'    | 25:BB:58:A:H5'     | 2.12                     | 0.49              |
| 26:BC:165:ALA:O   | 26:BC:172:THR:HG23 | 2.13                     | 0.49              |
| 30:BG:10:VAL:O    | 30:BG:10:VAL:CG2   | 2.58                     | 0.49              |
| 33:BJ:88:THR:HG21 | 33:BJ:90:GLU:HG3   | 1.94                     | 0.49              |
| 37:BN:18:GLN:HE21 | 37:BN:22:ARG:NH1   | 2.10                     | 0.49              |
| 49:BZ:40:THR:HG23 | 49:BZ:43:ILE:H     | 1.78                     | 0.49              |
| 8:CI:127:SER:HG   | 55:CA:1232:U:P     | 2.35                     | 0.49              |
| 55:CA:1453:G:H2'  | 55:CA:1454:G:O4'   | 2.13                     | 0.49              |
| 55:CA:582:C:H2'   | 55:CA:583:A:O4'    | 2.13                     | 0.49              |
| 55:CA:849:G:N1    | 55:CA:850:U:C2     | 2.81                     | 0.49              |
| 55:CA:887:G:H2'   | 55:CA:888:G:H5'    | 1.95                     | 0.49              |
| 6:CG:148:LYS:HB2  | 6:CG:148:LYS:HZ3   | 1.73                     | 0.49              |
| 6:CG:31:VAL:HG22  | 6:CG:32:ASP:OD1    | 2.12                     | 0.49              |
| 8:CI:44:ARG:CA    | 8:CI:46:VAL:HG22   | 2.42                     | 0.49              |
| 19:CT:70:LYS:HA   | 19:CT:73:ARG:NE    | 2.28                     | 0.49              |
| 51:D1:5:ARG:HH21  | 51:D1:23:THR:HB    | 1.75                     | 0.49              |
| 24:DA:1125:G:H4'  | 54:D4:37:GLN:NE2   | 2.28                     | 0.49              |
| 24:DA:1475:G:O2'  | 24:DA:1476:U:H6    | 1.95                     | 0.49              |
| 24:DA:1738:G:HO2' | 24:DA:1739:A:H8    | 1.53                     | 0.49              |
| 24:DA:1707:G:C5   | 24:DA:1756:G:C6    | 3.01                     | 0.49              |
| 24:DA:2056:G:N2   | 24:DA:2057:G:N9    | 2.61                     | 0.49              |
| 24:DA:233:A:C2'   | 24:DA:234:U:C6     | 2.96                     | 0.49              |
| 24:DA:2566:A:HO2' | 24:DA:2567:G:P     | 2.35                     | 0.49              |
| 24:DA:2566:A:O2'  | 24:DA:2567:G:OP2   | 2.28                     | 0.49              |
| 24:DA:2639:A:N6   | 24:DA:2640:G:C2    | 2.81                     | 0.49              |
| 24:DA:2737:G:H2'  | 24:DA:2738:A:O4'   | 2.13                     | 0.49              |
| 24:DA:2818:U:H2'  | 24:DA:2819:G:H8    | 1.78                     | 0.49              |
| 24:DA:2896:C:O2'  | 24:DA:2897:U:C5'   | 2.61                     | 0.49              |
| 24:DA:2902:C:O2'  | 24:DA:2903:U:O4'   | 2.29                     | 0.49              |
| 24:DA:449:A:H2'   | 24:DA:450:G:H8     | 1.77                     | 0.49              |
| 24:DA:481:G:H1'   | 24:DA:507:A:N6     | 2.28                     | 0.49              |
| 24:DA:532:A:H4'   | 24:DA:533:G:H8     | 1.74                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:655:A:O2'   | 24:DA:656:G:N7     | 2.46                     | 0.49              |
| 24:DA:983:A:H2'   | 24:DA:984:A:H5'    | 1.95                     | 0.49              |
| 27:DD:193:VAL:HB  | 27:DD:194:PRO:HD2  | 1.94                     | 0.49              |
| 28:DE:130:LYS:HG3 | 28:DE:133:LEU:HD13 | 1.95                     | 0.49              |
| 24:DA:674:G:H5''  | 28:DE:71:GLY:HA3   | 1.94                     | 0.49              |
| 31:DH:143:ILE:O   | 31:DH:144:VAL:HG13 | 2.11                     | 0.49              |
| 33:DJ:64:VAL:HG11 | 33:DJ:69:ARG:HA    | 1.95                     | 0.49              |
| 34:DK:111:LYS:HG2 | 34:DK:112:PHE:CD1  | 2.47                     | 0.49              |
| 37:DN:38:LEU:HB3  | 37:DN:39:PRO:CD    | 2.41                     | 0.49              |
| 37:DN:97:ILE:HD11 | 37:DN:99:LYS:NZ    | 2.28                     | 0.49              |
| 41:DR:36:ALA:HA   | 41:DR:58:VAL:HA    | 1.95                     | 0.49              |
| 24:DA:83:A:P      | 44:DU:91:LYS:HZ2   | 2.36                     | 0.49              |
| 47:DX:19:HIS:O    | 47:DX:20:ALA:HB3   | 2.13                     | 0.49              |
| 48:DY:23:ARG:O    | 48:DY:27:ASN:HB2   | 2.12                     | 0.49              |
| 1:AB:94:ARG:CG    | 21:AA:1100:C:OP1   | 2.61                     | 0.49              |
| 21:AA:1365:G:HO2' | 21:AA:1366:C:H6    | 1.61                     | 0.49              |
| 21:AA:389:A:H2'   | 21:AA:390:U:O4'    | 2.12                     | 0.49              |
| 21:AA:967:C:N3    | 21:AA:968:A:N6     | 2.60                     | 0.49              |
| 1:AB:52:ALA:HA    | 1:AB:197:PHE:CE1   | 2.48                     | 0.49              |
| 3:AD:25:ARG:HD2   | 3:AD:25:ARG:O      | 2.13                     | 0.49              |
| 4:AE:36:THR:HG23  | 4:AE:62:ALA:HB1    | 1.95                     | 0.49              |
| 5:AF:9:MET:HE1    | 17:AR:64:LEU:O     | 2.12                     | 0.49              |
| 6:AG:147:ASN:O    | 6:AG:150:PHE:CD1   | 2.66                     | 0.49              |
| 7:AH:40:LYS:HG3   | 7:AH:47:ASP:HA     | 1.94                     | 0.49              |
| 8:AI:8:THR:HG21   | 8:AI:10:ARG:NH2    | 2.25                     | 0.49              |
| 12:AM:58:GLU:HA   | 12:AM:61:LYS:HE3   | 1.95                     | 0.49              |
| 13:AN:87:ALA:HA   | 13:AN:92:ILE:HG13  | 1.95                     | 0.49              |
| 16:AQ:7:LEU:N     | 16:AQ:7:LEU:HD12   | 2.27                     | 0.49              |
| 20:AU:16:ARG:C    | 20:AU:18:PHE:H     | 2.15                     | 0.49              |
| 51:B1:24:LYS:HE2  | 51:B1:52:LYS:CB    | 2.43                     | 0.49              |
| 52:B2:13:ASN:O    | 52:B2:17:GLY:HA3   | 2.12                     | 0.49              |
| 24:BA:117:G:C6    | 24:BA:119:A:N6     | 2.81                     | 0.49              |
| 24:BA:1285:A:C2   | 24:BA:1328:A:H5''  | 2.47                     | 0.49              |
| 24:BA:1865:U:C5   | 24:BA:1875:G:N1    | 2.81                     | 0.49              |
| 24:BA:2015:A:O5'  | 24:BA:2015:A:H8    | 1.94                     | 0.49              |
| 24:BA:2198:A:O2'  | 24:BA:2224:G:N2    | 2.44                     | 0.49              |
| 24:BA:233:A:H61   | 24:BA:428:A:N6     | 2.10                     | 0.49              |
| 24:BA:2679:A:C2   | 24:BA:2729:G:C2    | 3.00                     | 0.49              |
| 24:BA:2809:A:H2'  | 24:BA:2810:A:C8    | 2.48                     | 0.49              |
| 24:BA:2816:G:C2   | 24:BA:2831:G:C4    | 3.01                     | 0.49              |
| 24:BA:513:A:C2    | 24:BA:514:A:C5     | 3.00                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:604:G:C6     | 24:BA:625:G:C2     | 3.00                     | 0.49              |
| 24:BA:67:U:O5'     | 24:BA:67:U:H6      | 1.95                     | 0.49              |
| 24:BA:86:G:O2'     | 24:BA:87:U:C5'     | 2.58                     | 0.49              |
| 24:BA:912:C:H2'    | 24:BA:913:U:C6     | 2.47                     | 0.49              |
| 26:BC:266:ILE:HD12 | 26:BC:266:ILE:N    | 2.27                     | 0.49              |
| 28:BE:26:ALA:O     | 28:BE:29:HIS:HB3   | 2.13                     | 0.49              |
| 32:BI:15:GLY:CA    | 32:BI:50:LYS:HB3   | 2.34                     | 0.49              |
| 34:BK:118:LEU:HD12 | 34:BK:118:LEU:N    | 2.28                     | 0.49              |
| 41:BR:33:VAL:HG21  | 41:BR:35:PHE:CZ    | 2.48                     | 0.49              |
| 46:BW:13:ARG:O     | 46:BW:14:ASP:C     | 2.51                     | 0.49              |
| 55:CA:1295:U:H2'   | 55:CA:1296:C:O4'   | 2.13                     | 0.49              |
| 55:CA:1367:C:H2'   | 55:CA:1368:A:O4'   | 2.12                     | 0.49              |
| 55:CA:1523:G:C4    | 55:CA:1524:C:C5    | 3.01                     | 0.49              |
| 55:CA:720:C:O5'    | 55:CA:720:C:H6     | 1.94                     | 0.49              |
| 55:CA:885:G:O2'    | 55:CA:886:G:O5'    | 2.28                     | 0.49              |
| 55:CA:962:C:C4     | 55:CA:974:A:N6     | 2.81                     | 0.49              |
| 2:CC:74:ILE:O      | 2:CC:74:ILE:HG12   | 2.13                     | 0.49              |
| 4:CE:122:VAL:O     | 4:CE:123:LEU:HD23  | 2.13                     | 0.49              |
| 8:CI:30:ASN:OD1    | 8:CI:65:THR:HG23   | 2.12                     | 0.49              |
| 8:CI:66:VAL:HG13   | 8:CI:66:VAL:O      | 2.13                     | 0.49              |
| 12:CM:53:ASP:HA    | 12:CM:56:ARG:CZ    | 2.43                     | 0.49              |
| 15:CP:32:PHE:CD1   | 15:CP:32:PHE:O     | 2.66                     | 0.49              |
| 20:CU:33:ARG:CZ    | 20:CU:34:ARG:HD3   | 2.43                     | 0.49              |
| 52:D2:11:LYS:O     | 52:D2:14:ARG:N     | 2.46                     | 0.49              |
| 24:DA:1014:A:C4    | 24:DA:1015:U:C5    | 3.00                     | 0.49              |
| 24:DA:1125:G:C6    | 24:DA:1126:A:N6    | 2.80                     | 0.49              |
| 24:DA:1331:G:N3    | 24:DA:1333:G:C8    | 2.81                     | 0.49              |
| 24:DA:1532:A:H2'   | 24:DA:1533:C:C6    | 2.47                     | 0.49              |
| 24:DA:1875:G:H8    | 24:DA:1875:G:OP2   | 1.95                     | 0.49              |
| 24:DA:1947:C:O2'   | 24:DA:1948:G:H5'   | 2.13                     | 0.49              |
| 24:DA:2496:C:N4    | 59:DA:3562:HOH:O   | 2.46                     | 0.49              |
| 24:DA:2550:G:O6    | 24:DA:2551:C:N4    | 2.45                     | 0.49              |
| 24:DA:2757:A:C2'   | 24:DA:2758:A:H5'   | 2.43                     | 0.49              |
| 24:DA:453:A:N3     | 24:DA:457:A:O2'    | 2.45                     | 0.49              |
| 24:DA:669:G:N2     | 24:DA:670:A:C2     | 2.80                     | 0.49              |
| 24:DA:83:A:N6      | 24:DA:101:A:C5'    | 2.73                     | 0.49              |
| 26:DC:166:ARG:HB2  | 26:DC:171:VAL:CG2  | 2.39                     | 0.49              |
| 28:DE:129:PRO:HG3  | 28:DE:159:LEU:HD23 | 1.93                     | 0.49              |
| 28:DE:98:LYS:O     | 28:DE:99:LYS:HB2   | 2.13                     | 0.49              |
| 31:DH:21:VAL:HG22  | 31:DH:22:LYS:H     | 1.77                     | 0.49              |
| 41:DR:6:GLN:HA     | 41:DR:6:GLN:HE21   | 1.78                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:1219:A:H2'  | 21:AA:1220:G:C8    | 2.47                     | 0.49              |
| 21:AA:1331:G:H2'  | 21:AA:1332:A:OP2   | 2.12                     | 0.49              |
| 21:AA:1386:G:C2   | 21:AA:1387:G:N7    | 2.81                     | 0.49              |
| 21:AA:147:G:H2'   | 21:AA:148:G:C8     | 2.47                     | 0.49              |
| 21:AA:570:G:C6    | 21:AA:873:A:C2     | 3.00                     | 0.49              |
| 21:AA:71:A:C6     | 21:AA:100:G:C8     | 3.00                     | 0.49              |
| 21:AA:664:G:H22   | 21:AA:741:G:H1     | 1.59                     | 0.49              |
| 21:AA:765:G:N2    | 21:AA:813:U:H5     | 2.11                     | 0.49              |
| 21:AA:967:C:N3    | 21:AA:968:A:C6     | 2.81                     | 0.49              |
| 1:AB:187:ASP:HB2  | 1:AB:203:ASP:OD1   | 2.13                     | 0.49              |
| 4:AE:80:LEU:HD23  | 4:AE:122:VAL:HG21  | 1.94                     | 0.49              |
| 4:AE:79:THR:OG1   | 4:AE:80:LEU:N      | 2.46                     | 0.49              |
| 5:AF:38:ARG:HH21  | 5:AF:97:THR:CA     | 2.26                     | 0.49              |
| 12:AM:3:ILE:HG13  | 12:AM:3:ILE:O      | 2.13                     | 0.49              |
| 15:AP:4:ILE:HG12  | 15:AP:21:VAL:HG22  | 1.94                     | 0.49              |
| 35:BL:57:LEU:HD22 | 53:B3:53:ASP:HB3   | 1.95                     | 0.49              |
| 24:BA:1083:U:H2'  | 24:BA:1084:A:O5'   | 2.13                     | 0.49              |
| 24:BA:1138:G:O2'  | 33:BJ:107:GLY:HA3  | 2.12                     | 0.49              |
| 24:BA:1452:G:C8   | 24:BA:1457:U:N3    | 2.81                     | 0.49              |
| 24:BA:1632:A:H2'  | 24:BA:1633:G:C8    | 2.47                     | 0.49              |
| 24:BA:164:C:H5'   | 24:BA:165:A:OP2    | 2.12                     | 0.49              |
| 24:BA:1675:C:O5'  | 24:BA:1675:C:H6    | 1.95                     | 0.49              |
| 24:BA:1831:G:H2'  | 24:BA:1832:C:H6    | 1.77                     | 0.49              |
| 24:BA:221:A:C4    | 24:BA:266:G:N7     | 2.81                     | 0.49              |
| 24:BA:2231:U:C4   | 24:BA:2232:C:C5    | 3.01                     | 0.49              |
| 24:BA:2468:A:O2'  | 24:BA:2469:A:P     | 2.71                     | 0.49              |
| 24:BA:322:A:O4'   | 24:BA:340:A:H1'    | 2.13                     | 0.49              |
| 24:BA:402:A:H2'   | 24:BA:403:U:O4'    | 2.13                     | 0.49              |
| 24:BA:418:C:C2'   | 24:BA:419:U:H5'    | 2.43                     | 0.49              |
| 24:BA:545:U:H2'   | 24:BA:546:U:C4'    | 2.39                     | 0.49              |
| 25:BB:35:C:H2'    | 25:BB:36:C:O4'     | 2.12                     | 0.49              |
| 27:BD:139:SER:HB3 | 27:BD:142:VAL:HG21 | 1.93                     | 0.49              |
| 29:BF:3:LEU:HD23  | 29:BF:100:GLU:HB2  | 1.95                     | 0.49              |
| 35:BL:80:SER:C    | 35:BL:81:ASP:O     | 2.49                     | 0.49              |
| 40:BQ:57:ARG:HH21 | 40:BQ:92:LYS:HD2   | 1.78                     | 0.49              |
| 40:BQ:91:ARG:CZ   | 40:BQ:93:ILE:HG21  | 2.43                     | 0.49              |
| 45:BV:42:LEU:HD12 | 45:BV:47:VAL:HG21  | 1.94                     | 0.49              |
| 46:BW:25:PHE:O    | 46:BW:27:GLY:N     | 2.45                     | 0.49              |
| 49:BZ:43:ILE:O    | 49:BZ:43:ILE:HD12  | 2.13                     | 0.49              |
| 55:CA:1004:A:C5   | 55:CA:1026:G:N7    | 2.81                     | 0.49              |
| 55:CA:1126:U:HO2' | 55:CA:1127:G:H8    | 1.61                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:CS:35:ARG:NE   | 55:CA:1221:G:H5'  | 2.28                     | 0.49              |
| 12:CM:102:LYS:CG  | 55:CA:1226:C:H41  | 2.19                     | 0.49              |
| 55:CA:1401:G:N2   | 55:CA:1402:C:H1'  | 2.28                     | 0.49              |
| 55:CA:927:G:C4'   | 55:CA:1503:A:N7   | 2.72                     | 0.49              |
| 55:CA:198:G:C6    | 55:CA:220:G:N3    | 2.81                     | 0.49              |
| 55:CA:588:G:C6    | 55:CA:589:U:C4    | 3.00                     | 0.49              |
| 55:CA:635:A:H2'   | 55:CA:636:U:C6    | 2.48                     | 0.49              |
| 55:CA:71:A:C2     | 55:CA:72:A:C8     | 3.00                     | 0.49              |
| 55:CA:752:G:H1'   | 55:CA:754:C:N4    | 2.27                     | 0.49              |
| 1:CB:64:GLY:HA2   | 1:CB:158:ASP:OD2  | 2.13                     | 0.49              |
| 2:CC:196:GLY:HA3  | 55:CA:1057:G:O3'  | 2.13                     | 0.49              |
| 3:CD:10:LEU:N     | 3:CD:10:LEU:HD12  | 2.28                     | 0.49              |
| 4:CE:63:MET:HA    | 4:CE:66:ALA:HB3   | 1.95                     | 0.49              |
| 6:CG:32:ASP:HB2   | 6:CG:34:LYS:HD3   | 1.94                     | 0.49              |
| 6:CG:70:PRO:O     | 6:CG:90:VAL:HG21  | 2.12                     | 0.49              |
| 8:CI:48:ARG:N     | 8:CI:48:ARG:HD2   | 2.28                     | 0.49              |
| 15:CP:36:VAL:HG21 | 15:CP:57:ILE:HD13 | 1.95                     | 0.49              |
| 16:CQ:17:GLU:O    | 55:CA:255:G:H5'   | 2.12                     | 0.49              |
| 17:CR:47:ARG:HD2  | 17:CR:50:TYR:CE2  | 2.48                     | 0.49              |
| 24:DA:1171:G:H2'  | 24:DA:1172:C:O4'  | 2.13                     | 0.49              |
| 24:DA:1272:A:N7   | 24:DA:1618:A:H1'  | 2.28                     | 0.49              |
| 24:DA:1906:G:N2   | 24:DA:1925:C:O2   | 2.46                     | 0.49              |
| 24:DA:2065:C:C4   | 24:DA:2066:C:N4   | 2.81                     | 0.49              |
| 24:DA:2106:U:H2'  | 24:DA:2107:G:C8   | 2.48                     | 0.49              |
| 24:DA:2141:G:H2'  | 24:DA:2142:A:C8   | 2.47                     | 0.49              |
| 24:DA:2152:G:N3   | 24:DA:2152:G:H2'  | 2.27                     | 0.49              |
| 24:DA:2199:A:H2'  | 24:DA:2200:C:C6   | 2.48                     | 0.49              |
| 24:DA:2331:G:C6   | 24:DA:2385:C:N4   | 2.81                     | 0.49              |
| 24:DA:1783:A:N1   | 24:DA:2587:A:H2'  | 2.27                     | 0.49              |
| 24:DA:2592:G:O2'  | 24:DA:2593:U:H5'  | 2.13                     | 0.49              |
| 24:DA:2074:U:H4'  | 24:DA:2598:A:O4'  | 2.11                     | 0.49              |
| 24:DA:2001:C:H1'  | 24:DA:2689:U:C4   | 2.47                     | 0.49              |
| 24:DA:2691:C:O2'  | 24:DA:2692:G:C5'  | 2.60                     | 0.49              |
| 24:DA:2779:U:O4'  | 24:DA:2781:A:N7   | 2.46                     | 0.49              |
| 24:DA:2861:U:H2'  | 24:DA:2862:G:H8   | 1.76                     | 0.49              |
| 24:DA:380:G:H2'   | 24:DA:381:G:O4'   | 2.12                     | 0.49              |
| 24:DA:446:G:H5''  | 24:DA:447:A:OP1   | 2.12                     | 0.49              |
| 24:DA:49:A:H1'    | 24:DA:51:G:C4     | 2.48                     | 0.49              |
| 24:DA:876:C:H3'   | 24:DA:877:A:C8    | 2.47                     | 0.49              |
| 24:DA:96:C:H2'    | 24:DA:97:C:C6     | 2.48                     | 0.49              |
| 26:DC:144:GLU:HG3 | 26:DC:151:GLY:CA  | 2.42                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:DC:93:VAL:HG13 | 26:DC:94:LEU:N     | 2.27                     | 0.49              |
| 29:DF:110:ILE:HB  | 29:DF:113:PHE:HB2  | 1.94                     | 0.49              |
| 32:DI:32:VAL:HG22 | 32:DI:58:ILE:HG21  | 1.95                     | 0.49              |
| 32:DI:61:TYR:HE2  | 32:DI:67:THR:H     | 1.61                     | 0.49              |
| 34:DK:87:LEU:HA   | 34:DK:95:ILE:H     | 1.78                     | 0.49              |
| 37:DN:114:GLU:HG2 | 37:DN:115:LEU:N    | 2.27                     | 0.49              |
| 38:DO:30:ARG:HG3  | 38:DO:30:ARG:NH1   | 2.23                     | 0.49              |
| 39:DP:20:ARG:HD2  | 39:DP:21:PRO:HD2   | 1.94                     | 0.49              |
| 43:DT:10:VAL:HG23 | 43:DT:11:LEU:H     | 1.78                     | 0.49              |
| 46:DW:16:GLU:O    | 46:DW:17:ALA:HB3   | 2.12                     | 0.49              |
| 21:AA:1142:G:C2   | 21:AA:1143:G:H1'   | 2.48                     | 0.49              |
| 21:AA:1220:G:N1   | 21:AA:1221:G:C5    | 2.81                     | 0.49              |
| 21:AA:1296:C:H4'  | 21:AA:1302:C:N3    | 2.28                     | 0.49              |
| 21:AA:198:G:O6    | 21:AA:220:G:C6     | 2.66                     | 0.49              |
| 21:AA:427:U:H2'   | 21:AA:428:G:C8     | 2.47                     | 0.49              |
| 21:AA:588:G:C5    | 21:AA:589:U:C5     | 3.01                     | 0.49              |
| 21:AA:604:G:C6    | 21:AA:605:U:N3     | 2.80                     | 0.49              |
| 1:AB:101:THR:HG23 | 1:AB:102:ASN:N     | 2.24                     | 0.49              |
| 1:AB:138:ARG:HA   | 1:AB:141:GLU:CD    | 2.33                     | 0.49              |
| 1:AB:216:VAL:HG12 | 1:AB:216:VAL:O     | 2.12                     | 0.49              |
| 2:AC:119:ILE:CG2  | 2:AC:197:VAL:HG11  | 2.42                     | 0.49              |
| 3:AD:71:PHE:O     | 3:AD:74:TYR:HB2    | 2.13                     | 0.49              |
| 4:AE:13:LYS:CE    | 4:AE:112:ALA:HA    | 2.43                     | 0.49              |
| 4:AE:14:LEU:HD13  | 4:AE:14:LEU:C      | 2.33                     | 0.49              |
| 6:AG:146:ALA:C    | 6:AG:148:LYS:H     | 2.14                     | 0.49              |
| 10:AK:126:ARG:HE  | 10:AK:126:ARG:HA   | 1.77                     | 0.49              |
| 14:AO:31:LEU:HD12 | 14:AO:62:ARG:HB2   | 1.94                     | 0.49              |
| 51:B1:13:SER:HB3  | 51:B1:47:ILE:O     | 2.13                     | 0.49              |
| 24:BA:1312:U:H4'  | 24:BA:1313:U:O2    | 2.13                     | 0.49              |
| 24:BA:1452:G:H3'  | 59:BA:3420:HOH:O   | 2.13                     | 0.49              |
| 24:BA:1781:U:O2'  | 24:BA:1782:U:P     | 2.71                     | 0.49              |
| 24:BA:1817:G:O2'  | 24:BA:1818:U:C5'   | 2.56                     | 0.49              |
| 24:BA:1965:C:H2'  | 24:BA:1966:A:H8    | 1.74                     | 0.49              |
| 24:BA:2886:A:N3   | 24:BA:2887:A:H1'   | 2.28                     | 0.49              |
| 24:BA:301:G:C5    | 24:BA:302:C:C4     | 3.01                     | 0.49              |
| 24:BA:778:G:C6    | 24:BA:779:U:N3     | 2.81                     | 0.49              |
| 29:BF:7:TYR:HD2   | 29:BF:11:VAL:HG11  | 1.77                     | 0.49              |
| 31:BH:80:ILE:HG23 | 31:BH:147:VAL:HG21 | 1.94                     | 0.49              |
| 32:BI:126:ARG:HA  | 32:BI:129:GLU:CB   | 2.42                     | 0.49              |
| 33:BJ:65:THR:CG2  | 33:BJ:66:GLY:N     | 2.74                     | 0.49              |
| 34:BK:7:MET:C     | 34:BK:8:LEU:HD23   | 2.33                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:BN:53:THR:HA   | 37:BN:56:LYS:HG3  | 1.95                     | 0.49              |
| 40:BQ:20:ALA:HB1  | 40:BQ:27:ARG:O    | 2.13                     | 0.49              |
| 44:BU:13:LEU:HD11 | 44:BU:70:ALA:HB2  | 1.95                     | 0.49              |
| 46:BW:31:LEU:HD23 | 46:BW:31:LEU:N    | 2.27                     | 0.49              |
| 48:BY:43:LEU:O    | 48:BY:47:ARG:HB2  | 2.12                     | 0.49              |
| 49:BZ:23:LEU:HD21 | 49:BZ:53:MET:CE   | 2.43                     | 0.49              |
| 55:CA:1050:G:O2'  | 55:CA:1051:C:O5'  | 2.31                     | 0.49              |
| 55:CA:1169:A:C2   | 55:CA:1170:A:C4   | 3.01                     | 0.49              |
| 55:CA:1502:A:O2'  | 55:CA:1503:A:OP1  | 2.26                     | 0.49              |
| 55:CA:345:C:H3'   | 39:DP:38:ARG:NH1  | 2.28                     | 0.49              |
| 55:CA:373:A:OP2   | 55:CA:373:A:H3'   | 2.13                     | 0.49              |
| 55:CA:428:G:H8    | 55:CA:428:G:OP1   | 1.96                     | 0.49              |
| 55:CA:792:A:C4    | 55:CA:794:A:N6    | 2.81                     | 0.49              |
| 55:CA:821:G:HO2'  | 55:CA:822:U:H6    | 1.54                     | 0.49              |
| 55:CA:93:U:H2'    | 55:CA:95:C:C5     | 2.47                     | 0.49              |
| 1:CB:170:ILE:HA   | 1:CB:173:LYS:HE2  | 1.95                     | 0.49              |
| 1:CB:73:ARG:HG3   | 1:CB:74:ALA:N     | 2.28                     | 0.49              |
| 2:CC:110:LEU:HD11 | 2:CC:203:LYS:HZ3  | 1.78                     | 0.49              |
| 3:CD:81:LEU:O     | 3:CD:83:GLY:N     | 2.45                     | 0.49              |
| 4:CE:79:THR:HA    | 4:CE:121:ASN:ND2  | 2.27                     | 0.49              |
| 6:CG:65:LEU:O     | 6:CG:69:ARG:HB2   | 2.13                     | 0.49              |
| 6:CG:94:ARG:O     | 6:CG:96:ASN:N     | 2.46                     | 0.49              |
| 13:CN:72:PHE:CG   | 13:CN:73:LEU:N    | 2.81                     | 0.49              |
| 53:D3:41:ARG:HG2  | 53:D3:44:ARG:HH22 | 1.78                     | 0.49              |
| 24:DA:1054:A:N3   | 24:DA:1055:G:H1'  | 2.27                     | 0.49              |
| 24:DA:1085:A:H2'  | 24:DA:1086:A:N3   | 2.28                     | 0.49              |
| 24:DA:1486:U:H2'  | 24:DA:1487:U:C6   | 2.47                     | 0.49              |
| 24:DA:1506:U:O5'  | 24:DA:1506:U:H6   | 1.96                     | 0.49              |
| 24:DA:1587:G:H2'  | 24:DA:1588:G:H8   | 1.78                     | 0.49              |
| 24:DA:1332:G:C6   | 24:DA:1609:A:N7   | 2.81                     | 0.49              |
| 24:DA:1659:G:C5   | 24:DA:1660:G:C8   | 3.01                     | 0.49              |
| 24:DA:2093:G:C6   | 24:DA:2225:A:N7   | 2.81                     | 0.49              |
| 24:DA:2227:A:H5'' | 26:DC:260:LYS:HD2 | 1.93                     | 0.49              |
| 24:DA:2340:A:H2'  | 24:DA:2341:G:H8   | 1.76                     | 0.49              |
| 24:DA:271:G:C4    | 24:DA:367:G:C2    | 3.01                     | 0.49              |
| 24:DA:303:G:C2    | 24:DA:304:U:C2    | 3.00                     | 0.49              |
| 24:DA:604:G:O2'   | 24:DA:605:G:C8    | 2.50                     | 0.49              |
| 24:DA:64:A:N1     | 24:DA:91:A:N6     | 2.60                     | 0.49              |
| 56:DB:76:G:H5''   | 45:DV:17:SER:CB   | 2.43                     | 0.49              |
| 26:DC:147:PRO:HD3 | 26:DC:184:GLU:CG  | 2.40                     | 0.49              |
| 27:DD:159:LYS:HE2 | 27:DD:160:LYS:N   | 2.27                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:DF:103:ILE:O   | 29:DF:103:ILE:HG22 | 2.13                     | 0.49              |
| 29:DF:35:LEU:HD11 | 29:DF:153:ILE:HG23 | 1.94                     | 0.49              |
| 56:DB:52:A:OP2    | 38:DO:64:TYR:CD1   | 2.66                     | 0.49              |
| 40:DQ:108:LEU:O   | 40:DQ:108:LEU:HD23 | 2.13                     | 0.49              |
| 40:DQ:42:GLY:O    | 40:DQ:45:ALA:HB3   | 2.12                     | 0.49              |
| 40:DQ:40:LYS:HD2  | 40:DQ:44:TYR:CE2   | 2.48                     | 0.49              |
| 45:DV:21:ARG:HE   | 45:DV:87:GLN:CB    | 2.26                     | 0.49              |
| 21:AA:1006:G:H2'  | 21:AA:1007:U:C6    | 2.48                     | 0.48              |
| 21:AA:1088:G:C2   | 21:AA:1089:G:C8    | 3.00                     | 0.48              |
| 21:AA:1304:G:H5'' | 21:AA:1305:G:OP1   | 2.13                     | 0.48              |
| 21:AA:1466:C:H2'  | 21:AA:1467:C:O4'   | 2.13                     | 0.48              |
| 21:AA:1513:A:H2'  | 21:AA:1514:G:H8    | 1.78                     | 0.48              |
| 21:AA:484:G:C4'   | 21:AA:485:U:O5'    | 2.56                     | 0.48              |
| 21:AA:655:A:H2'   | 21:AA:656:G:C8     | 2.48                     | 0.48              |
| 21:AA:954:G:C5    | 21:AA:955:U:C4     | 3.01                     | 0.48              |
| 1:AB:69:VAL:HB    | 1:AB:162:VAL:HG12  | 1.95                     | 0.48              |
| 1:AB:80:LYS:HG2   | 1:AB:80:LYS:O      | 2.12                     | 0.48              |
| 3:AD:195:ASN:CB   | 3:AD:198:LEU:HD12  | 2.43                     | 0.48              |
| 4:AE:75:LEU:HD21  | 4:AE:119:VAL:CG1   | 2.42                     | 0.48              |
| 8:AI:11:ARG:NE    | 8:AI:106:ASP:HB2   | 2.28                     | 0.48              |
| 8:AI:11:ARG:HD3   | 8:AI:106:ASP:HB2   | 1.94                     | 0.48              |
| 13:AN:63:CYS:HB3  | 13:AN:68:ARG:H     | 1.78                     | 0.48              |
| 16:AQ:17:GLU:O    | 16:AQ:17:GLU:HG2   | 2.13                     | 0.48              |
| 20:AU:36:PHE:HD1  | 20:AU:39:LYS:HG2   | 1.78                     | 0.48              |
| 24:BA:1059:G:C6   | 24:BA:1080:A:C6    | 3.01                     | 0.48              |
| 24:BA:1252:G:C2   | 24:BA:1253:A:C2    | 3.01                     | 0.48              |
| 24:BA:1520:U:C4   | 24:BA:1521:G:C6    | 3.01                     | 0.48              |
| 24:BA:1693:U:H4'  | 24:BA:1694:C:OP2   | 2.11                     | 0.48              |
| 24:BA:169:G:H2'   | 24:BA:170:U:C6     | 2.47                     | 0.48              |
| 24:BA:1805:A:N3   | 26:BC:49:THR:HG23  | 2.28                     | 0.48              |
| 24:BA:1786:A:H1'  | 24:BA:1938:A:N6    | 2.28                     | 0.48              |
| 24:BA:563:A:C6    | 24:BA:2018:G:C4    | 3.01                     | 0.48              |
| 24:BA:2063:C:C5   | 24:BA:2064:C:C5    | 3.01                     | 0.48              |
| 24:BA:2200:C:N4   | 24:BA:2224:G:C2    | 2.80                     | 0.48              |
| 24:BA:2316:G:H2'  | 24:BA:2317:A:H8    | 1.77                     | 0.48              |
| 24:BA:2405:G:H1'  | 24:BA:2412:A:H61   | 1.77                     | 0.48              |
| 24:BA:960:A:H2    | 24:BA:2495:G:N3    | 2.10                     | 0.48              |
| 24:BA:2842:G:C4   | 24:BA:2843:G:C8    | 3.01                     | 0.48              |
| 24:BA:728:G:C4    | 24:BA:730:A:C8     | 3.01                     | 0.48              |
| 24:BA:839:U:O2'   | 24:BA:840:C:H5'    | 2.13                     | 0.48              |
| 24:BA:995:C:OP2   | 40:BQ:53:LYS:CE    | 2.61                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:BL:30:THR:O    | 35:BL:33:ARG:HG2   | 2.12                     | 0.48              |
| 40:BQ:13:HIS:CD2  | 40:BQ:31:TYR:CD1   | 2.99                     | 0.48              |
| 55:CA:1070:U:H2'  | 55:CA:1071:C:C6    | 2.45                     | 0.48              |
| 55:CA:1213:A:C4   | 55:CA:1215:G:C8    | 3.01                     | 0.48              |
| 55:CA:1386:G:C2   | 55:CA:1387:G:N7    | 2.81                     | 0.48              |
| 55:CA:1524:C:H2'  | 55:CA:1525:G:C8    | 2.48                     | 0.48              |
| 55:CA:37:U:O2     | 55:CA:548:G:C2     | 2.66                     | 0.48              |
| 7:CH:29:SER:HB3   | 55:CA:589:U:H5''   | 1.95                     | 0.48              |
| 55:CA:80:A:C6     | 55:CA:81:A:O2'     | 2.66                     | 0.48              |
| 55:CA:885:G:HO2'  | 55:CA:886:G:H8     | 1.61                     | 0.48              |
| 1:CB:131:LYS:HD3  | 1:CB:131:LYS:O     | 2.13                     | 0.48              |
| 12:CM:69:ARG:HA   | 12:CM:72:ILE:CG2   | 2.42                     | 0.48              |
| 13:CN:30:ILE:O    | 13:CN:40:ARG:HA    | 2.13                     | 0.48              |
| 17:CR:33:THR:HG22 | 17:CR:39:VAL:HG22  | 1.94                     | 0.48              |
| 24:DA:1123:C:H2'  | 24:DA:1124:G:C8    | 2.47                     | 0.48              |
| 24:DA:1210:G:H5'  | 24:DA:1212:G:O4'   | 2.13                     | 0.48              |
| 24:DA:142:A:H5''  | 24:DA:142:A:H8     | 1.77                     | 0.48              |
| 24:DA:155:A:C6    | 24:DA:172:A:N6     | 2.81                     | 0.48              |
| 24:DA:1340:U:H1'  | 24:DA:1603:A:H5'   | 1.94                     | 0.48              |
| 24:DA:1889:A:N3   | 24:DA:2086:U:O2'   | 2.37                     | 0.48              |
| 24:DA:1:G:H2'     | 24:DA:2:G:H8       | 1.74                     | 0.48              |
| 24:DA:2093:G:O2'  | 24:DA:2094:A:C5'   | 2.61                     | 0.48              |
| 24:DA:2183:A:H2'  | 24:DA:2184:A:H8    | 1.78                     | 0.48              |
| 24:DA:2023:C:H4'  | 24:DA:2617:U:O2'   | 2.13                     | 0.48              |
| 24:DA:2880:C:H1'  | 37:DN:93:GLY:H     | 1.78                     | 0.48              |
| 24:DA:370:G:C6    | 24:DA:424:G:C5     | 3.01                     | 0.48              |
| 24:DA:526:A:C6    | 24:DA:2626:C:H4'   | 2.49                     | 0.48              |
| 24:DA:591:U:C2    | 24:DA:592:A:C8     | 3.01                     | 0.48              |
| 24:DA:815:C:H2'   | 24:DA:816:C:H6     | 1.78                     | 0.48              |
| 56:DB:45:A:C2'    | 56:DB:46:A:C8      | 2.92                     | 0.48              |
| 26:DC:173:LEU:N   | 26:DC:173:LEU:HD22 | 2.26                     | 0.48              |
| 24:DA:1566:A:C2   | 26:DC:212:TRP:HB2  | 2.48                     | 0.48              |
| 33:DJ:44:TYR:CD2  | 33:DJ:44:TYR:C     | 2.86                     | 0.48              |
| 36:DM:17:ASN:HB3  | 36:DM:38:ARG:NH2   | 2.28                     | 0.48              |
| 37:DN:32:GLU:OE1  | 37:DN:115:LEU:HD12 | 2.13                     | 0.48              |
| 40:DQ:57:ARG:O    | 40:DQ:61:ILE:HD13  | 2.12                     | 0.48              |
| 44:DU:47:PRO:HB3  | 44:DU:54:PRO:HG2   | 1.95                     | 0.48              |
| 56:DB:98:G:N1     | 45:DV:14:LYS:CB    | 2.75                     | 0.48              |
| 21:AA:230:G:O2'   | 21:AA:231:U:H5'    | 2.13                     | 0.48              |
| 21:AA:61:G:H2'    | 21:AA:62:U:C6      | 2.48                     | 0.48              |
| 21:AA:71:A:C2     | 21:AA:72:A:C8      | 3.01                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AF:98:GLU:O     | 5:AF:99:ALA:HB3   | 2.13                     | 0.48              |
| 7:AH:45:ILE:C     | 7:AH:63:LYS:HD2   | 2.32                     | 0.48              |
| 18:AS:36:ARG:HD3  | 21:AA:1318:A:O2'  | 2.13                     | 0.48              |
| 51:B1:11:VAL:O    | 51:B1:48:TYR:HA   | 2.13                     | 0.48              |
| 24:BA:1005:C:C2   | 24:BA:1143:A:C6   | 3.01                     | 0.48              |
| 24:BA:1190:G:H2'  | 24:BA:1191:G:C8   | 2.43                     | 0.48              |
| 24:BA:1231:U:H2'  | 24:BA:1232:G:H8   | 1.78                     | 0.48              |
| 24:BA:1356:G:C5   | 24:BA:1357:C:C5   | 3.01                     | 0.48              |
| 24:BA:1362:C:H2'  | 24:BA:1363:C:O4'  | 2.13                     | 0.48              |
| 24:BA:145:C:H2'   | 24:BA:146:A:C8    | 2.48                     | 0.48              |
| 24:BA:2231:U:P    | 47:BX:29:LEU:HD23 | 2.54                     | 0.48              |
| 24:BA:2378:A:N7   | 24:BA:2379:G:H1'  | 2.28                     | 0.48              |
| 24:BA:361:G:OP2   | 24:BA:361:G:H8    | 1.96                     | 0.48              |
| 24:BA:715:A:C6    | 24:BA:716:A:C6    | 3.01                     | 0.48              |
| 24:BA:726:G:O2'   | 24:BA:727:A:P     | 2.71                     | 0.48              |
| 24:BA:754:U:C2    | 24:BA:755:U:C5    | 3.01                     | 0.48              |
| 24:BA:976:G:N3    | 24:BA:977:G:C8    | 2.80                     | 0.48              |
| 25:BB:29:A:OP2    | 38:BO:32:PRO:HD2  | 2.13                     | 0.48              |
| 25:BB:41:G:H3'    | 25:BB:42:C:C5'    | 2.42                     | 0.48              |
| 26:BC:188:ARG:O   | 26:BC:189:ALA:HB2 | 2.12                     | 0.48              |
| 30:BG:59:ASP:O    | 30:BG:60:GLY:C    | 2.51                     | 0.48              |
| 34:BK:22:ILE:O    | 34:BK:23:LYS:HB2  | 2.13                     | 0.48              |
| 35:BL:55:MET:HE2  | 35:BL:56:PRO:CD   | 2.43                     | 0.48              |
| 35:BL:68:SER:HB3  | 35:BL:71:ALA:HB3  | 1.94                     | 0.48              |
| 35:BL:76:GLU:C    | 35:BL:77:ILE:HD12 | 2.33                     | 0.48              |
| 39:BP:67:GLU:HA   | 39:BP:67:GLU:OE1  | 2.13                     | 0.48              |
| 41:BR:98:ILE:HG22 | 41:BR:98:ILE:O    | 2.13                     | 0.48              |
| 42:BS:24:ILE:HD12 | 42:BS:32:ALA:HB1  | 1.96                     | 0.48              |
| 44:BU:73:ASN:HD22 | 44:BU:76:THR:HG23 | 1.78                     | 0.48              |
| 46:BW:37:VAL:HG22 | 46:BW:55:ASP:O    | 2.13                     | 0.48              |
| 47:BX:39:VAL:C    | 47:BX:41:SER:H    | 2.16                     | 0.48              |
| 55:CA:1162:C:C2   | 55:CA:1175:G:N2   | 2.81                     | 0.48              |
| 55:CA:1244:G:C6   | 55:CA:1245:C:C4   | 3.01                     | 0.48              |
| 55:CA:128:G:C2    | 55:CA:234:C:C2    | 3.01                     | 0.48              |
| 55:CA:459:A:H2'   | 55:CA:460:A:H8    | 1.78                     | 0.48              |
| 55:CA:792:A:O2'   | 55:CA:793:U:OP2   | 2.31                     | 0.48              |
| 1:CB:125:PHE:HA   | 1:CB:136:ARG:NH2  | 2.28                     | 0.48              |
| 20:AU:9:GLU:HB2   | 2:CC:48:LYS:NZ    | 2.28                     | 0.48              |
| 13:CN:9:GLU:HA    | 13:CN:12:ARG:HD2  | 1.95                     | 0.48              |
| 19:CT:62:ALA:HA   | 19:CT:67:HIS:CE1  | 2.48                     | 0.48              |
| 55:CA:530:G:O2'   | 22:CX:35:A:H4'    | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:D2:11:LYS:O    | 52:D2:12:ARG:C    | 2.51                     | 0.48              |
| 24:DA:1004:U:H1'  | 24:DA:1010:A:C4   | 2.47                     | 0.48              |
| 24:DA:1219:U:H2'  | 24:DA:1220:G:C8   | 2.47                     | 0.48              |
| 24:DA:1275:A:C4   | 37:DN:16:HIS:HD2  | 2.31                     | 0.48              |
| 24:DA:1278:C:H2'  | 24:DA:1279:G:H8   | 1.77                     | 0.48              |
| 24:DA:1412:U:H2'  | 24:DA:1413:A:O4'  | 2.12                     | 0.48              |
| 24:DA:1434:A:H2'  | 24:DA:1435:G:O4'  | 2.12                     | 0.48              |
| 24:DA:1570:A:C5   | 24:DA:1571:A:C6   | 3.00                     | 0.48              |
| 24:DA:1935:G:H1   | 24:DA:1962:C:H2'  | 1.78                     | 0.48              |
| 24:DA:1953:A:C2   | 24:DA:2550:G:O4'  | 2.66                     | 0.48              |
| 24:DA:2201:G:H2'  | 24:DA:2202:U:O4'  | 2.13                     | 0.48              |
| 24:DA:2229:U:H2'  | 24:DA:2230:G:H8   | 1.77                     | 0.48              |
| 24:DA:2270:A:H5'  | 46:DW:18:LYS:HG2  | 1.94                     | 0.48              |
| 24:DA:2283:C:N4   | 24:DA:2389:G:C6   | 2.81                     | 0.48              |
| 24:DA:40:U:C4     | 24:DA:41:C:C4     | 3.00                     | 0.48              |
| 24:DA:465:G:C4'   | 52:D2:16:HIS:HD2  | 2.24                     | 0.48              |
| 24:DA:574:A:H4'   | 24:DA:575:A:C5'   | 2.42                     | 0.48              |
| 24:DA:771:G:C4    | 24:DA:772:C:C5    | 3.00                     | 0.48              |
| 24:DA:78:U:C2'    | 24:DA:79:C:H5'    | 2.43                     | 0.48              |
| 56:DB:11:C:H3'    | 56:DB:12:C:H5'    | 1.94                     | 0.48              |
| 28:DE:148:ILE:HA  | 28:DE:187:VAL:HB  | 1.95                     | 0.48              |
| 30:DG:37:ASN:HD22 | 30:DG:40:VAL:CG2  | 2.25                     | 0.48              |
| 36:DM:3:GLN:NE2   | 36:DM:92:TRP:CD1  | 2.81                     | 0.48              |
| 38:DO:51:ALA:HB3  | 38:DO:78:VAL:HG22 | 1.95                     | 0.48              |
| 39:DP:107:ALA:O   | 39:DP:108:ARG:C   | 2.51                     | 0.48              |
| 39:DP:48:ALA:HB3  | 39:DP:59:THR:OG1  | 2.12                     | 0.48              |
| 24:DA:17:G:H4'    | 40:DQ:24:TYR:CE1  | 2.49                     | 0.48              |
| 21:AA:1049:U:O2'  | 21:AA:1050:G:P    | 2.71                     | 0.48              |
| 21:AA:1099:G:C5   | 21:AA:1100:C:C4   | 3.01                     | 0.48              |
| 9:AJ:37:ARG:HD2   | 21:AA:1125:U:OP1  | 2.13                     | 0.48              |
| 21:AA:1151:A:N6   | 21:AA:1152:A:N6   | 2.61                     | 0.48              |
| 21:AA:1169:A:O2'  | 21:AA:1170:A:C5'  | 2.62                     | 0.48              |
| 21:AA:1239:A:H1'  | 21:AA:1241:G:C5   | 2.48                     | 0.48              |
| 21:AA:465:A:H2'   | 21:AA:466:A:O4'   | 2.13                     | 0.48              |
| 21:AA:502:A:H2'   | 21:AA:503:C:H6    | 1.78                     | 0.48              |
| 21:AA:91:U:H2'    | 21:AA:92:U:C1'    | 2.42                     | 0.48              |
| 21:AA:947:G:C2    | 21:AA:948:C:C2    | 3.01                     | 0.48              |
| 21:AA:955:U:H2'   | 21:AA:956:U:C6    | 2.43                     | 0.48              |
| 1:AB:130:LYS:HA   | 1:AB:130:LYS:HZ3  | 1.77                     | 0.48              |
| 2:AC:139:ASN:N    | 2:AC:139:ASN:HD22 | 2.11                     | 0.48              |
| 2:AC:161:ILE:O    | 2:AC:161:ILE:HG13 | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AC:190:THR:HG21 | 2:AC:192:TYR:CZ   | 2.48                     | 0.48              |
| 16:AQ:46:HIS:CG   | 16:AQ:47:ASP:N    | 2.81                     | 0.48              |
| 16:AQ:51:GLU:HG2  | 16:AQ:52:CYS:SG   | 2.53                     | 0.48              |
| 19:AT:82:ILE:HD12 | 19:AT:82:ILE:C    | 2.33                     | 0.48              |
| 10:AK:113:THR:HB  | 20:AU:28:LEU:HD11 | 1.94                     | 0.48              |
| 20:AU:43:GLU:C    | 20:AU:45:LYS:H    | 2.16                     | 0.48              |
| 22:AV:37:A:C2     | 23:AW:1:U:C4      | 3.01                     | 0.48              |
| 24:BA:1001:A:H2'  | 24:BA:1002:G:O4'  | 2.13                     | 0.48              |
| 24:BA:1351:C:N3   | 24:BA:1381:G:C6   | 2.81                     | 0.48              |
| 24:BA:1374:G:C5   | 24:BA:1375:U:C5   | 3.01                     | 0.48              |
| 24:BA:1549:A:C6   | 24:BA:1550:C:N3   | 2.82                     | 0.48              |
| 24:BA:1858:A:O2'  | 24:BA:1859:U:H5'  | 2.13                     | 0.48              |
| 24:BA:2276:G:P    | 36:BM:83:GLY:O    | 2.71                     | 0.48              |
| 24:BA:2297:A:O2'  | 24:BA:2298:A:H5'  | 2.12                     | 0.48              |
| 24:BA:2318:G:C6   | 24:BA:2319:G:C6   | 3.01                     | 0.48              |
| 24:BA:2444:G:C6   | 24:BA:2445:G:C5   | 3.01                     | 0.48              |
| 24:BA:2486:C:H2'  | 24:BA:2487:G:O4'  | 2.13                     | 0.48              |
| 24:BA:2740:A:C6   | 24:BA:2741:A:C6   | 3.01                     | 0.48              |
| 24:BA:2887:A:H2'  | 24:BA:2887:A:N3   | 2.29                     | 0.48              |
| 24:BA:574:A:H4'   | 24:BA:575:A:H5'   | 1.95                     | 0.48              |
| 26:BC:169:ALA:O   | 26:BC:185:ALA:HB3 | 2.12                     | 0.48              |
| 27:BD:182:ALA:O   | 27:BD:184:ARG:N   | 2.46                     | 0.48              |
| 27:BD:70:LYS:O    | 27:BD:71:ALA:CB   | 2.61                     | 0.48              |
| 31:BH:5:LEU:O     | 31:BH:16:GLY:HA2  | 2.14                     | 0.48              |
| 32:BI:6:ALA:HB3   | 32:BI:60:VAL:H    | 1.79                     | 0.48              |
| 33:BJ:132:HIS:HB3 | 33:BJ:135:GLN:HG2 | 1.96                     | 0.48              |
| 33:BJ:37:ARG:HA   | 33:BJ:118:MET:CE  | 2.44                     | 0.48              |
| 33:BJ:64:VAL:HG13 | 33:BJ:65:THR:O    | 2.13                     | 0.48              |
| 37:BN:3:HIS:O     | 37:BN:4:ARG:HB2   | 2.13                     | 0.48              |
| 37:BN:93:GLY:C    | 37:BN:95:THR:H    | 2.15                     | 0.48              |
| 39:BP:8:GLU:O     | 39:BP:11:GLN:CB   | 2.60                     | 0.48              |
| 41:BR:49:ILE:HG22 | 41:BR:54:VAL:HG12 | 1.96                     | 0.48              |
| 47:BX:5:GLN:HG3   | 47:BX:49:ARG:O    | 2.13                     | 0.48              |
| 55:CA:1023:U:H2'  | 55:CA:1024:G:H8   | 1.71                     | 0.48              |
| 55:CA:1117:A:C2   | 55:CA:1184:G:C6   | 3.01                     | 0.48              |
| 55:CA:1275:A:H2'  | 55:CA:1276:G:H8   | 1.77                     | 0.48              |
| 55:CA:1254:A:C2   | 55:CA:1284:C:N3   | 2.82                     | 0.48              |
| 55:CA:1336:C:H4'  | 55:CA:1337:G:N3   | 2.27                     | 0.48              |
| 55:CA:247:G:O6    | 55:CA:278:G:C6    | 2.66                     | 0.48              |
| 55:CA:293:G:N1    | 55:CA:305:G:C2    | 2.81                     | 0.48              |
| 55:CA:476:U:C6    | 55:CA:476:U:OP2   | 2.66                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:855:U:H2'   | 55:CA:856:C:H6    | 1.78                     | 0.48              |
| 1:CB:208:ALA:HA   | 1:CB:211:LEU:HB3  | 1.94                     | 0.48              |
| 1:CB:59:ILE:HA    | 1:CB:62:ARG:CD    | 2.42                     | 0.48              |
| 7:CH:40:LYS:C     | 7:CH:40:LYS:HD3   | 2.32                     | 0.48              |
| 7:CH:77:VAL:HG21  | 7:CH:127:TYR:CE1  | 2.49                     | 0.48              |
| 11:CL:2:THR:HG22  | 11:CL:4:ASN:H     | 1.77                     | 0.48              |
| 11:CL:6:LEU:C     | 11:CL:8:ARG:H     | 2.16                     | 0.48              |
| 24:DA:1027:A:O2'  | 24:DA:1028:A:C8   | 2.64                     | 0.48              |
| 24:DA:1041:G:H2'  | 24:DA:1042:G:H8   | 1.79                     | 0.48              |
| 24:DA:1149:G:C2   | 24:DA:1150:C:C2   | 3.01                     | 0.48              |
| 24:DA:1376:C:H2'  | 24:DA:1377:G:C8   | 2.48                     | 0.48              |
| 24:DA:1936:A:H2   | 24:DA:1943:U:O4   | 1.96                     | 0.48              |
| 24:DA:2267:A:H3'  | 24:DA:2268:A:C5'  | 2.44                     | 0.48              |
| 24:DA:2339:C:O2'  | 24:DA:2340:A:O4'  | 2.30                     | 0.48              |
| 24:DA:2356:U:H2'  | 24:DA:2357:G:O4'  | 2.13                     | 0.48              |
| 24:DA:2418:A:H2'  | 24:DA:2419:U:O4'  | 2.13                     | 0.48              |
| 24:DA:2435:A:C2   | 24:DA:2436:G:C4   | 3.02                     | 0.48              |
| 24:DA:2662:A:H2'  | 24:DA:2663:G:O4'  | 2.13                     | 0.48              |
| 24:DA:2875:C:HO2' | 24:DA:2876:G:H8   | 1.59                     | 0.48              |
| 24:DA:324:A:N6    | 24:DA:338:G:C2'   | 2.75                     | 0.48              |
| 24:DA:361:G:HO2'  | 24:DA:362:A:P     | 2.37                     | 0.48              |
| 24:DA:480:A:HO2'  | 24:DA:499:U:HO2'  | 1.60                     | 0.48              |
| 24:DA:503:A:C2    | 24:DA:505:A:C4    | 3.02                     | 0.48              |
| 24:DA:924:G:O2'   | 24:DA:925:A:H5'   | 2.13                     | 0.48              |
| 56:DB:14:U:H3'    | 56:DB:15:A:H5''   | 1.94                     | 0.48              |
| 28:DE:5:LEU:HD13  | 28:DE:122:GLU:HB2 | 1.95                     | 0.48              |
| 31:DH:5:LEU:HD11  | 31:DH:13:GLY:HA3  | 1.95                     | 0.48              |
| 43:DT:30:ILE:O    | 43:DT:85:VAL:HG23 | 2.13                     | 0.48              |
| 44:DU:14:THR:HG23 | 44:DU:15:GLY:N    | 2.23                     | 0.48              |
| 21:AA:233:C:H2'   | 21:AA:234:C:C6    | 2.48                     | 0.48              |
| 21:AA:253:A:H2'   | 21:AA:254:G:C8    | 2.48                     | 0.48              |
| 21:AA:294:U:H2'   | 21:AA:295:C:C6    | 2.49                     | 0.48              |
| 21:AA:481:G:HO2'  | 21:AA:482:A:H8    | 1.57                     | 0.48              |
| 21:AA:552:U:H2'   | 21:AA:553:A:H8    | 1.78                     | 0.48              |
| 13:AN:70:HIS:CE1  | 21:AA:974:A:C1'   | 2.95                     | 0.48              |
| 15:AP:56:ARG:O    | 15:AP:59:HIS:HB3  | 2.14                     | 0.48              |
| 24:BA:1153:C:H2'  | 24:BA:1154:G:O4'  | 2.14                     | 0.48              |
| 24:BA:1406:U:H2'  | 24:BA:1407:G:H8   | 1.79                     | 0.48              |
| 24:BA:1553:A:C5   | 24:BA:1555:G:C5   | 3.00                     | 0.48              |
| 24:BA:2020:A:N1   | 24:BA:2022:U:C2   | 2.81                     | 0.48              |
| 24:BA:2097:A:H2'  | 24:BA:2098:U:O4'  | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:2093:G:C5   | 24:BA:2225:A:C8   | 3.01                     | 0.48              |
| 24:BA:228:C:H4'   | 24:BA:229:C:C5'   | 2.44                     | 0.48              |
| 24:BA:2578:G:C5   | 27:BD:145:SER:HB2 | 2.47                     | 0.48              |
| 24:BA:1672:A:C2   | 24:BA:2582:G:H5'  | 2.47                     | 0.48              |
| 24:BA:2725:A:C4   | 24:BA:2727:A:C8   | 3.01                     | 0.48              |
| 24:BA:2828:G:O2'  | 24:BA:2829:A:H5'  | 2.12                     | 0.48              |
| 24:BA:2856:A:O2'  | 24:BA:2857:G:H5'  | 2.13                     | 0.48              |
| 24:BA:684:G:C6    | 24:BA:774:G:C4    | 3.01                     | 0.48              |
| 24:BA:77:G:C4     | 24:BA:78:U:C5     | 3.01                     | 0.48              |
| 24:BA:797:G:C2    | 24:BA:798:G:C4    | 3.01                     | 0.48              |
| 24:BA:811:U:H2'   | 35:BL:21:ARG:HD3  | 1.94                     | 0.48              |
| 26:BC:221:GLY:O   | 26:BC:224:MET:HG3 | 2.13                     | 0.48              |
| 32:BI:12:VAL:HG23 | 32:BI:13:ALA:H    | 1.78                     | 0.48              |
| 35:BL:23:ILE:HG12 | 41:BR:82:HIS:CE1  | 2.48                     | 0.48              |
| 25:BB:90:C:H5'    | 36:BM:18:ARG:HG2  | 1.94                     | 0.48              |
| 41:BR:6:GLN:HE21  | 41:BR:9:GLY:CA    | 2.26                     | 0.48              |
| 55:CA:1170:A:H2'  | 55:CA:1171:A:O4'  | 2.13                     | 0.48              |
| 55:CA:1055:A:C6   | 55:CA:1206:G:C5   | 3.02                     | 0.48              |
| 55:CA:132:C:O2'   | 55:CA:133:U:C5'   | 2.61                     | 0.48              |
| 55:CA:1460:C:C5   | 55:CA:1461:G:N7   | 2.81                     | 0.48              |
| 55:CA:763:G:C2    | 55:CA:764:C:C6    | 3.01                     | 0.48              |
| 55:CA:764:C:N4    | 55:CA:812:G:C6    | 2.81                     | 0.48              |
| 55:CA:821:G:O2'   | 55:CA:822:U:C5'   | 2.61                     | 0.48              |
| 55:CA:821:G:O2'   | 55:CA:822:U:C6    | 2.59                     | 0.48              |
| 55:CA:82:G:C5     | 55:CA:89:U:C4     | 3.02                     | 0.48              |
| 1:CB:164:ASP:O    | 1:CB:168:GLU:HB2  | 2.13                     | 0.48              |
| 3:CD:55:ARG:HD2   | 3:CD:55:ARG:N     | 2.29                     | 0.48              |
| 6:CG:114:SER:HB2  | 6:CG:117:LEU:HD13 | 1.96                     | 0.48              |
| 6:CG:22:LEU:C     | 6:CG:22:LEU:HD23  | 2.34                     | 0.48              |
| 8:CI:24:ASN:HB2   | 8:CI:26:LYS:HZ3   | 1.76                     | 0.48              |
| 8:CI:90:ASP:HB3   | 8:CI:93:LEU:CD2   | 2.42                     | 0.48              |
| 9:CJ:11:LYS:HZ3   | 9:CJ:99:GLN:HB3   | 1.76                     | 0.48              |
| 12:CM:21:ILE:HG22 | 12:CM:23:GLY:H    | 1.79                     | 0.48              |
| 12:CM:1:ALA:N     | 12:CM:2:ARG:NH1   | 2.61                     | 0.48              |
| 16:CQ:46:HIS:HB2  | 16:CQ:70:LYS:HE3  | 1.94                     | 0.48              |
| 16:CQ:4:ILE:HG22  | 16:CQ:5:ARG:H     | 1.78                     | 0.48              |
| 19:CT:26:MET:CE   | 19:CT:30:PHE:HD1  | 2.25                     | 0.48              |
| 20:CU:23:GLU:O    | 20:CU:24:LYS:HB3  | 2.12                     | 0.48              |
| 24:DA:1059:G:C2   | 24:DA:1080:A:C2   | 3.02                     | 0.48              |
| 24:DA:1057:A:N3   | 24:DA:1082:U:C2   | 2.81                     | 0.48              |
| 24:DA:1142:A:C8   | 24:DA:1144:A:N7   | 2.82                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:156:A:H2'   | 24:DA:157:C:O4'   | 2.13                     | 0.48              |
| 24:DA:1669:A:O2'  | 24:DA:1670:C:H5'  | 2.13                     | 0.48              |
| 24:DA:1919:A:H2'  | 24:DA:1920:C:H5'  | 1.95                     | 0.48              |
| 24:DA:194:G:C6    | 24:DA:195:A:C6    | 3.01                     | 0.48              |
| 24:DA:2155:U:OP2  | 24:DA:2155:U:H6   | 1.96                     | 0.48              |
| 24:DA:2315:G:N1   | 24:DA:2316:G:C5   | 2.82                     | 0.48              |
| 24:DA:2616:C:HO2' | 24:DA:2617:U:H6   | 1.61                     | 0.48              |
| 24:DA:2653:U:C4   | 24:DA:2654:A:C5   | 3.01                     | 0.48              |
| 24:DA:227:A:H61   | 24:DA:410:G:H1'   | 1.78                     | 0.48              |
| 24:DA:777:G:N7    | 24:DA:793:A:C2    | 2.81                     | 0.48              |
| 24:DA:785:G:C6    | 24:DA:786:C:C4    | 3.01                     | 0.48              |
| 24:DA:807:U:H2'   | 24:DA:808:G:H8    | 1.78                     | 0.48              |
| 24:DA:92:U:O2'    | 24:DA:93:G:C5'    | 2.62                     | 0.48              |
| 24:DA:935:C:H2'   | 24:DA:936:A:H8    | 1.78                     | 0.48              |
| 56:DB:76:G:H5''   | 45:DV:17:SER:OG   | 2.13                     | 0.48              |
| 26:DC:62:ARG:NH2  | 26:DC:62:ARG:CG   | 2.77                     | 0.48              |
| 27:DD:114:LYS:HD2 | 27:DD:116:LYS:HZ2 | 1.79                     | 0.48              |
| 27:DD:17:GLU:H    | 27:DD:17:GLU:CD   | 2.17                     | 0.48              |
| 29:DF:1:ALA:HA    | 29:DF:97:GLU:HB3  | 1.95                     | 0.48              |
| 33:DJ:111:LYS:HB2 | 33:DJ:115:GLY:CA  | 2.43                     | 0.48              |
| 35:DL:90:VAL:HG13 | 35:DL:95:LEU:HD21 | 1.96                     | 0.48              |
| 36:DM:71:LYS:HD3  | 36:DM:95:LEU:CD1  | 2.43                     | 0.48              |
| 21:AA:1026:G:C5   | 21:AA:1027:C:N4   | 2.82                     | 0.48              |
| 21:AA:1219:A:C6   | 21:AA:1220:G:C6   | 3.01                     | 0.48              |
| 21:AA:1469:C:H2'  | 21:AA:1470:U:H5'  | 1.94                     | 0.48              |
| 21:AA:427:U:N3    | 21:AA:428:G:C6    | 2.82                     | 0.48              |
| 21:AA:987:G:C4    | 21:AA:988:G:C8    | 3.02                     | 0.48              |
| 1:AB:110:ILE:HA   | 1:AB:113:LEU:HB3  | 1.94                     | 0.48              |
| 2:AC:149:LYS:O    | 2:AC:200:TRP:HE3  | 1.95                     | 0.48              |
| 4:AE:109:ALA:C    | 4:AE:111:ARG:N    | 2.66                     | 0.48              |
| 4:AE:95:MET:CE    | 4:AE:114:LEU:HD11 | 2.44                     | 0.48              |
| 5:AF:36:ILE:HG22  | 5:AF:64:VAL:HG13  | 1.94                     | 0.48              |
| 5:AF:79:ARG:HE    | 5:AF:79:ARG:HA    | 1.78                     | 0.48              |
| 7:AH:17:GLN:NE2   | 7:AH:71:VAL:HG23  | 2.23                     | 0.48              |
| 10:AK:81:LEU:HD22 | 10:AK:104:PHE:HB3 | 1.94                     | 0.48              |
| 11:AL:24:GLU:O    | 11:AL:25:ALA:C    | 2.51                     | 0.48              |
| 14:AO:23:SER:HB3  | 14:AO:26:VAL:HG23 | 1.95                     | 0.48              |
| 24:BA:1142:A:C4   | 24:BA:1144:A:N7   | 2.82                     | 0.48              |
| 24:BA:1517:G:C6   | 24:BA:1518:C:C4   | 3.01                     | 0.48              |
| 24:BA:1967:C:H2'  | 24:BA:1968:G:H8   | 1.78                     | 0.48              |
| 24:BA:2250:G:O5'  | 24:BA:2250:G:C8   | 2.64                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:2689:U:C2    | 24:BA:2713:U:C6    | 3.02                     | 0.48              |
| 24:BA:49:A:C2      | 24:BA:118:A:C2     | 3.01                     | 0.48              |
| 24:BA:49:A:C2      | 24:BA:118:A:N1     | 2.82                     | 0.48              |
| 29:BF:107:VAL:HG11 | 29:BF:175:PRO:HG2  | 1.95                     | 0.48              |
| 29:BF:72:SER:HB2   | 29:BF:80:GLN:HB2   | 1.94                     | 0.48              |
| 31:BH:96:THR:HG23  | 31:BH:96:THR:O     | 2.14                     | 0.48              |
| 32:BI:107:GLU:HA   | 32:BI:110:GLN:HB3  | 1.95                     | 0.48              |
| 32:BI:56:VAL:HG11  | 32:BI:68:PHE:HD2   | 1.78                     | 0.48              |
| 33:BJ:23:LYS:O     | 33:BJ:63:ALA:HB3   | 2.13                     | 0.48              |
| 35:BL:82:LEU:C     | 35:BL:84:LYS:H     | 2.15                     | 0.48              |
| 39:BP:25:VAL:HG23  | 39:BP:83:ILE:HD11  | 1.95                     | 0.48              |
| 42:BS:63:GLY:O     | 42:BS:64:ALA:CB    | 2.61                     | 0.48              |
| 46:BW:45:HIS:HB2   | 46:BW:50:VAL:HG13  | 1.94                     | 0.48              |
| 24:BA:2232:C:OP1   | 47:BX:26:ARG:NH2   | 2.47                     | 0.48              |
| 55:CA:1227:A:H5''  | 55:CA:1227:A:N3    | 2.28                     | 0.48              |
| 55:CA:174:A:H2'    | 55:CA:175:C:C6     | 2.49                     | 0.48              |
| 55:CA:247:G:O6     | 55:CA:278:G:N1     | 2.47                     | 0.48              |
| 55:CA:519:C:O2'    | 55:CA:520:A:C5'    | 2.61                     | 0.48              |
| 55:CA:747:A:H2'    | 55:CA:748:G:O4'    | 2.12                     | 0.48              |
| 55:CA:915:A:O2'    | 55:CA:916:U:C5'    | 2.60                     | 0.48              |
| 2:CC:148:ILE:HG23  | 2:CC:169:GLU:HB3   | 1.95                     | 0.48              |
| 3:CD:113:ALA:O     | 3:CD:117:VAL:HG23  | 2.14                     | 0.48              |
| 3:CD:161:ALA:O     | 3:CD:164:ARG:HB2   | 2.13                     | 0.48              |
| 7:CH:64:TYR:HA     | 7:CH:69:ALA:HA     | 1.94                     | 0.48              |
| 11:CL:34:THR:C     | 11:CL:35:ARG:NE    | 2.67                     | 0.48              |
| 2:CC:19:SER:O      | 13:CN:93:PRO:HG3   | 2.13                     | 0.48              |
| 18:CS:39:ILE:HD11  | 18:CS:65:MET:HB2   | 1.95                     | 0.48              |
| 18:CS:50:VAL:CG2   | 18:CS:74:ALA:HB2   | 2.43                     | 0.48              |
| 53:D3:15:LYS:HZ2   | 53:D3:19:GLY:HA2   | 1.79                     | 0.48              |
| 24:DA:1571:A:H2'   | 24:DA:1572:A:C8    | 2.49                     | 0.48              |
| 24:DA:1910:G:C6    | 24:DA:1921:G:C6    | 3.01                     | 0.48              |
| 24:DA:964:C:O2'    | 24:DA:2273:A:H1'   | 2.14                     | 0.48              |
| 24:DA:227:A:H5'    | 24:DA:229:C:N4     | 2.28                     | 0.48              |
| 24:DA:2624:G:H2'   | 24:DA:2625:G:O4'   | 2.13                     | 0.48              |
| 24:DA:2811:G:H2'   | 24:DA:2812:G:H8    | 1.78                     | 0.48              |
| 24:DA:2838:G:OP1   | 59:DA:3795:HOH:O   | 2.20                     | 0.48              |
| 24:DA:2867:G:O2'   | 24:DA:2868:A:OP2   | 2.31                     | 0.48              |
| 24:DA:17:G:C6      | 24:DA:524:G:C6     | 3.01                     | 0.48              |
| 26:DC:245:THR:O    | 26:DC:247:TRP:N    | 2.47                     | 0.48              |
| 27:DD:36:GLN:HE21  | 27:DD:38:LYS:NZ    | 2.11                     | 0.48              |
| 28:DE:106:LYS:HG3  | 28:DE:200:LEU:HD12 | 1.96                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DE:48:THR:O     | 28:DE:52:VAL:HG23  | 2.14                     | 0.48              |
| 29:DF:134:GLN:HB2  | 29:DF:137:PHE:HE2  | 1.78                     | 0.48              |
| 30:DG:112:VAL:HG12 | 30:DG:114:HIS:HB3  | 1.96                     | 0.48              |
| 30:DG:8:VAL:O      | 30:DG:9:VAL:HB     | 2.14                     | 0.48              |
| 34:DK:118:LEU:O    | 34:DK:120:PRO:HD2  | 2.13                     | 0.48              |
| 35:DL:66:PHE:CG    | 35:DL:67:THR:N     | 2.81                     | 0.48              |
| 43:DT:50:LEU:HD23  | 43:DT:51:PHE:N     | 2.24                     | 0.48              |
| 21:AA:1036:A:H3'   | 21:AA:1037:C:C6    | 2.48                     | 0.48              |
| 4:AE:61:LYS:HD3    | 21:AA:1073:U:P     | 2.53                     | 0.48              |
| 21:AA:126:G:H2'    | 21:AA:127:G:O5'    | 2.14                     | 0.48              |
| 21:AA:636:U:H6     | 21:AA:636:U:O5'    | 1.97                     | 0.48              |
| 21:AA:901:A:N7     | 21:AA:902:G:H1'    | 2.28                     | 0.48              |
| 21:AA:944:G:C6     | 21:AA:1337:G:H2'   | 2.48                     | 0.48              |
| 1:AB:16:GLY:HA2    | 1:AB:202:ASN:ND2   | 2.29                     | 0.48              |
| 2:AC:70:ALA:HA     | 2:AC:105:VAL:HB    | 1.95                     | 0.48              |
| 3:AD:166:LYS:HA    | 3:AD:167:PRO:HD3   | 1.71                     | 0.48              |
| 4:AE:71:ILE:HD11   | 4:AE:144:GLU:HG3   | 1.96                     | 0.48              |
| 4:AE:14:LEU:HD22   | 4:AE:15:ILE:C      | 2.34                     | 0.48              |
| 9:AJ:74:VAL:O      | 9:AJ:75:ASP:HB3    | 2.13                     | 0.48              |
| 11:AL:27:PRO:O     | 11:AL:28:GLN:HB3   | 2.12                     | 0.48              |
| 11:AL:43:LYS:HB2   | 11:AL:44:PRO:CD    | 2.43                     | 0.48              |
| 24:BA:1025:G:H4'   | 24:BA:1026:G:OP2   | 2.14                     | 0.48              |
| 24:BA:1052:C:C2'   | 24:BA:1053:C:H5'   | 2.44                     | 0.48              |
| 24:BA:1147:A:C6    | 24:BA:1148:U:C4    | 3.02                     | 0.48              |
| 24:BA:2209:G:N1    | 24:BA:2210:U:O4    | 2.46                     | 0.48              |
| 24:BA:2217:G:H2'   | 24:BA:2218:G:C8    | 2.48                     | 0.48              |
| 24:BA:2415:G:C2    | 24:BA:2416:C:C2    | 3.01                     | 0.48              |
| 24:BA:2727:A:H2'   | 24:BA:2728:U:H6    | 1.78                     | 0.48              |
| 24:BA:471:A:O5'    | 24:BA:471:A:H8     | 1.97                     | 0.48              |
| 24:BA:484:C:H6     | 24:BA:484:C:O5'    | 1.95                     | 0.48              |
| 24:BA:48:G:N2      | 24:BA:177:G:N2     | 2.61                     | 0.48              |
| 24:BA:813:U:H2'    | 24:BA:814:C:C6     | 2.48                     | 0.48              |
| 24:BA:813:U:O2'    | 24:BA:1225:G:H1'   | 2.14                     | 0.48              |
| 24:BA:95:A:N1      | 24:BA:96:C:C2      | 2.81                     | 0.48              |
| 24:BA:994:C:H1'    | 41:BR:10:LYS:HZ3   | 1.76                     | 0.48              |
| 27:BD:61:THR:OG1   | 27:BD:63:PRO:HD2   | 2.14                     | 0.48              |
| 32:BI:105:LEU:HD23 | 32:BI:108:ILE:HG21 | 1.94                     | 0.48              |
| 32:BI:64:ARG:HG3   | 32:BI:65:SER:N     | 2.28                     | 0.48              |
| 33:BJ:45:THR:CG2   | 33:BJ:45:THR:O     | 2.60                     | 0.48              |
| 34:BK:57:VAL:C     | 34:BK:58:LEU:HD23  | 2.34                     | 0.48              |
| 35:BL:119:PRO:HA   | 35:BL:138:ALA:O    | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BM:101:VAL:CG1 | 36:BM:101:VAL:O   | 2.61                     | 0.48              |
| 24:BA:959:A:N6    | 36:BM:82:MET:CE   | 2.76                     | 0.48              |
| 37:BN:92:GLY:HA2  | 37:BN:94:TYR:CZ   | 2.49                     | 0.48              |
| 39:BP:105:LYS:CA  | 39:BP:108:ARG:HD3 | 2.44                     | 0.48              |
| 24:BA:493:G:O2'   | 42:BS:7:HIS:HA    | 2.14                     | 0.48              |
| 44:BU:53:GLN:N    | 44:BU:54:PRO:HD2  | 2.27                     | 0.48              |
| 24:BA:923:G:C1'   | 46:BW:23:LYS:HE2  | 2.42                     | 0.48              |
| 55:CA:1049:U:H4'  | 55:CA:1050:G:OP2  | 2.14                     | 0.48              |
| 55:CA:10:A:N1     | 55:CA:25:C:N3     | 2.62                     | 0.48              |
| 55:CA:370:C:O2'   | 55:CA:371:A:H5'   | 2.13                     | 0.48              |
| 55:CA:499:A:O2'   | 55:CA:500:G:H8    | 1.91                     | 0.48              |
| 55:CA:519:C:O2'   | 55:CA:520:A:C8    | 2.65                     | 0.48              |
| 55:CA:581:G:N2    | 55:CA:582:C:N4    | 2.62                     | 0.48              |
| 55:CA:588:G:C6    | 55:CA:589:U:N3    | 2.81                     | 0.48              |
| 55:CA:879:C:C2    | 55:CA:880:C:C6    | 3.01                     | 0.48              |
| 55:CA:95:C:O2'    | 55:CA:96:U:H5'    | 2.14                     | 0.48              |
| 2:CC:110:LEU:HD11 | 2:CC:203:LYS:HZ1  | 1.77                     | 0.48              |
| 2:CC:131:ARG:HA   | 2:CC:134:LYS:HD2  | 1.94                     | 0.48              |
| 6:CG:94:ARG:C     | 6:CG:96:ASN:H     | 2.17                     | 0.48              |
| 10:CK:15:VAL:HG13 | 10:CK:36:ARG:NH1  | 2.29                     | 0.48              |
| 12:CM:1:ALA:N     | 12:CM:2:ARG:CD    | 2.77                     | 0.48              |
| 12:CM:75:SER:C    | 12:CM:77:LYS:H    | 2.17                     | 0.48              |
| 13:CN:15:LEU:O    | 13:CN:54:SER:HB2  | 2.13                     | 0.48              |
| 17:CR:56:ARG:O    | 17:CR:60:ARG:HG3  | 2.14                     | 0.48              |
| 24:DA:1049:C:HO2' | 24:DA:1050:A:H8   | 1.61                     | 0.48              |
| 24:DA:1062:G:O2'  | 24:DA:1063:G:O5'  | 2.31                     | 0.48              |
| 24:DA:1152:C:H2'  | 24:DA:1153:C:H6   | 1.79                     | 0.48              |
| 24:DA:1259:G:H2'  | 24:DA:1260:A:H8   | 1.77                     | 0.48              |
| 24:DA:1293:C:H2'  | 24:DA:1294:U:O4'  | 2.13                     | 0.48              |
| 24:DA:1440:U:O2'  | 24:DA:1441:G:H5'  | 2.13                     | 0.48              |
| 24:DA:1535:A:H2'  | 24:DA:1535:A:N3   | 2.28                     | 0.48              |
| 24:DA:1941:C:O2'  | 24:DA:1942:C:H5'  | 2.13                     | 0.48              |
| 24:DA:1953:A:H4'  | 24:DA:2560:A:H5'  | 1.94                     | 0.48              |
| 24:DA:2061:G:H5'' | 24:DA:2503:A:C2   | 2.48                     | 0.48              |
| 24:DA:2303:G:C4   | 24:DA:2304:G:C8   | 3.01                     | 0.48              |
| 24:DA:2562:U:O2   | 24:DA:2562:U:H2'  | 2.14                     | 0.48              |
| 24:DA:2688:G:H1'  | 24:DA:2721:A:N6   | 2.28                     | 0.48              |
| 24:DA:2833:U:H3'  | 24:DA:2834:G:C5'  | 2.44                     | 0.48              |
| 24:DA:2901:C:N4   | 24:DA:2902:C:N4   | 2.62                     | 0.48              |
| 24:DA:860:U:HO2'  | 24:DA:861:A:C5'   | 2.26                     | 0.48              |
| 26:DC:7:PRO:HB3   | 26:DC:13:ARG:HB2  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:DE:151:GLY:HA3 | 28:DE:191:ASP:OD1 | 2.12                     | 0.48              |
| 29:DF:110:ILE:HB  | 29:DF:113:PHE:H   | 1.78                     | 0.48              |
| 31:DH:32:PRO:HA   | 47:DX:38:TRP:CD1  | 2.49                     | 0.48              |
| 32:DI:52:LEU:HD11 | 32:DI:78:LEU:CD2  | 2.44                     | 0.48              |
| 24:DA:2359:C:O2   | 35:DL:60:ARG:NH2  | 2.47                     | 0.48              |
| 42:DS:82:MET:HE1  | 42:DS:84:ARG:HH12 | 1.79                     | 0.48              |
| 44:DU:85:ARG:NE   | 44:DU:85:ARG:HA   | 2.29                     | 0.48              |
| 47:DX:53:LYS:CA   | 47:DX:56:ARG:HB3  | 2.25                     | 0.48              |
| 21:AA:1038:C:H2'  | 21:AA:1039:G:H8   | 1.78                     | 0.48              |
| 21:AA:1103:C:HO2' | 21:AA:1104:G:C4'  | 2.26                     | 0.48              |
| 21:AA:1106:G:C2   | 21:AA:1107:C:C6   | 3.02                     | 0.48              |
| 21:AA:1312:G:H2'  | 21:AA:1313:U:C6   | 2.49                     | 0.48              |
| 21:AA:1394:A:N6   | 21:AA:1501:C:C4'  | 2.76                     | 0.48              |
| 21:AA:394:G:C5    | 21:AA:395:C:C5    | 3.01                     | 0.48              |
| 21:AA:411:A:C5    | 21:AA:429:U:C5    | 3.02                     | 0.48              |
| 21:AA:415:A:O2'   | 21:AA:416:G:H5'   | 2.14                     | 0.48              |
| 21:AA:550:G:N2    | 21:AA:551:U:C2    | 2.82                     | 0.48              |
| 21:AA:596:A:O2'   | 21:AA:597:G:H5'   | 2.13                     | 0.48              |
| 21:AA:78:A:N6     | 21:AA:79:G:C6     | 2.81                     | 0.48              |
| 21:AA:842:U:H3'   | 21:AA:843:U:H5''  | 1.95                     | 0.48              |
| 21:AA:977:A:H2'   | 21:AA:977:A:N3    | 2.29                     | 0.48              |
| 1:AB:65:LYS:HG2   | 1:AB:153:MET:CG   | 2.43                     | 0.48              |
| 2:AC:148:ILE:HG12 | 2:AC:149:LYS:N    | 2.28                     | 0.48              |
| 2:AC:166:TRP:N    | 2:AC:166:TRP:CE3  | 2.71                     | 0.48              |
| 2:AC:99:GLN:O     | 2:AC:100:ILE:CB   | 2.58                     | 0.48              |
| 3:AD:164:ARG:HG2  | 3:AD:165:GLU:H    | 1.78                     | 0.48              |
| 3:AD:172:VAL:HG22 | 3:AD:173:ASP:N    | 2.20                     | 0.48              |
| 4:AE:37:VAL:HG11  | 4:AE:113:VAL:HG12 | 1.95                     | 0.48              |
| 6:AG:121:ASN:N    | 6:AG:121:ASN:HD22 | 2.11                     | 0.48              |
| 7:AH:74:ILE:HD13  | 7:AH:128:VAL:HG13 | 1.96                     | 0.48              |
| 9:AJ:53:ILE:HG22  | 9:AJ:62:ARG:H     | 1.79                     | 0.48              |
| 10:AK:125:LYS:O   | 10:AK:126:ARG:CB  | 2.62                     | 0.48              |
| 18:AS:39:ILE:HD11 | 18:AS:73:PHE:HE1  | 1.77                     | 0.48              |
| 19:AT:63:LYS:HE2  | 21:AA:176:C:OP1   | 2.14                     | 0.48              |
| 54:B4:25:VAL:CG2  | 54:B4:35:GLN:HB2  | 2.44                     | 0.48              |
| 24:BA:1054:A:C6   | 24:BA:1106:G:O6   | 2.67                     | 0.48              |
| 24:BA:1250:G:N7   | 35:BL:18:ARG:NH1  | 2.62                     | 0.48              |
| 24:BA:152:A:H2'   | 24:BA:153:U:C6    | 2.48                     | 0.48              |
| 24:BA:1873:G:H2'  | 24:BA:1874:C:H6   | 1.79                     | 0.48              |
| 24:BA:1892:C:H2'  | 24:BA:1893:C:C6   | 2.48                     | 0.48              |
| 24:BA:2488:G:C2   | 24:BA:2489:U:C2   | 3.02                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:2691:C:O2'   | 24:BA:2692:G:C5'   | 2.60                     | 0.48              |
| 24:BA:2845:U:H5''  | 39:BP:51:ASN:O     | 2.14                     | 0.48              |
| 24:BA:396:G:O3'    | 47:BX:30:PRO:HA    | 2.13                     | 0.48              |
| 24:BA:475:C:C4     | 24:BA:481:G:O6     | 2.67                     | 0.48              |
| 24:BA:668:A:C2'    | 24:BA:669:G:OP1    | 2.62                     | 0.48              |
| 27:BD:110:THR:OG1  | 27:BD:171:THR:CG2  | 2.61                     | 0.48              |
| 28:BE:147:LEU:O    | 28:BE:168:ASP:O    | 2.31                     | 0.48              |
| 30:BG:27:GLY:O     | 30:BG:29:ASN:O     | 2.32                     | 0.48              |
| 37:BN:60:VAL:O     | 37:BN:61:ALA:C     | 2.51                     | 0.48              |
| 37:BN:67:PHE:CE1   | 37:BN:73:ASN:OD1   | 2.66                     | 0.48              |
| 40:BQ:82:LEU:HD21  | 40:BQ:112:ALA:HB2  | 1.95                     | 0.48              |
| 42:BS:38:TYR:CD2   | 50:B0:38:LEU:HD21  | 2.48                     | 0.48              |
| 46:BW:17:ALA:HA    | 46:BW:35:ILE:CG2   | 2.27                     | 0.48              |
| 46:BW:24:ARG:C     | 46:BW:24:ARG:HD2   | 2.32                     | 0.48              |
| 46:BW:30:VAL:HA    | 46:BW:60:ALA:HB3   | 1.95                     | 0.48              |
| 46:BW:67:LYS:HG3   | 46:BW:69:GLU:HG3   | 1.94                     | 0.48              |
| 55:CA:1155:A:O2'   | 55:CA:1156:G:H5'   | 2.14                     | 0.48              |
| 55:CA:127:G:N2     | 55:CA:128:G:H1'    | 2.29                     | 0.48              |
| 55:CA:131:A:C2     | 55:CA:132:C:C2     | 3.02                     | 0.48              |
| 55:CA:942:G:C6     | 55:CA:1342:C:C4    | 3.01                     | 0.48              |
| 55:CA:259:G:C2     | 55:CA:268:U:C2     | 3.02                     | 0.48              |
| 55:CA:428:G:C1'    | 55:CA:430:A:C8     | 2.96                     | 0.48              |
| 55:CA:581:G:N2     | 55:CA:582:C:H41    | 2.12                     | 0.48              |
| 55:CA:601:G:H2'    | 55:CA:602:A:C8     | 2.43                     | 0.48              |
| 55:CA:95:C:H2'     | 55:CA:96:U:C5      | 2.47                     | 0.48              |
| 4:CE:114:LEU:HD13  | 4:CE:122:VAL:HG11  | 1.96                     | 0.48              |
| 8:CI:118:ARG:HH21  | 8:CI:122:ARG:HE    | 1.60                     | 0.48              |
| 9:CJ:7:ARG:HB2     | 9:CJ:101:SER:O     | 2.13                     | 0.48              |
| 9:CJ:35:GLN:OE1    | 9:CJ:77:VAL:HB     | 2.14                     | 0.48              |
| 10:CK:115:ILE:HD12 | 20:CU:23:GLU:CG    | 2.33                     | 0.48              |
| 19:CT:81:GLN:O     | 19:CT:82:ILE:HG23  | 2.13                     | 0.48              |
| 24:DA:1057:A:C4    | 24:DA:1082:U:N3    | 2.81                     | 0.48              |
| 24:DA:1254:A:H3'   | 24:DA:1255:U:H5''  | 1.96                     | 0.48              |
| 24:DA:1504:A:C2    | 24:DA:1505:A:C8    | 3.01                     | 0.48              |
| 24:DA:1809:A:O2'   | 24:DA:1810:A:O5'   | 2.31                     | 0.48              |
| 24:DA:2341:G:H2'   | 24:DA:2342:C:O4'   | 2.14                     | 0.48              |
| 24:DA:448:U:H4'    | 24:DA:449:A:OP2    | 2.14                     | 0.48              |
| 27:DD:118:PHE:O    | 27:DD:119:ALA:HB3  | 2.13                     | 0.48              |
| 28:DE:137:LYS:O    | 28:DE:140:ASP:HB2  | 2.13                     | 0.48              |
| 28:DE:164:LEU:HD12 | 28:DE:167:VAL:HG12 | 1.94                     | 0.48              |
| 30:DG:120:ILE:O    | 30:DG:120:ILE:HD13 | 2.13                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:DY:47:ARG:O    | 48:DY:50:VAL:N     | 2.45                     | 0.48              |
| 48:DY:53:VAL:O    | 48:DY:57:LEU:HB2   | 2.13                     | 0.48              |
| 21:AA:1257:A:H4'  | 21:AA:1258:G:OP2   | 2.11                     | 0.48              |
| 21:AA:1486:G:H2'  | 21:AA:1487:G:O4'   | 2.14                     | 0.48              |
| 21:AA:24:U:H2'    | 21:AA:25:C:H6      | 1.78                     | 0.48              |
| 21:AA:65:A:C2     | 21:AA:381:C:C6     | 3.02                     | 0.48              |
| 21:AA:414:A:N3    | 21:AA:414:A:H2'    | 2.29                     | 0.48              |
| 21:AA:415:A:H2'   | 21:AA:416:G:O4'    | 2.13                     | 0.48              |
| 21:AA:706:A:H2'   | 21:AA:707:U:O4'    | 2.14                     | 0.48              |
| 14:AO:22:GLY:O    | 21:AA:751:U:H1'    | 2.14                     | 0.48              |
| 21:AA:788:U:C4    | 21:AA:789:U:C4     | 3.02                     | 0.48              |
| 1:AB:130:LYS:O    | 1:AB:133:ALA:HB3   | 2.14                     | 0.48              |
| 3:AD:29:THR:HB    | 3:AD:30:LYS:NZ     | 2.29                     | 0.48              |
| 4:AE:95:MET:HE3   | 4:AE:114:LEU:HD11  | 1.95                     | 0.48              |
| 4:AE:40:ASP:OD1   | 4:AE:44:ARG:HB2    | 2.14                     | 0.48              |
| 7:AH:17:GLN:HB3   | 7:AH:69:ALA:HB2    | 1.94                     | 0.48              |
| 10:AK:61:ALA:O    | 10:AK:64:VAL:HG13  | 2.13                     | 0.48              |
| 11:AL:41:PRO:HB3  | 11:AL:49:ARG:HH12  | 1.77                     | 0.48              |
| 12:AM:74:MET:CA   | 12:AM:74:MET:CE    | 2.69                     | 0.48              |
| 14:AO:22:GLY:O    | 14:AO:27:GLN:NE2   | 2.47                     | 0.48              |
| 16:AQ:45:VAL:HG21 | 16:AQ:60:ILE:HD13  | 1.96                     | 0.48              |
| 19:AT:26:MET:HA   | 19:AT:29:THR:HG1   | 1.76                     | 0.48              |
| 24:BA:1022:G:C6   | 24:BA:1141:U:C5    | 3.01                     | 0.48              |
| 24:BA:1944:U:O4   | 24:BA:2557:G:N2    | 2.40                     | 0.48              |
| 24:BA:2207:C:H2'  | 24:BA:2208:C:C6    | 2.49                     | 0.48              |
| 24:BA:2082:A:N6   | 24:BA:2237:G:H1'   | 2.29                     | 0.48              |
| 24:BA:2291:U:C2   | 24:BA:2292:U:C4    | 3.01                     | 0.48              |
| 24:BA:2692:G:C4   | 24:BA:2718:G:N2    | 2.82                     | 0.48              |
| 24:BA:2204:G:H4'  | 26:BC:149:LYS:HG3  | 1.95                     | 0.48              |
| 27:BD:27:ILE:HG12 | 27:BD:201:LEU:HD23 | 1.96                     | 0.48              |
| 27:BD:4:LEU:HD23  | 27:BD:29:VAL:HG11  | 1.95                     | 0.48              |
| 29:BF:39:VAL:CG1  | 29:BF:49:LEU:HD13  | 2.44                     | 0.48              |
| 29:BF:66:ILE:O    | 29:BF:66:ILE:HG13  | 2.13                     | 0.48              |
| 29:BF:72:SER:HB2  | 29:BF:80:GLN:N     | 2.29                     | 0.48              |
| 30:BG:94:ARG:HG3  | 30:BG:127:GLN:OE1  | 2.13                     | 0.48              |
| 31:BH:100:ALA:O   | 31:BH:102:ALA:N    | 2.47                     | 0.48              |
| 33:BJ:5:THR:O     | 33:BJ:5:THR:HG22   | 2.13                     | 0.48              |
| 24:BA:1154:G:OP2  | 40:BQ:57:ARG:NH1   | 2.45                     | 0.48              |
| 43:BT:24:MET:HG3  | 43:BT:29:THR:HG23  | 1.96                     | 0.48              |
| 24:BA:856:G:C1'   | 46:BW:23:LYS:HB3   | 2.44                     | 0.48              |
| 55:CA:66:A:C2     | 55:CA:104:G:H1'    | 2.48                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:CE:22:LYS:CD    | 55:CA:1081:A:H5'   | 2.38                     | 0.48              |
| 55:CA:1270:G:H2'  | 55:CA:1271:A:C8    | 2.49                     | 0.48              |
| 55:CA:1426:G:N2   | 55:CA:1475:G:H1'   | 2.28                     | 0.48              |
| 55:CA:1449:C:O2'  | 55:CA:1450:U:C5'   | 2.62                     | 0.48              |
| 55:CA:27:G:H2'    | 55:CA:28:A:O4'     | 2.13                     | 0.48              |
| 55:CA:391:G:O6    | 55:CA:392:C:C4     | 2.67                     | 0.48              |
| 55:CA:463:U:H3    | 55:CA:469:C:H42    | 1.61                     | 0.48              |
| 55:CA:66:A:O2'    | 55:CA:67:C:H5'     | 2.12                     | 0.48              |
| 55:CA:848:C:H2'   | 55:CA:849:G:O5'    | 2.13                     | 0.48              |
| 55:CA:988:G:O2'   | 55:CA:989:U:H5'    | 2.14                     | 0.48              |
| 1:CB:72:LYS:HB2   | 1:CB:75:ALA:HB3    | 1.96                     | 0.48              |
| 1:CB:9:LEU:O      | 1:CB:10:LYS:CB     | 2.61                     | 0.48              |
| 3:CD:171:GLU:CG   | 3:CD:180:THR:HB    | 2.44                     | 0.48              |
| 6:CG:77:ARG:HG3   | 6:CG:77:ARG:HH11   | 1.79                     | 0.48              |
| 8:CI:51:LEU:HD11  | 8:CI:82:ILE:HG22   | 1.94                     | 0.48              |
| 11:CL:85:ARG:HA   | 11:CL:93:ARG:HA    | 1.95                     | 0.48              |
| 12:CM:14:ALA:HB1  | 12:CM:33:LEU:CD1   | 2.41                     | 0.48              |
| 19:CT:34:VAL:HG22 | 19:CT:49:ALA:HB1   | 1.95                     | 0.48              |
| 24:DA:1137:G:H2'  | 24:DA:1138:G:C8    | 2.49                     | 0.48              |
| 24:DA:1266:G:C8   | 42:DS:16:LYS:HE3   | 2.49                     | 0.48              |
| 24:DA:1802:A:H62  | 24:DA:1817:G:N2    | 2.12                     | 0.48              |
| 24:DA:190:A:H2'   | 24:DA:191:A:O4'    | 2.12                     | 0.48              |
| 24:DA:2037:A:H2'  | 24:DA:2038:G:C8    | 2.49                     | 0.48              |
| 24:DA:2446:G:H2'  | 24:DA:2447:G:H5''  | 1.96                     | 0.48              |
| 24:DA:2581:G:H5'' | 24:DA:2582:G:OP1   | 2.13                     | 0.48              |
| 24:DA:2721:A:C2   | 24:DA:2722:G:H1'   | 2.48                     | 0.48              |
| 24:DA:2838:G:C4   | 24:DA:2839:G:C8    | 3.01                     | 0.48              |
| 24:DA:471:A:H2'   | 24:DA:472:A:O4'    | 2.13                     | 0.48              |
| 24:DA:536:G:H2'   | 24:DA:537:G:H5'    | 1.94                     | 0.48              |
| 24:DA:556:A:H8    | 24:DA:556:A:OP2    | 1.95                     | 0.48              |
| 24:DA:831:G:H2'   | 24:DA:832:U:C6     | 2.49                     | 0.48              |
| 24:DA:845:A:N6    | 24:DA:932:U:C2     | 2.81                     | 0.48              |
| 24:DA:89:A:C2     | 24:DA:90:U:C2      | 3.02                     | 0.48              |
| 24:DA:2575:C:H4'  | 27:DD:148:GLN:O    | 2.14                     | 0.48              |
| 24:DA:675:A:OP1   | 28:DE:60:TRP:HZ2   | 1.95                     | 0.48              |
| 29:DF:76:PHE:CD2  | 29:DF:76:PHE:N     | 2.75                     | 0.48              |
| 31:DH:42:LYS:NZ   | 31:DH:42:LYS:HB3   | 2.29                     | 0.48              |
| 33:DJ:35:ARG:HH12 | 33:DJ:140:LEU:HD21 | 1.78                     | 0.48              |
| 33:DJ:2:LYS:HB2   | 33:DJ:2:LYS:NZ     | 2.29                     | 0.48              |
| 35:DL:71:ALA:HA   | 35:DL:74:THR:HB    | 1.96                     | 0.48              |
| 35:DL:76:GLU:O    | 35:DL:76:GLU:HG3   | 2.12                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:DJ:4:PHE:HB3    | 40:DQ:63:ARG:HH22  | 1.78                     | 0.48              |
| 46:DW:18:LYS:HZ3   | 46:DW:18:LYS:HB2   | 1.77                     | 0.48              |
| 48:DY:6:LEU:HD21   | 48:DY:56:LEU:HD12  | 1.95                     | 0.48              |
| 21:AA:1363:A:H2'   | 21:AA:1365:G:N7    | 2.29                     | 0.48              |
| 21:AA:1484:C:H2'   | 21:AA:1485:U:O4'   | 2.14                     | 0.48              |
| 21:AA:217:C:O2'    | 21:AA:218:U:H5'    | 2.14                     | 0.48              |
| 21:AA:332:G:C2     | 21:AA:333:U:C6     | 3.02                     | 0.48              |
| 21:AA:569:C:H5''   | 21:AA:570:G:OP1    | 2.14                     | 0.48              |
| 21:AA:622:A:H2'    | 21:AA:623:C:H5'    | 1.95                     | 0.48              |
| 1:AB:153:MET:HE1   | 1:AB:157:PRO:HG3   | 1.96                     | 0.48              |
| 1:AB:162:VAL:HG22  | 1:AB:184:ALA:HB2   | 1.95                     | 0.48              |
| 3:AD:191:SER:HA    | 3:AD:194:ILE:HD11  | 1.94                     | 0.48              |
| 4:AE:36:THR:HG23   | 4:AE:62:ALA:CB     | 2.44                     | 0.48              |
| 4:AE:82:HIS:HA     | 7:AH:98:LEU:HD12   | 1.96                     | 0.48              |
| 15:AP:42:ILE:C     | 15:AP:44:SER:H     | 2.16                     | 0.48              |
| 24:BA:1232:G:C6    | 24:BA:1233:C:C4    | 3.01                     | 0.48              |
| 24:BA:1759:A:H2'   | 24:BA:1760:C:C5    | 2.48                     | 0.48              |
| 24:BA:1773:A:H2'   | 24:BA:1774:C:O4'   | 2.13                     | 0.48              |
| 24:BA:2291:U:OP1   | 24:BA:2381:A:H5'   | 2.13                     | 0.48              |
| 24:BA:2643:G:H2'   | 24:BA:2644:G:O4'   | 2.14                     | 0.48              |
| 24:BA:2674:G:H2'   | 24:BA:2675:A:C8    | 2.49                     | 0.48              |
| 24:BA:2714:G:O2'   | 24:BA:2715:C:H5'   | 2.14                     | 0.48              |
| 24:BA:2798:U:H6    | 24:BA:2798:U:OP2   | 1.96                     | 0.48              |
| 24:BA:2818:U:H1'   | 24:BA:2829:A:C2    | 2.48                     | 0.48              |
| 24:BA:826:U:O2     | 24:BA:828:U:H4'    | 2.14                     | 0.48              |
| 24:BA:947:A:O2'    | 24:BA:984:A:C2     | 2.67                     | 0.48              |
| 24:BA:966:G:C6     | 24:BA:967:U:N3     | 2.82                     | 0.48              |
| 26:BC:77:VAL:O     | 26:BC:77:VAL:CG2   | 2.60                     | 0.48              |
| 28:BE:5:LEU:CD1    | 28:BE:10:SER:HB3   | 2.41                     | 0.48              |
| 28:BE:108:ILE:HD11 | 28:BE:180:LEU:HB3  | 1.94                     | 0.48              |
| 28:BE:148:ILE:HD13 | 28:BE:187:VAL:HG21 | 1.95                     | 0.48              |
| 28:BE:32:VAL:HG23  | 28:BE:33:VAL:N     | 2.29                     | 0.48              |
| 29:BF:110:ILE:O    | 29:BF:111:ARG:C    | 2.50                     | 0.48              |
| 29:BF:54:ALA:O     | 29:BF:57:ALA:HB3   | 2.13                     | 0.48              |
| 35:BL:100:ILE:HD12 | 35:BL:100:ILE:O    | 2.14                     | 0.48              |
| 35:BL:57:LEU:CD2   | 53:B3:53:ASP:HB3   | 2.44                     | 0.48              |
| 35:BL:81:ASP:O     | 35:BL:83:ALA:N     | 2.39                     | 0.48              |
| 37:BN:2:ARG:O      | 37:BN:3:HIS:C      | 2.52                     | 0.48              |
| 38:BO:74:VAL:HG12  | 38:BO:106:LEU:HD13 | 1.96                     | 0.48              |
| 43:BT:29:THR:HB    | 43:BT:86:THR:N     | 2.29                     | 0.48              |
| 55:CA:1250:A:C8    | 55:CA:1287:A:N7    | 2.82                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:238:A:H3'   | 55:CA:239:U:H5''  | 1.94                     | 0.48              |
| 55:CA:253:A:N3    | 55:CA:254:G:C8    | 2.82                     | 0.48              |
| 55:CA:327:A:C2    | 55:CA:329:A:C4    | 3.02                     | 0.48              |
| 55:CA:47:C:O2'    | 55:CA:48:C:H5'    | 2.13                     | 0.48              |
| 55:CA:533:A:H8    | 55:CA:533:A:OP2   | 1.97                     | 0.48              |
| 55:CA:954:G:C6    | 55:CA:955:U:N3    | 2.82                     | 0.48              |
| 55:CA:987:G:H2'   | 55:CA:988:G:C8    | 2.49                     | 0.48              |
| 4:CE:114:LEU:HB3  | 4:CE:119:VAL:HG23 | 1.96                     | 0.48              |
| 4:CE:94:PHE:CE2   | 4:CE:96:GLN:HB2   | 2.49                     | 0.48              |
| 9:CJ:64:GLN:HB2   | 13:CN:98:ALA:HB3  | 1.94                     | 0.48              |
| 11:CL:51:VAL:HG13 | 11:CL:64:SER:O    | 2.13                     | 0.48              |
| 12:CM:8:ILE:N     | 12:CM:9:PRO:HD2   | 2.26                     | 0.48              |
| 13:CN:80:ARG:CG   | 13:CN:81:ILE:N    | 2.77                     | 0.48              |
| 50:D0:28:SER:HB3  | 50:D0:39:ARG:HE   | 1.78                     | 0.48              |
| 53:D3:15:LYS:HZ1  | 53:D3:19:GLY:HA2  | 1.78                     | 0.48              |
| 54:D4:27:CYS:CB   | 54:D4:33:HIS:HB2  | 2.44                     | 0.48              |
| 24:DA:1009:A:C2   | 24:DA:1010:A:C2   | 3.02                     | 0.48              |
| 24:DA:1045:C:H1'  | 24:DA:1047:G:C2   | 2.49                     | 0.48              |
| 24:DA:1239:G:C2   | 24:DA:1240:U:H1'  | 2.49                     | 0.48              |
| 24:DA:132:G:N2    | 24:DA:148:U:C2    | 2.82                     | 0.48              |
| 24:DA:1448:G:C2   | 24:DA:1464:G:C2   | 3.02                     | 0.48              |
| 24:DA:49:A:N6     | 24:DA:177:G:C4    | 2.82                     | 0.48              |
| 24:DA:1997:C:O2'  | 24:DA:1998:A:H5'  | 2.14                     | 0.48              |
| 24:DA:2067:G:C4   | 24:DA:2444:G:N2   | 2.82                     | 0.48              |
| 24:DA:2069:G:C2   | 24:DA:2443:C:C2   | 3.01                     | 0.48              |
| 24:DA:2199:A:H2'  | 24:DA:2200:C:H6   | 1.79                     | 0.48              |
| 24:DA:232:G:O2'   | 24:DA:233:A:H5''  | 2.14                     | 0.48              |
| 24:DA:2408:U:O2'  | 24:DA:2409:G:O5'  | 2.32                     | 0.48              |
| 24:DA:2508:G:H2'  | 24:DA:2509:G:O4'  | 2.14                     | 0.48              |
| 24:DA:2544:G:H2'  | 24:DA:2545:G:H8   | 1.78                     | 0.48              |
| 24:DA:439:A:C5    | 24:DA:440:C:C4    | 3.02                     | 0.48              |
| 24:DA:537:G:N2    | 24:DA:557:C:H42   | 2.10                     | 0.48              |
| 24:DA:754:U:O2'   | 24:DA:755:U:C6    | 2.64                     | 0.48              |
| 24:DA:866:A:C8    | 24:DA:914:G:O6    | 2.67                     | 0.48              |
| 24:DA:88:G:C2     | 24:DA:89:A:C8     | 3.02                     | 0.48              |
| 56:DB:13:G:H21    | 56:DB:69:G:N2     | 2.11                     | 0.48              |
| 56:DB:8:C:H2'     | 56:DB:9:G:O4'     | 2.14                     | 0.48              |
| 24:DA:1807:G:OP1  | 26:DC:47:ARG:NH1  | 2.46                     | 0.48              |
| 27:DD:106:LYS:HD3 | 27:DD:106:LYS:N   | 2.28                     | 0.48              |
| 28:DE:130:LYS:O   | 28:DE:134:LEU:HB3 | 2.13                     | 0.48              |
| 29:DF:109:ARG:NH2 | 29:DF:109:ARG:CB  | 2.74                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:DF:43:ILE:HD13 | 29:DF:82:TYR:HE2  | 1.79                     | 0.48              |
| 30:DG:1:SER:C     | 30:DG:3:VAL:H     | 2.17                     | 0.48              |
| 24:DA:1011:G:OP1  | 40:DQ:76:SER:CB   | 2.62                     | 0.48              |
| 44:DU:20:LYS:HD2  | 44:DU:38:ILE:HD11 | 1.95                     | 0.48              |
| 46:DW:51:GLY:HA2  | 46:DW:59:PHE:HD2  | 1.79                     | 0.48              |
| 49:DZ:32:GLY:C    | 49:DZ:34:THR:N    | 2.66                     | 0.48              |
| 21:AA:1151:A:C4   | 21:AA:1152:A:N7   | 2.82                     | 0.48              |
| 21:AA:1171:A:H2'  | 21:AA:1172:C:H6   | 1.79                     | 0.48              |
| 21:AA:1172:C:H2'  | 21:AA:1173:U:C6   | 2.49                     | 0.48              |
| 21:AA:1183:U:HO2' | 21:AA:1184:G:P    | 2.37                     | 0.48              |
| 21:AA:158:G:C3'   | 21:AA:159:G:H5''  | 2.44                     | 0.48              |
| 21:AA:16:A:O2'    | 21:AA:17:U:H5'    | 2.14                     | 0.48              |
| 21:AA:184:G:C6    | 21:AA:194:C:N4    | 2.82                     | 0.48              |
| 21:AA:207:C:H2'   | 21:AA:208:U:C4    | 2.49                     | 0.48              |
| 21:AA:273:U:C4    | 21:AA:274:A:N7    | 2.82                     | 0.48              |
| 21:AA:543:U:H2'   | 21:AA:544:G:H5'   | 1.95                     | 0.48              |
| 21:AA:69:G:H2'    | 21:AA:69:G:N3     | 2.29                     | 0.48              |
| 21:AA:994:A:HO2'  | 21:AA:995:C:H5'   | 1.77                     | 0.48              |
| 1:AB:129:THR:O    | 1:AB:132:GLU:HB3  | 2.14                     | 0.48              |
| 1:AB:209:VAL:HG23 | 1:AB:210:THR:N    | 2.28                     | 0.48              |
| 5:AF:47:LEU:HD22  | 17:AR:65:SER:OG   | 2.14                     | 0.48              |
| 7:AH:6:ILE:HD12   | 7:AH:35:ILE:HD11  | 1.96                     | 0.48              |
| 8:AI:27:ILE:HG12  | 8:AI:34:LEU:HD13  | 1.96                     | 0.48              |
| 10:AK:30:ILE:CG2  | 10:AK:45:THR:HG22 | 2.42                     | 0.48              |
| 12:AM:109:LYS:HZ1 | 21:AA:1227:A:H5'  | 1.78                     | 0.48              |
| 15:AP:1:MET:HB2   | 21:AA:135:C:O2    | 2.13                     | 0.48              |
| 15:AP:38:PHE:O    | 15:AP:50:THR:HG23 | 2.14                     | 0.48              |
| 19:AT:74:HIS:O    | 19:AT:75:LYS:C    | 2.52                     | 0.48              |
| 52:B2:10:LEU:O    | 52:B2:10:LEU:HD12 | 2.14                     | 0.48              |
| 24:BA:1028:A:H2'  | 24:BA:1029:A:C8   | 2.49                     | 0.48              |
| 24:BA:55:G:N2     | 24:BA:116:C:C2    | 2.81                     | 0.48              |
| 24:BA:1338:G:O2'  | 43:BT:18:GLU:HG2  | 2.14                     | 0.48              |
| 24:BA:1570:A:C6   | 24:BA:1571:A:C6   | 3.02                     | 0.48              |
| 24:BA:1638:C:O2   | 24:BA:2698:U:O2'  | 2.30                     | 0.48              |
| 24:BA:1651:G:H4'  | 37:BN:39:PRO:HG2  | 1.94                     | 0.48              |
| 24:BA:2385:C:H6   | 24:BA:2385:C:H5'  | 1.79                     | 0.48              |
| 24:BA:684:G:C6    | 24:BA:774:G:C5    | 3.02                     | 0.48              |
| 24:BA:950:G:C6    | 24:BA:951:C:C4    | 3.02                     | 0.48              |
| 24:BA:962:G:N2    | 24:BA:2250:G:H1   | 2.11                     | 0.48              |
| 24:BA:995:C:O2'   | 24:BA:996:A:OP2   | 2.32                     | 0.48              |
| 26:BC:209:ALA:HA  | 26:BC:212:TRP:NE1 | 2.29                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BD:93:GLY:O     | 27:BD:94:GLN:C    | 2.51                     | 0.48              |
| 24:BA:616:A:H4'    | 28:BE:101:TYR:CE2 | 2.49                     | 0.48              |
| 28:BE:127:GLU:H    | 28:BE:127:GLU:CD  | 2.17                     | 0.48              |
| 28:BE:168:ASP:OD1  | 28:BE:169:VAL:N   | 2.47                     | 0.48              |
| 24:BA:2315:G:H1'   | 29:BF:122:ASP:OD2 | 2.14                     | 0.48              |
| 32:BI:76:ALA:HB2   | 32:BI:131:THR:CG2 | 2.40                     | 0.48              |
| 33:BJ:124:VAL:HG23 | 33:BJ:125:TYR:N   | 2.28                     | 0.48              |
| 33:BJ:44:TYR:C     | 33:BJ:44:TYR:CD1  | 2.87                     | 0.48              |
| 38:BO:3:LYS:CG     | 38:BO:4:LYS:H     | 2.27                     | 0.48              |
| 39:BP:33:GLU:OE2   | 39:BP:38:ARG:NH1  | 2.47                     | 0.48              |
| 24:BA:2720:U:H5''  | 39:BP:52:ARG:NH2  | 2.28                     | 0.48              |
| 55:CA:102:G:H2'    | 55:CA:103:U:H6    | 1.79                     | 0.48              |
| 55:CA:1296:C:O2'   | 55:CA:1302:C:N4   | 2.45                     | 0.48              |
| 55:CA:1309:G:C6    | 55:CA:1310:G:C6   | 3.02                     | 0.48              |
| 8:CI:108:ARG:HB3   | 55:CA:1347:G:C8   | 2.49                     | 0.48              |
| 55:CA:1498:U:C5    | 23:CW:2:U:H5'     | 2.49                     | 0.48              |
| 55:CA:1499:A:H2'   | 55:CA:1500:A:H8   | 1.78                     | 0.48              |
| 55:CA:1502:A:HO2'  | 55:CA:1503:A:P    | 2.34                     | 0.48              |
| 55:CA:785:G:H2'    | 55:CA:785:G:N3    | 2.29                     | 0.48              |
| 1:CB:142:LYS:HA    | 1:CB:145:ASN:HB2  | 1.94                     | 0.48              |
| 1:CB:186:VAL:HG11  | 1:CB:192:PRO:HB3  | 1.96                     | 0.48              |
| 3:CD:196:GLU:H     | 3:CD:196:GLU:CD   | 2.17                     | 0.48              |
| 5:CF:6:ILE:HD12    | 5:CF:6:ILE:H      | 1.79                     | 0.48              |
| 6:CG:96:ASN:O      | 6:CG:97:ALA:C     | 2.52                     | 0.48              |
| 7:CH:59:GLU:HG2    | 7:CH:60:LEU:N     | 2.29                     | 0.48              |
| 8:CI:48:ARG:C      | 8:CI:50:PRO:HD2   | 2.34                     | 0.48              |
| 16:CQ:44:HIS:CE1   | 55:CA:277:C:OP1   | 2.67                     | 0.48              |
| 16:CQ:46:HIS:HB3   | 16:CQ:66:LEU:HD13 | 1.96                     | 0.48              |
| 51:D1:47:ILE:N     | 51:D1:47:ILE:HD12 | 2.29                     | 0.48              |
| 24:DA:1078:U:H5''  | 24:DA:1079:C:OP1  | 2.14                     | 0.48              |
| 24:DA:1716:U:O2    | 24:DA:1717:A:C8   | 2.67                     | 0.48              |
| 24:DA:2067:G:C4'   | 24:DA:2068:U:OP2  | 2.62                     | 0.48              |
| 24:DA:2219:U:H2'   | 24:DA:2220:U:C6   | 2.48                     | 0.48              |
| 24:DA:2226:C:O2'   | 24:DA:2227:A:C5'  | 2.62                     | 0.48              |
| 24:DA:2269:G:H2'   | 24:DA:2270:A:H8   | 1.78                     | 0.48              |
| 24:DA:234:U:O2'    | 24:DA:235:U:O5'   | 2.32                     | 0.48              |
| 24:DA:2014:A:H2    | 24:DA:2613:U:C2   | 2.32                     | 0.48              |
| 24:DA:2624:G:H1'   | 50:D0:18:HIS:CE1  | 2.48                     | 0.48              |
| 24:DA:2748:A:N6    | 24:DA:2749:A:C6   | 2.82                     | 0.48              |
| 24:DA:27:G:C6      | 24:DA:512:G:C6    | 3.02                     | 0.48              |
| 24:DA:308:G:N1     | 24:DA:309:A:C2    | 2.82                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:571:U:O2'   | 24:DA:573:U:H5''  | 2.14                     | 0.48              |
| 24:DA:607:U:O4    | 24:DA:619:G:H2'   | 2.14                     | 0.48              |
| 24:DA:624:C:O2'   | 24:DA:657:U:H5''  | 2.14                     | 0.48              |
| 24:DA:647:G:O2'   | 24:DA:648:G:O4'   | 2.17                     | 0.48              |
| 24:DA:686:U:H2'   | 24:DA:788:A:N1    | 2.29                     | 0.48              |
| 24:DA:726:G:O2'   | 24:DA:727:A:P     | 2.72                     | 0.48              |
| 24:DA:1799:G:C8   | 26:DC:179:GLU:OE1 | 2.66                     | 0.48              |
| 26:DC:44:ASN:C    | 26:DC:46:GLY:H    | 2.18                     | 0.48              |
| 27:DD:122:VAL:HA  | 27:DD:127:PHE:H   | 1.78                     | 0.48              |
| 29:DF:118:ALA:HB2 | 29:DF:176:PHE:HB3 | 1.96                     | 0.48              |
| 29:DF:57:ALA:HB2  | 29:DF:64:PRO:HG2  | 1.96                     | 0.48              |
| 29:DF:7:TYR:O     | 29:DF:8:LYS:HG3   | 2.14                     | 0.48              |
| 46:DW:25:PHE:O    | 46:DW:27:GLY:N    | 2.46                     | 0.48              |
| 46:DW:37:VAL:C    | 46:DW:39:GLN:H    | 2.16                     | 0.48              |
| 21:AA:1051:C:O2'  | 21:AA:1052:U:O4'  | 2.31                     | 0.47              |
| 21:AA:1145:A:O2'  | 21:AA:1146:A:H8   | 1.96                     | 0.47              |
| 21:AA:960:U:C2    | 21:AA:1225:A:N7   | 2.82                     | 0.47              |
| 21:AA:654:G:O2'   | 21:AA:655:A:C5'   | 2.63                     | 0.47              |
| 21:AA:803:G:C5    | 21:AA:804:U:C4    | 3.02                     | 0.47              |
| 21:AA:895:G:H2'   | 21:AA:896:C:H6    | 1.79                     | 0.47              |
| 1:AB:86:CYS:SG    | 1:AB:221:ARG:HD3  | 2.53                     | 0.47              |
| 3:AD:49:ASP:O     | 3:AD:53:GLN:HB2   | 2.13                     | 0.47              |
| 4:AE:125:LYS:O    | 4:AE:127:TYR:CZ   | 2.67                     | 0.47              |
| 5:AF:42:TRP:HZ2   | 5:AF:61:LEU:HD22  | 1.78                     | 0.47              |
| 5:AF:99:ALA:O     | 5:AF:100:SER:CB   | 2.61                     | 0.47              |
| 50:B0:50:GLY:O    | 50:B0:51:ARG:O    | 2.32                     | 0.47              |
| 24:BA:1085:A:H3'  | 24:BA:1086:A:C2   | 2.48                     | 0.47              |
| 24:BA:1403:A:C4   | 24:BA:1404:C:C6   | 3.02                     | 0.47              |
| 24:BA:1867:G:O2'  | 24:BA:1868:C:C5'  | 2.56                     | 0.47              |
| 24:BA:2075:U:H2'  | 24:BA:2238:G:N2   | 2.28                     | 0.47              |
| 24:BA:2332:C:H4'  | 24:BA:2336:A:N6   | 2.29                     | 0.47              |
| 24:BA:199:A:C2    | 24:BA:2434:A:C2   | 3.02                     | 0.47              |
| 24:BA:249:C:O2'   | 24:BA:250:G:OP2   | 2.32                     | 0.47              |
| 24:BA:2628:C:O2'  | 24:BA:2781:A:H2'  | 2.14                     | 0.47              |
| 24:BA:2756:U:C4'  | 24:BA:2757:A:O5'  | 2.57                     | 0.47              |
| 24:BA:27:G:C4     | 24:BA:512:G:N2    | 2.82                     | 0.47              |
| 24:BA:30:G:C5     | 24:BA:31:C:C4     | 3.02                     | 0.47              |
| 24:BA:860:U:C5'   | 24:BA:860:U:C6    | 2.89                     | 0.47              |
| 24:BA:974:G:C6    | 24:BA:1186:G:C6   | 3.02                     | 0.47              |
| 24:BA:990:A:C6    | 24:BA:1186:G:H1'  | 2.49                     | 0.47              |
| 25:BB:28:C:H2'    | 25:BB:29:A:O4'    | 2.13                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BC:12:ARG:HG2  | 26:BC:12:ARG:NH1   | 2.25                     | 0.47              |
| 26:BC:203:VAL:O   | 26:BC:204:LEU:HB2  | 2.15                     | 0.47              |
| 24:BA:2052:A:C8   | 27:BD:146:ILE:HD11 | 2.48                     | 0.47              |
| 27:BD:53:GLY:HA3  | 27:BD:77:ARG:N     | 2.19                     | 0.47              |
| 28:BE:48:THR:C    | 28:BE:50:ALA:N     | 2.67                     | 0.47              |
| 29:BF:90:LEU:HA   | 29:BF:90:LEU:HD12  | 1.68                     | 0.47              |
| 30:BG:83:THR:HA   | 30:BG:84:LYS:CE    | 2.43                     | 0.47              |
| 30:BG:84:LYS:CG   | 30:BG:85:LYS:N     | 2.76                     | 0.47              |
| 31:BH:31:VAL:CG2  | 31:BH:32:PRO:HD2   | 2.44                     | 0.47              |
| 32:BI:21:PRO:HB2  | 32:BI:22:PRO:HD3   | 1.96                     | 0.47              |
| 35:BL:55:MET:HE3  | 35:BL:55:MET:HA    | 1.95                     | 0.47              |
| 40:BQ:91:ARG:HH21 | 40:BQ:93:ILE:HD13  | 1.76                     | 0.47              |
| 41:BR:14:VAL:CG1  | 41:BR:98:ILE:HD12  | 2.43                     | 0.47              |
| 55:CA:1050:G:C2   | 55:CA:1051:C:C4    | 3.02                     | 0.47              |
| 55:CA:11:G:C5     | 55:CA:12:U:C5      | 3.02                     | 0.47              |
| 55:CA:1400:C:C4   | 22:CV:34:G:C8      | 3.01                     | 0.47              |
| 55:CA:1484:C:H2'  | 55:CA:1485:U:O4'   | 2.13                     | 0.47              |
| 55:CA:293:G:C6    | 55:CA:305:G:C2     | 3.02                     | 0.47              |
| 55:CA:577:G:N2    | 55:CA:578:C:C2     | 2.82                     | 0.47              |
| 55:CA:612:C:C2    | 55:CA:629:A:C2     | 3.02                     | 0.47              |
| 10:CK:41:LEU:O    | 55:CA:685:G:H4'    | 2.14                     | 0.47              |
| 55:CA:927:G:C6    | 55:CA:1391:U:C2    | 3.02                     | 0.47              |
| 1:CB:114:LYS:CA   | 1:CB:117:GLU:HG2   | 2.36                     | 0.47              |
| 5:CF:3:HIS:HB2    | 5:CF:92:THR:HA     | 1.96                     | 0.47              |
| 4:CE:83:PRO:HG2   | 7:CH:95:MET:HA     | 1.96                     | 0.47              |
| 16:CQ:40:THR:HG23 | 55:CA:280:C:H42    | 1.79                     | 0.47              |
| 24:DA:978:G:O4'   | 24:DA:1001:A:C2    | 2.67                     | 0.47              |
| 24:DA:1056:G:C1'  | 24:DA:1103:A:H61   | 2.27                     | 0.47              |
| 24:DA:1278:C:O2'  | 24:DA:1279:G:H5'   | 2.13                     | 0.47              |
| 24:DA:140:C:O2'   | 24:DA:141:G:P      | 2.72                     | 0.47              |
| 24:DA:1429:G:O2'  | 24:DA:1430:G:C8    | 2.35                     | 0.47              |
| 24:DA:1633:G:C5   | 24:DA:1635:A:C5    | 3.02                     | 0.47              |
| 24:DA:15:G:C2     | 24:DA:16:C:C2      | 3.02                     | 0.47              |
| 24:DA:1255:U:H3   | 24:DA:2060:A:H5'   | 1.79                     | 0.47              |
| 24:DA:2283:C:C4   | 24:DA:2389:G:C6    | 3.02                     | 0.47              |
| 24:DA:2417:C:C2   | 24:DA:2418:A:C8    | 3.02                     | 0.47              |
| 24:DA:2466:C:H2'  | 24:DA:2467:C:H6    | 1.77                     | 0.47              |
| 24:DA:2478:A:N7   | 24:DA:2529:G:C6    | 2.82                     | 0.47              |
| 24:DA:2808:G:N2   | 24:DA:2891:U:C6    | 2.82                     | 0.47              |
| 24:DA:630:G:N2    | 24:DA:634:C:C4     | 2.82                     | 0.47              |
| 14:CO:88:ARG:NH2  | 24:DA:715:A:H4'    | 2.29                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:753:A:O2'    | 24:DA:754:U:O5'    | 2.32                     | 0.47              |
| 24:DA:776:G:H4'    | 24:DA:777:G:O5'    | 2.13                     | 0.47              |
| 24:DA:834:G:H2'    | 24:DA:835:C:O4'    | 2.14                     | 0.47              |
| 27:DD:124:ARG:HD3  | 27:DD:125:TRP:HE1  | 1.71                     | 0.47              |
| 31:DH:54:LEU:HA    | 31:DH:57:LYS:CG    | 2.44                     | 0.47              |
| 24:DA:636:G:H3'    | 35:DL:128:THR:HG21 | 1.95                     | 0.47              |
| 38:DO:31:THR:HG23  | 38:DO:34:HIS:O     | 2.14                     | 0.47              |
| 21:AA:1035:A:H2'   | 21:AA:1036:A:O4'   | 2.14                     | 0.47              |
| 21:AA:1227:A:N3    | 21:AA:1227:A:C2'   | 2.73                     | 0.47              |
| 3:AD:36:ALA:CB     | 21:AA:426:U:H5''   | 2.44                     | 0.47              |
| 21:AA:438:U:C4     | 21:AA:494:G:C5     | 3.02                     | 0.47              |
| 21:AA:550:G:C2     | 21:AA:551:U:C2     | 3.02                     | 0.47              |
| 3:AD:185:PRO:HB2   | 3:AD:190:LEU:HD23  | 1.96                     | 0.47              |
| 4:AE:112:ALA:O     | 4:AE:116:VAL:HG22  | 2.14                     | 0.47              |
| 4:AE:15:ILE:N      | 4:AE:15:ILE:HD12   | 2.28                     | 0.47              |
| 5:AF:67:PRO:HG2    | 5:AF:70:VAL:HG22   | 1.96                     | 0.47              |
| 8:AI:9:GLY:HA2     | 8:AI:80:HIS:HD2    | 1.78                     | 0.47              |
| 9:AJ:88:MET:C      | 9:AJ:90:LEU:H      | 2.17                     | 0.47              |
| 10:AK:43:TRP:CZ3   | 10:AK:45:THR:HG23  | 2.49                     | 0.47              |
| 10:AK:18:GLY:C     | 10:AK:81:LEU:HB2   | 2.34                     | 0.47              |
| 16:AQ:12:VAL:HG12  | 16:AQ:21:VAL:O     | 2.14                     | 0.47              |
| 17:AR:63:TYR:HE1   | 21:AA:673:A:H1'    | 1.79                     | 0.47              |
| 24:BA:1188:U:C2    | 24:BA:1189:A:C8    | 3.01                     | 0.47              |
| 24:BA:1471:G:C5    | 24:BA:1472:C:C5    | 3.02                     | 0.47              |
| 24:BA:2343:U:O3'   | 24:BA:2373:G:H4'   | 2.14                     | 0.47              |
| 24:BA:2407:A:C4    | 24:BA:2408:U:C5    | 3.02                     | 0.47              |
| 24:BA:2410:G:N2    | 24:BA:2411:A:H1'   | 2.28                     | 0.47              |
| 24:BA:10:A:C8      | 24:BA:2800:A:N6    | 2.83                     | 0.47              |
| 24:BA:506:G:H5''   | 24:BA:509:C:H1'    | 1.96                     | 0.47              |
| 24:BA:792:A:H5''   | 24:BA:793:A:H5'    | 1.96                     | 0.47              |
| 26:BC:141:HIS:HB2  | 26:BC:190:THR:CB   | 2.44                     | 0.47              |
| 27:BD:151:THR:CG2  | 27:BD:152:PRO:HD3  | 2.44                     | 0.47              |
| 27:BD:184:ARG:HH11 | 39:BP:6:GLN:CD     | 2.16                     | 0.47              |
| 31:BH:26:ALA:HA    | 31:BH:30:LEU:HB2   | 1.96                     | 0.47              |
| 24:BA:536:G:H21    | 33:BJ:47:HIS:CG    | 2.32                     | 0.47              |
| 24:BA:538:A:H4'    | 33:BJ:7:LYS:HB3    | 1.96                     | 0.47              |
| 36:BM:126:ILE:O    | 36:BM:126:ILE:HD12 | 2.14                     | 0.47              |
| 40:BQ:63:ARG:HD2   | 40:BQ:64:ILE:H     | 1.78                     | 0.47              |
| 41:BR:38:VAL:CG1   | 41:BR:59:ILE:HG13  | 2.44                     | 0.47              |
| 42:BS:18:ARG:O     | 42:BS:19:LEU:HB2   | 2.13                     | 0.47              |
| 55:CA:1043:G:C5    | 55:CA:1044:A:N7    | 2.82                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:CI:6:TYR:CE1    | 55:CA:1147:C:H4'  | 2.49                     | 0.47              |
| 55:CA:120:A:C3'   | 55:CA:121:U:C5'   | 2.90                     | 0.47              |
| 55:CA:1298:U:H4'  | 55:CA:1299:A:O5'  | 2.13                     | 0.47              |
| 55:CA:1475:G:H4'  | 24:DA:1689:A:H4'  | 1.95                     | 0.47              |
| 55:CA:254:G:O2'   | 55:CA:255:G:H5'   | 2.14                     | 0.47              |
| 55:CA:256:U:H2'   | 55:CA:257:G:O4'   | 2.14                     | 0.47              |
| 55:CA:330:C:H2'   | 55:CA:331:G:H8    | 1.79                     | 0.47              |
| 55:CA:601:G:C4    | 55:CA:602:A:C8    | 3.03                     | 0.47              |
| 2:CC:174:LEU:HD11 | 2:CC:200:TRP:NE1  | 2.29                     | 0.47              |
| 3:CD:47:LEU:HD23  | 3:CD:52:VAL:HA    | 1.95                     | 0.47              |
| 3:CD:78:ALA:C     | 3:CD:85:THR:HG23  | 2.34                     | 0.47              |
| 4:CE:149:PRO:HA   | 4:CE:152:VAL:HG23 | 1.95                     | 0.47              |
| 5:CF:47:LEU:HG    | 5:CF:55:HIS:C     | 2.34                     | 0.47              |
| 8:CI:24:ASN:O     | 8:CI:61:ASP:HA    | 2.13                     | 0.47              |
| 11:CL:45:ASN:OD1  | 55:CA:528:C:N4    | 2.43                     | 0.47              |
| 18:CS:35:ARG:HH12 | 18:CS:76:THR:HA   | 1.79                     | 0.47              |
| 24:DA:1021:A:C2'  | 24:DA:1022:G:H4'  | 2.43                     | 0.47              |
| 24:DA:1215:G:OP1  | 40:DQ:7:VAL:HG11  | 2.13                     | 0.47              |
| 24:DA:1327:A:O2'  | 24:DA:1328:A:O5'  | 2.32                     | 0.47              |
| 24:DA:1423:G:C4   | 24:DA:1424:G:C8   | 3.02                     | 0.47              |
| 24:DA:151:C:H2'   | 24:DA:152:A:C8    | 2.49                     | 0.47              |
| 24:DA:1649:G:C6   | 24:DA:2009:A:C6   | 3.02                     | 0.47              |
| 24:DA:1681:G:O2'  | 24:DA:1762:A:C2'  | 2.62                     | 0.47              |
| 24:DA:2100:G:C6   | 24:DA:2190:G:C5   | 3.02                     | 0.47              |
| 24:DA:2212:A:N7   | 24:DA:2214:C:N4   | 2.62                     | 0.47              |
| 24:DA:2386:A:O2'  | 24:DA:2387:U:O5'  | 2.31                     | 0.47              |
| 24:DA:251:A:C2'   | 24:DA:252:G:O4'   | 2.60                     | 0.47              |
| 24:DA:2543:G:C4   | 24:DA:2765:A:H2'  | 2.49                     | 0.47              |
| 24:DA:2550:G:C6   | 24:DA:2551:C:N4   | 2.82                     | 0.47              |
| 24:DA:1638:C:H1'  | 24:DA:2698:U:O2'  | 2.13                     | 0.47              |
| 24:DA:2875:C:H2'  | 24:DA:2876:G:C8   | 2.48                     | 0.47              |
| 24:DA:109:C:C4'   | 24:DA:348:A:H4'   | 2.38                     | 0.47              |
| 24:DA:379:G:C2    | 24:DA:396:G:C5    | 3.02                     | 0.47              |
| 24:DA:45:G:C4'    | 24:DA:46:G:H5'    | 2.44                     | 0.47              |
| 24:DA:49:A:C6     | 24:DA:177:G:C5    | 3.02                     | 0.47              |
| 24:DA:587:C:O2    | 24:DA:671:C:H5'   | 2.14                     | 0.47              |
| 24:DA:659:G:C6    | 24:DA:660:C:N4    | 2.82                     | 0.47              |
| 24:DA:92:U:O2'    | 24:DA:93:G:H5'    | 2.14                     | 0.47              |
| 30:DG:162:ARG:HB2 | 30:DG:166:GLU:CB  | 2.44                     | 0.47              |
| 35:DL:17:LYS:HZ1  | 35:DL:19:LEU:HD22 | 1.78                     | 0.47              |
| 38:DO:90:VAL:HB   | 38:DO:91:SER:H    | 1.52                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:DQ:10:ARG:O    | 40:DQ:14:LYS:HB2  | 2.14                     | 0.47              |
| 40:DQ:4:LYS:HE3   | 40:DQ:7:VAL:HG22  | 1.96                     | 0.47              |
| 21:AA:1074:G:C2   | 21:AA:1102:A:C5   | 3.02                     | 0.47              |
| 21:AA:1248:A:H2'  | 21:AA:1249:C:H6   | 1.79                     | 0.47              |
| 21:AA:255:G:H2'   | 21:AA:256:U:C6    | 2.49                     | 0.47              |
| 21:AA:251:G:C2    | 21:AA:266:G:O6    | 2.66                     | 0.47              |
| 21:AA:550:G:C6    | 21:AA:551:U:C4    | 3.02                     | 0.47              |
| 21:AA:996:A:H2'   | 21:AA:997:U:C6    | 2.49                     | 0.47              |
| 1:AB:22:TRP:CG    | 1:AB:22:TRP:O     | 2.67                     | 0.47              |
| 2:AC:6:PRO:HB3    | 2:AC:174:LEU:HD11 | 1.96                     | 0.47              |
| 3:AD:109:THR:HG23 | 3:AD:112:GLU:HB2  | 1.96                     | 0.47              |
| 4:AE:104:ILE:HD11 | 4:AE:111:ARG:HA   | 1.96                     | 0.47              |
| 5:AF:3:HIS:O      | 5:AF:92:THR:HA    | 2.12                     | 0.47              |
| 8:AI:43:ALA:HB1   | 8:AI:46:VAL:CG2   | 2.44                     | 0.47              |
| 24:BA:1046:A:H3'  | 24:BA:1047:G:C5'  | 2.43                     | 0.47              |
| 24:BA:1005:C:N3   | 24:BA:1143:A:C2   | 2.82                     | 0.47              |
| 24:BA:2391:G:O6   | 24:BA:2425:A:C8   | 2.56                     | 0.47              |
| 24:BA:242:G:N2    | 24:BA:255:A:OP2   | 2.39                     | 0.47              |
| 24:BA:310:A:HO2'  | 24:BA:311:A:P     | 2.38                     | 0.47              |
| 24:BA:369:U:O2'   | 24:BA:370:G:OP2   | 2.26                     | 0.47              |
| 24:BA:437:U:H2'   | 24:BA:438:G:H8    | 1.78                     | 0.47              |
| 25:BB:41:G:H3'    | 25:BB:42:C:H5''   | 1.97                     | 0.47              |
| 31:BH:82:SER:HA   | 31:BH:101:ASP:OD1 | 2.14                     | 0.47              |
| 31:BH:132:PHE:CG  | 31:BH:133:GLN:N   | 2.82                     | 0.47              |
| 32:BI:93:ASN:OD1  | 32:BI:136:GLY:HA2 | 2.14                     | 0.47              |
| 33:BJ:67:ASN:O    | 33:BJ:68:LYS:C    | 2.53                     | 0.47              |
| 38:BO:36:TYR:CD2  | 38:BO:36:TYR:N    | 2.82                     | 0.47              |
| 24:BA:1753:G:H5'' | 39:BP:92:ARG:HE   | 1.79                     | 0.47              |
| 41:BR:48:LYS:HD2  | 41:BR:48:LYS:O    | 2.15                     | 0.47              |
| 42:BS:96:ILE:CG1  | 42:BS:96:ILE:O    | 2.47                     | 0.47              |
| 47:BX:2:ARG:CD    | 47:BX:29:LEU:HD12 | 2.44                     | 0.47              |
| 55:CA:979:C:C6    | 55:CA:1318:A:N1   | 2.82                     | 0.47              |
| 55:CA:1324:A:C2'  | 55:CA:1325:C:H5'  | 2.44                     | 0.47              |
| 55:CA:482:A:H2'   | 55:CA:483:C:C6    | 2.49                     | 0.47              |
| 55:CA:801:U:H2'   | 55:CA:802:A:C8    | 2.49                     | 0.47              |
| 55:CA:837:U:H2'   | 55:CA:838:G:H8    | 1.79                     | 0.47              |
| 2:CC:106:ARG:CD   | 2:CC:106:ARG:H    | 2.19                     | 0.47              |
| 3:CD:164:ARG:HB3  | 3:CD:165:GLU:H    | 1.54                     | 0.47              |
| 3:CD:39:GLN:HA    | 55:CA:426:U:H4'   | 1.97                     | 0.47              |
| 4:CE:15:ILE:HD11  | 4:CE:37:VAL:CG2   | 2.44                     | 0.47              |
| 4:CE:59:ILE:O     | 4:CE:62:ALA:HB3   | 2.14                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CE:77:ASN:HB3    | 4:CE:79:THR:HG22   | 1.95                     | 0.47              |
| 8:CI:78:ILE:O      | 8:CI:82:ILE:HG13   | 2.14                     | 0.47              |
| 18:CS:33:TRP:HB2   | 55:CA:1014:A:N3    | 2.30                     | 0.47              |
| 22:CV:37:A:N6      | 22:CV:38:A:C6      | 2.83                     | 0.47              |
| 53:D3:41:ARG:HD2   | 53:D3:41:ARG:O     | 2.14                     | 0.47              |
| 24:DA:1180:U:C4    | 24:DA:1181:U:N3    | 2.83                     | 0.47              |
| 24:DA:1254:A:N1    | 28:DE:77:ILE:HD12  | 2.29                     | 0.47              |
| 24:DA:1269:A:H2'   | 24:DA:1270:C:H6    | 1.79                     | 0.47              |
| 24:DA:1427:A:H4'   | 24:DA:1428:C:O4'   | 2.14                     | 0.47              |
| 24:DA:159:G:O2'    | 24:DA:160:A:H5''   | 2.14                     | 0.47              |
| 24:DA:1635:A:HO2'  | 24:DA:1636:U:H5'   | 1.77                     | 0.47              |
| 24:DA:1715:G:H8    | 24:DA:1715:G:OP1   | 1.98                     | 0.47              |
| 24:DA:2136:G:H5'   | 24:DA:2137:U:OP2   | 2.15                     | 0.47              |
| 24:DA:2142:A:C2'   | 24:DA:2143:C:H4'   | 2.44                     | 0.47              |
| 24:DA:2189:U:C2    | 24:DA:2190:G:C8    | 3.02                     | 0.47              |
| 24:DA:2234:G:C6    | 24:DA:2235:G:C5    | 3.03                     | 0.47              |
| 24:DA:2345:G:C4    | 24:DA:2381:A:C2    | 3.02                     | 0.47              |
| 24:DA:2393:U:H2'   | 24:DA:2394:C:O4'   | 2.14                     | 0.47              |
| 24:DA:2428:G:H4'   | 24:DA:2429:G:C4    | 2.49                     | 0.47              |
| 24:DA:2449:U:H4'   | 24:DA:2450:A:OP1   | 2.15                     | 0.47              |
| 24:DA:2686:G:C6    | 24:DA:2687:U:N3    | 2.83                     | 0.47              |
| 24:DA:478:A:C6     | 24:DA:480:A:C6     | 3.03                     | 0.47              |
| 24:DA:49:A:C6      | 24:DA:177:G:C6     | 3.02                     | 0.47              |
| 24:DA:836:G:C6     | 24:DA:837:C:C4     | 3.01                     | 0.47              |
| 24:DA:8:C:C2'      | 24:DA:9:G:H5'      | 2.44                     | 0.47              |
| 24:DA:922:C:H1'    | 46:DW:22:VAL:CG2   | 2.40                     | 0.47              |
| 56:DB:28:C:H2'     | 56:DB:29:A:O4'     | 2.15                     | 0.47              |
| 56:DB:37:C:N3      | 56:DB:49:C:O4'     | 2.47                     | 0.47              |
| 26:DC:159:THR:N    | 26:DC:194:VAL:CG1  | 2.78                     | 0.47              |
| 26:DC:14:HIS:O     | 26:DC:203:VAL:HG11 | 2.14                     | 0.47              |
| 27:DD:12:THR:HG22  | 27:DD:13:ARG:O     | 2.14                     | 0.47              |
| 28:DE:112:LEU:HD13 | 28:DE:112:LEU:O    | 2.14                     | 0.47              |
| 29:DF:134:GLN:HG3  | 29:DF:149:ARG:O    | 2.13                     | 0.47              |
| 32:DI:102:ARG:HG2  | 32:DI:141:ASP:O    | 2.14                     | 0.47              |
| 34:DK:19:VAL:CG1   | 34:DK:41:ILE:HG12  | 2.43                     | 0.47              |
| 34:DK:97:THR:O     | 34:DK:98:ARG:HB2   | 2.14                     | 0.47              |
| 35:DL:81:ASP:C     | 35:DL:82:LEU:HD12  | 2.35                     | 0.47              |
| 36:DM:71:LYS:HD3   | 36:DM:95:LEU:HD13  | 1.96                     | 0.47              |
| 38:DO:30:ARG:CG    | 38:DO:30:ARG:NH1   | 2.76                     | 0.47              |
| 41:DR:26:ASP:O     | 41:DR:27:ILE:HD13  | 2.14                     | 0.47              |
| 41:DR:72:VAL:O     | 41:DR:72:VAL:HG23  | 2.13                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 43:DT:55:VAL:HG23  | 43:DT:86:THR:O    | 2.14                     | 0.47              |
| 43:DT:69:ARG:NE    | 43:DT:70:HIS:CD2  | 2.82                     | 0.47              |
| 44:DU:3:LYS:HD3    | 44:DU:82:VAL:CG2  | 2.44                     | 0.47              |
| 44:DU:91:LYS:O     | 44:DU:92:VAL:HG22 | 2.13                     | 0.47              |
| 21:AA:1058:G:C6    | 21:AA:1059:C:C4   | 3.02                     | 0.47              |
| 4:AE:89:THR:HG21   | 21:AA:1078:U:C2   | 2.49                     | 0.47              |
| 21:AA:1095:U:H5'   | 21:AA:1109:C:O2   | 2.14                     | 0.47              |
| 21:AA:1122:U:H2'   | 21:AA:1123:U:H6   | 1.79                     | 0.47              |
| 12:AM:69:ARG:HH22  | 21:AA:1330:U:H5'' | 1.77                     | 0.47              |
| 21:AA:1459:G:H8    | 21:AA:1459:G:O5'  | 1.97                     | 0.47              |
| 21:AA:14:U:H2'     | 21:AA:16:A:OP2    | 2.13                     | 0.47              |
| 21:AA:208:U:H3     | 21:AA:212:G:N2    | 2.13                     | 0.47              |
| 21:AA:551:U:H2'    | 21:AA:552:U:O4'   | 2.15                     | 0.47              |
| 21:AA:763:G:H2'    | 21:AA:764:C:H6    | 1.79                     | 0.47              |
| 21:AA:696:A:H1'    | 21:AA:786:G:O2'   | 2.14                     | 0.47              |
| 21:AA:6:G:O2'      | 21:AA:7:A:P       | 2.72                     | 0.47              |
| 21:AA:82:G:H2'     | 21:AA:83:C:C4'    | 2.44                     | 0.47              |
| 21:AA:97:G:O2'     | 21:AA:98:A:H5'    | 2.13                     | 0.47              |
| 1:AB:34:ARG:HG2    | 1:AB:35:ASN:H     | 1.77                     | 0.47              |
| 2:AC:168:ARG:HD2   | 2:AC:169:GLU:N    | 2.29                     | 0.47              |
| 8:AI:56:MET:SD     | 8:AI:57:VAL:N     | 2.84                     | 0.47              |
| 11:AL:62:VAL:HG21  | 11:AL:94:TYR:CE2  | 2.36                     | 0.47              |
| 11:AL:74:GLN:CG    | 11:AL:75:GLU:HG2  | 2.44                     | 0.47              |
| 13:AN:58:ARG:HH21  | 21:AA:980:C:H5'   | 1.80                     | 0.47              |
| 19:AT:82:ILE:HD11  | 19:AT:83:ASN:ND2  | 2.29                     | 0.47              |
| 10:AK:124:LYS:HG2  | 20:AU:34:ARG:HG2  | 1.97                     | 0.47              |
| 24:BA:1024:G:H5''  | 24:BA:1025:G:H3'  | 1.96                     | 0.47              |
| 24:BA:1185:G:H5''  | 24:BA:1186:G:OP1  | 2.14                     | 0.47              |
| 24:BA:1310:G:H3'   | 24:BA:1311:G:C8   | 2.49                     | 0.47              |
| 24:BA:1538:G:O2'   | 24:BA:1539:U:H5'  | 2.14                     | 0.47              |
| 24:BA:1987:A:C2    | 24:BA:1988:G:C8   | 3.02                     | 0.47              |
| 24:BA:1996:C:H4'   | 24:BA:1997:C:OP1  | 2.13                     | 0.47              |
| 24:BA:2226:C:H2'   | 24:BA:2227:A:H8   | 1.79                     | 0.47              |
| 24:BA:2580:U:H5''  | 27:BD:135:GLY:O   | 2.15                     | 0.47              |
| 24:BA:2691:C:H2'   | 24:BA:2692:G:H8   | 1.78                     | 0.47              |
| 24:BA:271:G:C2     | 24:BA:272:A:C5    | 3.02                     | 0.47              |
| 24:BA:664:G:H4'    | 24:BA:941:A:OP1   | 2.14                     | 0.47              |
| 26:BC:144:GLU:CA   | 26:BC:151:GLY:HA2 | 2.44                     | 0.47              |
| 26:BC:21:PRO:C     | 26:BC:23:LEU:H    | 2.17                     | 0.47              |
| 29:BF:15:LEU:O     | 29:BF:18:GLU:N    | 2.46                     | 0.47              |
| 29:BF:168:LEU:HD12 | 29:BF:168:LEU:C   | 2.35                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:BG:73:SER:HA   | 30:BG:76:ILE:HG22 | 1.95                     | 0.47              |
| 38:BO:33:ARG:HG2  | 38:BO:34:HIS:ND1  | 2.29                     | 0.47              |
| 39:BP:50:ARG:HD3  | 39:BP:56:SER:HB3  | 1.97                     | 0.47              |
| 43:BT:29:THR:HA   | 43:BT:86:THR:H    | 1.79                     | 0.47              |
| 43:BT:39:THR:O    | 43:BT:40:LYS:HB2  | 2.14                     | 0.47              |
| 43:BT:29:THR:H    | 43:BT:91:GLN:HE22 | 1.59                     | 0.47              |
| 44:BU:58:VAL:O    | 44:BU:58:VAL:HG12 | 2.15                     | 0.47              |
| 55:CA:1299:A:O2'  | 55:CA:1300:G:H4'  | 2.14                     | 0.47              |
| 55:CA:1497:G:HO2' | 55:CA:1518:A:H2   | 1.60                     | 0.47              |
| 55:CA:200:G:H2'   | 55:CA:200:G:N3    | 2.29                     | 0.47              |
| 55:CA:275:G:N3    | 55:CA:276:G:C8    | 2.82                     | 0.47              |
| 55:CA:364:A:C2    | 55:CA:365:U:O4    | 2.68                     | 0.47              |
| 55:CA:369:G:O2'   | 55:CA:370:C:H6    | 1.97                     | 0.47              |
| 55:CA:50:A:N1     | 55:CA:360:G:O2'   | 2.33                     | 0.47              |
| 55:CA:544:G:C6    | 55:CA:545:C:C4    | 3.02                     | 0.47              |
| 55:CA:766:A:H2'   | 55:CA:767:A:O4'   | 2.15                     | 0.47              |
| 55:CA:775:G:O2'   | 55:CA:776:G:H5'   | 2.14                     | 0.47              |
| 55:CA:981:U:C5    | 55:CA:982:U:C2    | 3.02                     | 0.47              |
| 1:CB:115:ASP:O    | 1:CB:119:GLN:HB2  | 2.13                     | 0.47              |
| 1:CB:71:THR:HG22  | 1:CB:71:THR:O     | 2.13                     | 0.47              |
| 4:CE:45:VAL:O     | 4:CE:71:ILE:HG22  | 2.13                     | 0.47              |
| 6:CG:30:MET:HA    | 6:CG:38:ALA:HB2   | 1.96                     | 0.47              |
| 4:CE:156:ARG:HH11 | 7:CH:43:GLY:HA3   | 1.78                     | 0.47              |
| 8:CI:123:ARG:HG3  | 8:CI:124:PRO:O    | 2.13                     | 0.47              |
| 16:CQ:45:VAL:HA   | 16:CQ:72:TRP:O    | 2.15                     | 0.47              |
| 18:CS:20:LYS:C    | 18:CS:20:LYS:HD3  | 2.35                     | 0.47              |
| 24:DA:1121:C:H2'  | 24:DA:1122:G:O4'  | 2.13                     | 0.47              |
| 24:DA:1140:C:OP2  | 33:DJ:68:LYS:HE3  | 2.13                     | 0.47              |
| 24:DA:1172:C:H2'  | 24:DA:1173:U:O4'  | 2.14                     | 0.47              |
| 24:DA:1672:A:N6   | 24:DA:1673:G:C6   | 2.83                     | 0.47              |
| 24:DA:1760:C:O2'  | 24:DA:1761:C:C5'  | 2.62                     | 0.47              |
| 24:DA:1833:C:H2'  | 24:DA:1834:U:H6   | 1.78                     | 0.47              |
| 24:DA:2026:U:C2   | 24:DA:2038:G:N2   | 2.82                     | 0.47              |
| 24:DA:2068:U:H5'' | 24:DA:2068:U:H6   | 1.78                     | 0.47              |
| 24:DA:20:C:H2'    | 24:DA:21:A:H8     | 1.79                     | 0.47              |
| 24:DA:2287:A:N7   | 24:DA:2289:G:C8   | 2.82                     | 0.47              |
| 24:DA:2064:C:C2   | 24:DA:2450:A:N6   | 2.82                     | 0.47              |
| 24:DA:2603:G:C2   | 24:DA:2604:U:C2   | 3.02                     | 0.47              |
| 24:DA:2656:U:O2'  | 24:DA:2657:A:H5'  | 2.13                     | 0.47              |
| 24:DA:2672:U:H6   | 24:DA:2672:U:O5'  | 1.97                     | 0.47              |
| 24:DA:2748:A:C6   | 24:DA:2749:A:C5   | 3.02                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:379:G:C5    | 24:DA:396:G:C6     | 3.02                     | 0.47              |
| 24:DA:396:G:O2'   | 24:DA:397:U:C5'    | 2.62                     | 0.47              |
| 24:DA:40:U:C4     | 24:DA:41:C:N4      | 2.83                     | 0.47              |
| 56:DB:13:G:N2     | 56:DB:16:G:C4      | 2.83                     | 0.47              |
| 27:DD:169:ARG:O   | 27:DD:170:VAL:O    | 2.32                     | 0.47              |
| 28:DE:115:GLN:O   | 28:DE:117:ARG:N    | 2.47                     | 0.47              |
| 28:DE:144:GLU:O   | 28:DE:145:ASP:C    | 2.53                     | 0.47              |
| 28:DE:175:ILE:O   | 28:DE:175:ILE:HG23 | 2.14                     | 0.47              |
| 28:DE:79:ARG:HG2  | 28:DE:80:SER:N     | 2.25                     | 0.47              |
| 29:DF:90:LEU:HB3  | 29:DF:95:MET:HG3   | 1.96                     | 0.47              |
| 33:DJ:89:PHE:HE2  | 33:DJ:100:VAL:HG11 | 1.79                     | 0.47              |
| 36:DM:111:GLU:O   | 36:DM:115:GLU:HB2  | 2.13                     | 0.47              |
| 42:DS:44:ALA:O    | 42:DS:48:LYS:HB2   | 2.14                     | 0.47              |
| 45:DV:17:SER:HA   | 45:DV:20:LEU:HG    | 1.95                     | 0.47              |
| 21:AA:1031:C:H1'  | 21:AA:1032:G:C2    | 2.49                     | 0.47              |
| 21:AA:1095:U:H5'' | 21:AA:1109:C:O2    | 2.14                     | 0.47              |
| 21:AA:1172:C:H2'  | 21:AA:1173:U:H6    | 1.78                     | 0.47              |
| 21:AA:594:U:H2'   | 21:AA:595:A:O4'    | 2.14                     | 0.47              |
| 1:AB:9:LEU:HD12   | 1:AB:42:LEU:HD13   | 1.97                     | 0.47              |
| 1:AB:89:PHE:CZ    | 1:AB:153:MET:HB2   | 2.48                     | 0.47              |
| 4:AE:109:ALA:O    | 4:AE:110:MET:C     | 2.53                     | 0.47              |
| 4:AE:59:ILE:HA    | 4:AE:62:ALA:HB3    | 1.97                     | 0.47              |
| 6:AG:96:ASN:O     | 6:AG:100:MET:HG3   | 2.15                     | 0.47              |
| 10:AK:80:ASN:HA   | 10:AK:105:ARG:O    | 2.15                     | 0.47              |
| 14:AO:73:ASP:CG   | 14:AO:76:ARG:HG3   | 2.35                     | 0.47              |
| 10:AK:126:ARG:HB2 | 20:AU:33:ARG:NH1   | 2.30                     | 0.47              |
| 52:B2:29:GLN:O    | 52:B2:33:ARG:HG3   | 2.13                     | 0.47              |
| 24:BA:32:C:P      | 24:BA:1238:G:H5''  | 2.55                     | 0.47              |
| 24:BA:1344:U:O2'  | 24:BA:1345:C:OP1   | 2.28                     | 0.47              |
| 24:BA:1413:A:H2'  | 24:BA:1414:C:O4'   | 2.14                     | 0.47              |
| 24:BA:1556:C:O2'  | 24:BA:1557:C:C5'   | 2.63                     | 0.47              |
| 24:BA:1707:G:H2'  | 24:BA:1708:C:C6    | 2.50                     | 0.47              |
| 24:BA:2018:G:N1   | 24:BA:2019:A:C5    | 2.83                     | 0.47              |
| 24:BA:2027:G:H2'  | 24:BA:2028:U:H6    | 1.79                     | 0.47              |
| 24:BA:2385:C:O2'  | 24:BA:2386:A:H5'   | 2.14                     | 0.47              |
| 24:BA:2599:G:C2   | 24:BA:2600:A:C8    | 3.02                     | 0.47              |
| 24:BA:2740:A:C6   | 24:BA:2764:A:C8    | 3.03                     | 0.47              |
| 24:BA:301:G:C5    | 24:BA:302:C:N4     | 2.81                     | 0.47              |
| 24:BA:487:C:N4    | 24:BA:494:G:C6     | 2.82                     | 0.47              |
| 24:BA:581:C:C2    | 24:BA:582:A:N7     | 2.82                     | 0.47              |
| 24:BA:608:A:C4    | 24:BA:621:A:C6     | 3.02                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:90:U:H2'    | 24:BA:91:A:H8     | 1.79                     | 0.47              |
| 24:BA:920:A:C6    | 24:BA:921:C:C4    | 3.02                     | 0.47              |
| 24:BA:95:A:C2     | 24:BA:96:C:H1'    | 2.49                     | 0.47              |
| 25:BB:46:A:H2'    | 25:BB:47:C:C6     | 2.49                     | 0.47              |
| 24:BA:1820:U:OP1  | 26:BC:176:ARG:HG2 | 2.14                     | 0.47              |
| 26:BC:229:HIS:CD2 | 26:BC:246:PRO:CB  | 2.97                     | 0.47              |
| 26:BC:64:VAL:HG11 | 26:BC:66:PHE:CZ   | 2.50                     | 0.47              |
| 27:BD:111:GLY:O   | 27:BD:169:ARG:O   | 2.32                     | 0.47              |
| 30:BG:112:VAL:O   | 30:BG:113:ASP:HB2 | 2.15                     | 0.47              |
| 31:BH:68:ARG:HH22 | 31:BH:72:ILE:HG21 | 1.77                     | 0.47              |
| 33:BJ:64:VAL:CG1  | 33:BJ:65:THR:N    | 2.77                     | 0.47              |
| 36:BM:45:GLN:HE22 | 36:BM:125:PRO:HG3 | 1.78                     | 0.47              |
| 36:BM:2:LEU:HD23  | 36:BM:69:PRO:HD2  | 1.97                     | 0.47              |
| 24:BA:1011:G:H5'' | 40:BQ:76:SER:OG   | 2.15                     | 0.47              |
| 41:BR:1:MET:HB2   | 41:BR:43:ASN:ND2  | 2.29                     | 0.47              |
| 48:BY:21:LEU:O    | 48:BY:22:LEU:C    | 2.52                     | 0.47              |
| 55:CA:1154:G:H2'  | 55:CA:1155:A:H8   | 1.80                     | 0.47              |
| 55:CA:1239:A:H1'  | 55:CA:1241:G:C4   | 2.50                     | 0.47              |
| 55:CA:1256:A:N9   | 55:CA:1278:G:C6   | 2.83                     | 0.47              |
| 6:CG:77:ARG:NH1   | 55:CA:1381:U:N3   | 2.63                     | 0.47              |
| 55:CA:1453:G:C2'  | 55:CA:1453:G:N3   | 2.77                     | 0.47              |
| 55:CA:168:G:C2'   | 55:CA:169:C:H5'   | 2.44                     | 0.47              |
| 55:CA:210:C:O2'   | 55:CA:211:G:P     | 2.73                     | 0.47              |
| 55:CA:708:C:H2'   | 55:CA:709:U:C6    | 2.43                     | 0.47              |
| 55:CA:709:U:H2'   | 55:CA:710:G:C8    | 2.50                     | 0.47              |
| 2:CC:45:GLU:C     | 2:CC:47:ALA:H     | 2.17                     | 0.47              |
| 3:CD:180:THR:O    | 3:CD:182:LYS:N    | 2.47                     | 0.47              |
| 6:CG:108:ARG:CZ   | 55:CA:1240:U:H6   | 2.26                     | 0.47              |
| 10:CK:124:LYS:HD2 | 20:CU:34:ARG:HD2  | 1.96                     | 0.47              |
| 11:CL:109:ARG:O   | 11:CL:110:LYS:HD2 | 2.14                     | 0.47              |
| 12:CM:12:LYS:HE2  | 12:CM:16:ILE:HG22 | 1.97                     | 0.47              |
| 12:CM:99:GLN:HE22 | 55:CA:1307:U:H5'  | 1.78                     | 0.47              |
| 16:CQ:3:LYS:HZ3   | 16:CQ:6:THR:HG21  | 1.80                     | 0.47              |
| 18:CS:18:VAL:HG21 | 18:CS:42:ASN:HB3  | 1.96                     | 0.47              |
| 19:CT:77:ASN:OD1  | 19:CT:77:ASN:N    | 2.37                     | 0.47              |
| 50:D0:55:ALA:HB3  | 50:D0:56:LYS:NZ   | 2.29                     | 0.47              |
| 53:D3:57:VAL:O    | 53:D3:60:CYS:HB2  | 2.15                     | 0.47              |
| 24:DA:1343:G:C4   | 24:DA:1597:A:C6   | 3.03                     | 0.47              |
| 24:DA:740:C:H5''  | 24:DA:1784:A:OP1  | 2.14                     | 0.47              |
| 24:DA:1930:G:HO2' | 24:DA:1968:G:H1   | 1.56                     | 0.47              |
| 24:DA:2239:G:C4   | 24:DA:2240:U:C5   | 3.02                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:DA:2516:A:C2    | 24:DA:2569:G:N3   | 2.82                     | 0.47              |
| 24:DA:335:C:H2'    | 24:DA:336:C:H6    | 1.80                     | 0.47              |
| 24:DA:527:C:H4'    | 24:DA:528:A:H5'   | 1.96                     | 0.47              |
| 24:DA:607:U:C5     | 24:DA:619:G:C4    | 3.01                     | 0.47              |
| 24:DA:625:G:H5'    | 24:DA:657:U:OP1   | 2.14                     | 0.47              |
| 24:DA:705:A:O5'    | 24:DA:705:A:H8    | 1.97                     | 0.47              |
| 24:DA:740:C:O2'    | 24:DA:741:U:C5'   | 2.47                     | 0.47              |
| 56:DB:75:G:H22     | 56:DB:102:G:N2    | 2.12                     | 0.47              |
| 56:DB:43:C:O2'     | 56:DB:45:A:N7     | 2.46                     | 0.47              |
| 24:DA:2574:G:HO2'  | 27:DD:148:GLN:HB2 | 1.78                     | 0.47              |
| 29:DF:109:ARG:HH11 | 29:DF:135:ILE:CG2 | 2.27                     | 0.47              |
| 30:DG:116:LEU:HA   | 30:DG:117:PRO:HD3 | 1.68                     | 0.47              |
| 33:DJ:124:VAL:HG22 | 33:DJ:125:TYR:O   | 2.14                     | 0.47              |
| 35:DL:117:THR:HG22 | 35:DL:118:THR:N   | 2.27                     | 0.47              |
| 24:DA:2415:G:C4'   | 35:DL:66:PHE:HB2  | 2.37                     | 0.47              |
| 39:DP:37:LYS:O     | 39:DP:38:ARG:HB3  | 2.15                     | 0.47              |
| 42:DS:51:LEU:HG    | 42:DS:55:ILE:HD13 | 1.97                     | 0.47              |
| 43:DT:12:ARG:HB2   | 43:DT:33:LYS:HG2  | 1.97                     | 0.47              |
| 21:AA:104:G:C2     | 21:AA:105:G:C5    | 3.02                     | 0.47              |
| 21:AA:1266:G:C6    | 21:AA:1270:G:C6   | 3.02                     | 0.47              |
| 21:AA:1390:U:H2'   | 21:AA:1391:U:C6   | 2.49                     | 0.47              |
| 21:AA:244:U:C2     | 21:AA:894:G:C2    | 3.02                     | 0.47              |
| 21:AA:302:G:O2'    | 21:AA:556:C:H5'   | 2.14                     | 0.47              |
| 21:AA:707:U:C4     | 21:AA:708:C:N4    | 2.82                     | 0.47              |
| 21:AA:981:U:H2'    | 21:AA:982:U:C5    | 2.50                     | 0.47              |
| 1:AB:119:GLN:O     | 1:AB:120:SER:C    | 2.53                     | 0.47              |
| 2:AC:125:ARG:O     | 2:AC:126:ARG:HB3  | 2.15                     | 0.47              |
| 5:AF:31:GLY:C      | 5:AF:33:GLU:H     | 2.18                     | 0.47              |
| 7:AH:79:ARG:HB2    | 7:AH:80:PRO:HD2   | 1.96                     | 0.47              |
| 9:AJ:6:ILE:HD11    | 9:AJ:79:PRO:CA    | 2.44                     | 0.47              |
| 13:AN:89:ARG:HB2   | 13:AN:91:GLU:HG2  | 1.97                     | 0.47              |
| 14:AO:42:PHE:CD2   | 14:AO:52:ARG:HD3  | 2.50                     | 0.47              |
| 15:AP:1:MET:SD     | 15:AP:66:THR:HG21 | 2.55                     | 0.47              |
| 16:AQ:30:HIS:HB2   | 16:AQ:35:LYS:O    | 2.14                     | 0.47              |
| 18:AS:35:ARG:HD2   | 18:AS:51:HIS:O    | 2.14                     | 0.47              |
| 24:BA:1005:C:O2    | 24:BA:1143:A:C6   | 2.67                     | 0.47              |
| 24:BA:1315:C:O2'   | 24:BA:1316:U:H5'  | 2.15                     | 0.47              |
| 24:BA:1422:G:C5    | 24:BA:1423:G:N7   | 2.83                     | 0.47              |
| 24:BA:1497:U:H2'   | 24:BA:1578:U:OP1  | 2.14                     | 0.47              |
| 24:BA:1479:G:N2    | 24:BA:1513:U:H1'  | 2.30                     | 0.47              |
| 24:BA:1672:A:N6    | 24:BA:1673:G:C6   | 2.83                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:BA:1833:C:H2'   | 24:BA:1834:U:H6   | 1.79                     | 0.47              |
| 24:BA:1859:U:H2'   | 24:BA:1860:G:O4'  | 2.15                     | 0.47              |
| 24:BA:237:C:C2'    | 24:BA:238:C:H5'   | 2.44                     | 0.47              |
| 24:BA:197:A:C6     | 24:BA:2430:A:N3   | 2.82                     | 0.47              |
| 24:BA:2526:G:C6    | 24:BA:2527:C:N3   | 2.83                     | 0.47              |
| 24:BA:2657:A:C6    | 24:BA:2665:A:C8   | 3.02                     | 0.47              |
| 24:BA:2720:U:H2'   | 24:BA:2721:A:C8   | 2.50                     | 0.47              |
| 24:BA:855:G:H1'    | 46:BW:23:LYS:CD   | 2.42                     | 0.47              |
| 24:BA:841:G:C4     | 24:BA:938:G:N2    | 2.82                     | 0.47              |
| 26:BC:141:HIS:HB3  | 26:BC:142:ASN:H   | 1.34                     | 0.47              |
| 28:BE:159:LEU:HD12 | 28:BE:159:LEU:HA  | 1.55                     | 0.47              |
| 34:BK:21:CYS:SG    | 34:BK:39:ILE:HD11 | 2.54                     | 0.47              |
| 36:BM:136:MET:HE2  | 45:BV:57:TYR:CE2  | 2.50                     | 0.47              |
| 37:BN:55:ALA:HB1   | 37:BN:80:PHE:H    | 1.77                     | 0.47              |
| 40:BQ:59:LEU:O     | 40:BQ:60:TRP:C    | 2.51                     | 0.47              |
| 42:BS:36:LEU:HA    | 42:BS:36:LEU:HD12 | 1.49                     | 0.47              |
| 45:BV:26:PHE:CD1   | 45:BV:26:PHE:C    | 2.87                     | 0.47              |
| 46:BW:22:VAL:O     | 46:BW:25:PHE:HD2  | 1.96                     | 0.47              |
| 46:BW:28:GLU:CG    | 46:BW:29:SER:N    | 2.78                     | 0.47              |
| 55:CA:1051:C:O2'   | 55:CA:1052:U:O4'  | 2.32                     | 0.47              |
| 55:CA:1069:C:O2'   | 55:CA:1192:C:H1'  | 2.15                     | 0.47              |
| 55:CA:9:G:C2       | 55:CA:10:A:C8     | 3.03                     | 0.47              |
| 55:CA:1170:A:O2'   | 55:CA:1171:A:H5'  | 2.15                     | 0.47              |
| 55:CA:1202:U:O2'   | 55:CA:1203:C:H5'  | 2.14                     | 0.47              |
| 55:CA:1460:C:N4    | 55:CA:1461:G:C6   | 2.83                     | 0.47              |
| 55:CA:247:G:C5     | 55:CA:278:G:C2    | 3.03                     | 0.47              |
| 55:CA:327:A:C2     | 55:CA:329:A:N3    | 2.82                     | 0.47              |
| 10:CK:70:ALA:HB1   | 10:CK:104:PHE:CZ  | 2.49                     | 0.47              |
| 15:CP:8:ARG:NH2    | 15:CP:15:PRO:HD3  | 2.30                     | 0.47              |
| 18:CS:5:LYS:H      | 18:CS:5:LYS:HD3   | 1.79                     | 0.47              |
| 23:CW:5:U:H2'      | 23:CW:6:U:C6      | 2.49                     | 0.47              |
| 24:DA:1022:G:O2'   | 24:DA:1023:U:OP2  | 2.25                     | 0.47              |
| 24:DA:112:U:H5'    | 48:DY:58:ASN:ND2  | 2.29                     | 0.47              |
| 24:DA:1331:G:H2'   | 24:DA:1333:G:N7   | 2.29                     | 0.47              |
| 24:DA:1889:A:H2    | 24:DA:2086:U:H1'  | 1.79                     | 0.47              |
| 24:DA:222:A:C6     | 24:DA:224:U:C2    | 3.02                     | 0.47              |
| 24:DA:244:A:H2'    | 24:DA:245:G:O4'   | 2.14                     | 0.47              |
| 24:DA:2061:G:H8    | 24:DA:2501:C:H4'  | 1.78                     | 0.47              |
| 24:DA:2527:C:H2'   | 24:DA:2528:U:O4'  | 2.13                     | 0.47              |
| 24:DA:2568:U:H2'   | 24:DA:2569:G:C8   | 2.49                     | 0.47              |
| 24:DA:296:U:C2     | 24:DA:297:G:C8    | 3.03                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:562:U:H2'    | 24:DA:572:A:O4'    | 2.14                     | 0.47              |
| 24:DA:971:G:O6     | 24:DA:972:A:C2     | 2.67                     | 0.47              |
| 56:DB:102:G:C6     | 56:DB:103:U:C4     | 3.03                     | 0.47              |
| 26:DC:62:ARG:HH21  | 26:DC:62:ARG:CG    | 2.18                     | 0.47              |
| 28:DE:108:ILE:HD13 | 28:DE:108:ILE:O    | 2.15                     | 0.47              |
| 30:DG:7:PRO:HB3    | 30:DG:48:THR:HB    | 1.97                     | 0.47              |
| 30:DG:84:LYS:O     | 30:DG:85:LYS:CB    | 2.62                     | 0.47              |
| 31:DH:90:LEU:CB    | 31:DH:123:ARG:HB3  | 2.39                     | 0.47              |
| 31:DH:75:LEU:O     | 31:DH:76:GLU:HB2   | 2.14                     | 0.47              |
| 32:DI:57:VAL:HG21  | 32:DI:69:VAL:H     | 1.78                     | 0.47              |
| 35:DL:100:ILE:O    | 35:DL:101:ILE:CB   | 2.62                     | 0.47              |
| 36:DM:72:PRO:O     | 36:DM:73:ILE:CB    | 2.59                     | 0.47              |
| 40:DQ:63:ARG:HH12  | 40:DQ:99:VAL:HG21  | 1.79                     | 0.47              |
| 44:DU:92:VAL:CB    | 44:DU:101:THR:HG21 | 2.41                     | 0.47              |
| 44:DU:95:PHE:N     | 44:DU:95:PHE:HD1   | 2.09                     | 0.47              |
| 49:DZ:38:GLU:CD    | 49:DZ:39:ASP:H     | 2.18                     | 0.47              |
| 21:AA:143:A:H5'    | 21:AA:144:G:H5'    | 1.96                     | 0.47              |
| 3:AD:109:THR:HG21  | 21:AA:408:A:O5'    | 2.14                     | 0.47              |
| 21:AA:415:A:C8     | 21:AA:416:G:N7     | 2.82                     | 0.47              |
| 21:AA:481:G:O2'    | 21:AA:482:A:C8     | 2.65                     | 0.47              |
| 21:AA:821:G:H2'    | 21:AA:822:U:H6     | 1.78                     | 0.47              |
| 1:AB:170:ILE:HD13  | 1:AB:170:ILE:H     | 1.79                     | 0.47              |
| 1:AB:186:VAL:O     | 1:AB:186:VAL:HG23  | 2.15                     | 0.47              |
| 3:AD:98:ASP:HB2    | 3:AD:114:ARG:HG2   | 1.97                     | 0.47              |
| 4:AE:37:VAL:HG21   | 4:AE:113:VAL:CG1   | 2.37                     | 0.47              |
| 10:AK:51:PHE:HZ    | 10:AK:64:VAL:HG11  | 1.79                     | 0.47              |
| 14:AO:34:GLN:O     | 14:AO:38:LEU:HD23  | 2.15                     | 0.47              |
| 24:BA:1498:C:O2'   | 24:BA:1499:C:O4'   | 2.30                     | 0.47              |
| 24:BA:1539:U:O2'   | 24:BA:1540:G:O5'   | 2.32                     | 0.47              |
| 24:BA:1819:A:H5''  | 26:BC:159:THR:CG2  | 2.44                     | 0.47              |
| 24:BA:184:C:H2'    | 24:BA:185:G:H8     | 1.80                     | 0.47              |
| 24:BA:1936:A:C2    | 24:BA:1943:U:O4    | 2.67                     | 0.47              |
| 24:BA:2510:C:C4    | 24:BA:2511:U:C4    | 3.03                     | 0.47              |
| 24:BA:2552:U:H2'   | 24:BA:2554:U:OP2   | 2.13                     | 0.47              |
| 24:BA:2513:A:C6    | 24:BA:2574:G:C6    | 3.02                     | 0.47              |
| 24:BA:2595:G:N2    | 24:BA:2599:G:C5    | 2.83                     | 0.47              |
| 24:BA:2748:A:N6    | 24:BA:2749:A:C6    | 2.82                     | 0.47              |
| 24:BA:2796:U:H3    | 24:BA:2799:A:N6    | 2.05                     | 0.47              |
| 24:BA:2870:C:O2'   | 24:BA:2871:U:H5'   | 2.14                     | 0.47              |
| 24:BA:27:G:O2'     | 24:BA:28:A:OP2     | 2.33                     | 0.47              |
| 24:BA:911:A:H2'    | 36:BM:9:PHE:CZ     | 2.49                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:946:C:H2'    | 24:BA:947:A:C8     | 2.47                     | 0.47              |
| 25:BB:88:C:H3'     | 25:BB:88:C:OP2     | 2.14                     | 0.47              |
| 32:BI:100:ILE:HG22 | 32:BI:101:SER:N    | 2.22                     | 0.47              |
| 32:BI:60:VAL:HG22  | 32:BI:66:PHE:CB    | 2.45                     | 0.47              |
| 41:BR:83:TYR:C     | 41:BR:83:TYR:CD1   | 2.87                     | 0.47              |
| 43:BT:15:HIS:HB3   | 43:BT:31:VAL:HG22  | 1.97                     | 0.47              |
| 47:BX:53:LYS:C     | 47:BX:53:LYS:HD3   | 2.35                     | 0.47              |
| 55:CA:1009:U:H2'   | 55:CA:1010:U:C5    | 2.49                     | 0.47              |
| 55:CA:1486:G:H2'   | 55:CA:1487:G:O4'   | 2.14                     | 0.47              |
| 55:CA:212:G:O2'    | 55:CA:213:G:O5'    | 2.33                     | 0.47              |
| 55:CA:126:G:C2     | 55:CA:236:A:C2     | 3.03                     | 0.47              |
| 55:CA:265:G:C2'    | 55:CA:266:G:H5'    | 2.44                     | 0.47              |
| 55:CA:397:A:H5''   | 55:CA:397:A:N3     | 2.29                     | 0.47              |
| 55:CA:774:G:C5     | 55:CA:775:G:C8     | 3.03                     | 0.47              |
| 55:CA:90:C:H2'     | 55:CA:91:U:C5      | 2.49                     | 0.47              |
| 1:CB:127:LYS:O     | 1:CB:132:GLU:HB2   | 2.14                     | 0.47              |
| 1:CB:164:ASP:HB3   | 1:CB:167:HIS:H     | 1.79                     | 0.47              |
| 4:CE:80:LEU:O      | 4:CE:81:GLN:C      | 2.53                     | 0.47              |
| 5:CF:73:GLU:OE1    | 5:CF:73:GLU:HA     | 2.14                     | 0.47              |
| 6:CG:68:VAL:HG22   | 6:CG:134:VAL:HG12  | 1.97                     | 0.47              |
| 10:CK:104:PHE:N    | 10:CK:104:PHE:HD1  | 2.13                     | 0.47              |
| 12:CM:23:GLY:HA3   | 12:CM:64:VAL:HG13  | 1.96                     | 0.47              |
| 12:CM:66:GLY:O     | 12:CM:70:ARG:HB2   | 2.15                     | 0.47              |
| 13:CN:63:CYS:O     | 13:CN:67:GLY:HA2   | 2.14                     | 0.47              |
| 18:CS:43:MET:CE    | 18:CS:43:MET:H     | 2.27                     | 0.47              |
| 24:DA:2285:C:H5    | 51:D1:5:ARG:CZ     | 2.27                     | 0.47              |
| 24:DA:138:U:H2'    | 24:DA:140:C:C1'    | 2.45                     | 0.47              |
| 24:DA:1783:A:C5'   | 24:DA:2608:G:H4'   | 2.45                     | 0.47              |
| 24:DA:2547:A:C8    | 24:DA:2566:A:N7    | 2.82                     | 0.47              |
| 24:DA:2623:G:C2'   | 24:DA:2624:G:H5'   | 2.45                     | 0.47              |
| 24:DA:2523:G:H1'   | 24:DA:2765:A:N7    | 2.30                     | 0.47              |
| 24:DA:405:U:H3'    | 24:DA:406:G:H5'    | 1.96                     | 0.47              |
| 24:DA:54:G:C6      | 24:DA:117:G:N2     | 2.83                     | 0.47              |
| 24:DA:571:U:C2     | 24:DA:575:A:N7     | 2.83                     | 0.47              |
| 24:DA:828:U:C5     | 24:DA:829:A:N6     | 2.83                     | 0.47              |
| 56:DB:77:U:OP1     | 45:DV:18:ARG:CG    | 2.60                     | 0.47              |
| 27:DD:51:THR:HG21  | 27:DD:76:GLY:HA3   | 1.94                     | 0.47              |
| 28:DE:77:ILE:H     | 28:DE:77:ILE:HG12  | 1.51                     | 0.47              |
| 30:DG:104:LEU:HG   | 30:DG:112:VAL:HG21 | 1.95                     | 0.47              |
| 32:DI:48:ILE:HG13  | 32:DI:49:GLU:N     | 2.29                     | 0.47              |
| 24:DA:1669:A:H8    | 34:DK:5:GLN:HG3    | 1.79                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:DK:6:THR:O     | 34:DK:8:LEU:CD1   | 2.62                     | 0.47              |
| 47:DX:31:ASN:HB2  | 47:DX:33:HIS:CE1  | 2.49                     | 0.47              |
| 21:AA:103:U:N3    | 21:AA:104:G:C8    | 2.83                     | 0.47              |
| 21:AA:1065:U:C4   | 21:AA:1190:G:O4'  | 2.68                     | 0.47              |
| 21:AA:131:A:C2    | 21:AA:132:C:N3    | 2.83                     | 0.47              |
| 21:AA:339:C:H2'   | 21:AA:340:U:H6    | 1.79                     | 0.47              |
| 21:AA:692:U:O2    | 21:AA:694:A:H3'   | 2.15                     | 0.47              |
| 21:AA:962:C:H2'   | 21:AA:963:G:O4'   | 2.15                     | 0.47              |
| 21:AA:987:G:N1    | 21:AA:988:G:C5    | 2.83                     | 0.47              |
| 1:AB:150:ILE:O    | 1:AB:150:ILE:HG12 | 2.15                     | 0.47              |
| 1:AB:69:VAL:CG2   | 1:AB:160:LEU:HD21 | 2.44                     | 0.47              |
| 3:AD:55:ARG:HH12  | 3:AD:58:GLN:HB3   | 1.79                     | 0.47              |
| 7:AH:3:GLN:OE1    | 21:AA:878:A:H1'   | 2.15                     | 0.47              |
| 10:AK:63:GLN:HG3  | 10:AK:98:ALA:HB3  | 1.96                     | 0.47              |
| 12:AM:27:THR:HG21 | 21:AA:1328:C:H5'' | 1.97                     | 0.47              |
| 17:AR:21:ASP:OD1  | 17:AR:23:LYS:HG3  | 2.15                     | 0.47              |
| 19:AT:5:SER:OG    | 19:AT:6:ALA:N     | 2.46                     | 0.47              |
| 50:B0:9:ARG:CG    | 50:B0:9:ARG:NH2   | 2.76                     | 0.47              |
| 51:B1:16:THR:HG21 | 51:B1:39:ASP:OD1  | 2.14                     | 0.47              |
| 24:BA:241:A:O2'   | 53:B3:2:LYS:NZ    | 2.48                     | 0.47              |
| 24:BA:1107:G:H2'  | 24:BA:1108:U:H6   | 1.80                     | 0.47              |
| 24:BA:1247:A:C5   | 24:BA:1249:U:C4   | 3.03                     | 0.47              |
| 24:BA:1253:A:H3'  | 24:BA:1254:A:H5'  | 1.95                     | 0.47              |
| 24:BA:1274:A:H8   | 24:BA:1274:A:O5'  | 1.98                     | 0.47              |
| 24:BA:1553:A:C8   | 24:BA:1555:G:C5   | 3.02                     | 0.47              |
| 24:BA:1663:G:C6   | 24:BA:1998:A:C6   | 3.03                     | 0.47              |
| 24:BA:1937:A:H5'' | 59:BA:3469:HOH:O  | 2.14                     | 0.47              |
| 24:BA:2525:G:C2   | 24:BA:2539:C:C2   | 3.02                     | 0.47              |
| 24:BA:2776:A:C2   | 24:BA:2778:A:C4   | 3.02                     | 0.47              |
| 24:BA:2800:A:C2   | 24:BA:2895:G:C1'  | 2.96                     | 0.47              |
| 24:BA:387:U:C5    | 24:BA:388:G:O6    | 2.68                     | 0.47              |
| 24:BA:960:A:C8    | 24:BA:962:G:C8    | 3.02                     | 0.47              |
| 26:BC:124:LYS:HB3 | 26:BC:127:ASN:ND2 | 2.30                     | 0.47              |
| 27:BD:34:VAL:CG2  | 27:BD:91:THR:HA   | 2.43                     | 0.47              |
| 28:BE:58:LYS:O    | 28:BE:59:PRO:C    | 2.52                     | 0.47              |
| 30:BG:54:ARG:HG3  | 30:BG:57:TYR:HD1  | 1.80                     | 0.47              |
| 32:BI:123:ALA:C   | 32:BI:125:THR:H   | 2.17                     | 0.47              |
| 41:BR:29:THR:HG22 | 41:BR:29:THR:O    | 2.15                     | 0.47              |
| 55:CA:1266:G:C6   | 55:CA:1270:G:O6   | 2.68                     | 0.47              |
| 55:CA:1370:G:H2'  | 55:CA:1371:G:H8   | 1.78                     | 0.47              |
| 55:CA:161:A:C4    | 55:CA:162:A:C8    | 3.03                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:204:G:H2'   | 55:CA:205:A:O4'   | 2.14                     | 0.47              |
| 55:CA:251:G:C2    | 55:CA:266:G:C6    | 3.03                     | 0.47              |
| 55:CA:722:G:H2'   | 55:CA:724:G:C8    | 2.50                     | 0.47              |
| 55:CA:723:U:O2'   | 55:CA:724:G:OP1   | 2.26                     | 0.47              |
| 55:CA:749:A:C6    | 55:CA:750:C:C4    | 3.03                     | 0.47              |
| 55:CA:969:A:C2'   | 55:CA:970:C:H5'   | 2.44                     | 0.47              |
| 1:CB:14:HIS:HE1   | 1:CB:42:LEU:HD11  | 1.80                     | 0.47              |
| 1:CB:65:LYS:HE2   | 1:CB:153:MET:HG3  | 1.97                     | 0.47              |
| 1:CB:80:LYS:O     | 1:CB:83:ALA:N     | 2.48                     | 0.47              |
| 8:CI:47:VAL:HG23  | 8:CI:48:ARG:HD2   | 1.96                     | 0.47              |
| 10:CK:121:ARG:HD3 | 55:CA:778:G:H21   | 1.80                     | 0.47              |
| 11:CL:26:CYS:HB2  | 11:CL:29:LYS:HE2  | 1.95                     | 0.47              |
| 11:CL:65:TYR:CD1  | 11:CL:66:ILE:N    | 2.79                     | 0.47              |
| 15:CP:13:LYS:HE2  | 55:CA:483:C:O2    | 2.15                     | 0.47              |
| 17:CR:72:ARG:HA   | 20:CU:4:LYS:HE3   | 1.96                     | 0.47              |
| 18:CS:35:ARG:HD2  | 18:CS:71:GLY:HA2  | 1.97                     | 0.47              |
| 24:DA:1019:U:C5   | 24:DA:1020:A:N7   | 2.83                     | 0.47              |
| 24:DA:100:U:O2'   | 24:DA:101:A:C5'   | 2.63                     | 0.47              |
| 24:DA:1248:G:O2'  | 40:DQ:2:ARG:HA    | 2.15                     | 0.47              |
| 24:DA:126:A:OP2   | 52:D2:19:ARG:HB2  | 2.15                     | 0.47              |
| 24:DA:1378:A:N7   | 24:DA:1380:G:C6   | 2.83                     | 0.47              |
| 24:DA:155:A:O2'   | 24:DA:156:A:H5'   | 2.15                     | 0.47              |
| 24:DA:1693:U:O4   | 24:DA:1977:A:C5   | 2.67                     | 0.47              |
| 24:DA:2370:G:C6   | 24:DA:2371:G:C5   | 3.03                     | 0.47              |
| 24:DA:2439:A:H2'  | 24:DA:2439:A:N3   | 2.29                     | 0.47              |
| 24:DA:2571:U:O4   | 24:DA:2574:G:C8   | 2.67                     | 0.47              |
| 24:DA:2023:C:C5'  | 24:DA:2617:U:H4'  | 2.45                     | 0.47              |
| 24:DA:449:A:O2'   | 24:DA:450:G:C5'   | 2.59                     | 0.47              |
| 24:DA:617:G:H2'   | 24:DA:618:G:H8    | 1.80                     | 0.47              |
| 24:DA:636:G:H4'   | 24:DA:638:G:O3'   | 2.15                     | 0.47              |
| 24:DA:675:A:N6    | 24:DA:676:A:N6    | 2.63                     | 0.47              |
| 24:DA:771:G:C5    | 24:DA:772:C:C5    | 3.03                     | 0.47              |
| 24:DA:78:U:O2'    | 24:DA:79:C:H5'    | 2.14                     | 0.47              |
| 24:DA:910:A:N6    | 24:DA:911:A:C6    | 2.82                     | 0.47              |
| 56:DB:16:G:H2'    | 56:DB:17:C:C6     | 2.50                     | 0.47              |
| 27:DD:127:PHE:CZ  | 27:DD:160:LYS:HD2 | 2.49                     | 0.47              |
| 38:DO:7:ARG:HH21  | 38:DO:95:SER:HB3  | 1.78                     | 0.47              |
| 41:DR:51:VAL:HB   | 41:DR:52:PRO:HD2  | 1.97                     | 0.47              |
| 48:DY:28:LEU:HD22 | 48:DY:28:LEU:O    | 2.15                     | 0.47              |
| 21:AA:123:U:H2'   | 21:AA:124:C:H6    | 1.79                     | 0.47              |
| 21:AA:1256:A:O2'  | 21:AA:1257:A:OP2  | 2.29                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 21:AA:1337:G:H5''  | 21:AA:1338:G:OP1  | 2.15                     | 0.47              |
| 21:AA:1416:G:C2'   | 21:AA:1417:G:H5'  | 2.44                     | 0.47              |
| 21:AA:1468:A:C2'   | 21:AA:1469:C:H5'' | 2.43                     | 0.47              |
| 21:AA:155:A:C6     | 21:AA:156:C:C4    | 3.03                     | 0.47              |
| 21:AA:298:A:H2'    | 21:AA:299:G:C8    | 2.50                     | 0.47              |
| 21:AA:499:A:O2'    | 21:AA:500:G:N7    | 2.45                     | 0.47              |
| 11:AL:109:ARG:NH2  | 21:AA:537:G:OP1   | 2.45                     | 0.47              |
| 21:AA:721:G:H4'    | 21:AA:722:G:H5''  | 1.96                     | 0.47              |
| 21:AA:764:C:C2     | 21:AA:765:G:C8    | 3.03                     | 0.47              |
| 21:AA:841:C:H3'    | 21:AA:843:U:OP2   | 2.15                     | 0.47              |
| 21:AA:855:U:N3     | 21:AA:856:C:C5    | 2.83                     | 0.47              |
| 9:AJ:59:LYS:CG     | 21:AA:972:C:H4'   | 2.45                     | 0.47              |
| 1:AB:56:LEU:O      | 1:AB:59:ILE:HG13  | 2.15                     | 0.47              |
| 3:AD:57:LYS:HD2    | 3:AD:57:LYS:C     | 2.35                     | 0.47              |
| 4:AE:13:LYS:HE2    | 4:AE:112:ALA:HB2  | 1.95                     | 0.47              |
| 6:AG:26:VAL:HG12   | 6:AG:42:VAL:HG11  | 1.96                     | 0.47              |
| 8:AI:24:ASN:HB3    | 8:AI:58:GLU:OE1   | 2.15                     | 0.47              |
| 11:AL:43:LYS:N     | 11:AL:43:LYS:HD3  | 2.15                     | 0.47              |
| 15:AP:16:PHE:CE2   | 21:AA:625:U:H4'   | 2.50                     | 0.47              |
| 16:AQ:60:ILE:HG22  | 16:AQ:61:ARG:H    | 1.80                     | 0.47              |
| 22:AV:34:G:H2'     | 22:AV:35:A:H8     | 1.80                     | 0.47              |
| 54:B4:9:LYS:HB3    | 54:B4:14:CYS:CB   | 2.45                     | 0.47              |
| 24:BA:1048:A:C6    | 24:BA:1049:C:C4   | 3.03                     | 0.47              |
| 24:BA:1343:G:H2'   | 24:BA:1344:U:C5   | 2.50                     | 0.47              |
| 24:BA:1427:A:H1'   | 24:BA:1428:C:C5   | 2.50                     | 0.47              |
| 24:BA:1570:A:H5'   | 26:BC:35:LYS:HG2  | 1.97                     | 0.47              |
| 24:BA:1809:A:O2'   | 24:BA:1810:A:O5'  | 2.32                     | 0.47              |
| 24:BA:1945:G:H2'   | 24:BA:1946:U:C6   | 2.50                     | 0.47              |
| 24:BA:215:G:C4'    | 24:BA:216:A:H4'   | 2.45                     | 0.47              |
| 24:BA:2410:G:C2    | 24:BA:2411:A:C1'  | 2.98                     | 0.47              |
| 24:BA:2492:U:C2    | 24:BA:2493:U:C5   | 3.03                     | 0.47              |
| 24:BA:2720:U:H2'   | 24:BA:2721:A:H8   | 1.80                     | 0.47              |
| 24:BA:383:C:H5'    | 24:BA:385:C:OP2   | 2.14                     | 0.47              |
| 24:BA:783:A:C4'    | 24:BA:1779:U:O2   | 2.62                     | 0.47              |
| 24:BA:84:A:C6      | 24:BA:103:A:N6    | 2.83                     | 0.47              |
| 25:BB:62:C:H2'     | 25:BB:63:C:C6     | 2.37                     | 0.47              |
| 24:BA:1820:U:C5    | 26:BC:158:GLY:HA3 | 2.50                     | 0.47              |
| 26:BC:194:VAL:HG22 | 26:BC:195:GLY:N   | 2.30                     | 0.47              |
| 26:BC:229:HIS:CD2  | 26:BC:246:PRO:CA  | 2.98                     | 0.47              |
| 32:BI:19:PRO:HG2   | 32:BI:23:VAL:HG22 | 1.96                     | 0.47              |
| 32:BI:33:ASN:HB3   | 32:BI:36:GLU:CB   | 2.41                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:BJ:64:VAL:HG22 | 33:BJ:68:LYS:HD2  | 1.97                     | 0.47              |
| 33:BJ:77:HIS:CD2  | 33:BJ:79:GLY:H    | 2.31                     | 0.47              |
| 40:BQ:97:ILE:HG13 | 40:BQ:98:ALA:N    | 2.27                     | 0.47              |
| 47:BX:36:ARG:HG2  | 47:BX:45:PHE:HB3  | 1.96                     | 0.47              |
| 24:BA:96:C:H4'    | 48:BY:41:HIS:ND1  | 2.30                     | 0.47              |
| 48:BY:57:LEU:CA   | 48:BY:60:LYS:HB3  | 2.42                     | 0.47              |
| 55:CA:1020:G:C6   | 55:CA:1021:A:C6   | 3.03                     | 0.47              |
| 55:CA:1256:A:C5   | 55:CA:1278:G:C5   | 3.03                     | 0.47              |
| 55:CA:1306:A:C5   | 55:CA:1307:U:C5   | 3.03                     | 0.47              |
| 55:CA:1322:C:HO2' | 55:CA:1323:G:H5'  | 1.74                     | 0.47              |
| 55:CA:1342:C:O2'  | 55:CA:1343:G:H5'  | 2.15                     | 0.47              |
| 55:CA:161:A:H2'   | 55:CA:162:A:H8    | 1.78                     | 0.47              |
| 55:CA:486:U:H2'   | 55:CA:487:A:H8    | 1.79                     | 0.47              |
| 55:CA:702:A:O2'   | 55:CA:703:G:OP1   | 2.31                     | 0.47              |
| 6:CG:26:VAL:O     | 6:CG:30:MET:HG3   | 2.15                     | 0.47              |
| 6:CG:94:ARG:HB3   | 6:CG:98:LEU:CD1   | 2.45                     | 0.47              |
| 2:CC:22:PHE:CD1   | 9:CJ:13:PHE:CE1   | 3.02                     | 0.47              |
| 10:CK:104:PHE:N   | 10:CK:104:PHE:CD1 | 2.83                     | 0.47              |
| 14:CO:54:GLY:O    | 14:CO:58:MET:HG3  | 2.14                     | 0.47              |
| 15:CP:43:ALA:HB1  | 15:CP:46:LYS:HZ3  | 1.80                     | 0.47              |
| 20:CU:3:ILE:O     | 20:CU:4:LYS:O     | 2.33                     | 0.47              |
| 22:CV:30:G:C2     | 22:CV:31:A:C8     | 3.03                     | 0.47              |
| 24:DA:56:A:C2     | 24:DA:115:C:C2    | 3.03                     | 0.47              |
| 24:DA:1179:G:O2'  | 24:DA:1180:U:H5'  | 2.15                     | 0.47              |
| 24:DA:1247:A:C5   | 24:DA:1249:U:C4   | 3.02                     | 0.47              |
| 24:DA:1345:C:O2'  | 24:DA:1346:G:C5'  | 2.62                     | 0.47              |
| 24:DA:1613:G:H1   | 24:DA:1617:C:HO2' | 1.63                     | 0.47              |
| 24:DA:1832:C:C4   | 24:DA:1833:C:C5   | 3.02                     | 0.47              |
| 24:DA:1833:C:H2'  | 24:DA:1834:U:C6   | 2.50                     | 0.47              |
| 24:DA:2023:C:H5'  | 24:DA:2617:U:H4'  | 1.97                     | 0.47              |
| 24:DA:2630:G:O2'  | 24:DA:2631:G:C8   | 2.66                     | 0.47              |
| 24:DA:2645:G:H3'  | 24:DA:2646:C:C5'  | 2.44                     | 0.47              |
| 24:DA:2765:A:H3'  | 24:DA:2766:A:H5'  | 1.97                     | 0.47              |
| 24:DA:527:C:N3    | 24:DA:2779:U:H2'  | 2.30                     | 0.47              |
| 24:DA:2825:G:C4   | 24:DA:2826:A:C8   | 3.03                     | 0.47              |
| 24:DA:2848:G:N3   | 24:DA:2849:U:C5   | 2.83                     | 0.47              |
| 24:DA:2849:U:O4   | 24:DA:2867:G:C8   | 2.68                     | 0.47              |
| 24:DA:586:A:O5'   | 24:DA:586:A:C8    | 2.68                     | 0.47              |
| 24:DA:588:U:O4    | 24:DA:670:A:H1'   | 2.15                     | 0.47              |
| 24:DA:77:G:H2'    | 24:DA:78:U:C6     | 2.49                     | 0.47              |
| 24:DA:1789:A:OP1  | 26:DC:220:ARG:HD3 | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DE:153:LEU:HD22 | 28:DE:158:PHE:HD2  | 1.79                     | 0.47              |
| 28:DE:16:GLU:O     | 28:DE:16:GLU:HG3   | 2.15                     | 0.47              |
| 31:DH:24:GLY:O     | 31:DH:28:ASN:HB2   | 2.14                     | 0.47              |
| 24:DA:1140:C:OP1   | 33:DJ:25:LEU:HD13  | 2.14                     | 0.47              |
| 34:DK:66:LYS:O     | 34:DK:66:LYS:HG2   | 2.15                     | 0.47              |
| 35:DL:89:VAL:HG21  | 35:DL:123:ARG:HE   | 1.79                     | 0.47              |
| 38:DO:28:VAL:HG23  | 38:DO:106:LEU:HD23 | 1.95                     | 0.47              |
| 39:DP:63:ILE:CA    | 39:DP:68:GLY:HA2   | 2.36                     | 0.47              |
| 42:DS:68:ASP:N     | 42:DS:68:ASP:OD1   | 2.48                     | 0.47              |
| 45:DV:63:ILE:HD13  | 45:DV:72:VAL:CG2   | 2.45                     | 0.47              |
| 46:DW:49:ASN:HB3   | 46:DW:81:ILE:HG12  | 1.96                     | 0.47              |
| 24:DA:380:G:O3'    | 47:DX:15:ASN:HB2   | 2.15                     | 0.47              |
| 21:AA:1161:C:O2'   | 21:AA:1162:C:O4'   | 2.31                     | 0.47              |
| 21:AA:438:U:O2'    | 21:AA:439:U:H5     | 1.97                     | 0.47              |
| 21:AA:449:G:N1     | 21:AA:450:G:C6     | 2.83                     | 0.47              |
| 21:AA:511:C:O2'    | 21:AA:512:U:O5'    | 2.33                     | 0.47              |
| 21:AA:615:G:C2     | 21:AA:616:G:C8     | 3.03                     | 0.47              |
| 21:AA:737:C:N4     | 21:AA:738:C:N4     | 2.63                     | 0.47              |
| 21:AA:75:G:N1      | 21:AA:96:U:N3      | 2.63                     | 0.47              |
| 1:AB:19:THR:HA     | 1:AB:37:VAL:HG23   | 1.97                     | 0.47              |
| 2:AC:89:VAL:O      | 2:AC:93:ILE:HG13   | 2.14                     | 0.47              |
| 8:AI:42:THR:O      | 8:AI:43:ALA:HB2    | 2.15                     | 0.47              |
| 8:AI:60:LEU:HD23   | 8:AI:60:LEU:N      | 2.30                     | 0.47              |
| 18:AS:19:GLU:O     | 18:AS:22:VAL:HB    | 2.15                     | 0.47              |
| 50:B0:53:VAL:O     | 50:B0:54:ILE:C     | 2.53                     | 0.47              |
| 24:BA:1869:G:H8    | 24:BA:1869:G:OP2   | 1.97                     | 0.47              |
| 24:BA:1899:A:H2'   | 24:BA:1900:A:OP2   | 2.15                     | 0.47              |
| 24:BA:189:G:P      | 47:BX:13:THR:HG21  | 2.54                     | 0.47              |
| 24:BA:2330:G:C2    | 24:BA:2386:A:C2    | 3.03                     | 0.47              |
| 24:BA:580:U:O2'    | 24:BA:581:C:H5'    | 2.15                     | 0.47              |
| 24:BA:617:G:O2'    | 24:BA:618:G:H5'    | 2.15                     | 0.47              |
| 26:BC:129:LEU:HD22 | 26:BC:133:ASN:HB2  | 1.96                     | 0.47              |
| 24:BA:1805:A:N3    | 26:BC:49:THR:HG21  | 2.30                     | 0.47              |
| 27:BD:53:GLY:O     | 27:BD:54:ALA:HB2   | 2.15                     | 0.47              |
| 33:BJ:12:LYS:O     | 33:BJ:13:ARG:CB    | 2.61                     | 0.47              |
| 35:BL:135:ILE:HG22 | 35:BL:136:GLU:N    | 2.29                     | 0.47              |
| 35:BL:93:ASN:O     | 35:BL:95:LEU:N     | 2.47                     | 0.47              |
| 39:BP:24:THR:O     | 39:BP:25:VAL:O     | 2.33                     | 0.47              |
| 40:BQ:91:ARG:HB3   | 40:BQ:93:ILE:CG2   | 2.42                     | 0.47              |
| 55:CA:1090:U:N3    | 55:CA:1091:U:C5    | 2.83                     | 0.47              |
| 55:CA:1241:G:C2    | 55:CA:1242:G:C5    | 3.03                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:CA:321:A:O2'   | 55:CA:1436:U:H5'   | 2.15                     | 0.47              |
| 55:CA:1446:A:N6   | 55:CA:1447:A:N6    | 2.62                     | 0.47              |
| 55:CA:197:A:C5    | 55:CA:221:C:H4'    | 2.50                     | 0.47              |
| 31:BH:97:ARG:NH1  | 55:CA:368:U:OP1    | 2.48                     | 0.47              |
| 55:CA:373:A:C2'   | 55:CA:374:A:H8     | 2.27                     | 0.47              |
| 55:CA:76:G:OP2    | 55:CA:76:G:H8      | 1.97                     | 0.47              |
| 55:CA:781:A:H2'   | 55:CA:782:A:C5'    | 2.42                     | 0.47              |
| 55:CA:872:A:C5    | 55:CA:874:G:C8     | 3.02                     | 0.47              |
| 55:CA:90:C:H2'    | 55:CA:91:U:C6      | 2.50                     | 0.47              |
| 55:CA:98:A:H2'    | 55:CA:99:C:O4'     | 2.15                     | 0.47              |
| 1:CB:19:THR:HG23  | 1:CB:20:ARG:H      | 1.79                     | 0.47              |
| 1:CB:28:PRO:HB2   | 1:CB:29:PHE:CE1    | 2.50                     | 0.47              |
| 2:CC:161:ILE:O    | 2:CC:161:ILE:HG12  | 2.14                     | 0.47              |
| 3:CD:105:GLY:HA3  | 3:CD:158:LEU:CD2   | 2.44                     | 0.47              |
| 3:CD:98:ASP:OD2   | 3:CD:132:ALA:HB1   | 2.15                     | 0.47              |
| 5:CF:2:ARG:HH22   | 5:CF:91:ARG:HB2    | 1.78                     | 0.47              |
| 8:CI:11:ARG:HD3   | 8:CI:106:ASP:OD1   | 2.15                     | 0.47              |
| 9:CJ:42:LEU:HD22  | 9:CJ:71:LEU:CD2    | 2.40                     | 0.47              |
| 9:CJ:42:LEU:CB    | 9:CJ:43:PRO:HD2    | 2.44                     | 0.47              |
| 9:CJ:5:ARG:CZ     | 9:CJ:7:ARG:HH12    | 2.27                     | 0.47              |
| 10:CK:96:ILE:HD13 | 10:CK:109:ILE:HD13 | 1.95                     | 0.47              |
| 10:CK:115:ILE:O   | 10:CK:115:ILE:HG23 | 2.15                     | 0.47              |
| 13:CN:60:ARG:HH22 | 13:CN:70:HIS:HD2   | 1.61                     | 0.47              |
| 15:CP:8:ARG:CZ    | 15:CP:15:PRO:HB3   | 2.45                     | 0.47              |
| 24:DA:1031:G:O2'  | 54:D4:7:VAL:HG12   | 2.14                     | 0.47              |
| 24:DA:740:C:C4    | 24:DA:1981:A:C2    | 3.03                     | 0.47              |
| 24:DA:2053:G:C2   | 24:DA:2054:A:C4    | 3.02                     | 0.47              |
| 24:DA:2331:G:C2   | 24:DA:2332:C:C2    | 3.03                     | 0.47              |
| 24:DA:2250:G:H21  | 24:DA:2496:C:H5''  | 1.78                     | 0.47              |
| 24:DA:2520:C:N4   | 24:DA:2567:G:C5    | 2.83                     | 0.47              |
| 24:DA:2660:A:C2   | 24:DA:2661:G:C5    | 3.03                     | 0.47              |
| 24:DA:223:A:C6    | 24:DA:422:A:N7     | 2.83                     | 0.47              |
| 24:DA:61:C:HO2'   | 24:DA:62:U:H5'     | 1.78                     | 0.47              |
| 24:DA:775:G:C2    | 24:DA:794:A:C8     | 3.03                     | 0.47              |
| 24:DA:807:U:O4'   | 24:DA:2445:G:H4'   | 2.15                     | 0.47              |
| 56:DB:109:A:C5    | 56:DB:110:C:C4     | 3.03                     | 0.47              |
| 26:DC:260:LYS:HA  | 26:DC:263:ASP:OD1  | 2.15                     | 0.47              |
| 28:DE:40:ARG:NH2  | 28:DE:92:HIS:NE2   | 2.63                     | 0.47              |
| 31:DH:99:ILE:HG22 | 31:DH:100:ALA:N    | 2.28                     | 0.47              |
| 31:DH:120:GLY:O   | 31:DH:121:VAL:HB   | 2.15                     | 0.47              |
| 34:DK:14:SER:OG   | 34:DK:51:LYS:N     | 2.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:DL:23:ILE:HG13 | 41:DR:82:HIS:HE1  | 1.69                     | 0.47              |
| 38:DO:31:THR:HG21 | 38:DO:36:TYR:HE2  | 1.80                     | 0.47              |
| 40:DQ:60:TRP:CZ2  | 40:DQ:93:ILE:HB   | 2.50                     | 0.47              |
| 41:DR:48:LYS:H    | 41:DR:48:LYS:CD   | 2.23                     | 0.47              |
| 43:DT:62:VAL:HG12 | 43:DT:63:VAL:H    | 1.77                     | 0.47              |
| 45:DV:26:PHE:CE2  | 45:DV:42:LEU:HD12 | 2.49                     | 0.47              |
| 21:AA:104:G:O2'   | 21:AA:105:G:H5'   | 2.15                     | 0.47              |
| 21:AA:1185:G:C6   | 21:AA:1186:G:C5   | 3.03                     | 0.47              |
| 21:AA:1184:G:O2'  | 21:AA:1185:G:H5'  | 2.14                     | 0.47              |
| 21:AA:1410:A:C4   | 21:AA:1491:G:N2   | 2.84                     | 0.47              |
| 21:AA:1446:A:C2'  | 21:AA:1447:A:H5'  | 2.45                     | 0.47              |
| 21:AA:261:U:C2    | 21:AA:263:A:OP2   | 2.67                     | 0.47              |
| 21:AA:274:A:H4'   | 21:AA:275:G:O5'   | 2.15                     | 0.47              |
| 17:AR:37:LYS:HA   | 21:AA:719:C:O2    | 2.14                     | 0.47              |
| 21:AA:766:A:H2'   | 21:AA:767:A:H8    | 1.76                     | 0.47              |
| 21:AA:860:A:H8    | 21:AA:860:A:O5'   | 1.98                     | 0.47              |
| 21:AA:76:G:C2     | 21:AA:95:C:N3     | 2.83                     | 0.47              |
| 21:AA:987:G:C5    | 21:AA:988:G:N7    | 2.83                     | 0.47              |
| 1:AB:184:ALA:HB3  | 1:AB:195:VAL:CG2  | 2.45                     | 0.47              |
| 1:AB:199:ILE:O    | 1:AB:200:PRO:O    | 2.33                     | 0.47              |
| 4:AE:104:ILE:O    | 4:AE:104:ILE:HG12 | 2.14                     | 0.47              |
| 13:AN:81:ILE:HD13 | 21:AA:1202:U:C6   | 2.49                     | 0.47              |
| 9:AJ:65:TYR:CB    | 13:AN:95:LEU:HD11 | 2.42                     | 0.47              |
| 18:AS:20:LYS:CB   | 18:AS:20:LYS:HZ2  | 2.27                     | 0.47              |
| 19:AT:27:MET:HG3  | 19:AT:28:ARG:N    | 2.29                     | 0.47              |
| 24:BA:1065:U:P    | 24:BA:1065:U:H3'  | 2.55                     | 0.47              |
| 24:BA:1348:C:H2'  | 24:BA:1349:C:H5'  | 1.97                     | 0.47              |
| 24:BA:1429:G:H2'  | 24:BA:1430:G:C8   | 2.50                     | 0.47              |
| 24:BA:1579:A:H2'  | 24:BA:1580:A:H8   | 1.79                     | 0.47              |
| 24:BA:171:U:H2'   | 24:BA:172:A:C8    | 2.50                     | 0.47              |
| 24:BA:2042:A:H2'  | 24:BA:2043:C:H5'  | 1.96                     | 0.47              |
| 24:BA:211:C:O2'   | 24:BA:212:G:H5'   | 2.14                     | 0.47              |
| 24:BA:2549:G:N2   | 24:BA:2560:A:C4   | 2.83                     | 0.47              |
| 24:BA:2691:C:C4   | 24:BA:2719:G:N2   | 2.82                     | 0.47              |
| 24:BA:2843:G:N2   | 24:BA:2844:G:H1'  | 2.29                     | 0.47              |
| 24:BA:479:A:C2    | 24:BA:480:A:C5    | 3.03                     | 0.47              |
| 24:BA:667:U:H2'   | 24:BA:668:A:O4'   | 2.15                     | 0.47              |
| 24:BA:80:G:C2'    | 24:BA:81:G:H5'    | 2.44                     | 0.47              |
| 24:BA:84:A:H4'    | 24:BA:85:G:O5'    | 2.14                     | 0.47              |
| 24:BA:866:A:HO2'  | 24:BA:867:C:H5'   | 1.80                     | 0.47              |
| 24:BA:925:A:H2'   | 24:BA:926:G:O4'   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BD:101:PHE:HD1 | 27:BD:101:PHE:N   | 2.13                     | 0.47              |
| 29:BF:128:SER:HA  | 29:BF:154:THR:HA  | 1.96                     | 0.47              |
| 30:BG:163:TYR:O   | 30:BG:164:ALA:CB  | 2.63                     | 0.47              |
| 31:BH:12:LEU:HB2  | 31:BH:19:VAL:HG11 | 1.97                     | 0.47              |
| 31:BH:8:LYS:O     | 31:BH:13:GLY:CA   | 2.62                     | 0.47              |
| 36:BM:6:ARG:HD2   | 36:BM:8:LYS:NZ    | 2.30                     | 0.47              |
| 39:BP:80:VAL:O    | 39:BP:81:ASP:HB3  | 2.14                     | 0.47              |
| 24:BA:1392:A:H61  | 43:BT:18:GLU:CD   | 2.18                     | 0.47              |
| 24:BA:855:G:C1'   | 46:BW:23:LYS:HD3  | 2.42                     | 0.47              |
| 49:BZ:9:THR:HG23  | 49:BZ:10:ARG:HB2  | 1.97                     | 0.47              |
| 55:CA:1218:C:H2'  | 55:CA:1219:A:H8   | 1.74                     | 0.47              |
| 55:CA:1304:G:O2'  | 55:CA:1333:A:N6   | 2.47                     | 0.47              |
| 55:CA:1452:C:H4'  | 55:CA:1453:G:H5'' | 1.97                     | 0.47              |
| 55:CA:197:A:C4'   | 55:CA:198:G:O5'   | 2.55                     | 0.47              |
| 55:CA:355:C:H2'   | 55:CA:356:A:O4'   | 2.15                     | 0.47              |
| 55:CA:722:G:C2    | 55:CA:724:G:C5    | 3.03                     | 0.47              |
| 55:CA:790:A:OP1   | 22:CV:38:A:O2'    | 2.33                     | 0.47              |
| 1:CB:128:LEU:HD13 | 1:CB:132:GLU:HG3  | 1.96                     | 0.47              |
| 1:CB:160:LEU:O    | 1:CB:183:PHE:CD1  | 2.68                     | 0.47              |
| 1:CB:59:ILE:HA    | 1:CB:62:ARG:CG    | 2.44                     | 0.47              |
| 2:CC:127:VAL:O    | 2:CC:128:MET:HB2  | 2.15                     | 0.47              |
| 4:CE:15:ILE:HD11  | 4:CE:37:VAL:HG23  | 1.97                     | 0.47              |
| 6:CG:30:MET:SD    | 6:CG:35:LYS:HB2   | 2.54                     | 0.47              |
| 7:CH:87:ARG:HB3   | 55:CA:600:A:OP1   | 2.14                     | 0.47              |
| 8:CI:30:ASN:O     | 8:CI:31:GLN:HG3   | 2.15                     | 0.47              |
| 11:CL:122:LYS:O   | 11:CL:123:ALA:CB  | 2.63                     | 0.47              |
| 11:CL:98:ARG:CB   | 11:CL:116:TYR:HA  | 2.43                     | 0.47              |
| 12:CM:69:ARG:HD2  | 12:CM:69:ARG:H    | 1.80                     | 0.47              |
| 17:CR:32:ILE:HD12 | 17:CR:33:THR:O    | 2.14                     | 0.47              |
| 19:CT:20:ASN:O    | 19:CT:24:ARG:HB2  | 2.15                     | 0.47              |
| 19:CT:58:ASP:O    | 19:CT:61:ALA:HB3  | 2.15                     | 0.47              |
| 50:D0:11:LYS:HD2  | 50:D0:14:MET:HB2  | 1.97                     | 0.47              |
| 24:DA:1026:G:O2'  | 24:DA:1027:A:C5'  | 2.60                     | 0.47              |
| 24:DA:1056:G:O5'  | 24:DA:1085:A:H2   | 1.98                     | 0.47              |
| 24:DA:1113:U:O2'  | 24:DA:1114:C:O5'  | 2.33                     | 0.47              |
| 24:DA:1476:U:C5   | 24:DA:1514:G:C2   | 3.03                     | 0.47              |
| 24:DA:1435:G:C2   | 24:DA:1558:C:N4   | 2.83                     | 0.47              |
| 24:DA:1570:A:C2   | 24:DA:1571:A:C2   | 3.03                     | 0.47              |
| 24:DA:2067:G:C6   | 24:DA:2069:G:N7   | 2.83                     | 0.47              |
| 24:DA:2394:C:H5'' | 35:DL:63:LYS:HE3  | 1.97                     | 0.47              |
| 24:DA:2590:A:H2'  | 24:DA:2591:C:H6   | 1.80                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:2868:A:O2'   | 24:DA:2869:G:O4'   | 2.31                     | 0.47              |
| 24:DA:571:U:C4     | 24:DA:2030:A:C6    | 3.02                     | 0.47              |
| 24:DA:658:U:O2'    | 24:DA:659:G:O4'    | 2.24                     | 0.47              |
| 24:DA:963:U:O2'    | 24:DA:964:C:O5'    | 2.32                     | 0.47              |
| 24:DA:85:G:C5      | 24:DA:98:G:C2      | 3.03                     | 0.47              |
| 56:DB:48:U:C4      | 56:DB:49:C:N4      | 2.83                     | 0.47              |
| 56:DB:98:G:H1      | 45:DV:14:LYS:HB3   | 1.80                     | 0.47              |
| 26:DC:161:VAL:HG13 | 26:DC:174:ARG:O    | 2.15                     | 0.47              |
| 29:DF:122:ASP:HB2  | 29:DF:126:ASN:HB2  | 1.97                     | 0.47              |
| 31:DH:2:GLN:HB3    | 31:DH:18:GLN:HG2   | 1.97                     | 0.47              |
| 31:DH:62:LEU:HD12  | 31:DH:63:ALA:N     | 2.29                     | 0.47              |
| 32:DI:18:ASN:HB3   | 32:DI:19:PRO:HD3   | 1.97                     | 0.47              |
| 32:DI:58:ILE:HG23  | 32:DI:66:PHE:CD2   | 2.50                     | 0.47              |
| 33:DJ:104:ALA:O    | 33:DJ:108:MET:HG3  | 2.15                     | 0.47              |
| 24:DA:2392:A:C2    | 35:DL:55:MET:SD    | 3.03                     | 0.47              |
| 36:DM:34:LYS:HD3   | 36:DM:131:VAL:CG2  | 2.44                     | 0.47              |
| 27:DD:116:LYS:CD   | 37:DN:1:MET:HE1    | 2.45                     | 0.47              |
| 40:DQ:78:PHE:CE2   | 40:DQ:109:VAL:HG22 | 2.50                     | 0.47              |
| 42:DS:8:ARG:HA     | 42:DS:102:HIS:ND1  | 2.29                     | 0.47              |
| 46:DW:46:ALA:HA    | 46:DW:50:VAL:HG12  | 1.96                     | 0.47              |
| 21:AA:103:U:H2'    | 21:AA:103:U:O2     | 2.15                     | 0.46              |
| 21:AA:1082:A:N1    | 21:AA:1083:U:N3    | 2.63                     | 0.46              |
| 21:AA:1461:G:H2'   | 21:AA:1462:C:C6    | 2.50                     | 0.46              |
| 21:AA:17:U:H2'     | 21:AA:18:C:H6      | 1.80                     | 0.46              |
| 21:AA:722:G:N3     | 21:AA:722:G:C2'    | 2.78                     | 0.46              |
| 21:AA:978:A:C6     | 21:AA:1318:A:C6    | 3.03                     | 0.46              |
| 2:AC:156:LEU:CD1   | 2:AC:156:LEU:H     | 2.28                     | 0.46              |
| 4:AE:94:PHE:CE1    | 4:AE:96:GLN:HG2    | 2.49                     | 0.46              |
| 8:AI:80:HIS:HE1    | 8:AI:103:VAL:O     | 1.97                     | 0.46              |
| 9:AJ:67:ILE:HG23   | 13:AN:94:GLY:O     | 2.15                     | 0.46              |
| 10:AK:95:THR:HG23  | 10:AK:96:ILE:N     | 2.30                     | 0.46              |
| 50:B0:42:ILE:CD1   | 50:B0:48:TYR:HB2   | 2.44                     | 0.46              |
| 51:B1:47:ILE:HD12  | 51:B1:47:ILE:N     | 2.20                     | 0.46              |
| 51:B1:5:ARG:HG2    | 51:B1:23:THR:HB    | 1.96                     | 0.46              |
| 24:BA:1303:G:H2'   | 24:BA:1304:A:C8    | 2.45                     | 0.46              |
| 24:BA:1475:G:O2'   | 24:BA:1476:U:P     | 2.73                     | 0.46              |
| 24:BA:1779:U:C6    | 24:BA:1783:A:N7    | 2.83                     | 0.46              |
| 24:BA:1829:A:H2'   | 24:BA:1830:C:C6    | 2.51                     | 0.46              |
| 24:BA:1835:G:C4    | 24:BA:1931:U:C4    | 3.03                     | 0.46              |
| 24:BA:2793:C:H2'   | 24:BA:2794:C:H6    | 1.75                     | 0.46              |
| 24:BA:2902:C:O2'   | 24:BA:2903:U:C5'   | 2.63                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:2902:C:O2'  | 24:BA:2903:U:H5'  | 2.16                     | 0.46              |
| 24:BA:825:A:H1'   | 35:BL:54:GLN:HE22 | 1.71                     | 0.46              |
| 24:BA:7:G:C5      | 24:BA:8:C:C4      | 3.03                     | 0.46              |
| 25:BB:46:A:H2'    | 25:BB:47:C:H6     | 1.80                     | 0.46              |
| 26:BC:12:ARG:HA   | 26:BC:15:VAL:HG23 | 1.97                     | 0.46              |
| 26:BC:259:ASN:C   | 26:BC:261:ARG:N   | 2.68                     | 0.46              |
| 26:BC:90:ILE:CG2  | 26:BC:91:ALA:N    | 2.78                     | 0.46              |
| 28:BE:101:TYR:O   | 28:BE:102:ARG:C   | 2.51                     | 0.46              |
| 29:BF:31:GLU:HB3  | 29:BF:156:THR:O   | 2.15                     | 0.46              |
| 33:BJ:49:ASP:OD2  | 33:BJ:49:ASP:C    | 2.54                     | 0.46              |
| 33:BJ:60:ASP:OD1  | 33:BJ:61:LYS:HG3  | 2.15                     | 0.46              |
| 55:CA:1432:G:O2'  | 55:CA:1433:A:C8   | 2.68                     | 0.46              |
| 55:CA:163:C:H6    | 55:CA:163:C:O5'   | 1.98                     | 0.46              |
| 55:CA:298:A:H2'   | 55:CA:299:G:O4'   | 2.15                     | 0.46              |
| 55:CA:486:U:H2'   | 55:CA:487:A:C8    | 2.50                     | 0.46              |
| 55:CA:764:C:H3'   | 55:CA:765:G:N2    | 2.23                     | 0.46              |
| 55:CA:813:U:H3'   | 55:CA:816:A:N6    | 2.29                     | 0.46              |
| 55:CA:914:A:H2'   | 55:CA:915:A:H8    | 1.79                     | 0.46              |
| 55:CA:982:U:O2    | 55:CA:1222:G:O6   | 2.33                     | 0.46              |
| 1:CB:209:VAL:O    | 1:CB:213:LEU:HB2  | 2.15                     | 0.46              |
| 1:CB:47:PRO:HA    | 1:CB:50:ASN:CB    | 2.39                     | 0.46              |
| 4:CE:111:ARG:C    | 4:CE:113:VAL:H    | 2.18                     | 0.46              |
| 7:CH:36:ALA:O     | 7:CH:45:ILE:HD11  | 2.15                     | 0.46              |
| 12:CM:6:ILE:O     | 12:CM:6:ILE:HD12  | 2.15                     | 0.46              |
| 20:CU:35:GLU:O    | 20:CU:36:PHE:HD2  | 1.97                     | 0.46              |
| 24:DA:1092:C:H2'  | 24:DA:1093:G:O4'  | 2.15                     | 0.46              |
| 24:DA:1190:G:H5'' | 35:DL:32:GLY:HA2  | 1.97                     | 0.46              |
| 24:DA:1214:A:O2'  | 24:DA:1215:G:H5'  | 2.15                     | 0.46              |
| 24:DA:1553:A:C8   | 24:DA:1555:G:C5   | 3.03                     | 0.46              |
| 24:DA:1760:C:O2'  | 24:DA:1761:C:O4'  | 2.31                     | 0.46              |
| 24:DA:1651:G:N2   | 24:DA:2007:U:C2   | 2.83                     | 0.46              |
| 24:DA:202:U:C4    | 24:DA:203:A:N1    | 2.83                     | 0.46              |
| 24:DA:858:G:H2'   | 24:DA:2268:A:N3   | 2.30                     | 0.46              |
| 24:DA:2261:C:C2   | 24:DA:2280:G:N2   | 2.83                     | 0.46              |
| 24:DA:233:A:H2'   | 24:DA:234:U:C5    | 2.49                     | 0.46              |
| 24:DA:2378:A:C2'  | 38:DO:21:LEU:HD13 | 2.45                     | 0.46              |
| 24:DA:2411:A:H2'  | 24:DA:2412:A:H8   | 1.80                     | 0.46              |
| 24:DA:2484:G:OP1  | 36:DM:44:ARG:HD3  | 2.15                     | 0.46              |
| 24:DA:747:U:C2    | 24:DA:2613:U:O4   | 2.68                     | 0.46              |
| 24:DA:2682:A:N6   | 24:DA:2728:U:H1'  | 2.23                     | 0.46              |
| 24:DA:2836:U:O2'  | 24:DA:2837:A:C5'  | 2.63                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:311:A:O2'    | 24:DA:312:G:H5'    | 2.15                     | 0.46              |
| 24:DA:335:C:O2'    | 24:DA:336:C:C5'    | 2.63                     | 0.46              |
| 24:DA:476:G:HO2'   | 24:DA:477:A:H3'    | 1.80                     | 0.46              |
| 24:DA:536:G:C2'    | 24:DA:537:G:H5'    | 2.45                     | 0.46              |
| 24:DA:54:G:C6      | 24:DA:55:G:C5      | 3.03                     | 0.46              |
| 24:DA:661:A:H2'    | 24:DA:662:G:O4'    | 2.15                     | 0.46              |
| 24:DA:836:G:C5     | 24:DA:837:C:C4     | 3.03                     | 0.46              |
| 56:DB:79:G:N7      | 45:DV:14:LYS:NZ    | 2.45                     | 0.46              |
| 24:DA:2771:C:H5''  | 27:DD:207:VAL:HG11 | 1.97                     | 0.46              |
| 28:DE:5:LEU:HD12   | 28:DE:10:SER:HB2   | 1.97                     | 0.46              |
| 28:DE:131:THR:HG22 | 28:DE:161:ALA:N    | 2.28                     | 0.46              |
| 33:DJ:57:LEU:HD11  | 33:DJ:129:GLU:H    | 1.79                     | 0.46              |
| 35:DL:98:ALA:O     | 35:DL:100:ILE:HG22 | 2.15                     | 0.46              |
| 36:DM:15:GLY:O     | 36:DM:16:ARG:HB3   | 2.15                     | 0.46              |
| 37:DN:22:ARG:O     | 37:DN:22:ARG:HG2   | 2.15                     | 0.46              |
| 39:DP:32:VAL:HA    | 39:DP:37:LYS:HA    | 1.96                     | 0.46              |
| 40:DQ:77:LYS:HE2   | 40:DQ:116:LEU:HD21 | 1.97                     | 0.46              |
| 41:DR:2:TYR:H      | 41:DR:42:ALA:CB    | 2.28                     | 0.46              |
| 21:AA:1053:G:P     | 21:AA:1054:C:H3'   | 2.55                     | 0.46              |
| 8:AI:105:ARG:NE    | 21:AA:1117:A:H4'   | 2.29                     | 0.46              |
| 21:AA:119:A:H5''   | 21:AA:120:A:O4'    | 2.15                     | 0.46              |
| 21:AA:1426:G:N2    | 21:AA:1475:G:H1'   | 2.31                     | 0.46              |
| 21:AA:587:G:C2     | 21:AA:755:G:C5     | 3.03                     | 0.46              |
| 14:AO:21:THR:HG23  | 21:AA:657:U:O2     | 2.15                     | 0.46              |
| 21:AA:735:C:O2'    | 21:AA:736:C:H5'    | 2.15                     | 0.46              |
| 4:AE:14:LEU:HA     | 4:AE:36:THR:HA     | 1.97                     | 0.46              |
| 6:AG:146:ALA:C     | 6:AG:148:LYS:N     | 2.69                     | 0.46              |
| 8:AI:55:ASP:CG     | 8:AI:56:MET:H      | 2.19                     | 0.46              |
| 9:AJ:80:THR:HB     | 9:AJ:83:THR:HG22   | 1.97                     | 0.46              |
| 14:AO:40:GLY:HA2   | 14:AO:43:ALA:HB2   | 1.98                     | 0.46              |
| 18:AS:17:LYS:O     | 18:AS:20:LYS:HB3   | 2.15                     | 0.46              |
| 53:B3:62:PRO:HG2   | 53:B3:63:TYR:CD2   | 2.51                     | 0.46              |
| 24:BA:1061:U:H1'   | 24:BA:1070:A:O4'   | 2.15                     | 0.46              |
| 24:BA:1970:A:H4'   | 24:BA:1971:U:O5'   | 2.15                     | 0.46              |
| 24:BA:2063:C:H6    | 24:BA:2063:C:H5'   | 1.79                     | 0.46              |
| 24:BA:2273:A:C2    | 24:BA:2274:A:C5    | 3.03                     | 0.46              |
| 24:BA:2523:G:C2'   | 24:BA:2524:G:H5'   | 2.45                     | 0.46              |
| 24:BA:2581:G:H2'   | 24:BA:2610:C:H41   | 1.79                     | 0.46              |
| 24:BA:2856:A:C6    | 24:BA:2857:G:C6    | 3.03                     | 0.46              |
| 24:BA:93:G:N2      | 24:BA:94:A:H1'     | 2.29                     | 0.46              |
| 25:BB:90:C:C2'     | 25:BB:91:C:O5'     | 2.63                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:1803:A:H4'   | 26:BC:256:THR:OG1  | 2.15                     | 0.46              |
| 26:BC:268:ARG:HB3  | 26:BC:268:ARG:HH11 | 1.80                     | 0.46              |
| 26:BC:42:ARG:HG2   | 26:BC:48:ILE:HA    | 1.97                     | 0.46              |
| 27:BD:151:THR:HG22 | 27:BD:152:PRO:HD3  | 1.97                     | 0.46              |
| 29:BF:168:LEU:HD12 | 29:BF:168:LEU:O    | 2.15                     | 0.46              |
| 30:BG:120:ILE:HD11 | 30:BG:132:LEU:CB   | 2.42                     | 0.46              |
| 33:BJ:74:TYR:HB2   | 33:BJ:87:ALA:O     | 2.15                     | 0.46              |
| 35:BL:122:VAL:HG22 | 35:BL:122:VAL:O    | 2.15                     | 0.46              |
| 36:BM:59:ARG:O     | 36:BM:60:GLN:O     | 2.33                     | 0.46              |
| 40:BQ:114:ALA:C    | 40:BQ:116:LEU:H    | 2.17                     | 0.46              |
| 43:BT:14:PRO:HA    | 43:BT:32:LEU:HB3   | 1.96                     | 0.46              |
| 45:BV:68:LYS:O     | 45:BV:69:GLU:C     | 2.53                     | 0.46              |
| 55:CA:51:A:C6      | 55:CA:116:A:C8     | 3.03                     | 0.46              |
| 2:CC:2:GLN:HE21    | 55:CA:1191:A:P     | 2.38                     | 0.46              |
| 55:CA:1253:G:N1    | 55:CA:1285:A:N6    | 2.62                     | 0.46              |
| 55:CA:1276:G:O2'   | 55:CA:1277:C:H5'   | 2.15                     | 0.46              |
| 55:CA:1324:A:O2'   | 55:CA:1325:C:H5'   | 2.15                     | 0.46              |
| 55:CA:403:C:H2'    | 55:CA:404:G:H8     | 1.81                     | 0.46              |
| 55:CA:57:G:H2'     | 55:CA:58:C:H6      | 1.78                     | 0.46              |
| 55:CA:631:C:H3'    | 55:CA:632:U:H5'    | 1.97                     | 0.46              |
| 55:CA:702:A:H8     | 55:CA:702:A:OP1    | 1.97                     | 0.46              |
| 55:CA:861:G:C5     | 55:CA:862:C:C5     | 3.03                     | 0.46              |
| 55:CA:888:G:N1     | 55:CA:889:A:N6     | 2.63                     | 0.46              |
| 55:CA:890:G:O2'    | 55:CA:891:U:P      | 2.73                     | 0.46              |
| 55:CA:89:U:O2'     | 55:CA:90:C:O5'     | 2.34                     | 0.46              |
| 1:CB:101:THR:HG22  | 1:CB:178:LEU:HD13  | 1.97                     | 0.46              |
| 1:CB:71:THR:HA     | 1:CB:92:ASN:O      | 2.15                     | 0.46              |
| 2:CC:120:THR:CG2   | 2:CC:187:GLU:O     | 2.63                     | 0.46              |
| 5:CF:38:ARG:HD2    | 5:CF:63:ASN:HB2    | 1.96                     | 0.46              |
| 6:CG:115:MET:HA    | 6:CG:118:ARG:HD2   | 1.98                     | 0.46              |
| 6:CG:75:LYS:HG3    | 6:CG:76:SER:N      | 2.30                     | 0.46              |
| 4:CE:83:PRO:HD2    | 7:CH:95:MET:O      | 2.15                     | 0.46              |
| 9:CJ:15:HIS:HE1    | 9:CJ:68:ARG:HD3    | 1.80                     | 0.46              |
| 15:CP:20:VAL:HA    | 15:CP:36:VAL:HG12  | 1.96                     | 0.46              |
| 20:CU:16:ARG:O     | 20:CU:20:ARG:HG2   | 2.15                     | 0.46              |
| 53:D3:41:ARG:HG2   | 53:D3:44:ARG:NH2   | 2.30                     | 0.46              |
| 24:DA:1084:A:C2'   | 24:DA:1085:A:H5'   | 2.44                     | 0.46              |
| 24:DA:1286:A:O2'   | 24:DA:1288:G:N2    | 2.47                     | 0.46              |
| 24:DA:1470:A:C8    | 24:DA:1470:A:OP2   | 2.65                     | 0.46              |
| 24:DA:1519:G:N3    | 24:DA:1519:G:H2'   | 2.28                     | 0.46              |
| 24:DA:1633:G:C6    | 24:DA:1635:A:C6    | 3.03                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:1633:G:C6   | 24:DA:1635:A:C5    | 3.03                     | 0.46              |
| 24:DA:1665:A:N6   | 59:DA:3440:HOH:O   | 2.47                     | 0.46              |
| 24:DA:193:U:H4'   | 24:DA:803:U:H5'    | 1.97                     | 0.46              |
| 24:DA:2202:U:H5'' | 24:DA:2203:U:OP1   | 2.16                     | 0.46              |
| 24:DA:197:A:C8    | 24:DA:2430:A:N7    | 2.83                     | 0.46              |
| 24:DA:2611:C:H2'  | 24:DA:2612:C:H6    | 1.80                     | 0.46              |
| 24:DA:2725:A:C4   | 24:DA:2727:A:C8    | 3.03                     | 0.46              |
| 24:DA:2812:G:H2'  | 24:DA:2813:A:C8    | 2.49                     | 0.46              |
| 24:DA:2630:G:C6   | 24:DA:2894:G:O6    | 2.68                     | 0.46              |
| 24:DA:292:U:H2'   | 24:DA:293:U:H6     | 1.79                     | 0.46              |
| 24:DA:532:A:C2'   | 24:DA:532:A:N3     | 2.78                     | 0.46              |
| 24:DA:776:G:C8    | 24:DA:793:A:C5     | 3.03                     | 0.46              |
| 24:DA:831:G:O2'   | 24:DA:832:U:H5'    | 2.15                     | 0.46              |
| 26:DC:196:ASN:O   | 26:DC:197:ALA:HB3  | 2.15                     | 0.46              |
| 27:DD:105:LYS:HA  | 27:DD:177:VAL:CG2  | 2.40                     | 0.46              |
| 24:DA:674:G:H5''  | 28:DE:71:GLY:N     | 2.30                     | 0.46              |
| 30:DG:152:ARG:HD2 | 30:DG:153:PRO:HD2  | 1.97                     | 0.46              |
| 24:DA:1287:A:OP1  | 37:DN:103:ARG:HD2  | 2.15                     | 0.46              |
| 21:AA:1064:G:H1'  | 21:AA:1066:C:C6    | 2.50                     | 0.46              |
| 21:AA:1078:U:H3'  | 21:AA:1079:G:C8    | 2.50                     | 0.46              |
| 21:AA:15:G:C2     | 21:AA:16:A:C4      | 3.03                     | 0.46              |
| 21:AA:22:G:C6     | 21:AA:23:C:C4      | 3.03                     | 0.46              |
| 21:AA:265:G:H2'   | 21:AA:267:C:H5     | 1.81                     | 0.46              |
| 21:AA:540:G:C6    | 21:AA:541:G:C5     | 3.03                     | 0.46              |
| 21:AA:681:A:C2    | 21:AA:710:G:C2     | 3.03                     | 0.46              |
| 2:AC:33:ASP:O     | 2:AC:37:LYS:HB2    | 2.16                     | 0.46              |
| 3:AD:68:GLU:O     | 3:AD:72:ARG:HG2    | 2.15                     | 0.46              |
| 5:AF:45:ARG:HG2   | 5:AF:46:GLN:N      | 2.29                     | 0.46              |
| 7:AH:123:GLU:O    | 7:AH:125:ILE:HD12  | 2.15                     | 0.46              |
| 12:AM:106:ARG:HG3 | 12:AM:112:ARG:HH21 | 1.80                     | 0.46              |
| 12:AM:74:MET:HE2  | 12:AM:77:LYS:HB3   | 1.95                     | 0.46              |
| 10:AK:126:ARG:C   | 20:AU:33:ARG:HH12  | 2.19                     | 0.46              |
| 51:B1:10:LEU:HB3  | 51:B1:48:TYR:HB3   | 1.97                     | 0.46              |
| 24:BA:1020:A:C2   | 24:BA:1141:U:O2    | 2.69                     | 0.46              |
| 24:BA:1090:A:C6   | 24:BA:1102:C:C2    | 3.03                     | 0.46              |
| 24:BA:1347:A:O2'  | 24:BA:1348:C:H5'   | 2.15                     | 0.46              |
| 24:BA:1653:G:O6   | 37:BN:11:ASN:N     | 2.39                     | 0.46              |
| 24:BA:1659:G:C5   | 24:BA:1660:G:C8    | 3.03                     | 0.46              |
| 24:BA:1839:G:H2'  | 24:BA:1840:G:H8    | 1.81                     | 0.46              |
| 24:BA:1964:G:O2'  | 24:BA:1967:C:OP2   | 2.34                     | 0.46              |
| 24:BA:2418:A:H2'  | 24:BA:2419:U:O4'   | 2.16                     | 0.46              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 24:BA:2077:A:C8  | 24:BA:2435:A:C4    | 3.04                     | 0.46              |
| 24:BA:2461:A:H2' | 24:BA:2462:C:C6    | 2.49                     | 0.46              |
| 24:BA:292:U:C4   | 24:BA:293:U:C5     | 3.03                     | 0.46              |
| 24:BA:625:G:O2'  | 24:BA:626:A:H5'    | 2.14                     | 0.46              |
| 24:BA:745:G:H2'  | 24:BA:746:U:H5'    | 1.97                     | 0.46              |
| 24:BA:799:G:H2'  | 24:BA:800:A:H8     | 1.80                     | 0.46              |
| 27:BD:114:LYS:CD | 27:BD:116:LYS:HE2  | 2.45                     | 0.46              |
| 24:BA:2512:C:H1' | 27:BD:145:SER:O    | 2.15                     | 0.46              |
| 29:BF:3:LEU:HD12 | 29:BF:172:PHE:CD2  | 2.50                     | 0.46              |
| 29:BF:172:PHE:O  | 29:BF:173:ASP:C    | 2.53                     | 0.46              |
| 31:BH:41:LYS:HA  | 31:BH:44:ILE:CG1   | 2.41                     | 0.46              |
| 31:BH:89:LYS:O   | 31:BH:90:LEU:HD12  | 2.15                     | 0.46              |
| 35:BL:73:ILE:C   | 35:BL:105:ILE:HD13 | 2.35                     | 0.46              |
| 37:BN:82:GLU:O   | 37:BN:85:PRO:HG2   | 2.16                     | 0.46              |
| 40:BQ:104:ALA:O  | 40:BQ:108:LEU:HD12 | 2.16                     | 0.46              |
| 41:BR:24:LYS:HA  | 41:BR:94:THR:HG23  | 1.97                     | 0.46              |
| 42:BS:18:ARG:H   | 42:BS:18:ARG:HG3   | 1.56                     | 0.46              |
| 46:BW:28:GLU:H   | 46:BW:31:LEU:CD1   | 2.28                     | 0.46              |
| 55:CA:104:G:C2   | 55:CA:105:G:C8     | 3.03                     | 0.46              |
| 4:CE:88:HIS:HE1  | 55:CA:1078:U:O4'   | 1.98                     | 0.46              |
| 55:CA:1207:G:C5  | 55:CA:1208:C:C5    | 3.03                     | 0.46              |
| 55:CA:960:U:C4   | 55:CA:1225:A:H1'   | 2.49                     | 0.46              |
| 55:CA:1292:G:C5  | 55:CA:1293:C:C4    | 3.03                     | 0.46              |
| 55:CA:1399:C:O2  | 55:CA:1401:G:C5    | 2.67                     | 0.46              |
| 55:CA:426:U:C2   | 55:CA:427:U:C5     | 3.04                     | 0.46              |
| 55:CA:502:A:H2'  | 55:CA:503:C:O4'    | 2.15                     | 0.46              |
| 55:CA:585:G:C5   | 55:CA:586:C:C5     | 3.04                     | 0.46              |
| 2:CC:10:ARG:O    | 2:CC:13:ILE:O      | 2.32                     | 0.46              |
| 3:CD:176:LYS:O   | 3:CD:176:LYS:HG3   | 2.15                     | 0.46              |
| 8:CI:121:ARG:HG3 | 55:CA:1348:U:H4'   | 1.97                     | 0.46              |
| 11:CL:4:ASN:HA   | 11:CL:7:VAL:HG23   | 1.97                     | 0.46              |
| 16:CQ:26:ARG:HG3 | 16:CQ:39:ARG:HB2   | 1.98                     | 0.46              |
| 18:CS:35:ARG:HA  | 18:CS:70:LEU:CB    | 2.42                     | 0.46              |
| 24:DA:1011:G:C6  | 24:DA:1013:C:N3    | 2.83                     | 0.46              |
| 24:DA:1090:A:C6  | 24:DA:1102:C:O2    | 2.68                     | 0.46              |
| 24:DA:110:G:C2   | 24:DA:111:A:C8     | 3.04                     | 0.46              |
| 24:DA:1450:G:C2  | 24:DA:1462:C:N3    | 2.83                     | 0.46              |
| 24:DA:1534:U:O2  | 24:DA:1534:U:H2'   | 2.15                     | 0.46              |
| 24:DA:1539:U:H2' | 24:DA:1540:G:C8    | 2.50                     | 0.46              |
| 24:DA:1873:G:N2  | 24:DA:1874:C:C2    | 2.84                     | 0.46              |
| 24:DA:2093:G:C8  | 24:DA:2225:A:C4    | 3.03                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:2413:G:N2   | 24:DA:2414:G:H1'  | 2.31                     | 0.46              |
| 24:DA:2473:U:P    | 24:DA:2473:U:H6   | 2.38                     | 0.46              |
| 24:DA:2513:A:H2'  | 24:DA:2514:U:C6   | 2.51                     | 0.46              |
| 24:DA:2592:G:C4   | 24:DA:2593:U:C6   | 3.03                     | 0.46              |
| 24:DA:224:U:C5    | 24:DA:420:C:H4'   | 2.49                     | 0.46              |
| 24:DA:33:C:N4     | 24:DA:446:G:O2'   | 2.48                     | 0.46              |
| 24:DA:616:A:O2'   | 24:DA:617:G:O4'   | 2.28                     | 0.46              |
| 24:DA:779:U:C2'   | 24:DA:780:G:H5'   | 2.45                     | 0.46              |
| 24:DA:95:A:O2'    | 48:DY:41:HIS:HD2  | 1.99                     | 0.46              |
| 26:DC:75:ALA:HA   | 26:DC:95:TYR:HA   | 1.97                     | 0.46              |
| 27:DD:193:VAL:O   | 27:DD:194:PRO:O   | 2.33                     | 0.46              |
| 30:DG:8:VAL:HG11  | 30:DG:49:LEU:HD23 | 1.97                     | 0.46              |
| 31:DH:62:LEU:C    | 31:DH:64:ALA:H    | 2.18                     | 0.46              |
| 36:DM:136:MET:HE1 | 45:DV:75:GLN:C    | 2.35                     | 0.46              |
| 37:DN:1:MET:O     | 37:DN:2:ARG:CB    | 2.62                     | 0.46              |
| 38:DO:18:LEU:HD21 | 38:DO:91:SER:HB2  | 1.96                     | 0.46              |
| 42:DS:71:VAL:HG23 | 42:DS:107:VAL:HB  | 1.96                     | 0.46              |
| 44:DU:7:ASP:O     | 44:DU:8:ASP:HB2   | 2.15                     | 0.46              |
| 47:DX:65:THR:O    | 47:DX:68:ALA:HB3  | 2.15                     | 0.46              |
| 21:AA:1061:G:N7   | 21:AA:1062:U:C4   | 2.84                     | 0.46              |
| 21:AA:1096:C:H2'  | 21:AA:1097:C:O4'  | 2.16                     | 0.46              |
| 21:AA:1163:A:H2'  | 21:AA:1164:G:C8   | 2.51                     | 0.46              |
| 21:AA:115:G:H1'   | 21:AA:116:A:N7    | 2.30                     | 0.46              |
| 21:AA:1181:G:N2   | 21:AA:1182:G:N2   | 2.63                     | 0.46              |
| 21:AA:1185:G:C4   | 21:AA:1186:G:C8   | 3.04                     | 0.46              |
| 21:AA:1054:C:OP1  | 21:AA:1198:G:OP2  | 2.34                     | 0.46              |
| 21:AA:1352:C:H2'  | 21:AA:1353:G:C8   | 2.51                     | 0.46              |
| 21:AA:1441:A:N6   | 21:AA:1461:G:H21  | 2.13                     | 0.46              |
| 21:AA:41:G:N3     | 21:AA:42:G:C8     | 2.84                     | 0.46              |
| 21:AA:481:G:O2'   | 21:AA:482:A:H8    | 1.98                     | 0.46              |
| 1:AB:52:ALA:HA    | 1:AB:197:PHE:CD1  | 2.51                     | 0.46              |
| 2:AC:39:ARG:CG    | 2:AC:54:ILE:HD11  | 2.45                     | 0.46              |
| 3:AD:109:THR:CG2  | 3:AD:112:GLU:HB2  | 2.46                     | 0.46              |
| 7:AH:4:ASP:OD2    | 7:AH:76:ARG:NH1   | 2.49                     | 0.46              |
| 8:AI:14:SER:OG    | 8:AI:69:GLY:HA3   | 2.15                     | 0.46              |
| 15:AP:22:ALA:HB2  | 15:AP:32:PHE:HA   | 1.97                     | 0.46              |
| 24:BA:1927:A:H2'  | 24:BA:1928:A:C8   | 2.50                     | 0.46              |
| 24:BA:2536:G:C5   | 24:BA:2537:U:C5   | 3.03                     | 0.46              |
| 24:BA:2742:G:C2'  | 24:BA:2743:U:H5'  | 2.46                     | 0.46              |
| 24:BA:2828:G:H2'  | 24:BA:2829:A:H5'  | 1.97                     | 0.46              |
| 24:BA:312:G:H2'   | 24:BA:313:G:C8    | 2.47                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:763:G:O2'   | 24:BA:765:C:H5'   | 2.15                     | 0.46              |
| 25:BB:37:C:H6     | 25:BB:37:C:C5'    | 2.28                     | 0.46              |
| 26:BC:106:PRO:N   | 26:BC:141:HIS:HE1 | 2.14                     | 0.46              |
| 27:BD:121:THR:O   | 27:BD:122:VAL:CG2 | 2.64                     | 0.46              |
| 28:BE:37:ALA:O    | 28:BE:39:ALA:N    | 2.47                     | 0.46              |
| 33:BJ:110:PRO:HB2 | 33:BJ:111:LYS:HG3 | 1.96                     | 0.46              |
| 40:BQ:4:LYS:HZ3   | 40:BQ:7:VAL:HG13  | 1.78                     | 0.46              |
| 41:BR:4:VAL:HG23  | 41:BR:39:LEU:HG   | 1.97                     | 0.46              |
| 44:BU:38:ILE:HG22 | 44:BU:39:ASN:H    | 1.79                     | 0.46              |
| 47:BX:39:VAL:HG13 | 47:BX:46:VAL:HG22 | 1.96                     | 0.46              |
| 55:CA:1153:G:N2   | 55:CA:1154:G:H1'  | 2.29                     | 0.46              |
| 55:CA:1160:G:O2'  | 55:CA:1161:C:C5'  | 2.63                     | 0.46              |
| 55:CA:1201:A:H5'  | 55:CA:1203:C:OP2  | 2.16                     | 0.46              |
| 55:CA:1210:C:H1'  | 55:CA:1214:C:C4   | 2.50                     | 0.46              |
| 55:CA:1255:G:C5   | 55:CA:1279:G:C6   | 3.04                     | 0.46              |
| 55:CA:1433:A:C4   | 55:CA:1468:A:C2   | 3.03                     | 0.46              |
| 16:CQ:68:LYS:HE2  | 55:CA:253:A:OP1   | 2.15                     | 0.46              |
| 55:CA:813:U:H2'   | 55:CA:814:A:H5'   | 1.96                     | 0.46              |
| 1:CB:185:ILE:HG22 | 1:CB:199:ILE:HG13 | 1.97                     | 0.46              |
| 1:CB:221:ARG:HG3  | 1:CB:222:GLU:H    | 1.79                     | 0.46              |
| 3:CD:30:LYS:HB2   | 3:CD:30:LYS:NZ    | 2.31                     | 0.46              |
| 11:CL:91:GLY:O    | 11:CL:92:VAL:C    | 2.53                     | 0.46              |
| 12:CM:12:LYS:O    | 12:CM:44:ILE:HG13 | 2.15                     | 0.46              |
| 52:D2:15:SER:O    | 52:D2:16:HIS:ND1  | 2.48                     | 0.46              |
| 52:D2:46:LYS:N    | 52:D2:46:LYS:HD2  | 2.31                     | 0.46              |
| 24:DA:1126:A:H4'  | 24:DA:1127:A:C5'  | 2.46                     | 0.46              |
| 24:DA:1212:G:H1'  | 24:DA:1236:G:N2   | 2.31                     | 0.46              |
| 24:DA:1325:U:O2'  | 24:DA:1326:U:H5'  | 2.15                     | 0.46              |
| 24:DA:1413:A:C6   | 24:DA:1414:C:N4   | 2.83                     | 0.46              |
| 24:DA:1722:A:C6   | 24:DA:1739:A:C8   | 3.03                     | 0.46              |
| 24:DA:389:G:N9    | 24:DA:2413:G:H4'  | 2.31                     | 0.46              |
| 24:DA:2458:G:H4'  | 24:DA:2459:A:C8   | 2.50                     | 0.46              |
| 24:DA:687:C:O2'   | 24:DA:688:U:C5'   | 2.64                     | 0.46              |
| 24:DA:751:A:C5'   | 42:DS:90:LYS:HA   | 2.46                     | 0.46              |
| 24:DA:811:U:O4    | 35:DL:21:ARG:NH1  | 2.46                     | 0.46              |
| 24:DA:963:U:O2'   | 24:DA:964:C:H6    | 1.98                     | 0.46              |
| 24:DA:972:A:C6    | 24:DA:973:A:N6    | 2.84                     | 0.46              |
| 24:DA:982:C:H5''  | 24:DA:983:A:OP1   | 2.14                     | 0.46              |
| 35:DL:79:LEU:HD23 | 35:DL:82:LEU:CD1  | 2.45                     | 0.46              |
| 37:DN:37:THR:HA   | 37:DN:110:MET:HE2 | 1.96                     | 0.46              |
| 37:DN:82:GLU:C    | 37:DN:85:PRO:HD2  | 2.35                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:DO:49:VAL:CG1  | 38:DO:81:ARG:HB3  | 2.45                     | 0.46              |
| 38:DO:62:LEU:C    | 38:DO:62:LEU:HD13 | 2.36                     | 0.46              |
| 42:DS:70:LYS:HD2  | 42:DS:110:ARG:O   | 2.16                     | 0.46              |
| 56:DB:73:A:C2     | 45:DV:37:PRO:HB3  | 2.50                     | 0.46              |
| 46:DW:14:ASP:O    | 46:DW:15:SER:HB2  | 2.15                     | 0.46              |
| 46:DW:42:THR:O    | 46:DW:43:LYS:HG2  | 2.15                     | 0.46              |
| 21:AA:1036:A:H5'  | 21:AA:1037:C:P    | 2.56                     | 0.46              |
| 21:AA:1050:G:O2'  | 21:AA:1051:C:C5'  | 2.63                     | 0.46              |
| 12:AM:112:ARG:HA  | 21:AA:1228:C:OP1  | 2.16                     | 0.46              |
| 21:AA:1403:C:H1'  | 21:AA:1500:A:N1   | 2.30                     | 0.46              |
| 21:AA:370:C:O2'   | 21:AA:371:A:H5'   | 2.15                     | 0.46              |
| 21:AA:386:C:C2'   | 21:AA:387:U:H5'   | 2.46                     | 0.46              |
| 5:AF:49:TYR:HE2   | 5:AF:51:ILE:HB    | 1.81                     | 0.46              |
| 5:AF:91:ARG:HG3   | 5:AF:92:THR:H     | 1.81                     | 0.46              |
| 5:AF:3:HIS:ND1    | 5:AF:95:ALA:HB2   | 2.29                     | 0.46              |
| 6:AG:119:LEU:HD23 | 6:AG:119:LEU:C    | 2.35                     | 0.46              |
| 7:AH:91:LEU:HD23  | 7:AH:92:PRO:HD2   | 1.97                     | 0.46              |
| 8:AI:9:GLY:HA2    | 8:AI:80:HIS:CD2   | 2.50                     | 0.46              |
| 9:AJ:15:HIS:CG    | 9:AJ:16:ARG:N     | 2.83                     | 0.46              |
| 51:B1:25:ASN:O    | 51:B1:26:LYS:C    | 2.53                     | 0.46              |
| 53:B3:14:LYS:O    | 53:B3:15:LYS:C    | 2.54                     | 0.46              |
| 54:B4:36:ARG:O    | 54:B4:37:GLN:C    | 2.54                     | 0.46              |
| 24:BA:1082:U:H2'  | 24:BA:1083:U:O2   | 2.16                     | 0.46              |
| 24:BA:1097:U:H3'  | 24:BA:1098:A:C4'  | 2.45                     | 0.46              |
| 24:BA:1229:C:H2'  | 24:BA:1230:A:H8   | 1.79                     | 0.46              |
| 24:BA:151:C:O2    | 24:BA:176:A:H2    | 1.99                     | 0.46              |
| 24:BA:1620:G:C2'  | 24:BA:1621:U:H5'  | 2.46                     | 0.46              |
| 24:BA:945:A:C5    | 24:BA:2448:A:C2   | 3.04                     | 0.46              |
| 24:BA:2555:U:C5   | 24:BA:2556:C:N1   | 2.83                     | 0.46              |
| 24:BA:2827:C:H2'  | 24:BA:2828:G:H8   | 1.80                     | 0.46              |
| 24:BA:595:C:H2'   | 24:BA:596:U:C6    | 2.50                     | 0.46              |
| 24:BA:66:C:C4     | 24:BA:67:U:C4     | 3.04                     | 0.46              |
| 24:BA:72:U:C4     | 24:BA:112:U:H4'   | 2.50                     | 0.46              |
| 24:BA:778:G:C6    | 24:BA:779:U:C4    | 3.03                     | 0.46              |
| 24:BA:820:A:H8    | 24:BA:820:A:O5'   | 1.98                     | 0.46              |
| 26:BC:114:GLN:O   | 26:BC:115:ILE:CD1 | 2.64                     | 0.46              |
| 27:BD:182:ALA:C   | 27:BD:184:ARG:N   | 2.68                     | 0.46              |
| 29:BF:13:LYS:HD2  | 29:BF:13:LYS:O    | 2.15                     | 0.46              |
| 29:BF:173:ASP:O   | 29:BF:174:PHE:C   | 2.53                     | 0.46              |
| 30:BG:166:GLU:OE2 | 30:BG:166:GLU:C   | 2.53                     | 0.46              |
| 33:BJ:117:ALA:HA  | 33:BJ:120:ARG:NH2 | 2.30                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BK:85:VAL:HG11  | 34:BK:115:ILE:HD11 | 1.98                     | 0.46              |
| 36:BM:53:MET:O     | 36:BM:56:ALA:HB3   | 2.16                     | 0.46              |
| 37:BN:71:ARG:HH21  | 37:BN:71:ARG:HG3   | 1.79                     | 0.46              |
| 41:BR:1:MET:HG3    | 41:BR:1:MET:O      | 2.15                     | 0.46              |
| 24:BA:747:U:O2'    | 42:BS:88:ARG:NH2   | 2.49                     | 0.46              |
| 43:BT:32:LEU:O     | 43:BT:34:VAL:HG13  | 2.15                     | 0.46              |
| 55:CA:1349:A:C4    | 55:CA:1350:A:C8    | 3.03                     | 0.46              |
| 55:CA:768:A:H5'    | 55:CA:1524:C:H1'   | 1.98                     | 0.46              |
| 1:CB:127:LYS:HG3   | 1:CB:128:LEU:HD13  | 1.97                     | 0.46              |
| 2:CC:140:ALA:O     | 2:CC:145:ALA:HB3   | 2.15                     | 0.46              |
| 2:CC:149:LYS:CG    | 2:CC:168:ARG:HB2   | 2.46                     | 0.46              |
| 2:CC:172:VAL:O     | 2:CC:172:VAL:HG12  | 2.15                     | 0.46              |
| 2:CC:183:TYR:HE1   | 2:CC:200:TRP:CZ2   | 2.34                     | 0.46              |
| 4:CE:114:LEU:HD13  | 4:CE:122:VAL:HG21  | 1.97                     | 0.46              |
| 5:CF:92:THR:C      | 5:CF:93:LYS:HG2    | 2.36                     | 0.46              |
| 6:CG:61:PHE:HE2    | 6:CG:123:LEU:HD11  | 1.80                     | 0.46              |
| 7:CH:42:GLU:O      | 7:CH:42:GLU:OE2    | 2.34                     | 0.46              |
| 7:CH:93:LYS:H      | 7:CH:93:LYS:HD3    | 1.79                     | 0.46              |
| 10:CK:94:SER:O     | 10:CK:97:ARG:HB2   | 2.15                     | 0.46              |
| 13:CN:87:ALA:HB1   | 13:CN:95:LEU:HD23  | 1.97                     | 0.46              |
| 24:DA:1060:U:O4'   | 24:DA:1061:U:H2'   | 2.15                     | 0.46              |
| 24:DA:1152:C:H2'   | 24:DA:1153:C:C6    | 2.50                     | 0.46              |
| 24:DA:1512:C:C4    | 24:DA:1513:U:C4    | 3.02                     | 0.46              |
| 24:DA:1926:U:H2'   | 24:DA:1928:A:N7    | 2.31                     | 0.46              |
| 24:DA:1946:U:O2'   | 24:DA:1947:C:H5'   | 2.15                     | 0.46              |
| 24:DA:2348:U:H2'   | 24:DA:2349:G:H8    | 1.80                     | 0.46              |
| 24:DA:2407:A:H2'   | 24:DA:2408:U:C5    | 2.50                     | 0.46              |
| 24:DA:2422:C:H2'   | 24:DA:2423:U:H5''  | 1.97                     | 0.46              |
| 24:DA:2455:G:C6    | 24:DA:2498:C:N4    | 2.84                     | 0.46              |
| 24:DA:576:U:H4'    | 24:DA:2502:G:C8    | 2.50                     | 0.46              |
| 24:DA:784:G:OP1    | 24:DA:2588:G:H5''  | 2.16                     | 0.46              |
| 24:DA:2593:U:N3    | 24:DA:2594:C:C5    | 2.83                     | 0.46              |
| 24:DA:296:U:H2'    | 24:DA:297:G:C8     | 2.51                     | 0.46              |
| 24:DA:365:U:H2'    | 24:DA:366:C:C6     | 2.51                     | 0.46              |
| 24:DA:439:A:H2'    | 24:DA:440:C:O4'    | 2.14                     | 0.46              |
| 56:DB:49:C:OP1     | 38:DO:102:ARG:HB2  | 2.15                     | 0.46              |
| 56:DB:21:G:C2      | 56:DB:63:C:C2      | 3.03                     | 0.46              |
| 26:DC:103:ILE:HD12 | 26:DC:104:LEU:H    | 1.81                     | 0.46              |
| 27:DD:16:THR:HG23  | 27:DD:18:ASP:H     | 1.80                     | 0.46              |
| 27:DD:38:LYS:HD2   | 27:DD:45:TYR:OH    | 2.16                     | 0.46              |
| 28:DE:24:ASN:O     | 28:DE:28:VAL:HG13  | 2.16                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DH:5:LEU:O     | 31:DH:6:LEU:HD12   | 2.15                     | 0.46              |
| 36:DM:118:LYS:O   | 36:DM:118:LYS:HD3  | 2.16                     | 0.46              |
| 37:DN:51:LEU:HD21 | 37:DN:69:ARG:HG3   | 1.98                     | 0.46              |
| 40:DQ:111:LYS:HE3 | 41:DR:48:LYS:HD3   | 1.96                     | 0.46              |
| 40:DQ:15:LYS:HD2  | 40:DQ:19:GLN:HE21  | 1.81                     | 0.46              |
| 43:DT:10:VAL:HG23 | 43:DT:11:LEU:CD1   | 2.45                     | 0.46              |
| 43:DT:69:ARG:HD2  | 43:DT:70:HIS:H     | 1.79                     | 0.46              |
| 47:DX:4:CYS:O     | 47:DX:4:CYS:SG     | 2.73                     | 0.46              |
| 21:AA:112:G:C2    | 21:AA:113:G:C8     | 3.04                     | 0.46              |
| 21:AA:15:G:C5     | 21:AA:1396:A:N1    | 2.83                     | 0.46              |
| 17:AR:49:LYS:HB2  | 21:AA:835:U:OP1    | 2.16                     | 0.46              |
| 1:AB:187:ASP:HB2  | 1:AB:203:ASP:CG    | 2.36                     | 0.46              |
| 4:AE:117:ALA:HB3  | 4:AE:119:VAL:HG22  | 1.97                     | 0.46              |
| 4:AE:76:ASN:O     | 4:AE:77:ASN:CB     | 2.62                     | 0.46              |
| 6:AG:68:VAL:HG12  | 6:AG:102:TRP:CE3   | 2.50                     | 0.46              |
| 9:AJ:91:ASP:O     | 9:AJ:92:LEU:HG     | 2.16                     | 0.46              |
| 12:AM:74:MET:CE   | 12:AM:77:LYS:HD3   | 2.45                     | 0.46              |
| 14:AO:40:GLY:O    | 14:AO:43:ALA:HB3   | 2.15                     | 0.46              |
| 14:AO:50:HIS:CE1  | 21:AA:667:G:H4'    | 2.51                     | 0.46              |
| 15:AP:31:ARG:HH21 | 21:AA:230:G:H5''   | 1.81                     | 0.46              |
| 18:AS:30:LEU:N    | 18:AS:30:LEU:HD12  | 2.31                     | 0.46              |
| 18:AS:51:HIS:CD2  | 18:AS:53:GLY:H     | 2.32                     | 0.46              |
| 21:AA:1054:C:N4   | 22:AX:34:G:C4      | 2.84                     | 0.46              |
| 24:BA:111:A:N1    | 24:BA:112:U:C2     | 2.84                     | 0.46              |
| 24:BA:1235:G:C2   | 24:BA:1236:G:N2    | 2.84                     | 0.46              |
| 24:BA:1328:A:HO2' | 24:BA:1329:U:H6    | 1.63                     | 0.46              |
| 24:BA:1429:G:N3   | 24:BA:1568:G:N2    | 2.63                     | 0.46              |
| 24:BA:1569:A:N6   | 24:BA:1570:A:N1    | 2.64                     | 0.46              |
| 24:BA:2106:U:C4   | 24:BA:2107:G:N7    | 2.84                     | 0.46              |
| 24:BA:2136:G:H2'  | 24:BA:2137:U:C6    | 2.45                     | 0.46              |
| 24:BA:2594:C:O2'  | 24:BA:2595:G:H5'   | 2.16                     | 0.46              |
| 24:BA:264:C:C2'   | 24:BA:265:A:H5''   | 2.46                     | 0.46              |
| 24:BA:2673:G:C2   | 24:BA:2674:G:N7    | 2.83                     | 0.46              |
| 24:BA:2776:A:H4'  | 24:BA:2777:G:O5'   | 2.15                     | 0.46              |
| 24:BA:445:C:H5''  | 40:BQ:2:ARG:HB2    | 1.98                     | 0.46              |
| 24:BA:551:G:C6    | 24:BA:552:U:C4     | 3.03                     | 0.46              |
| 30:BG:72:ASN:C    | 30:BG:72:ASN:HD22  | 2.18                     | 0.46              |
| 32:BI:107:GLU:O   | 32:BI:111:THR:HG23 | 2.16                     | 0.46              |
| 34:BK:12:ASP:OD1  | 34:BK:12:ASP:C     | 2.53                     | 0.46              |
| 35:BL:80:SER:O    | 35:BL:81:ASP:O     | 2.34                     | 0.46              |
| 41:BR:49:ILE:CG1  | 41:BR:51:VAL:O     | 2.63                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:BW:17:ALA:O    | 46:BW:18:LYS:CB    | 2.64                     | 0.46              |
| 49:BZ:52:PHE:CE2  | 49:BZ:53:MET:HG2   | 2.51                     | 0.46              |
| 55:CA:1134:G:C2   | 55:CA:1135:U:O2'   | 2.66                     | 0.46              |
| 55:CA:119:A:H5'   | 55:CA:120:A:O4'    | 2.16                     | 0.46              |
| 55:CA:1415:G:N2   | 55:CA:1486:G:C4    | 2.84                     | 0.46              |
| 55:CA:200:G:N1    | 55:CA:201:G:C5     | 2.84                     | 0.46              |
| 55:CA:246:A:O3'   | 55:CA:247:G:H4'    | 2.16                     | 0.46              |
| 55:CA:317:U:C2'   | 55:CA:318:G:H8     | 2.26                     | 0.46              |
| 55:CA:33:A:H2'    | 55:CA:34:C:H6      | 1.78                     | 0.46              |
| 55:CA:369:G:O2'   | 55:CA:370:C:C6     | 2.67                     | 0.46              |
| 55:CA:32:A:C6     | 55:CA:553:A:N1     | 2.83                     | 0.46              |
| 55:CA:565:U:H2'   | 55:CA:566:G:C8     | 2.50                     | 0.46              |
| 55:CA:767:A:C5    | 55:CA:768:A:N7     | 2.83                     | 0.46              |
| 55:CA:770:C:H1'   | 55:CA:899:C:H42    | 1.80                     | 0.46              |
| 55:CA:813:U:H3'   | 55:CA:816:A:H62    | 1.81                     | 0.46              |
| 55:CA:938:A:C6    | 55:CA:939:G:C5     | 3.03                     | 0.46              |
| 1:CB:120:SER:HA   | 1:CB:125:PHE:CZ    | 2.51                     | 0.46              |
| 1:CB:14:HIS:O     | 1:CB:14:HIS:CG     | 2.68                     | 0.46              |
| 2:CC:179:ALA:O    | 2:CC:180:ASP:C     | 2.54                     | 0.46              |
| 5:CF:2:ARG:NH2    | 5:CF:91:ARG:HB2    | 2.30                     | 0.46              |
| 8:CI:33:SER:N     | 8:CI:36:GLN:HG3    | 2.30                     | 0.46              |
| 11:CL:49:ARG:HG3  | 11:CL:65:TYR:OH    | 2.15                     | 0.46              |
| 15:CP:10:GLY:HA2  | 55:CA:624:C:O3'    | 2.16                     | 0.46              |
| 24:DA:1004:U:H1'  | 24:DA:1010:A:N3    | 2.30                     | 0.46              |
| 24:DA:83:A:C6     | 24:DA:101:A:OP1    | 2.68                     | 0.46              |
| 24:DA:1059:G:C5   | 24:DA:1060:U:N3    | 2.84                     | 0.46              |
| 24:DA:122:G:O2'   | 24:DA:123:G:C5'    | 2.64                     | 0.46              |
| 24:DA:1331:G:C4   | 24:DA:1333:G:C8    | 3.03                     | 0.46              |
| 24:DA:1695:G:HO2' | 24:DA:1696:G:P     | 2.39                     | 0.46              |
| 24:DA:1832:C:H2'  | 24:DA:1833:C:O4'   | 2.16                     | 0.46              |
| 24:DA:858:G:C4    | 24:DA:2268:A:C2    | 3.03                     | 0.46              |
| 24:DA:2660:A:C2   | 24:DA:2661:G:C8    | 3.03                     | 0.46              |
| 24:DA:284:U:OP2   | 24:DA:284:U:H6     | 1.98                     | 0.46              |
| 24:DA:2900:A:C2   | 24:DA:2901:C:C2    | 3.04                     | 0.46              |
| 24:DA:482:A:N6    | 24:DA:506:G:N9     | 2.63                     | 0.46              |
| 24:DA:51:G:N3     | 24:DA:119:A:C2     | 2.84                     | 0.46              |
| 24:DA:734:A:C5    | 24:DA:735:A:C8     | 3.04                     | 0.46              |
| 24:DA:777:G:N2    | 24:DA:778:G:C4     | 2.84                     | 0.46              |
| 24:DA:838:C:C2    | 24:DA:941:A:C2     | 3.04                     | 0.46              |
| 26:DC:128:THR:C   | 26:DC:129:LEU:HD23 | 2.35                     | 0.46              |
| 24:DA:1797:G:O3'  | 26:DC:255:LYS:O    | 2.33                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:DF:135:ILE:HD12 | 29:DF:135:ILE:N   | 2.31                     | 0.46              |
| 24:DA:812:C:O5'    | 35:DL:22:GLY:HA2  | 2.16                     | 0.46              |
| 47:DX:3:VAL:O      | 47:DX:3:VAL:HG23  | 2.14                     | 0.46              |
| 21:AA:1224:U:C4'   | 21:AA:1225:A:OP2  | 2.57                     | 0.46              |
| 21:AA:1239:A:H62   | 21:AA:1299:A:N6   | 2.13                     | 0.46              |
| 21:AA:261:U:H2'    | 21:AA:263:A:OP2   | 2.14                     | 0.46              |
| 21:AA:414:A:N3     | 21:AA:414:A:C2'   | 2.79                     | 0.46              |
| 21:AA:544:G:C6     | 21:AA:545:C:C4    | 3.04                     | 0.46              |
| 21:AA:683:G:N1     | 21:AA:684:U:C2    | 2.83                     | 0.46              |
| 21:AA:736:C:H2'    | 21:AA:737:C:C6    | 2.51                     | 0.46              |
| 21:AA:803:G:H2'    | 21:AA:804:U:C6    | 2.51                     | 0.46              |
| 21:AA:892:A:C6     | 21:AA:893:C:C4    | 3.03                     | 0.46              |
| 21:AA:918:A:H2'    | 21:AA:919:A:O4'   | 2.15                     | 0.46              |
| 21:AA:956:U:H2'    | 21:AA:956:U:O2    | 2.15                     | 0.46              |
| 1:AB:106:VAL:O     | 1:AB:106:VAL:HG12 | 2.16                     | 0.46              |
| 1:AB:15:PHE:HB2    | 1:AB:39:ILE:CG2   | 2.44                     | 0.46              |
| 3:AD:104:MET:HE3   | 3:AD:170:LEU:HD22 | 1.97                     | 0.46              |
| 3:AD:43:ARG:HA     | 3:AD:43:ARG:CZ    | 2.46                     | 0.46              |
| 3:AD:54:LEU:O      | 3:AD:58:GLN:HB2   | 2.16                     | 0.46              |
| 4:AE:76:ASN:CB     | 4:AE:81:GLN:HG2   | 2.43                     | 0.46              |
| 5:AF:70:VAL:HA     | 5:AF:73:GLU:HB3   | 1.98                     | 0.46              |
| 6:AG:144:ALA:O     | 6:AG:146:ALA:N    | 2.49                     | 0.46              |
| 7:AH:48:PHE:O      | 7:AH:49:LYS:HG3   | 2.15                     | 0.46              |
| 8:AI:14:SER:HB3    | 8:AI:74:GLN:HA    | 1.97                     | 0.46              |
| 10:AK:57:SER:O     | 10:AK:90:PRO:HG3  | 2.16                     | 0.46              |
| 11:AL:33:CYS:CA    | 11:AL:54:VAL:HA   | 2.26                     | 0.46              |
| 11:AL:54:VAL:HG21  | 11:AL:79:ILE:HD11 | 1.97                     | 0.46              |
| 11:AL:84:GLY:O     | 11:AL:95:HIS:HD2  | 1.99                     | 0.46              |
| 17:AR:44:THR:OG1   | 17:AR:46:THR:HG22 | 2.16                     | 0.46              |
| 22:AX:30:G:C2      | 22:AX:31:A:C8     | 3.04                     | 0.46              |
| 24:BA:1310:G:N2    | 24:BA:1313:U:C5   | 2.83                     | 0.46              |
| 24:BA:1320:C:C6    | 24:BA:1329:U:OP2  | 2.69                     | 0.46              |
| 24:BA:1327:A:O2'   | 24:BA:1328:A:H5'  | 2.15                     | 0.46              |
| 24:BA:1425:G:N1    | 24:BA:1426:G:C2   | 2.83                     | 0.46              |
| 24:BA:1445:G:O2'   | 24:BA:1446:C:H5'  | 2.16                     | 0.46              |
| 24:BA:1746:A:C4    | 24:BA:1747:U:C5   | 3.04                     | 0.46              |
| 24:BA:2273:A:H2'   | 24:BA:2274:A:C8   | 2.51                     | 0.46              |
| 24:BA:2404:U:C2    | 24:BA:2414:G:N1   | 2.83                     | 0.46              |
| 24:BA:2625:G:H2'   | 24:BA:2626:C:O4'  | 2.16                     | 0.46              |
| 24:BA:272:A:O2'    | 24:BA:273:G:C5'   | 2.64                     | 0.46              |
| 24:BA:2805:C:C5    | 24:BA:2806:C:C5   | 3.04                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:BA:2816:G:O3'   | 37:BN:99:LYS:HE2  | 2.15                     | 0.46              |
| 24:BA:396:G:OP2    | 47:BX:9:LYS:NZ    | 2.46                     | 0.46              |
| 24:BA:68:G:C5      | 24:BA:69:C:C5     | 3.04                     | 0.46              |
| 24:BA:752:A:O2'    | 24:BA:753:A:OP2   | 2.31                     | 0.46              |
| 24:BA:763:G:C8     | 24:BA:765:C:C6    | 3.04                     | 0.46              |
| 24:BA:857:G:H2'    | 24:BA:858:G:O4'   | 2.15                     | 0.46              |
| 24:BA:96:C:H2'     | 24:BA:97:C:H6     | 1.81                     | 0.46              |
| 27:BD:125:TRP:CD2  | 27:BD:160:LYS:HG2 | 2.50                     | 0.46              |
| 28:BE:109:LEU:HD13 | 28:BE:109:LEU:HA  | 1.75                     | 0.46              |
| 31:BH:101:ASP:C    | 31:BH:104:THR:HB  | 2.36                     | 0.46              |
| 24:BA:1063:G:OP1   | 32:BI:76:ALA:HB3  | 2.16                     | 0.46              |
| 33:BJ:128:ASN:O    | 33:BJ:128:ASN:CG  | 2.54                     | 0.46              |
| 35:BL:47:ARG:CG    | 35:BL:50:PHE:HB2  | 2.45                     | 0.46              |
| 36:BM:24:THR:O     | 36:BM:34:LYS:CE   | 2.63                     | 0.46              |
| 39:BP:25:VAL:CG2   | 39:BP:83:ILE:HD11 | 2.46                     | 0.46              |
| 40:BQ:86:SER:O     | 40:BQ:87:VAL:C    | 2.54                     | 0.46              |
| 42:BS:72:THR:HG21  | 42:BS:108:SER:OG  | 2.15                     | 0.46              |
| 43:BT:50:LEU:O     | 43:BT:51:PHE:HB2  | 2.15                     | 0.46              |
| 44:BU:38:ILE:O     | 44:BU:40:LEU:N    | 2.49                     | 0.46              |
| 46:BW:66:VAL:HG12  | 46:BW:67:LYS:N    | 2.31                     | 0.46              |
| 55:CA:1072:G:H2'   | 55:CA:1073:U:C6   | 2.50                     | 0.46              |
| 55:CA:1144:G:H2'   | 55:CA:1145:A:O4'  | 2.16                     | 0.46              |
| 55:CA:1160:G:O2'   | 55:CA:1161:C:H6   | 1.98                     | 0.46              |
| 55:CA:814:A:H5'    | 55:CA:1511:G:H4'  | 1.98                     | 0.46              |
| 55:CA:247:G:OP1    | 55:CA:247:G:H4'   | 2.12                     | 0.46              |
| 55:CA:254:G:HO2'   | 55:CA:255:G:H5'   | 1.81                     | 0.46              |
| 55:CA:391:G:C6     | 55:CA:392:C:N3    | 2.83                     | 0.46              |
| 55:CA:548:G:O2'    | 55:CA:549:C:C5'   | 2.64                     | 0.46              |
| 55:CA:724:G:C4     | 55:CA:725:G:C8    | 3.03                     | 0.46              |
| 55:CA:71:A:O2'     | 55:CA:72:A:O4'    | 2.23                     | 0.46              |
| 55:CA:754:C:H2'    | 55:CA:754:C:O2    | 2.16                     | 0.46              |
| 55:CA:756:C:O2'    | 55:CA:757:U:H5'   | 2.16                     | 0.46              |
| 55:CA:914:A:O2'    | 55:CA:915:A:H5'   | 2.16                     | 0.46              |
| 55:CA:95:C:H6      | 55:CA:95:C:H5''   | 1.80                     | 0.46              |
| 1:CB:26:MET:HG2    | 1:CB:188:THR:HA   | 1.98                     | 0.46              |
| 1:CB:71:THR:HG23   | 1:CB:92:ASN:O     | 2.15                     | 0.46              |
| 3:CD:105:GLY:CA    | 3:CD:158:LEU:HD23 | 2.44                     | 0.46              |
| 3:CD:56:GLU:OE2    | 3:CD:194:ILE:HA   | 2.16                     | 0.46              |
| 3:CD:81:LEU:HB2    | 3:CD:88:ASN:ND2   | 2.31                     | 0.46              |
| 4:CE:37:VAL:HG12   | 4:CE:38:VAL:O     | 2.15                     | 0.46              |
| 24:DA:1080:A:C5    | 24:DA:1081:U:C4   | 3.03                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:1157:G:H2'   | 24:DA:1158:C:H6    | 1.79                     | 0.46              |
| 24:DA:940:G:N3     | 24:DA:1191:G:H4'   | 2.30                     | 0.46              |
| 24:DA:1213:A:C2'   | 24:DA:1214:A:H8    | 2.27                     | 0.46              |
| 24:DA:1249:U:H2'   | 35:DL:18:ARG:HH12  | 1.79                     | 0.46              |
| 24:DA:1281:G:N1    | 24:DA:1290:C:C4    | 2.83                     | 0.46              |
| 24:DA:1378:A:H2'   | 24:DA:1380:G:N7    | 2.31                     | 0.46              |
| 24:DA:1450:G:C2    | 24:DA:1462:C:C2    | 3.04                     | 0.46              |
| 24:DA:1533:C:C4    | 24:DA:1534:U:H5    | 2.33                     | 0.46              |
| 24:DA:1553:A:H2'   | 24:DA:1555:G:N7    | 2.31                     | 0.46              |
| 24:DA:1787:A:C2    | 24:DA:1788:C:C5    | 3.03                     | 0.46              |
| 24:DA:1889:A:O2'   | 24:DA:2087:G:H5'   | 2.15                     | 0.46              |
| 24:DA:1930:G:C4    | 24:DA:1968:G:C6    | 3.03                     | 0.46              |
| 24:DA:2107:G:H2'   | 24:DA:2108:A:H8    | 1.81                     | 0.46              |
| 24:DA:2184:A:H2'   | 24:DA:2185:U:O4'   | 2.14                     | 0.46              |
| 24:DA:2524:G:H21   | 24:DA:2741:A:H1'   | 1.81                     | 0.46              |
| 24:DA:2748:A:C6    | 24:DA:2749:A:C6    | 3.03                     | 0.46              |
| 24:DA:2811:G:C4    | 24:DA:2812:G:C8    | 3.03                     | 0.46              |
| 24:DA:450:G:O6     | 59:DA:3239:HOH:O   | 2.20                     | 0.46              |
| 24:DA:570:G:O6     | 24:DA:2499:C:OP1   | 2.34                     | 0.46              |
| 24:DA:571:U:O2'    | 24:DA:573:U:H6     | 1.97                     | 0.46              |
| 24:DA:632:A:H4'    | 35:DL:68:SER:HA    | 1.98                     | 0.46              |
| 24:DA:638:G:O2'    | 24:DA:639:U:H5'    | 2.16                     | 0.46              |
| 24:DA:837:C:H2'    | 24:DA:838:C:H5'    | 1.98                     | 0.46              |
| 24:DA:950:G:C6     | 24:DA:968:C:N3     | 2.84                     | 0.46              |
| 56:DB:10:G:C6      | 56:DB:11:C:N3      | 2.84                     | 0.46              |
| 56:DB:6:G:H4'      | 56:DB:28:C:H4'     | 1.97                     | 0.46              |
| 28:DE:126:VAL:HG13 | 28:DE:127:GLU:N    | 2.30                     | 0.46              |
| 29:DF:56:LEU:O     | 29:DF:60:SER:HB3   | 2.15                     | 0.46              |
| 30:DG:138:GLN:HG2  | 30:DG:138:GLN:O    | 2.16                     | 0.46              |
| 31:DH:125:THR:CG2  | 31:DH:146:VAL:HG11 | 2.45                     | 0.46              |
| 31:DH:54:LEU:HA    | 31:DH:57:LYS:HG3   | 1.97                     | 0.46              |
| 36:DM:41:LEU:HD11  | 36:DM:126:ILE:HD11 | 1.97                     | 0.46              |
| 36:DM:42:THR:HG22  | 36:DM:44:ARG:N     | 2.22                     | 0.46              |
| 37:DN:12:ARG:HG2   | 37:DN:16:HIS:CG    | 2.51                     | 0.46              |
| 37:DN:37:THR:HG22  | 37:DN:39:PRO:CD    | 2.32                     | 0.46              |
| 44:DU:86:PHE:CG    | 44:DU:87:GLU:N     | 2.83                     | 0.46              |
| 46:DW:23:LYS:HD2   | 46:DW:24:ARG:H     | 1.77                     | 0.46              |
| 18:AS:77:ARG:NH2   | 21:AA:1322:C:OP1   | 2.49                     | 0.46              |
| 21:AA:1338:G:N2    | 21:AA:1339:A:N3    | 2.63                     | 0.46              |
| 21:AA:1348:U:H2'   | 21:AA:1349:A:C8    | 2.50                     | 0.46              |
| 21:AA:1234:C:H4'   | 21:AA:1364:U:H1'   | 1.97                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 21:AA:1444:U:H1' | 21:AA:1459:G:H22  | 1.77                     | 0.46              |
| 21:AA:158:G:H3'  | 21:AA:159:G:H5''  | 1.98                     | 0.46              |
| 21:AA:182:A:N6   | 21:AA:194:C:N4    | 2.63                     | 0.46              |
| 21:AA:295:C:H2'  | 21:AA:296:U:H6    | 1.81                     | 0.46              |
| 21:AA:409:U:O4   | 21:AA:410:G:C6    | 2.69                     | 0.46              |
| 21:AA:51:A:H4'   | 21:AA:52:C:H5'    | 1.96                     | 0.46              |
| 21:AA:720:C:H2'  | 21:AA:721:G:C8    | 2.51                     | 0.46              |
| 21:AA:741:G:C2   | 21:AA:742:G:C4    | 3.04                     | 0.46              |
| 21:AA:6:G:O2'    | 21:AA:7:A:OP2     | 2.29                     | 0.46              |
| 21:AA:80:A:C2    | 21:AA:90:C:C2     | 3.04                     | 0.46              |
| 21:AA:828:U:H2'  | 21:AA:829:G:O5'   | 2.16                     | 0.46              |
| 21:AA:833:G:O2'  | 21:AA:834:U:H5'   | 2.16                     | 0.46              |
| 21:AA:833:G:C5   | 21:AA:834:U:C5    | 3.04                     | 0.46              |
| 21:AA:824:G:N1   | 21:AA:877:G:C6    | 2.84                     | 0.46              |
| 3:AD:61:ARG:NH1  | 3:AD:68:GLU:HG2   | 2.31                     | 0.46              |
| 3:AD:78:ALA:C    | 3:AD:85:THR:HG23  | 2.36                     | 0.46              |
| 5:AF:97:THR:HG22 | 5:AF:98:GLU:H     | 1.81                     | 0.46              |
| 6:AG:87:PRO:HG2  | 6:AG:87:PRO:O     | 2.16                     | 0.46              |
| 10:AK:30:ILE:C   | 10:AK:30:ILE:HD12 | 2.36                     | 0.46              |
| 11:AL:1:ALA:HB2  | 21:AA:568:G:O6    | 2.15                     | 0.46              |
| 14:AO:6:ALA:O    | 14:AO:10:ILE:HG13 | 2.15                     | 0.46              |
| 15:AP:23:ASP:HB3 | 15:AP:26:ASN:OD1  | 2.16                     | 0.46              |
| 15:AP:5:ARG:HH12 | 15:AP:24:SER:HA   | 1.81                     | 0.46              |
| 24:BA:1005:C:C2  | 24:BA:1143:A:C5   | 3.03                     | 0.46              |
| 24:BA:1026:G:O2' | 24:BA:1027:A:H8   | 1.98                     | 0.46              |
| 24:BA:1139:G:C2' | 24:BA:1140:C:H5'  | 2.46                     | 0.46              |
| 24:BA:1313:U:O3' | 24:BA:1332:G:H5'' | 2.15                     | 0.46              |
| 24:BA:1839:G:C8  | 24:BA:1927:A:C1'  | 2.98                     | 0.46              |
| 24:BA:1900:A:N1  | 24:BA:1970:A:C5   | 2.83                     | 0.46              |
| 24:BA:1945:G:H2' | 24:BA:1946:U:C5   | 2.51                     | 0.46              |
| 24:BA:2394:C:OP1 | 53:B3:29:ARG:NH2  | 2.48                     | 0.46              |
| 24:BA:2496:C:OP1 | 36:BM:82:MET:HB2  | 2.15                     | 0.46              |
| 24:BA:406:G:H2'  | 24:BA:407:G:H8    | 1.81                     | 0.46              |
| 24:BA:436:C:O2'  | 24:BA:437:U:H6    | 1.97                     | 0.46              |
| 24:BA:491:G:C2   | 24:BA:492:A:C1'   | 2.99                     | 0.46              |
| 24:BA:3:U:H2'    | 24:BA:4:U:C6      | 2.50                     | 0.46              |
| 24:BA:503:A:C6   | 24:BA:506:G:C6    | 3.04                     | 0.46              |
| 24:BA:630:G:N2   | 24:BA:632:A:H3'   | 2.31                     | 0.46              |
| 24:BA:62:U:C4'   | 24:BA:63:A:OP1    | 2.62                     | 0.46              |
| 24:BA:96:C:C2    | 24:BA:97:C:C5     | 3.04                     | 0.46              |
| 29:BF:24:VAL:O   | 29:BF:27:VAL:HG12 | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:BF:7:TYR:CD2   | 29:BF:11:VAL:HG11 | 2.51                     | 0.46              |
| 31:BH:2:GLN:HA    | 31:BH:20:ASN:HA   | 1.97                     | 0.46              |
| 24:BA:1064:C:C4'  | 32:BI:90:GLY:H    | 2.24                     | 0.46              |
| 33:BJ:124:VAL:O   | 33:BJ:125:TYR:HB2 | 2.16                     | 0.46              |
| 37:BN:35:LYS:HB2  | 37:BN:112:TYR:CE1 | 2.51                     | 0.46              |
| 37:BN:117:ASP:O   | 37:BN:119:SER:N   | 2.47                     | 0.46              |
| 37:BN:13:ASN:O    | 37:BN:14:SER:C    | 2.54                     | 0.46              |
| 37:BN:38:LEU:CD1  | 37:BN:42:LYS:HD2  | 2.45                     | 0.46              |
| 42:BS:28:LYS:HE3  | 42:BS:28:LYS:HB3  | 1.62                     | 0.46              |
| 42:BS:73:LYS:CE   | 42:BS:73:LYS:HA   | 2.41                     | 0.46              |
| 24:BA:26:G:OP1    | 42:BS:80:PRO:HB3  | 2.16                     | 0.46              |
| 55:CA:1005:A:N7   | 55:CA:1006:G:H1'  | 2.31                     | 0.46              |
| 55:CA:1520:C:H2'  | 55:CA:1521:C:H6   | 1.79                     | 0.46              |
| 55:CA:414:A:C2    | 55:CA:415:A:C4    | 3.04                     | 0.46              |
| 55:CA:429:U:H1'   | 55:CA:430:A:H5''  | 1.97                     | 0.46              |
| 1:CB:22:TRP:HE1   | 55:CA:830:G:H5''  | 1.80                     | 0.46              |
| 1:CB:46:VAL:HG13  | 1:CB:47:PRO:HD3   | 1.98                     | 0.46              |
| 3:CD:102:TYR:HB2  | 3:CD:113:ALA:HB2  | 1.96                     | 0.46              |
| 4:CE:47:PHE:CD2   | 4:CE:48:GLY:N     | 2.84                     | 0.46              |
| 5:CF:6:ILE:HD12   | 5:CF:6:ILE:N      | 2.31                     | 0.46              |
| 6:CG:104:VAL:HA   | 6:CG:107:ALA:HB2  | 1.98                     | 0.46              |
| 10:CK:19:VAL:N    | 10:CK:34:THR:O    | 2.48                     | 0.46              |
| 11:CL:6:LEU:HD21  | 11:CL:11:ARG:NE   | 2.31                     | 0.46              |
| 16:CQ:3:LYS:NZ    | 16:CQ:6:THR:HG21  | 2.31                     | 0.46              |
| 20:CU:31:VAL:C    | 20:CU:33:ARG:H    | 2.19                     | 0.46              |
| 50:D0:39:ARG:O    | 50:D0:40:HIS:HB2  | 2.15                     | 0.46              |
| 24:DA:1231:U:H2'  | 24:DA:1232:G:H8   | 1.81                     | 0.46              |
| 24:DA:1388:G:C2   | 24:DA:1389:G:C8   | 3.04                     | 0.46              |
| 24:DA:1445:G:C2   | 24:DA:1547:C:N3   | 2.83                     | 0.46              |
| 24:DA:2142:A:H3'  | 24:DA:2143:C:H4'  | 1.97                     | 0.46              |
| 24:DA:237:C:C2    | 24:DA:261:G:C2    | 3.03                     | 0.46              |
| 24:DA:323:C:H2'   | 28:DE:163:ASN:CG  | 2.37                     | 0.46              |
| 24:DA:352:A:C2    | 24:DA:353:C:H1'   | 2.51                     | 0.46              |
| 24:DA:399:U:C4    | 24:DA:400:G:C6    | 3.03                     | 0.46              |
| 24:DA:604:G:C6    | 24:DA:625:G:N1    | 2.84                     | 0.46              |
| 24:DA:607:U:H3    | 24:DA:620:G:H1'   | 1.80                     | 0.46              |
| 24:DA:764:A:O4'   | 26:DC:211:ARG:HG3 | 2.16                     | 0.46              |
| 24:DA:818:G:O2'   | 24:DA:819:A:H5''  | 2.15                     | 0.46              |
| 24:DA:949:G:C2    | 24:DA:969:G:C2    | 3.04                     | 0.46              |
| 26:DC:77:VAL:CG2  | 26:DC:112:GLY:H   | 2.25                     | 0.46              |
| 26:DC:124:LYS:HB3 | 26:DC:124:LYS:HZ3 | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:DC:134:ILE:O   | 26:DC:166:ARG:NH1 | 2.46                     | 0.46              |
| 24:DA:1655:A:H4'  | 27:DD:118:PHE:CD1 | 2.51                     | 0.46              |
| 29:DF:122:ASP:HB3 | 29:DF:123:GLY:H   | 1.45                     | 0.46              |
| 29:DF:58:ALA:HB1  | 29:DF:139:GLU:CG  | 2.46                     | 0.46              |
| 56:DB:42:C:C5     | 29:DF:87:LYS:NZ   | 2.84                     | 0.46              |
| 43:DT:76:ARG:HG2  | 43:DT:77:ARG:N    | 2.31                     | 0.46              |
| 21:AA:1016:A:H3'  | 21:AA:1017:U:O4'  | 2.16                     | 0.46              |
| 21:AA:1123:U:H5'' | 21:AA:1124:G:OP2  | 2.15                     | 0.46              |
| 21:AA:212:G:N2    | 21:AA:213:G:C5    | 2.84                     | 0.46              |
| 21:AA:230:G:C2'   | 21:AA:231:U:H5'   | 2.46                     | 0.46              |
| 21:AA:250:A:H1'   | 21:AA:252:U:C4    | 2.51                     | 0.46              |
| 21:AA:546:A:H4'   | 21:AA:548:G:H4'   | 1.98                     | 0.46              |
| 21:AA:94:G:N1     | 21:AA:98:A:C2     | 2.84                     | 0.46              |
| 1:AB:138:ARG:HB2  | 1:AB:138:ARG:NH1  | 2.30                     | 0.46              |
| 1:AB:165:ALA:CB   | 1:AB:186:VAL:HG12 | 2.44                     | 0.46              |
| 2:AC:72:PRO:O     | 2:AC:76:ILE:HG13  | 2.15                     | 0.46              |
| 4:AE:13:LYS:HE2   | 4:AE:112:ALA:CB   | 2.45                     | 0.46              |
| 4:AE:71:ILE:CD1   | 4:AE:144:GLU:HG3  | 2.46                     | 0.46              |
| 4:AE:81:GLN:H     | 4:AE:81:GLN:CD    | 2.18                     | 0.46              |
| 6:AG:91:ARG:C     | 6:AG:93:VAL:H     | 2.18                     | 0.46              |
| 18:AS:28:LYS:HB3  | 18:AS:29:PRO:HD2  | 1.97                     | 0.46              |
| 22:AV:27:G:O2'    | 22:AV:28:G:H5'    | 2.16                     | 0.46              |
| 24:BA:137:U:HO2'  | 24:BA:138:U:P     | 2.39                     | 0.46              |
| 24:BA:1892:C:H2'  | 24:BA:1893:C:H6   | 1.80                     | 0.46              |
| 24:BA:192:C:O5'   | 24:BA:192:C:H6    | 1.99                     | 0.46              |
| 24:BA:2734:A:N6   | 24:BA:2770:G:H1'  | 2.31                     | 0.46              |
| 24:BA:2692:G:H1'  | 24:BA:2847:U:H1'  | 1.96                     | 0.46              |
| 24:BA:31:C:H4'    | 24:BA:1238:G:H4'  | 1.98                     | 0.46              |
| 24:BA:542:C:O2    | 24:BA:542:C:H2'   | 2.16                     | 0.46              |
| 24:BA:763:G:O2'   | 24:BA:764:A:H3'   | 2.15                     | 0.46              |
| 26:BC:8:THR:O     | 26:BC:9:SER:HB3   | 2.15                     | 0.46              |
| 33:BJ:109:LEU:HB3 | 33:BJ:110:PRO:HD2 | 1.97                     | 0.46              |
| 33:BJ:76:HIS:O    | 33:BJ:84:ILE:HD12 | 2.16                     | 0.46              |
| 34:BK:47:ILE:HD12 | 34:BK:47:ILE:HA   | 1.76                     | 0.46              |
| 37:BN:30:ARG:HE   | 37:BN:30:ARG:HB2  | 1.57                     | 0.46              |
| 37:BN:33:ILE:HG13 | 37:BN:118:ARG:CD  | 2.46                     | 0.46              |
| 55:CA:1005:A:C5   | 55:CA:1006:G:H1'  | 2.51                     | 0.46              |
| 55:CA:1053:G:N7   | 55:CA:1199:U:H3'  | 2.31                     | 0.46              |
| 55:CA:268:U:C4    | 55:CA:269:C:N4    | 2.83                     | 0.46              |
| 55:CA:382:A:O2'   | 55:CA:383:A:C5'   | 2.64                     | 0.46              |
| 55:CA:580:C:H2'   | 55:CA:581:G:O4'   | 2.16                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:CA:597:G:C6    | 55:CA:598:U:C2     | 3.04                     | 0.46              |
| 55:CA:610:U:H5'   | 55:CA:611:C:OP2    | 2.16                     | 0.46              |
| 55:CA:743:A:C2    | 55:CA:744:C:C2     | 3.03                     | 0.46              |
| 55:CA:835:U:H1'   | 55:CA:852:G:N2     | 2.31                     | 0.46              |
| 2:CC:133:MET:HB2  | 2:CC:150:VAL:CG2   | 2.46                     | 0.46              |
| 2:CC:188:ALA:O    | 2:CC:194:VAL:HA    | 2.16                     | 0.46              |
| 6:CG:115:MET:C    | 6:CG:117:LEU:H     | 2.18                     | 0.46              |
| 6:CG:73:GLU:HA    | 6:CG:140:VAL:HG11  | 1.97                     | 0.46              |
| 7:CH:54:THR:HG23  | 7:CH:55:LYS:N      | 2.31                     | 0.46              |
| 12:CM:21:ILE:HB   | 12:CM:24:VAL:HG23  | 1.98                     | 0.46              |
| 12:CM:89:ARG:HE   | 12:CM:94:LEU:HB2   | 1.80                     | 0.46              |
| 13:CN:62:ARG:HA   | 13:CN:68:ARG:O     | 2.16                     | 0.46              |
| 15:CP:40:ASN:OD1  | 15:CP:42:ILE:HG12  | 2.16                     | 0.46              |
| 18:CS:35:ARG:HH12 | 18:CS:52:ASN:HA    | 1.79                     | 0.46              |
| 12:CM:82:LEU:HD21 | 18:CS:60:PHE:HB3   | 1.98                     | 0.46              |
| 24:DA:1358:G:C8   | 24:DA:1371:G:O6    | 2.68                     | 0.46              |
| 24:DA:1476:U:O2'  | 24:DA:1477:A:H8    | 1.99                     | 0.46              |
| 24:DA:1665:A:C2   | 24:DA:1666:G:C4    | 3.04                     | 0.46              |
| 24:DA:1835:G:H2'  | 24:DA:1836:C:C6    | 2.50                     | 0.46              |
| 24:DA:1884:G:H8   | 24:DA:1884:G:OP2   | 1.99                     | 0.46              |
| 24:DA:1923:U:H2'  | 24:DA:1924:C:C6    | 2.48                     | 0.46              |
| 24:DA:2093:G:C2   | 24:DA:2094:A:C5    | 3.03                     | 0.46              |
| 24:DA:2252:G:H2'  | 24:DA:2253:G:O4'   | 2.16                     | 0.46              |
| 24:DA:2315:G:C2   | 24:DA:2316:G:N9    | 2.84                     | 0.46              |
| 24:DA:2386:A:O2'  | 24:DA:2387:U:H6    | 1.89                     | 0.46              |
| 24:DA:2547:A:C8   | 24:DA:2566:A:C5    | 3.04                     | 0.46              |
| 24:DA:2692:G:H2'  | 24:DA:2693:G:H8    | 1.78                     | 0.46              |
| 24:DA:297:G:C6    | 24:DA:342:A:N1     | 2.84                     | 0.46              |
| 24:DA:412:A:H61   | 24:DA:2411:A:C2'   | 2.29                     | 0.46              |
| 24:DA:495:G:H4'   | 42:DS:4:ILE:O      | 2.16                     | 0.46              |
| 24:DA:528:A:HO2'  | 24:DA:529:A:P      | 2.39                     | 0.46              |
| 24:DA:538:A:H2'   | 24:DA:539:G:C8     | 2.49                     | 0.46              |
| 24:DA:464:U:C2    | 24:DA:788:A:N6     | 2.84                     | 0.46              |
| 24:DA:811:U:C4    | 35:DL:21:ARG:NH2   | 2.84                     | 0.46              |
| 24:DA:863:A:H2'   | 24:DA:864:G:H8     | 1.80                     | 0.46              |
| 24:DA:956:G:H1'   | 36:DM:82:MET:HE1   | 1.97                     | 0.46              |
| 56:DB:49:C:H2'    | 56:DB:50:A:H8      | 1.81                     | 0.46              |
| 26:DC:202:ARG:HE  | 26:DC:204:LEU:HD21 | 1.81                     | 0.46              |
| 30:DG:104:LEU:HB3 | 30:DG:106:LEU:HD21 | 1.97                     | 0.46              |
| 31:DH:21:VAL:HG22 | 31:DH:22:LYS:N     | 2.31                     | 0.46              |
| 31:DH:38:PRO:O    | 31:DH:40:THR:N     | 2.49                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DK:113:MET:SD   | 34:DK:116:ILE:HD11 | 2.56                     | 0.46              |
| 34:DK:17:ARG:HG2   | 34:DK:18:ARG:H     | 1.80                     | 0.46              |
| 35:DL:47:ARG:CG    | 35:DL:47:ARG:NH2   | 2.77                     | 0.46              |
| 35:DL:7:SER:HB2    | 35:DL:8:PRO:HD2    | 1.97                     | 0.46              |
| 39:DP:52:ARG:HH11  | 39:DP:52:ARG:HG2   | 1.81                     | 0.46              |
| 42:DS:10:ALA:O     | 42:DS:100:THR:HB   | 2.16                     | 0.46              |
| 43:DT:29:THR:CA    | 43:DT:87:LEU:HB2   | 2.46                     | 0.46              |
| 21:AA:1395:C:C5'   | 21:AA:1401:G:H21   | 2.26                     | 0.46              |
| 21:AA:13:U:O2'     | 21:AA:14:U:H5'     | 2.16                     | 0.46              |
| 15:AP:25:ARG:HH22  | 21:AA:230:G:H4'    | 1.81                     | 0.46              |
| 21:AA:367:U:C6     | 21:AA:394:G:N2     | 2.84                     | 0.46              |
| 21:AA:64:G:C8      | 21:AA:99:C:N4      | 2.84                     | 0.46              |
| 21:AA:575:G:N1     | 21:AA:821:G:C5     | 2.83                     | 0.46              |
| 21:AA:833:G:C6     | 21:AA:834:U:C4     | 3.04                     | 0.46              |
| 5:AF:88:MET:HG2    | 5:AF:89:VAL:N      | 2.31                     | 0.46              |
| 6:AG:102:TRP:CD1   | 6:AG:136:LYS:HG2   | 2.50                     | 0.46              |
| 6:AG:52:ARG:HH12   | 6:AG:121:ASN:ND2   | 2.14                     | 0.46              |
| 6:AG:4:ARG:NE      | 6:AG:4:ARG:HA      | 2.30                     | 0.46              |
| 7:AH:104:SER:O     | 7:AH:122:GLY:HA3   | 2.16                     | 0.46              |
| 8:AI:56:MET:CE     | 8:AI:57:VAL:H      | 2.29                     | 0.46              |
| 13:AN:76:PHE:CE2   | 13:AN:92:ILE:HG21  | 2.51                     | 0.46              |
| 16:AQ:16:MET:HB2   | 16:AQ:19:SER:HB3   | 1.98                     | 0.46              |
| 24:BA:16:C:O3'     | 50:B0:10:SER:OG    | 2.33                     | 0.46              |
| 24:BA:1059:G:OP2   | 24:BA:1060:U:O3'   | 2.35                     | 0.46              |
| 24:BA:1071:G:C8    | 24:BA:1089:A:C6    | 3.04                     | 0.46              |
| 24:BA:1131:G:C5    | 33:BJ:77:HIS:CE1   | 3.04                     | 0.46              |
| 24:BA:1387:A:H5'   | 24:BA:1469:A:H1'   | 1.98                     | 0.46              |
| 24:BA:1423:G:C2    | 24:BA:1424:G:C8    | 3.05                     | 0.46              |
| 24:BA:1432:G:H2'   | 24:BA:1433:A:C8    | 2.51                     | 0.46              |
| 24:BA:1487:U:H2'   | 24:BA:1488:C:O4'   | 2.15                     | 0.46              |
| 24:BA:2318:G:C6    | 24:BA:2319:G:N1    | 2.84                     | 0.46              |
| 24:BA:2425:A:H5'   | 24:BA:2427:C:H5'   | 1.98                     | 0.46              |
| 24:BA:2624:G:H1'   | 50:B0:18:HIS:CE1   | 2.51                     | 0.46              |
| 24:BA:272:A:H2'    | 24:BA:273:G:C8     | 2.51                     | 0.46              |
| 24:BA:2847:U:C2'   | 24:BA:2848:G:H5'   | 2.46                     | 0.46              |
| 24:BA:831:G:C5     | 24:BA:832:U:C5     | 3.03                     | 0.46              |
| 24:BA:918:A:O5'    | 24:BA:918:A:H8     | 1.99                     | 0.46              |
| 25:BB:54:G:C4      | 25:BB:55:U:C5      | 3.04                     | 0.46              |
| 26:BC:20:ASN:HA    | 26:BC:21:PRO:HD2   | 1.82                     | 0.46              |
| 26:BC:67:LYS:HG2   | 26:BC:150:GLY:HA2  | 1.97                     | 0.46              |
| 27:BD:151:THR:HG22 | 27:BD:152:PRO:N    | 2.31                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BD:107:VAL:N   | 27:BD:206:ALA:H    | 2.02                     | 0.46              |
| 28:BE:12:LEU:HD21 | 28:BE:190:ALA:HB1  | 1.98                     | 0.46              |
| 28:BE:96:VAL:O    | 28:BE:96:VAL:HG12  | 2.16                     | 0.46              |
| 29:BF:134:GLN:CG  | 29:BF:135:ILE:N    | 2.70                     | 0.46              |
| 29:BF:7:TYR:OH    | 29:BF:29:ARG:HB3   | 2.16                     | 0.46              |
| 34:BK:17:ARG:HG3  | 34:BK:47:ILE:HD13  | 1.97                     | 0.46              |
| 38:BO:41:ALA:HB2  | 38:BO:48:LEU:HD21  | 1.98                     | 0.46              |
| 42:BS:37:THR:CG2  | 42:BS:37:THR:O     | 2.64                     | 0.46              |
| 46:BW:22:VAL:HG13 | 46:BW:25:PHE:CE2   | 2.51                     | 0.46              |
| 46:BW:47:GLY:C    | 46:BW:49:ASN:H     | 2.19                     | 0.46              |
| 55:CA:1101:A:H1'  | 55:CA:1102:A:O4'   | 2.15                     | 0.46              |
| 55:CA:1113:C:H2'  | 55:CA:1114:C:O4'   | 2.15                     | 0.46              |
| 8:CI:10:ARG:NH2   | 55:CA:1119:C:OP2   | 2.49                     | 0.46              |
| 55:CA:1183:U:O2'  | 55:CA:1184:G:P     | 2.73                     | 0.46              |
| 13:CN:2:LYS:HE2   | 55:CA:1216:A:OP1   | 2.15                     | 0.46              |
| 55:CA:1266:G:N1   | 55:CA:1270:G:C6    | 2.84                     | 0.46              |
| 55:CA:204:G:H2'   | 55:CA:205:A:C8     | 2.51                     | 0.46              |
| 55:CA:377:G:N2    | 55:CA:387:U:H1'    | 2.30                     | 0.46              |
| 55:CA:61:G:C6     | 55:CA:107:G:C6     | 3.04                     | 0.46              |
| 55:CA:96:U:O2'    | 55:CA:97:G:H8      | 1.98                     | 0.46              |
| 1:CB:147:LEU:N    | 1:CB:147:LEU:HD12  | 2.31                     | 0.46              |
| 1:CB:156:LEU:HD23 | 1:CB:156:LEU:H     | 1.80                     | 0.46              |
| 3:CD:106:PHE:CE1  | 3:CD:144:ILE:HD11  | 2.51                     | 0.46              |
| 3:CD:23:GLY:HA2   | 3:CD:160:LEU:HD12  | 1.97                     | 0.46              |
| 4:CE:148:SER:H    | 4:CE:151:MET:CE    | 2.21                     | 0.46              |
| 5:CF:14:GLN:HB3   | 5:CF:17:GLN:HE22   | 1.79                     | 0.46              |
| 10:CK:22:ILE:HB   | 10:CK:85:VAL:HG22  | 1.98                     | 0.46              |
| 12:CM:86:ARG:C    | 12:CM:88:LEU:H     | 2.20                     | 0.46              |
| 18:CS:34:SER:O    | 18:CS:36:ARG:N     | 2.48                     | 0.46              |
| 19:CT:67:HIS:CG   | 19:CT:68:LYS:H     | 2.25                     | 0.46              |
| 22:CV:30:G:C4     | 22:CV:31:A:C8      | 3.04                     | 0.46              |
| 24:DA:1071:G:C8   | 24:DA:1089:A:C5    | 3.04                     | 0.46              |
| 24:DA:1149:G:C6   | 24:DA:1150:C:N4    | 2.84                     | 0.46              |
| 24:DA:1277:G:H5'  | 37:DN:20:MET:CE    | 2.46                     | 0.46              |
| 24:DA:136:G:H2'   | 24:DA:137:U:O4'    | 2.16                     | 0.46              |
| 24:DA:1422:G:H4'  | 24:DA:1493:C:OP1   | 2.16                     | 0.46              |
| 24:DA:1430:G:H2'  | 24:DA:1431:A:H8    | 1.80                     | 0.46              |
| 24:DA:1731:G:C4'  | 24:DA:1732:C:OP1   | 2.63                     | 0.46              |
| 24:DA:1800:C:C2   | 24:DA:1802:A:C8    | 3.04                     | 0.46              |
| 24:DA:2011:U:H2'  | 24:DA:2012:G:O4'   | 2.16                     | 0.46              |
| 24:DA:2050:C:O2'  | 27:DD:146:ILE:HG21 | 2.16                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:2104:C:O2   | 24:DA:2105:U:C5    | 2.68                     | 0.46              |
| 24:DA:2214:C:H2'  | 24:DA:2215:C:C6    | 2.50                     | 0.46              |
| 24:DA:2230:G:H2'  | 24:DA:2231:U:C6    | 2.51                     | 0.46              |
| 24:DA:30:G:C6     | 24:DA:511:U:O2     | 2.69                     | 0.46              |
| 24:DA:325:G:O2'   | 24:DA:326:G:C5'    | 2.63                     | 0.46              |
| 24:DA:628:G:C6    | 24:DA:636:G:N1     | 2.84                     | 0.46              |
| 24:DA:72:U:O2'    | 24:DA:73:A:H5'     | 2.16                     | 0.46              |
| 24:DA:845:A:H2'   | 24:DA:847:U:O2     | 2.16                     | 0.46              |
| 24:DA:950:G:O2'   | 24:DA:951:C:H5'    | 2.16                     | 0.46              |
| 26:DC:128:THR:HA  | 26:DC:190:THR:HA   | 1.98                     | 0.46              |
| 26:DC:211:ARG:C   | 26:DC:213:ARG:H    | 2.19                     | 0.46              |
| 24:DA:782:A:N7    | 26:DC:219:VAL:HG21 | 2.31                     | 0.46              |
| 24:DA:1993:U:H4'  | 27:DD:133:THR:HG21 | 1.96                     | 0.46              |
| 29:DF:131:VAL:O   | 29:DF:132:ARG:HB2  | 2.16                     | 0.46              |
| 29:DF:160:LYS:HD3 | 29:DF:161:SER:H    | 1.80                     | 0.46              |
| 31:DH:104:THR:O   | 31:DH:104:THR:HG23 | 2.16                     | 0.46              |
| 31:DH:89:LYS:HD2  | 31:DH:124:THR:HA   | 1.96                     | 0.46              |
| 31:DH:61:VAL:HG13 | 31:DH:62:LEU:N     | 2.31                     | 0.46              |
| 34:DK:92:GLU:O    | 34:DK:93:GLN:O     | 2.34                     | 0.46              |
| 37:DN:56:LYS:HD3  | 37:DN:88:ALA:HA    | 1.98                     | 0.46              |
| 38:DO:49:VAL:HG11 | 38:DO:81:ARG:HB3   | 1.97                     | 0.46              |
| 40:DQ:60:TRP:CH2  | 40:DQ:93:ILE:HB    | 2.50                     | 0.46              |
| 40:DQ:46:TYR:HD1  | 41:DR:74:ILE:HG23  | 1.80                     | 0.46              |
| 43:DT:10:VAL:HG23 | 43:DT:11:LEU:HD12  | 1.97                     | 0.46              |
| 43:DT:19:LYS:HA   | 43:DT:19:LYS:HD3   | 1.64                     | 0.46              |
| 43:DT:39:THR:OG1  | 43:DT:42:GLU:HG3   | 2.14                     | 0.46              |
| 21:AA:1140:C:O2'  | 21:AA:1141:C:O5'   | 2.34                     | 0.45              |
| 21:AA:1054:C:P    | 21:AA:1197:A:OP2   | 2.74                     | 0.45              |
| 21:AA:588:G:C6    | 21:AA:589:U:C4     | 3.04                     | 0.45              |
| 21:AA:763:G:C5    | 21:AA:764:C:C5     | 3.04                     | 0.45              |
| 21:AA:80:A:C2     | 21:AA:81:A:H1'     | 2.51                     | 0.45              |
| 21:AA:872:A:C2    | 21:AA:874:G:C6     | 3.04                     | 0.45              |
| 1:AB:117:GLU:C    | 1:AB:119:GLN:H     | 2.20                     | 0.45              |
| 1:AB:96:LEU:O     | 1:AB:99:MET:HB3    | 2.16                     | 0.45              |
| 2:AC:179:ALA:HB1  | 2:AC:202:PHE:CE1   | 2.50                     | 0.45              |
| 3:AD:2:ARG:HB2    | 3:AD:4:LEU:HD13    | 1.98                     | 0.45              |
| 4:AE:120:HIS:O    | 4:AE:121:ASN:HB3   | 2.16                     | 0.45              |
| 4:AE:94:PHE:CZ    | 4:AE:95:MET:O      | 2.69                     | 0.45              |
| 5:AF:38:ARG:HH22  | 5:AF:96:VAL:HG23   | 1.80                     | 0.45              |
| 11:AL:23:LEU:HG   | 11:AL:24:GLU:N     | 2.12                     | 0.45              |
| 11:AL:33:CYS:CB   | 11:AL:54:VAL:HG22  | 2.33                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:AT:53:MET:HA   | 19:AT:56:ILE:HG22 | 1.98                     | 0.45              |
| 20:AU:18:PHE:O    | 20:AU:21:SER:HB3  | 2.15                     | 0.45              |
| 52:B2:12:ARG:HE   | 52:B2:44:VAL:HG11 | 1.80                     | 0.45              |
| 53:B3:46:LYS:HD3  | 53:B3:46:LYS:HA   | 1.78                     | 0.45              |
| 24:BA:1060:U:H5'' | 24:BA:1061:U:OP1  | 2.16                     | 0.45              |
| 24:BA:1224:U:O4   | 24:BA:1225:G:C6   | 2.69                     | 0.45              |
| 24:BA:1399:C:C2   | 24:BA:1400:U:C5   | 3.05                     | 0.45              |
| 24:BA:142:A:H2'   | 24:BA:143:C:C5    | 2.50                     | 0.45              |
| 24:BA:1471:G:H2'  | 24:BA:1472:C:H6   | 1.81                     | 0.45              |
| 24:BA:1631:G:H1'  | 24:BA:1635:A:N6   | 2.31                     | 0.45              |
| 24:BA:49:A:N6     | 24:BA:177:G:C4    | 2.84                     | 0.45              |
| 24:BA:1936:A:H2   | 24:BA:1943:U:C5   | 2.35                     | 0.45              |
| 24:BA:2082:A:H61  | 24:BA:2237:G:H1'  | 1.80                     | 0.45              |
| 24:BA:2413:G:C4   | 24:BA:2414:G:C8   | 3.04                     | 0.45              |
| 24:BA:24:G:C6     | 24:BA:25:U:C4     | 3.04                     | 0.45              |
| 24:BA:308:G:H2'   | 24:BA:309:A:O4'   | 2.16                     | 0.45              |
| 24:BA:310:A:H5''  | 44:BU:14:THR:HG22 | 1.97                     | 0.45              |
| 24:BA:821:A:N7    | 24:BA:946:C:N3    | 2.64                     | 0.45              |
| 24:BA:919:U:C2    | 24:BA:920:A:C8    | 3.03                     | 0.45              |
| 24:BA:957:C:C5    | 24:BA:959:A:C5    | 3.04                     | 0.45              |
| 24:BA:96:C:O2'    | 24:BA:97:C:H5'    | 2.15                     | 0.45              |
| 31:BH:27:ARG:HH12 | 31:BH:38:PRO:HG3  | 1.81                     | 0.45              |
| 34:BK:19:VAL:HG22 | 34:BK:41:ILE:CG1  | 2.42                     | 0.45              |
| 39:BP:15:ASP:OD1  | 39:BP:15:ASP:C    | 2.52                     | 0.45              |
| 43:BT:18:GLU:HA   | 43:BT:18:GLU:OE2  | 2.16                     | 0.45              |
| 44:BU:27:VAL:HG22 | 44:BU:28:LEU:N    | 2.31                     | 0.45              |
| 45:BV:65:VAL:O    | 45:BV:66:ASP:OD1  | 2.34                     | 0.45              |
| 46:BW:18:LYS:N    | 46:BW:36:ILE:HG12 | 2.30                     | 0.45              |
| 47:BX:69:GLU:O    | 47:BX:71:ARG:N    | 2.47                     | 0.45              |
| 48:BY:22:LEU:O    | 48:BY:23:ARG:O    | 2.34                     | 0.45              |
| 55:CA:1319:A:C5   | 55:CA:1323:G:C5   | 3.05                     | 0.45              |
| 55:CA:1381:U:O2'  | 55:CA:1382:C:H6   | 1.99                     | 0.45              |
| 55:CA:156:C:OP2   | 55:CA:156:C:H6    | 1.99                     | 0.45              |
| 16:CQ:18:LYS:HD2  | 55:CA:255:G:O3'   | 2.16                     | 0.45              |
| 55:CA:286:C:H2'   | 55:CA:287:U:O4'   | 2.16                     | 0.45              |
| 55:CA:612:C:C2    | 55:CA:629:A:H2    | 2.34                     | 0.45              |
| 55:CA:783:C:H2'   | 55:CA:784:A:H8    | 1.80                     | 0.45              |
| 55:CA:977:A:O3'   | 55:CA:980:C:N4    | 2.49                     | 0.45              |
| 2:CC:166:TRP:CE3  | 2:CC:166:TRP:N    | 2.82                     | 0.45              |
| 6:CG:148:LYS:HD3  | 6:CG:148:LYS:O    | 2.16                     | 0.45              |
| 6:CG:62:GLU:OE2   | 6:CG:65:LEU:HD12  | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:CL:83:GLY:HA2  | 11:CL:94:TYR:HD1  | 1.80                     | 0.45              |
| 15:CP:1:MET:HG3   | 15:CP:1:MET:O     | 2.16                     | 0.45              |
| 22:CV:38:A:N7     | 22:CV:39:U:C5     | 2.84                     | 0.45              |
| 22:CX:38:A:H2'    | 22:CX:39:U:H6     | 1.81                     | 0.45              |
| 50:D0:38:LEU:HB2  | 50:D0:41:HIS:CE1  | 2.51                     | 0.45              |
| 54:D4:7:VAL:CG1   | 54:D4:8:LYS:N     | 2.79                     | 0.45              |
| 24:DA:1056:G:N2   | 24:DA:1102:C:H5   | 2.14                     | 0.45              |
| 24:DA:1183:U:H2'  | 24:DA:1184:U:H6   | 1.81                     | 0.45              |
| 24:DA:1364:G:H1'  | 24:DA:1368:G:N2   | 2.31                     | 0.45              |
| 24:DA:1603:A:H2'  | 24:DA:1604:C:O4'  | 2.15                     | 0.45              |
| 24:DA:1715:G:N2   | 24:DA:1743:G:H2'  | 2.31                     | 0.45              |
| 24:DA:1895:C:N3   | 24:DA:1896:G:N7   | 2.65                     | 0.45              |
| 24:DA:827:U:H1'   | 24:DA:2246:G:O2'  | 2.16                     | 0.45              |
| 24:DA:2435:A:N1   | 24:DA:2436:G:C5   | 2.84                     | 0.45              |
| 24:DA:2519:U:C6   | 24:DA:2542:A:C6   | 3.04                     | 0.45              |
| 24:DA:2516:A:N3   | 24:DA:2569:G:N2   | 2.64                     | 0.45              |
| 24:DA:2687:U:H2'  | 24:DA:2688:G:C8   | 2.50                     | 0.45              |
| 24:DA:2842:G:C6   | 24:DA:2843:G:C5   | 3.04                     | 0.45              |
| 24:DA:304:U:H2'   | 24:DA:305:C:C6    | 2.51                     | 0.45              |
| 24:DA:372:G:P     | 47:DX:61:LYS:HZ1  | 2.38                     | 0.45              |
| 24:DA:755:U:H2'   | 24:DA:756:A:H8    | 1.81                     | 0.45              |
| 24:DA:903:C:C2    | 24:DA:904:G:C8    | 3.04                     | 0.45              |
| 27:DD:121:THR:CG2 | 27:DD:127:PHE:CD1 | 2.99                     | 0.45              |
| 27:DD:60:VAL:O    | 27:DD:60:VAL:HG13 | 2.15                     | 0.45              |
| 27:DD:61:THR:HB   | 27:DD:63:PRO:HD2  | 1.97                     | 0.45              |
| 29:DF:113:PHE:HE2 | 29:DF:116:LEU:HB2 | 1.81                     | 0.45              |
| 35:DL:85:VAL:O    | 35:DL:85:VAL:HG22 | 2.16                     | 0.45              |
| 40:DQ:82:LEU:HD23 | 40:DQ:112:ALA:HB2 | 1.97                     | 0.45              |
| 46:DW:20:LEU:HD11 | 46:DW:35:ILE:HD11 | 1.98                     | 0.45              |
| 46:DW:37:VAL:CG2  | 46:DW:38:ARG:NH1  | 2.79                     | 0.45              |
| 21:AA:109:A:C4    | 21:AA:326:G:C2    | 3.04                     | 0.45              |
| 21:AA:1171:A:C2   | 21:AA:1172:C:C2   | 3.04                     | 0.45              |
| 21:AA:1353:G:C2   | 21:AA:1370:G:C2   | 3.05                     | 0.45              |
| 21:AA:756:C:H2'   | 21:AA:757:U:O4'   | 2.15                     | 0.45              |
| 21:AA:815:A:C2    | 21:AA:1529:G:C4   | 3.05                     | 0.45              |
| 1:AB:136:ARG:HD2  | 1:AB:136:ARG:O    | 2.16                     | 0.45              |
| 1:AB:160:LEU:HB3  | 1:AB:182:VAL:CG1  | 2.44                     | 0.45              |
| 1:AB:182:VAL:CG1  | 1:AB:183:PHE:N    | 2.79                     | 0.45              |
| 1:AB:52:ALA:C     | 1:AB:54:ALA:N     | 2.69                     | 0.45              |
| 3:AD:137:SER:HB3  | 3:AD:138:PRO:HD2  | 1.98                     | 0.45              |
| 4:AE:20:VAL:O     | 4:AE:30:PHE:HA    | 2.17                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:AE:56:PRO:C      | 4:AE:58:ALA:N     | 2.70                     | 0.45              |
| 6:AG:52:ARG:HH12   | 6:AG:121:ASN:HD21 | 1.63                     | 0.45              |
| 7:AH:75:GLN:O      | 7:AH:126:CYS:HB2  | 2.17                     | 0.45              |
| 9:AJ:57:VAL:HG22   | 9:AJ:58:ASN:N     | 2.23                     | 0.45              |
| 15:AP:19:VAL:HG22  | 15:AP:36:VAL:CG1  | 2.47                     | 0.45              |
| 19:AT:27:MET:SD    | 19:AT:66:ILE:HD13 | 2.56                     | 0.45              |
| 22:AV:40:C:C2      | 22:AV:41:C:C5     | 3.03                     | 0.45              |
| 53:B3:7:ARG:HD2    | 53:B3:7:ARG:HA    | 1.52                     | 0.45              |
| 24:BA:1274:A:H8    | 24:BA:1274:A:C5'  | 2.29                     | 0.45              |
| 24:BA:1369:G:C6    | 24:BA:1370:C:C4   | 3.05                     | 0.45              |
| 24:BA:2061:G:C2    | 24:BA:2063:C:C4   | 3.04                     | 0.45              |
| 24:BA:2418:A:C2    | 24:BA:2419:U:C2   | 3.05                     | 0.45              |
| 24:BA:2778:A:H4'   | 24:BA:2779:U:OP2  | 2.17                     | 0.45              |
| 24:BA:404:A:O2'    | 24:BA:405:U:P     | 2.74                     | 0.45              |
| 24:BA:812:C:C2     | 24:BA:1250:G:N1   | 2.84                     | 0.45              |
| 24:BA:923:G:C4'    | 46:BW:25:PHE:CZ   | 2.99                     | 0.45              |
| 25:BB:66:A:H4'     | 25:BB:67:G:OP1    | 2.15                     | 0.45              |
| 29:BF:103:ILE:HG12 | 29:BF:103:ILE:H   | 1.54                     | 0.45              |
| 29:BF:133:GLU:H    | 29:BF:150:GLY:HA3 | 1.81                     | 0.45              |
| 30:BG:31:GLU:O     | 30:BG:32:LEU:C    | 2.54                     | 0.45              |
| 30:BG:53:PRO:HD3   | 30:BG:61:TRP:CE3  | 2.52                     | 0.45              |
| 32:BI:52:LEU:HD12  | 32:BI:52:LEU:N    | 2.31                     | 0.45              |
| 33:BJ:80:HIS:O     | 33:BJ:81:ILE:C    | 2.54                     | 0.45              |
| 34:BK:2:ILE:HG21   | 34:BK:39:ILE:CD1  | 2.46                     | 0.45              |
| 36:BM:108:VAL:HG13 | 36:BM:112:LEU:HB3 | 1.98                     | 0.45              |
| 36:BM:2:LEU:HD22   | 36:BM:46:ILE:HD13 | 1.98                     | 0.45              |
| 37:BN:71:ARG:NH2   | 37:BN:71:ARG:CG   | 2.71                     | 0.45              |
| 39:BP:8:GLU:O      | 39:BP:11:GLN:N    | 2.49                     | 0.45              |
| 39:BP:61:ARG:HG2   | 39:BP:70:GLU:CG   | 2.36                     | 0.45              |
| 39:BP:91:VAL:O     | 39:BP:92:ARG:HG2  | 2.16                     | 0.45              |
| 41:BR:49:ILE:HG21  | 41:BR:53:PHE:N    | 2.31                     | 0.45              |
| 42:BS:28:LYS:O     | 42:BS:29:VAL:C    | 2.54                     | 0.45              |
| 24:BA:2013:A:OP1   | 42:BS:96:ILE:HA   | 2.17                     | 0.45              |
| 24:BA:856:G:N2     | 46:BW:19:ARG:HH22 | 2.09                     | 0.45              |
| 46:BW:29:SER:CA    | 46:BW:63:ASP:HB3  | 2.45                     | 0.45              |
| 46:BW:72:GLY:N     | 46:BW:73:PRO:CD   | 2.78                     | 0.45              |
| 47:BX:69:GLU:O     | 47:BX:70:LEU:HB2  | 2.16                     | 0.45              |
| 49:BZ:23:LEU:HD13  | 49:BZ:23:LEU:HA   | 1.72                     | 0.45              |
| 55:CA:1415:G:C2    | 55:CA:1486:G:C5   | 3.03                     | 0.45              |
| 55:CA:367:U:C6     | 55:CA:394:G:N2    | 2.84                     | 0.45              |
| 55:CA:458:U:H2'    | 55:CA:459:A:C8    | 2.51                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:CA:202:G:O2'   | 55:CA:468:A:C8     | 2.68                     | 0.45              |
| 55:CA:542:G:H2'   | 55:CA:543:U:C6     | 2.51                     | 0.45              |
| 55:CA:652:U:O2'   | 55:CA:653:U:P      | 2.74                     | 0.45              |
| 55:CA:655:A:N6    | 55:CA:752:G:N2     | 2.64                     | 0.45              |
| 55:CA:587:G:C6    | 55:CA:755:G:O6     | 2.70                     | 0.45              |
| 55:CA:813:U:C2'   | 55:CA:814:A:H5'    | 2.46                     | 0.45              |
| 1:CB:100:LEU:C    | 1:CB:102:ASN:H     | 2.20                     | 0.45              |
| 1:CB:100:LEU:O    | 1:CB:102:ASN:N     | 2.49                     | 0.45              |
| 1:CB:39:ILE:HD13  | 1:CB:40:ILE:H      | 1.81                     | 0.45              |
| 3:CD:3:TYR:OH     | 3:CD:10:LEU:HD11   | 2.16                     | 0.45              |
| 4:CE:88:HIS:O     | 4:CE:89:THR:C      | 2.54                     | 0.45              |
| 6:CG:136:LYS:O    | 6:CG:140:VAL:HG23  | 2.16                     | 0.45              |
| 6:CG:2:ARG:HA     | 55:CA:1380:U:C5    | 2.51                     | 0.45              |
| 7:CH:102:VAL:O    | 7:CH:125:ILE:HB    | 2.16                     | 0.45              |
| 10:CK:22:ILE:HG12 | 10:CK:95:THR:HG21  | 1.98                     | 0.45              |
| 18:CS:21:ALA:HB2  | 18:CS:27:LYS:HZ3   | 1.80                     | 0.45              |
| 24:DA:2015:A:C5   | 50:D0:2:VAL:HG11   | 2.50                     | 0.45              |
| 24:DA:1021:A:H2'  | 24:DA:1022:G:H4'   | 1.98                     | 0.45              |
| 24:DA:1034:G:O2'  | 24:DA:1035:U:O4'   | 2.20                     | 0.45              |
| 24:DA:1040:A:H2'  | 24:DA:1041:G:O4'   | 2.17                     | 0.45              |
| 24:DA:1159:U:O2'  | 24:DA:1160:G:H5'   | 2.16                     | 0.45              |
| 24:DA:1205:A:C5   | 28:DE:165:HIS:CE1  | 3.05                     | 0.45              |
| 24:DA:1303:G:C2'  | 24:DA:1304:A:H8    | 2.28                     | 0.45              |
| 24:DA:1661:G:O2'  | 24:DA:1662:U:H5'   | 2.16                     | 0.45              |
| 24:DA:1884:G:N3   | 24:DA:1884:G:H2'   | 2.31                     | 0.45              |
| 24:DA:204:A:C8    | 24:DA:206:U:N3     | 2.84                     | 0.45              |
| 24:DA:192:C:OP1   | 24:DA:2243:U:OP1   | 2.34                     | 0.45              |
| 24:DA:917:A:H5''  | 24:DA:2268:A:H61   | 1.81                     | 0.45              |
| 24:DA:197:A:C5    | 24:DA:2430:A:C5    | 3.05                     | 0.45              |
| 24:DA:2599:G:OP2  | 26:DC:234:GLY:HA2  | 2.16                     | 0.45              |
| 24:DA:2772:C:N3   | 24:DA:2773:C:C5    | 2.84                     | 0.45              |
| 24:DA:2869:G:C6   | 24:DA:2870:C:C4    | 3.04                     | 0.45              |
| 24:DA:322:A:H3'   | 28:DE:163:ASN:HD21 | 1.82                     | 0.45              |
| 24:DA:298:G:H2'   | 24:DA:339:U:O4     | 2.17                     | 0.45              |
| 24:DA:353:C:N4    | 24:DA:354:A:N6     | 2.64                     | 0.45              |
| 24:DA:413:C:O2'   | 24:DA:414:C:H5'    | 2.16                     | 0.45              |
| 24:DA:581:C:N3    | 24:DA:582:A:C5     | 2.84                     | 0.45              |
| 24:DA:660:C:H5''  | 28:DE:94:GLN:OE1   | 2.15                     | 0.45              |
| 24:DA:719:C:C2    | 24:DA:720:U:C6     | 3.04                     | 0.45              |
| 24:DA:725:G:C6    | 24:DA:726:G:N1     | 2.84                     | 0.45              |
| 24:DA:857:G:H1'   | 46:DW:19:ARG:HE    | 1.79                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:DB:75:G:H22     | 56:DB:102:G:H21    | 1.64                     | 0.45              |
| 56:DB:43:C:C2'     | 56:DB:45:A:N7      | 2.80                     | 0.45              |
| 32:DI:102:ARG:HD3  | 32:DI:140:GLU:O    | 2.16                     | 0.45              |
| 36:DM:40:ARG:HB2   | 36:DM:93:VAL:HG21  | 1.97                     | 0.45              |
| 40:DQ:12:ARG:H     | 40:DQ:12:ARG:HD2   | 1.80                     | 0.45              |
| 41:DR:37:GLU:HB2   | 41:DR:53:PHE:CD2   | 2.51                     | 0.45              |
| 41:DR:98:ILE:N     | 41:DR:98:ILE:HD12  | 2.32                     | 0.45              |
| 21:AA:113:G:H2'    | 21:AA:114:U:C6     | 2.50                     | 0.45              |
| 21:AA:1346:A:C4    | 21:AA:1348:U:C4    | 3.04                     | 0.45              |
| 21:AA:570:G:C6     | 21:AA:571:U:O4     | 2.70                     | 0.45              |
| 21:AA:802:A:H5''   | 21:AA:803:G:OP2    | 2.17                     | 0.45              |
| 21:AA:914:A:H2'    | 21:AA:915:A:C8     | 2.48                     | 0.45              |
| 1:AB:63:LYS:HG2    | 1:AB:224:ARG:CZ    | 2.46                     | 0.45              |
| 3:AD:158:LEU:O     | 3:AD:161:ALA:HB3   | 2.16                     | 0.45              |
| 3:AD:57:LYS:HG2    | 3:AD:202:LEU:CD2   | 2.45                     | 0.45              |
| 4:AE:152:VAL:HB    | 4:AE:155:LYS:NZ    | 2.31                     | 0.45              |
| 9:AJ:5:ARG:HG2     | 9:AJ:79:PRO:CD     | 2.46                     | 0.45              |
| 10:AK:121:ARG:HH21 | 20:AU:35:GLU:HB2   | 1.82                     | 0.45              |
| 11:AL:86:VAL:O     | 11:AL:88:ASP:N     | 2.43                     | 0.45              |
| 13:AN:40:ARG:NH1   | 13:AN:44:VAL:HG21  | 2.18                     | 0.45              |
| 16:AQ:32:ILE:HG22  | 16:AQ:33:TYR:CD2   | 2.52                     | 0.45              |
| 51:B1:3:GLY:C      | 51:B1:5:ARG:H      | 2.19                     | 0.45              |
| 24:BA:1060:U:C5'   | 24:BA:1061:U:OP1   | 2.64                     | 0.45              |
| 24:BA:1322:A:N7    | 24:BA:1323:C:C5    | 2.85                     | 0.45              |
| 24:BA:1342:A:C6    | 24:BA:1345:C:C2    | 3.05                     | 0.45              |
| 24:BA:1471:G:C6    | 24:BA:1472:C:C4    | 3.05                     | 0.45              |
| 24:BA:1724:G:C6    | 24:BA:1725:U:C4    | 3.04                     | 0.45              |
| 24:BA:1850:G:O2'   | 24:BA:1851:U:H5'   | 2.17                     | 0.45              |
| 24:BA:18:U:H2'     | 24:BA:19:A:O4'     | 2.16                     | 0.45              |
| 24:BA:2305:U:H2'   | 24:BA:2306:C:C6    | 2.51                     | 0.45              |
| 24:BA:1758:U:H2'   | 24:BA:2696:U:O4'   | 2.16                     | 0.45              |
| 24:BA:2895:G:H2'   | 24:BA:2896:C:C6    | 2.51                     | 0.45              |
| 24:BA:736:C:H2'    | 24:BA:737:C:H6     | 1.81                     | 0.45              |
| 24:BA:919:U:C4'    | 24:BA:919:U:C6     | 2.94                     | 0.45              |
| 25:BB:66:A:N6      | 25:BB:107:G:H3'    | 2.32                     | 0.45              |
| 27:BD:12:THR:CG2   | 27:BD:13:ARG:H     | 2.29                     | 0.45              |
| 28:BE:164:LEU:HB3  | 28:BE:167:VAL:HG12 | 1.97                     | 0.45              |
| 33:BJ:55:ILE:HA    | 33:BJ:123:LYS:O    | 2.16                     | 0.45              |
| 33:BJ:18:VAL:HG23  | 33:BJ:54:ILE:HD13  | 1.99                     | 0.45              |
| 35:BL:4:ASN:N      | 35:BL:4:ASN:ND2    | 2.63                     | 0.45              |
| 36:BM:132:THR:CG2  | 36:BM:133:LYS:H    | 2.24                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BM:32:GLY:CA    | 36:BM:131:VAL:HG23 | 2.46                     | 0.45              |
| 36:BM:71:LYS:HD3   | 36:BM:95:LEU:HD13  | 1.97                     | 0.45              |
| 38:BO:104:GLN:C    | 38:BO:105:ALA:O    | 2.54                     | 0.45              |
| 38:BO:11:ALA:HB2   | 38:BO:96:GLY:CA    | 2.47                     | 0.45              |
| 41:BR:37:GLU:CD    | 41:BR:37:GLU:H     | 2.20                     | 0.45              |
| 43:BT:61:LEU:HA    | 59:BT:201:HOH:O    | 2.16                     | 0.45              |
| 47:BX:33:HIS:O     | 47:BX:34:SER:C     | 2.55                     | 0.45              |
| 55:CA:1090:U:C4    | 55:CA:1091:U:C5    | 3.04                     | 0.45              |
| 18:CS:76:THR:HB    | 55:CA:1221:G:O3'   | 2.16                     | 0.45              |
| 55:CA:1236:A:H2'   | 55:CA:1237:C:C6    | 2.52                     | 0.45              |
| 55:CA:1246:A:O2'   | 55:CA:1247:U:H5'   | 2.17                     | 0.45              |
| 55:CA:1315:U:H3'   | 55:CA:1316:G:C8    | 2.51                     | 0.45              |
| 55:CA:1496:C:H2'   | 55:CA:1497:G:O4'   | 2.17                     | 0.45              |
| 55:CA:395:C:H2'    | 55:CA:396:C:H6     | 1.80                     | 0.45              |
| 55:CA:397:A:H5'    | 55:CA:398:U:OP1    | 2.16                     | 0.45              |
| 55:CA:648:A:H2'    | 55:CA:649:A:H8     | 1.81                     | 0.45              |
| 55:CA:790:A:H2'    | 55:CA:791:G:O4'    | 2.16                     | 0.45              |
| 8:CI:12:LYS:HG2    | 8:CI:12:LYS:O      | 2.15                     | 0.45              |
| 16:CQ:46:HIS:CB    | 16:CQ:66:LEU:HD13  | 2.46                     | 0.45              |
| 35:DL:62:PRO:HG2   | 53:D3:24:LYS:CB    | 2.47                     | 0.45              |
| 24:DA:1085:A:H3'   | 24:DA:1086:A:N3    | 2.32                     | 0.45              |
| 24:DA:1153:C:H2'   | 24:DA:1154:G:H8    | 1.81                     | 0.45              |
| 24:DA:171:U:O2     | 24:DA:172:A:C8     | 2.70                     | 0.45              |
| 24:DA:1826:G:C5    | 24:DA:1827:U:C4    | 3.04                     | 0.45              |
| 24:DA:1830:C:H2'   | 24:DA:1831:G:C8    | 2.48                     | 0.45              |
| 24:DA:2031:A:O2'   | 24:DA:2032:G:P     | 2.74                     | 0.45              |
| 24:DA:2056:G:N2    | 24:DA:2057:G:C8    | 2.84                     | 0.45              |
| 24:DA:2108:A:C8    | 24:DA:2108:A:OP2   | 2.69                     | 0.45              |
| 24:DA:2248:C:H3'   | 24:DA:2249:U:H6    | 1.81                     | 0.45              |
| 24:DA:230:G:C2     | 24:DA:231:A:C8     | 3.04                     | 0.45              |
| 24:DA:2386:A:H2    | 46:DW:38:ARG:HG2   | 1.81                     | 0.45              |
| 24:DA:2259:U:C2    | 24:DA:2427:C:N3    | 2.85                     | 0.45              |
| 24:DA:2520:C:O2'   | 24:DA:2521:C:C5'   | 2.64                     | 0.45              |
| 24:DA:2881:U:O4'   | 37:DN:93:GLY:HA3   | 2.16                     | 0.45              |
| 24:DA:247:G:H5''   | 24:DA:386:G:H2'    | 1.97                     | 0.45              |
| 24:DA:770:G:O4'    | 24:DA:1379:U:C5    | 2.70                     | 0.45              |
| 56:DB:11:C:H5      | 56:DB:12:C:H5      | 1.63                     | 0.45              |
| 56:DB:42:C:O2'     | 56:DB:43:C:H5'     | 2.16                     | 0.45              |
| 26:DC:206:LYS:HG3  | 26:DC:209:ALA:H    | 1.82                     | 0.45              |
| 29:DF:134:GLN:HE22 | 29:DF:136:ILE:H    | 1.64                     | 0.45              |
| 31:DH:31:VAL:HB    | 31:DH:32:PRO:HD3   | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DH:49:ALA:C    | 31:DH:53:GLU:HB2  | 2.37                     | 0.45              |
| 33:DJ:106:LYS:HE2 | 33:DJ:106:LYS:HA  | 1.98                     | 0.45              |
| 34:DK:16:ALA:HB3  | 34:DK:46:ALA:N    | 2.31                     | 0.45              |
| 34:DK:88:ASN:CB   | 34:DK:91:SER:HB2  | 2.46                     | 0.45              |
| 34:DK:92:GLU:O    | 34:DK:93:GLN:C    | 2.54                     | 0.45              |
| 39:DP:64:SER:O    | 39:DP:66:GLY:N    | 2.47                     | 0.45              |
| 42:DS:55:ILE:O    | 42:DS:59:GLU:HG2  | 2.17                     | 0.45              |
| 44:DU:73:ASN:CB   | 44:DU:95:PHE:HE2  | 2.29                     | 0.45              |
| 45:DV:57:TYR:CD2  | 45:DV:74:ALA:HB1  | 2.51                     | 0.45              |
| 24:DA:2264:C:H41  | 46:DW:11:ASN:ND2  | 2.14                     | 0.45              |
| 21:AA:1131:G:H1   | 21:AA:1144:G:H4'  | 1.80                     | 0.45              |
| 21:AA:1169:A:O2'  | 21:AA:1170:A:O4'  | 2.35                     | 0.45              |
| 21:AA:1322:C:O4'  | 21:AA:1322:C:O2   | 2.30                     | 0.45              |
| 21:AA:1348:U:O2'  | 21:AA:1349:A:C5'  | 2.64                     | 0.45              |
| 21:AA:1386:G:N3   | 21:AA:1387:G:C8   | 2.84                     | 0.45              |
| 21:AA:1462:C:C4   | 21:AA:1463:U:C4   | 3.04                     | 0.45              |
| 21:AA:199:A:O2'   | 21:AA:200:G:O5'   | 2.35                     | 0.45              |
| 15:AP:17:TYR:CE2  | 21:AA:375:U:H4'   | 2.52                     | 0.45              |
| 21:AA:423:G:O2'   | 21:AA:424:G:O4'   | 2.33                     | 0.45              |
| 21:AA:652:U:HO2'  | 21:AA:653:U:H6    | 1.61                     | 0.45              |
| 4:AE:95:MET:HA    | 4:AE:124:ALA:CB   | 2.46                     | 0.45              |
| 9:AJ:10:LEU:HD21  | 9:AJ:25:ILE:HD11  | 1.98                     | 0.45              |
| 16:AQ:60:ILE:HG22 | 16:AQ:61:ARG:N    | 2.32                     | 0.45              |
| 24:BA:107:G:H1'   | 24:BA:294:A:H1'   | 1.97                     | 0.45              |
| 24:BA:1179:G:OP2  | 24:BA:1180:U:H5'' | 2.15                     | 0.45              |
| 24:BA:1223:G:N2   | 24:BA:1226:A:OP2  | 2.47                     | 0.45              |
| 24:BA:1315:C:N3   | 24:BA:1338:G:C2   | 2.85                     | 0.45              |
| 24:BA:1429:G:H2'  | 24:BA:1430:G:H8   | 1.82                     | 0.45              |
| 24:BA:1544:A:C6   | 24:BA:1545:A:C6   | 3.04                     | 0.45              |
| 24:BA:1850:G:C2'  | 24:BA:1851:U:H5'  | 2.46                     | 0.45              |
| 24:BA:1914:C:H2'  | 24:BA:1915:U:C6   | 2.51                     | 0.45              |
| 24:BA:1989:G:O5'  | 24:BA:1989:G:H8   | 2.00                     | 0.45              |
| 24:BA:1989:G:H2'  | 24:BA:1990:C:C5'  | 2.46                     | 0.45              |
| 24:BA:2023:C:H4'  | 24:BA:2617:U:O3'  | 2.15                     | 0.45              |
| 24:BA:2297:A:C8   | 24:BA:2320:U:N3   | 2.84                     | 0.45              |
| 24:BA:2528:U:H2'  | 24:BA:2530:A:O5'  | 2.16                     | 0.45              |
| 24:BA:2603:G:C6   | 24:BA:2604:U:C4   | 3.05                     | 0.45              |
| 24:BA:2682:A:H2'  | 24:BA:2683:C:C6   | 2.52                     | 0.45              |
| 24:BA:2679:A:C2   | 24:BA:2729:G:N1   | 2.84                     | 0.45              |
| 24:BA:527:C:C5    | 24:BA:2779:U:C5   | 3.04                     | 0.45              |
| 24:BA:27:G:H1'    | 24:BA:513:A:H62   | 1.82                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:2897:U:H2'   | 24:BA:2898:U:O4'   | 2.16                     | 0.45              |
| 24:BA:320:A:H4'    | 24:BA:322:A:N7     | 2.32                     | 0.45              |
| 24:BA:608:A:N6     | 24:BA:609:A:C6     | 2.84                     | 0.45              |
| 24:BA:631:A:H3'    | 24:BA:632:A:H8     | 1.82                     | 0.45              |
| 24:BA:669:G:C5     | 24:BA:801:G:C6     | 3.05                     | 0.45              |
| 24:BA:81:G:H2'     | 24:BA:82:U:O4'     | 2.16                     | 0.45              |
| 24:BA:919:U:C4     | 24:BA:920:A:N7     | 2.84                     | 0.45              |
| 25:BB:37:C:C5      | 25:BB:38:C:C5      | 3.04                     | 0.45              |
| 26:BC:114:GLN:C    | 26:BC:115:ILE:HD13 | 2.35                     | 0.45              |
| 26:BC:5:CYS:HB3    | 26:BC:12:ARG:NH1   | 2.31                     | 0.45              |
| 27:BD:90:PHE:C     | 27:BD:92:VAL:N     | 2.70                     | 0.45              |
| 28:BE:31:VAL:HG21  | 28:BE:104:ALA:HB3  | 1.98                     | 0.45              |
| 29:BF:153:ILE:HG13 | 29:BF:153:ILE:H    | 1.57                     | 0.45              |
| 29:BF:174:PHE:CD1  | 29:BF:176:PHE:CE1  | 3.05                     | 0.45              |
| 31:BH:101:ASP:O    | 31:BH:104:THR:HB   | 2.16                     | 0.45              |
| 24:BA:1059:G:C2'   | 32:BI:131:THR:OG1  | 2.64                     | 0.45              |
| 32:BI:19:PRO:HB2   | 32:BI:22:PRO:HD2   | 1.99                     | 0.45              |
| 36:BM:32:GLY:HA3   | 36:BM:131:VAL:HG23 | 1.98                     | 0.45              |
| 38:BO:3:LYS:CG     | 38:BO:4:LYS:N      | 2.79                     | 0.45              |
| 40:BQ:105:PHE:HA   | 40:BQ:108:LEU:HD12 | 1.98                     | 0.45              |
| 24:BA:994:C:O2     | 41:BR:10:LYS:CE    | 2.64                     | 0.45              |
| 41:BR:53:PHE:CD1   | 41:BR:53:PHE:N     | 2.80                     | 0.45              |
| 42:BS:68:ASP:O     | 42:BS:109:ASP:HB3  | 2.16                     | 0.45              |
| 49:BZ:43:ILE:C     | 49:BZ:43:ILE:HD12  | 2.36                     | 0.45              |
| 55:CA:1157:A:C4'   | 55:CA:1158:C:O5'   | 2.56                     | 0.45              |
| 55:CA:1217:C:H2'   | 55:CA:1218:C:C6    | 2.52                     | 0.45              |
| 55:CA:1386:G:C2    | 55:CA:1387:G:C8    | 3.05                     | 0.45              |
| 55:CA:245:U:O2'    | 55:CA:246:A:H5'    | 2.16                     | 0.45              |
| 55:CA:405:U:OP1    | 55:CA:406:G:O2'    | 2.32                     | 0.45              |
| 55:CA:51:A:H4'     | 55:CA:52:C:H5'     | 1.98                     | 0.45              |
| 55:CA:636:U:H2'    | 55:CA:637:C:C6     | 2.51                     | 0.45              |
| 55:CA:669:G:H2'    | 55:CA:670:G:C8     | 2.51                     | 0.45              |
| 55:CA:77:A:H3'     | 55:CA:77:A:OP2     | 2.17                     | 0.45              |
| 55:CA:961:U:O2'    | 55:CA:962:C:O4'    | 2.30                     | 0.45              |
| 55:CA:977:A:H2'    | 55:CA:1224:U:C4    | 2.45                     | 0.45              |
| 1:CB:103:TRP:HD1   | 1:CB:107:ARG:HB3   | 1.81                     | 0.45              |
| 2:CC:168:ARG:NH1   | 55:CA:1106:G:O2'   | 2.49                     | 0.45              |
| 3:CD:77:GLU:OE1    | 3:CD:80:ARG:NH2    | 2.48                     | 0.45              |
| 9:CJ:31:ARG:NH1    | 9:CJ:32:THR:HB     | 2.32                     | 0.45              |
| 9:CJ:42:LEU:HB3    | 9:CJ:43:PRO:CD     | 2.45                     | 0.45              |
| 9:CJ:5:ARG:CG      | 9:CJ:79:PRO:HG3    | 2.47                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:CL:34:THR:C    | 11:CL:35:ARG:HE    | 2.19                     | 0.45              |
| 13:CN:15:LEU:HD22 | 13:CN:19:TYR:HE1   | 1.82                     | 0.45              |
| 9:CJ:65:TYR:HB3   | 13:CN:95:LEU:HD11  | 1.98                     | 0.45              |
| 15:CP:38:PHE:O    | 15:CP:50:THR:HG23  | 2.15                     | 0.45              |
| 19:CT:22:SER:O    | 19:CT:26:MET:HB2   | 2.17                     | 0.45              |
| 19:CT:61:ALA:O    | 19:CT:67:HIS:HA    | 2.16                     | 0.45              |
| 50:D0:29:VAL:HG21 | 50:D0:34:GLY:HA2   | 1.97                     | 0.45              |
| 24:DA:2419:U:OP2  | 53:D3:32:LEU:HD13  | 2.16                     | 0.45              |
| 24:DA:1520:U:O4   | 24:DA:1521:G:C6    | 2.69                     | 0.45              |
| 24:DA:1684:G:C2   | 24:DA:1705:A:C2    | 3.04                     | 0.45              |
| 24:DA:170:U:H6    | 24:DA:170:U:O5'    | 1.99                     | 0.45              |
| 24:DA:1731:G:N3   | 24:DA:1731:G:O4'   | 2.46                     | 0.45              |
| 24:DA:1821:A:H5'  | 26:DC:156:SER:OG   | 2.16                     | 0.45              |
| 24:DA:1857:G:C4   | 24:DA:1884:G:N1    | 2.85                     | 0.45              |
| 24:DA:2603:G:C6   | 24:DA:2604:U:C4    | 3.05                     | 0.45              |
| 24:DA:2619:C:H5'  | 27:DD:157:LYS:HD3  | 1.97                     | 0.45              |
| 24:DA:2826:A:H2'  | 24:DA:2827:C:O4'   | 2.16                     | 0.45              |
| 24:DA:294:A:H2'   | 24:DA:295:G:O5'    | 2.16                     | 0.45              |
| 24:DA:539:G:C6    | 24:DA:540:C:C4     | 3.04                     | 0.45              |
| 24:DA:571:U:C5    | 24:DA:575:A:C5     | 3.05                     | 0.45              |
| 24:DA:68:G:N2     | 24:DA:69:C:H1'     | 2.32                     | 0.45              |
| 24:DA:838:C:C2    | 24:DA:941:A:N1     | 2.84                     | 0.45              |
| 24:DA:866:A:N7    | 24:DA:914:G:N7     | 2.64                     | 0.45              |
| 24:DA:996:A:C4'   | 40:DQ:91:ARG:HH11  | 2.30                     | 0.45              |
| 56:DB:9:G:C2      | 56:DB:112:G:C2     | 3.04                     | 0.45              |
| 56:DB:49:C:H2'    | 56:DB:50:A:C8      | 2.51                     | 0.45              |
| 26:DC:17:LYS:HD3  | 26:DC:17:LYS:C     | 2.37                     | 0.45              |
| 28:DE:45:ALA:O    | 28:DE:46:GLN:CB    | 2.64                     | 0.45              |
| 29:DF:11:VAL:HG12 | 29:DF:12:VAL:H     | 1.81                     | 0.45              |
| 29:DF:28:PRO:HB2  | 29:DF:168:LEU:CD2  | 2.42                     | 0.45              |
| 33:DJ:35:ARG:HH11 | 33:DJ:140:LEU:HD11 | 1.80                     | 0.45              |
| 43:DT:63:VAL:HG21 | 43:DT:80:TRP:CE2   | 2.51                     | 0.45              |
| 44:DU:48:VAL:HG22 | 44:DU:50:ALA:H     | 1.81                     | 0.45              |
| 48:DY:50:VAL:HA   | 48:DY:53:VAL:HG23  | 1.97                     | 0.45              |
| 49:DZ:29:ARG:H    | 49:DZ:29:ARG:CZ    | 2.29                     | 0.45              |
| 21:AA:1163:A:N1   | 21:AA:1174:G:C6    | 2.85                     | 0.45              |
| 21:AA:1253:G:C2   | 21:AA:1285:A:N6    | 2.85                     | 0.45              |
| 21:AA:1428:A:C5   | 21:AA:1429:A:N7    | 2.84                     | 0.45              |
| 21:AA:1463:U:H2'  | 21:AA:1464:U:C6    | 2.52                     | 0.45              |
| 16:AQ:18:LYS:HE3  | 21:AA:255:G:H4'    | 1.97                     | 0.45              |
| 21:AA:346:G:P     | 39:BP:33:GLU:OE2   | 2.74                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 21:AA:462:G:OP1    | 21:AA:463:U:H5    | 2.00                     | 0.45              |
| 21:AA:579:A:C4     | 21:AA:580:C:C5    | 3.05                     | 0.45              |
| 21:AA:845:A:H5''   | 21:AA:846:G:C1'   | 2.46                     | 0.45              |
| 2:AC:144:GLY:O     | 2:AC:145:ALA:O    | 2.35                     | 0.45              |
| 7:AH:106:SER:HB2   | 21:AA:640:A:O2'   | 2.17                     | 0.45              |
| 10:AK:81:LEU:CD2   | 10:AK:104:PHE:HB3 | 2.46                     | 0.45              |
| 11:AL:38:THR:HG22  | 11:AL:50:LYS:HA   | 1.99                     | 0.45              |
| 17:AR:62:ARG:HA    | 17:AR:67:LEU:O    | 2.16                     | 0.45              |
| 24:BA:1016:G:N2    | 24:BA:1147:A:C4   | 2.84                     | 0.45              |
| 24:BA:1179:G:N1    | 24:BA:1180:U:O2'  | 2.50                     | 0.45              |
| 24:BA:1190:G:OP1   | 35:BL:32:GLY:CA   | 2.64                     | 0.45              |
| 24:BA:1216:G:C5    | 24:BA:1217:U:C5   | 3.05                     | 0.45              |
| 24:BA:1331:G:C2    | 24:BA:1333:G:C8   | 3.05                     | 0.45              |
| 24:BA:1419:A:C8    | 24:BA:1421:G:C6   | 3.05                     | 0.45              |
| 24:BA:1509:A:C4    | 24:BA:1510:G:C8   | 3.04                     | 0.45              |
| 24:BA:1550:C:H2'   | 24:BA:1551:A:O4'  | 2.16                     | 0.45              |
| 24:BA:192:C:O2'    | 24:BA:802:A:H1'   | 2.17                     | 0.45              |
| 24:BA:2069:G:O2'   | 24:BA:2070:A:H5'  | 2.16                     | 0.45              |
| 24:BA:2196:C:H5''  | 3:CD:150:LYS:HB3  | 1.99                     | 0.45              |
| 24:BA:2517:C:H2'   | 24:BA:2542:A:N7   | 2.32                     | 0.45              |
| 24:BA:272:A:H2'    | 24:BA:273:G:H8    | 1.80                     | 0.45              |
| 24:BA:271:G:O2'    | 24:BA:272:A:H8    | 1.99                     | 0.45              |
| 24:BA:2799:A:H2'   | 24:BA:2799:A:H8   | 1.58                     | 0.45              |
| 24:BA:2863:C:C2    | 24:BA:2864:G:C8   | 3.05                     | 0.45              |
| 24:BA:536:G:C6     | 24:BA:537:G:C4    | 3.05                     | 0.45              |
| 24:BA:668:A:H2'    | 24:BA:669:G:OP1   | 2.17                     | 0.45              |
| 24:BA:909:A:C6     | 24:BA:912:C:C2    | 3.05                     | 0.45              |
| 24:BA:956:G:N2     | 24:BA:959:A:H3'   | 2.32                     | 0.45              |
| 25:BB:32:U:O2'     | 25:BB:33:G:H5'    | 2.17                     | 0.45              |
| 25:BB:44:G:H1'     | 25:BB:47:C:N4     | 2.32                     | 0.45              |
| 27:BD:151:THR:HG22 | 27:BD:152:PRO:CD  | 2.47                     | 0.45              |
| 32:BI:18:ASN:ND2   | 32:BI:38:CYS:HB3  | 2.31                     | 0.45              |
| 24:BA:2881:U:O2'   | 37:BN:96:ARG:HA   | 2.17                     | 0.45              |
| 39:BP:26:GLU:CB    | 39:BP:43:GLU:HB2  | 2.47                     | 0.45              |
| 43:BT:14:PRO:HA    | 43:BT:32:LEU:CB   | 2.45                     | 0.45              |
| 43:BT:40:LYS:O     | 43:BT:44:LYS:N    | 2.50                     | 0.45              |
| 44:BU:82:VAL:O     | 44:BU:94:PHE:O    | 2.34                     | 0.45              |
| 46:BW:46:ALA:O     | 46:BW:47:GLY:O    | 2.33                     | 0.45              |
| 47:BX:16:ASN:HB2   | 47:BX:24:THR:OG1  | 2.17                     | 0.45              |
| 49:BZ:22:THR:O     | 49:BZ:23:LEU:C    | 2.54                     | 0.45              |
| 18:CS:33:TRP:CB    | 55:CA:1014:A:C2   | 3.00                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:CA:1460:C:N4   | 55:CA:1461:G:C5    | 2.85                     | 0.45              |
| 55:CA:374:A:P     | 55:CA:452:A:H61    | 2.39                     | 0.45              |
| 55:CA:488:C:H2'   | 55:CA:489:C:C6     | 2.51                     | 0.45              |
| 55:CA:512:U:C2    | 55:CA:513:C:C5     | 3.05                     | 0.45              |
| 55:CA:557:G:C6    | 55:CA:558:G:C2     | 3.04                     | 0.45              |
| 55:CA:688:G:H2'   | 55:CA:689:C:C6     | 2.52                     | 0.45              |
| 55:CA:728:A:H2'   | 55:CA:729:A:H8     | 1.80                     | 0.45              |
| 55:CA:767:A:N6    | 55:CA:768:A:C6     | 2.84                     | 0.45              |
| 55:CA:807:A:H2'   | 55:CA:808:C:C6     | 2.52                     | 0.45              |
| 55:CA:951:G:C2    | 55:CA:1231:G:C5    | 3.05                     | 0.45              |
| 1:CB:23:ASN:ND2   | 1:CB:191:ASP:OD1   | 2.46                     | 0.45              |
| 2:CC:80:GLY:O     | 2:CC:83:VAL:HG22   | 2.16                     | 0.45              |
| 3:CD:124:VAL:O    | 3:CD:125:ASN:C     | 2.54                     | 0.45              |
| 7:CH:112:ASP:OD2  | 7:CH:116:ARG:HG3   | 2.15                     | 0.45              |
| 11:CL:6:LEU:C     | 11:CL:8:ARG:N      | 2.70                     | 0.45              |
| 15:CP:6:LEU:HB2   | 15:CP:17:TYR:HB3   | 1.97                     | 0.45              |
| 7:CH:85:TYR:CD1   | 16:CQ:36:PHE:HE2   | 2.35                     | 0.45              |
| 16:CQ:68:LYS:O    | 55:CA:254:G:OP1    | 2.35                     | 0.45              |
| 17:CR:44:THR:OG1  | 17:CR:46:THR:HG22  | 2.16                     | 0.45              |
| 18:CS:10:ILE:HG22 | 18:CS:14:LEU:HD11  | 1.98                     | 0.45              |
| 19:CT:34:VAL:O    | 19:CT:38:ILE:HG13  | 2.17                     | 0.45              |
| 24:DA:1050:A:O2'  | 24:DA:1051:G:C5'   | 2.64                     | 0.45              |
| 24:DA:1255:U:H2'  | 28:DE:68:ALA:HB2   | 1.98                     | 0.45              |
| 24:DA:1341:G:OP2  | 24:DA:1394:U:O2'   | 2.34                     | 0.45              |
| 24:DA:1439:A:N6   | 24:DA:1552:A:C8    | 2.84                     | 0.45              |
| 24:DA:160:A:N1    | 24:DA:161:A:C2     | 2.85                     | 0.45              |
| 24:DA:1710:G:H2'  | 24:DA:1711:A:C8    | 2.51                     | 0.45              |
| 24:DA:2210:U:H4'  | 24:DA:2211:A:H5'   | 1.97                     | 0.45              |
| 24:DA:2250:G:OP1  | 24:DA:2275:C:H2'   | 2.16                     | 0.45              |
| 24:DA:2418:A:C6   | 24:DA:2419:U:C4    | 3.04                     | 0.45              |
| 24:DA:2425:A:H4'  | 24:DA:2426:A:O5'   | 2.16                     | 0.45              |
| 24:DA:2456:C:H2'  | 24:DA:2457:U:O4'   | 2.16                     | 0.45              |
| 24:DA:2474:U:H2'  | 24:DA:2475:C:O5'   | 2.17                     | 0.45              |
| 24:DA:2718:G:H2'  | 24:DA:2719:G:O4'   | 2.16                     | 0.45              |
| 24:DA:296:U:H2'   | 24:DA:297:G:H8     | 1.82                     | 0.45              |
| 24:DA:30:G:H2'    | 24:DA:31:C:O4'     | 2.16                     | 0.45              |
| 24:DA:500:G:C2    | 24:DA:503:A:C8     | 3.05                     | 0.45              |
| 24:DA:90:U:OP2    | 24:DA:91:A:H3'     | 2.15                     | 0.45              |
| 24:DA:975:A:C5    | 24:DA:990:A:N7     | 2.85                     | 0.45              |
| 24:DA:995:C:H1'   | 40:DQ:60:TRP:HZ2   | 1.81                     | 0.45              |
| 26:DC:68:ARG:HH12 | 26:DC:115:ILE:HD12 | 1.82                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 28:DE:194:LYS:O  | 28:DE:197:GLU:HB3 | 2.17                     | 0.45              |
| 30:DG:58:ALA:O   | 30:DG:59:ASP:C    | 2.55                     | 0.45              |
| 32:DI:22:PRO:HB2 | 32:DI:23:VAL:H    | 1.57                     | 0.45              |
| 41:DR:13:ARG:HE  | 41:DR:13:ARG:C    | 2.19                     | 0.45              |
| 41:DR:38:VAL:O   | 41:DR:53:PHE:HA   | 2.16                     | 0.45              |
| 42:DS:33:LEU:O   | 42:DS:36:LEU:HB2  | 2.17                     | 0.45              |
| 43:DT:34:VAL:O   | 43:DT:35:ALA:HB3  | 2.17                     | 0.45              |
| 45:DV:32:GLY:O   | 45:DV:33:GLY:C    | 2.55                     | 0.45              |
| 47:DX:70:LEU:O   | 47:DX:74:GLY:N    | 2.49                     | 0.45              |
| 9:AJ:39:PRO:HD2  | 21:AA:1123:U:H4'  | 1.97                     | 0.45              |
| 21:AA:1144:G:C8  | 21:AA:1144:G:OP2  | 2.69                     | 0.45              |
| 21:AA:1195:C:C4  | 21:AA:1197:A:N7   | 2.85                     | 0.45              |
| 21:AA:1202:U:H2' | 21:AA:1203:C:C6   | 2.52                     | 0.45              |
| 21:AA:1250:A:C8  | 21:AA:1287:A:N7   | 2.85                     | 0.45              |
| 21:AA:1384:C:H2' | 21:AA:1385:G:C8   | 2.46                     | 0.45              |
| 21:AA:1423:G:H2' | 21:AA:1424:U:H6   | 1.80                     | 0.45              |
| 21:AA:1449:C:O2' | 21:AA:1450:U:C5'  | 2.64                     | 0.45              |
| 21:AA:1452:C:H4' | 21:AA:1453:G:C4   | 2.51                     | 0.45              |
| 21:AA:1462:C:C4  | 21:AA:1463:U:C5   | 3.05                     | 0.45              |
| 21:AA:264:C:N4   | 21:AA:265:G:C6    | 2.85                     | 0.45              |
| 21:AA:401:C:C2   | 21:AA:402:G:C8    | 3.05                     | 0.45              |
| 21:AA:632:U:O2   | 21:AA:632:U:H2'   | 2.15                     | 0.45              |
| 21:AA:682:G:N2   | 21:AA:709:U:C2    | 2.85                     | 0.45              |
| 21:AA:844:G:C6   | 21:AA:847:G:H5'   | 2.52                     | 0.45              |
| 21:AA:908:A:H2'  | 21:AA:909:A:C8    | 2.51                     | 0.45              |
| 21:AA:914:A:O2'  | 21:AA:915:A:H8    | 1.98                     | 0.45              |
| 1:AB:108:GLN:CA  | 1:AB:111:LYS:HB3  | 2.40                     | 0.45              |
| 1:AB:160:LEU:O   | 1:AB:183:PHE:CD2  | 2.66                     | 0.45              |
| 1:AB:161:PHE:CZ  | 1:AB:216:VAL:HG21 | 2.51                     | 0.45              |
| 1:AB:30:ILE:HD11 | 1:AB:188:THR:CG2  | 2.47                     | 0.45              |
| 2:AC:8:GLY:HA2   | 2:AC:11:LEU:HG    | 1.98                     | 0.45              |
| 3:AD:194:ILE:C   | 3:AD:195:ASN:HD22 | 2.19                     | 0.45              |
| 4:AE:15:ILE:CD1  | 4:AE:37:VAL:HG23  | 2.44                     | 0.45              |
| 6:AG:134:VAL:O   | 6:AG:137:ARG:HB3  | 2.17                     | 0.45              |
| 6:AG:43:TYR:O    | 6:AG:47:GLU:HB2   | 2.16                     | 0.45              |
| 7:AH:124:ILE:H   | 7:AH:124:ILE:HG12 | 1.49                     | 0.45              |
| 10:AK:13:LYS:O   | 10:AK:14:GLN:HB3  | 2.16                     | 0.45              |
| 16:AQ:49:ASN:O   | 16:AQ:51:GLU:N    | 2.50                     | 0.45              |
| 54:B4:19:ARG:O   | 54:B4:20:ASP:C    | 2.54                     | 0.45              |
| 24:BA:1063:G:C2  | 24:BA:1064:C:C2   | 3.05                     | 0.45              |
| 24:BA:1549:A:C5  | 24:BA:1550:C:C4   | 3.05                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:BA:1615:C:O2'   | 24:BA:1616:A:P    | 2.74                     | 0.45              |
| 24:BA:2315:G:H2'   | 24:BA:2316:G:O4'  | 2.16                     | 0.45              |
| 24:BA:2364:C:C2'   | 24:BA:2365:G:H5'  | 2.47                     | 0.45              |
| 24:BA:2683:C:H2'   | 24:BA:2684:U:H6   | 1.81                     | 0.45              |
| 24:BA:2824:C:C5    | 24:BA:2825:G:C6   | 3.05                     | 0.45              |
| 24:BA:2824:C:C5    | 24:BA:2825:G:C5   | 3.05                     | 0.45              |
| 24:BA:56:A:C2      | 24:BA:57:C:C2     | 3.05                     | 0.45              |
| 24:BA:602:A:N3     | 24:BA:655:A:C2    | 2.85                     | 0.45              |
| 24:BA:729:G:C4     | 24:BA:1775:U:C2   | 3.04                     | 0.45              |
| 24:BA:746:U:O2'    | 24:BA:747:U:P     | 2.75                     | 0.45              |
| 24:BA:994:C:H3'    | 40:BQ:53:LYS:HE2  | 1.99                     | 0.45              |
| 26:BC:114:GLN:HE21 | 26:BC:114:GLN:HB2 | 1.59                     | 0.45              |
| 27:BD:182:ALA:C    | 27:BD:183:GLU:HG3 | 2.37                     | 0.45              |
| 27:BD:97:SER:OG    | 27:BD:98:VAL:N    | 2.50                     | 0.45              |
| 28:BE:119:ILE:CD1  | 28:BE:187:VAL:HA  | 2.47                     | 0.45              |
| 30:BG:123:GLU:CD   | 30:BG:124:CYS:N   | 2.70                     | 0.45              |
| 30:BG:33:THR:CA    | 30:BG:34:ARG:HD3  | 2.47                     | 0.45              |
| 32:BI:32:VAL:HG22  | 32:BI:66:PHE:CD1  | 2.52                     | 0.45              |
| 33:BJ:64:VAL:O     | 33:BJ:65:THR:CB   | 2.65                     | 0.45              |
| 35:BL:79:LEU:HB3   | 35:BL:116:VAL:HB  | 1.99                     | 0.45              |
| 40:BQ:94:LEU:HD22  | 40:BQ:94:LEU:HA   | 1.64                     | 0.45              |
| 41:BR:81:LYS:O     | 41:BR:82:HIS:C    | 2.54                     | 0.45              |
| 42:BS:25:ARG:CD    | 42:BS:73:LYS:NZ   | 2.80                     | 0.45              |
| 44:BU:78:LYS:HG2   | 44:BU:79:ALA:H    | 1.81                     | 0.45              |
| 46:BW:28:GLU:HG3   | 46:BW:29:SER:N    | 2.28                     | 0.45              |
| 46:BW:29:SER:O     | 46:BW:30:VAL:HB   | 2.17                     | 0.45              |
| 46:BW:28:GLU:O     | 46:BW:30:VAL:N    | 2.50                     | 0.45              |
| 55:CA:1391:U:H2'   | 55:CA:1392:G:C8   | 2.52                     | 0.45              |
| 55:CA:161:A:H2'    | 55:CA:162:A:C8    | 2.51                     | 0.45              |
| 55:CA:275:G:H2'    | 55:CA:276:G:H8    | 1.80                     | 0.45              |
| 55:CA:391:G:C6     | 55:CA:392:C:C4    | 3.04                     | 0.45              |
| 55:CA:557:G:O6     | 55:CA:558:G:N1    | 2.50                     | 0.45              |
| 55:CA:596:A:N3     | 55:CA:597:G:C8    | 2.84                     | 0.45              |
| 55:CA:792:A:C4     | 55:CA:794:A:C6    | 3.05                     | 0.45              |
| 4:CE:43:GLY:O      | 4:CE:73:VAL:HB    | 2.16                     | 0.45              |
| 7:CH:110:MET:HB2   | 7:CH:111:THR:H    | 1.65                     | 0.45              |
| 9:CJ:15:HIS:CE1    | 9:CJ:68:ARG:HD3   | 2.52                     | 0.45              |
| 9:CJ:77:VAL:O      | 9:CJ:79:PRO:HD3   | 2.16                     | 0.45              |
| 50:D0:47:TYR:CE2   | 50:D0:52:LYS:HG3  | 2.51                     | 0.45              |
| 24:DA:1158:C:HO2'  | 24:DA:1159:U:H6   | 1.63                     | 0.45              |
| 24:DA:1188:U:O2'   | 24:DA:1189:A:H5'  | 2.17                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:1425:G:H8   | 24:DA:1425:G:O5'   | 1.99                     | 0.45              |
| 24:DA:153:U:O2'   | 24:DA:154:U:H5'    | 2.16                     | 0.45              |
| 24:DA:1783:A:C2   | 24:DA:2588:G:O4'   | 2.69                     | 0.45              |
| 24:DA:1853:A:C1'  | 24:DA:2234:G:H5'   | 2.46                     | 0.45              |
| 24:DA:2233:U:H2'  | 24:DA:2234:G:C8    | 2.45                     | 0.45              |
| 24:DA:2312:U:OP1  | 29:DF:70:ARG:HB2   | 2.16                     | 0.45              |
| 24:DA:244:A:C2    | 24:DA:255:A:C4     | 3.04                     | 0.45              |
| 24:DA:2552:U:C2   | 24:DA:2554:U:H5'   | 2.52                     | 0.45              |
| 24:DA:271:G:O4'   | 24:DA:367:G:N2     | 2.49                     | 0.45              |
| 24:DA:2738:A:C2   | 24:DA:2766:A:N6    | 2.83                     | 0.45              |
| 24:DA:2902:C:O2'  | 24:DA:2903:U:H5'   | 2.17                     | 0.45              |
| 24:DA:455:C:H3'   | 24:DA:456:C:H5'    | 1.99                     | 0.45              |
| 24:DA:628:G:H2'   | 24:DA:629:G:H8     | 1.76                     | 0.45              |
| 24:DA:684:G:OP1   | 52:D2:16:HIS:CD2   | 2.70                     | 0.45              |
| 24:DA:691:C:O5'   | 24:DA:691:C:H6     | 1.99                     | 0.45              |
| 24:DA:742:A:H2'   | 24:DA:743:A:C8     | 2.52                     | 0.45              |
| 24:DA:753:A:C2    | 24:DA:754:U:C4     | 3.04                     | 0.45              |
| 24:DA:962:G:N2    | 36:DM:82:MET:HE2   | 2.31                     | 0.45              |
| 56:DB:81:G:C5     | 56:DB:82:U:C5      | 3.04                     | 0.45              |
| 26:DC:119:VAL:CG1 | 26:DC:133:ASN:HD21 | 2.22                     | 0.45              |
| 26:DC:244:VAL:HB  | 26:DC:249:VAL:N    | 2.32                     | 0.45              |
| 26:DC:62:ARG:N    | 26:DC:62:ARG:HD2   | 2.31                     | 0.45              |
| 27:DD:149:ASN:OD1 | 27:DD:150:GLN:N    | 2.49                     | 0.45              |
| 29:DF:113:PHE:CZ  | 29:DF:116:LEU:HD22 | 2.52                     | 0.45              |
| 32:DI:28:GLY:O    | 32:DI:29:GLN:C     | 2.54                     | 0.45              |
| 45:DV:21:ARG:C    | 45:DV:23:ALA:H     | 2.20                     | 0.45              |
| 45:DV:49:ASN:O    | 45:DV:52:ALA:HB3   | 2.17                     | 0.45              |
| 47:DX:67:LEU:O    | 47:DX:77:TYR:OH    | 2.33                     | 0.45              |
| 21:AA:1082:A:C5   | 21:AA:1083:U:C4    | 3.05                     | 0.45              |
| 21:AA:1151:A:O2'  | 21:AA:1152:A:O5'   | 2.31                     | 0.45              |
| 21:AA:138:G:C2    | 21:AA:226:G:C4     | 3.04                     | 0.45              |
| 21:AA:233:C:H2'   | 21:AA:234:C:H6     | 1.82                     | 0.45              |
| 21:AA:329:A:O2'   | 21:AA:330:C:H5'    | 2.16                     | 0.45              |
| 21:AA:622:A:H2'   | 21:AA:623:C:C5'    | 2.46                     | 0.45              |
| 21:AA:815:A:O2'   | 21:AA:816:A:P      | 2.75                     | 0.45              |
| 21:AA:872:A:O2'   | 21:AA:873:A:H3'    | 2.17                     | 0.45              |
| 1:AB:110:ILE:HG13 | 1:AB:147:LEU:HD13  | 1.99                     | 0.45              |
| 1:AB:138:ARG:HH21 | 21:AA:1170:A:P     | 2.39                     | 0.45              |
| 1:AB:20:ARG:O     | 1:AB:21:TYR:C      | 2.54                     | 0.45              |
| 3:AD:57:LYS:HA    | 3:AD:199:ILE:HD12  | 1.99                     | 0.45              |
| 4:AE:121:ASN:HD22 | 4:AE:122:VAL:N     | 2.15                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:AI:24:ASN:C     | 8:AI:26:LYS:H     | 2.19                     | 0.45              |
| 9:AJ:53:ILE:HG22  | 9:AJ:62:ARG:N     | 2.31                     | 0.45              |
| 9:AJ:57:VAL:O     | 9:AJ:58:ASN:HB2   | 2.16                     | 0.45              |
| 53:B3:54:LEU:HD12 | 53:B3:54:LEU:HA   | 1.82                     | 0.45              |
| 24:BA:563:A:C6    | 24:BA:2018:G:C5   | 3.05                     | 0.45              |
| 24:BA:2067:G:O3'  | 24:BA:2068:U:H4'  | 2.17                     | 0.45              |
| 24:BA:225:C:H2'   | 24:BA:226:A:O4'   | 2.17                     | 0.45              |
| 24:BA:2287:A:C6   | 24:BA:2289:G:C5   | 3.05                     | 0.45              |
| 24:BA:2333:A:C6   | 24:BA:2335:A:N6   | 2.85                     | 0.45              |
| 24:BA:235:U:H2'   | 24:BA:236:C:O4'   | 2.16                     | 0.45              |
| 24:BA:2581:G:C5   | 24:BA:2610:C:C4   | 3.04                     | 0.45              |
| 24:BA:2639:A:H2'  | 24:BA:2640:G:O4'  | 2.17                     | 0.45              |
| 24:BA:355:U:H2'   | 24:BA:356:G:H8    | 1.78                     | 0.45              |
| 24:BA:35:G:C4     | 24:BA:454:A:C2    | 3.05                     | 0.45              |
| 24:BA:522:A:C5    | 24:BA:523:C:C4    | 3.04                     | 0.45              |
| 24:BA:587:C:C6    | 24:BA:671:C:HI'   | 2.52                     | 0.45              |
| 24:BA:715:A:OP1   | 24:BA:715:A:H8    | 2.00                     | 0.45              |
| 24:BA:753:A:O2'   | 24:BA:754:U:H5'   | 2.16                     | 0.45              |
| 24:BA:841:G:C2    | 24:BA:938:G:C2    | 3.05                     | 0.45              |
| 24:BA:973:A:O4'   | 24:BA:1188:U:C6   | 2.69                     | 0.45              |
| 31:BH:31:VAL:O    | 31:BH:33:GLN:N    | 2.50                     | 0.45              |
| 32:BI:79:LEU:HD22 | 32:BI:137:LEU:CD1 | 2.47                     | 0.45              |
| 34:BK:35:VAL:HG12 | 34:BK:36:GLY:N    | 2.32                     | 0.45              |
| 37:BN:67:PHE:HE1  | 37:BN:73:ASN:OD1  | 2.00                     | 0.45              |
| 39:BP:104:GLY:O   | 39:BP:106:ALA:N   | 2.50                     | 0.45              |
| 45:BV:41:GLU:OE1  | 45:BV:41:GLU:O    | 2.35                     | 0.45              |
| 46:BW:45:HIS:N    | 46:BW:45:HIS:ND1  | 2.57                     | 0.45              |
| 55:CA:1013:G:N2   | 55:CA:1015:G:H3'  | 2.32                     | 0.45              |
| 55:CA:1026:G:N2   | 55:CA:1036:A:H61  | 2.14                     | 0.45              |
| 55:CA:994:A:N7    | 55:CA:1216:A:O4'  | 2.49                     | 0.45              |
| 55:CA:1250:A:C5   | 55:CA:1251:A:C8   | 3.04                     | 0.45              |
| 55:CA:1305:G:N2   | 55:CA:1331:G:H2'  | 2.28                     | 0.45              |
| 55:CA:316:C:C5    | 55:CA:351:G:C5    | 3.04                     | 0.45              |
| 55:CA:369:G:C6    | 55:CA:393:A:C2    | 3.05                     | 0.45              |
| 55:CA:464:U:O2'   | 55:CA:465:A:O5'   | 2.28                     | 0.45              |
| 55:CA:607:A:C6    | 55:CA:608:A:C6    | 3.05                     | 0.45              |
| 55:CA:722:G:N3    | 55:CA:722:G:C2'   | 2.79                     | 0.45              |
| 55:CA:994:A:O2'   | 55:CA:995:C:H5'   | 2.17                     | 0.45              |
| 3:CD:176:LYS:HE2  | 3:CD:178:GLU:OE1  | 2.16                     | 0.45              |
| 3:CD:57:LYS:CA    | 3:CD:199:ILE:HG22 | 2.47                     | 0.45              |
| 17:CR:34:GLU:HB2  | 20:CU:18:PHE:HZ   | 1.81                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:CS:9:PHE:HB3   | 55:CA:1319:A:OP1  | 2.16                     | 0.45              |
| 19:CT:14:GLU:OE1  | 19:CT:18:LYS:HE2  | 2.17                     | 0.45              |
| 53:D3:61:LEU:HB2  | 53:D3:64:ALA:HB3  | 1.98                     | 0.45              |
| 24:DA:1088:A:H4'  | 24:DA:1089:A:H8   | 1.81                     | 0.45              |
| 24:DA:1376:C:H6   | 59:DA:3412:HOH:O  | 2.00                     | 0.45              |
| 24:DA:1430:G:O2'  | 24:DA:1431:A:O4'  | 2.32                     | 0.45              |
| 24:DA:1475:G:O2'  | 24:DA:1476:U:OP2  | 2.35                     | 0.45              |
| 24:DA:1534:U:H2'  | 24:DA:1536:C:O2   | 2.17                     | 0.45              |
| 24:DA:1776:G:H21  | 24:DA:1789:A:H1'  | 1.82                     | 0.45              |
| 24:DA:1793:C:H2'  | 24:DA:1794:A:H8   | 1.82                     | 0.45              |
| 24:DA:1940:U:H1'  | 24:DA:1942:C:N4   | 2.31                     | 0.45              |
| 24:DA:2297:A:H1'  | 24:DA:2322:A:N3   | 2.32                     | 0.45              |
| 24:DA:2428:G:H4'  | 24:DA:2429:G:C5   | 2.52                     | 0.45              |
| 24:DA:2788:C:H2'  | 24:DA:2789:C:H6   | 1.79                     | 0.45              |
| 24:DA:413:C:O2'   | 24:DA:414:C:O4'   | 2.34                     | 0.45              |
| 24:DA:181:A:H2    | 24:DA:434:U:H1'   | 1.82                     | 0.45              |
| 24:DA:510:C:O2'   | 24:DA:511:U:H5'   | 2.16                     | 0.45              |
| 24:DA:749:A:C4    | 24:DA:750:A:C8    | 3.05                     | 0.45              |
| 24:DA:690:G:O2'   | 24:DA:780:G:OP1   | 2.23                     | 0.45              |
| 56:DB:48:U:H5'    | 38:DO:30:ARG:HE   | 1.80                     | 0.45              |
| 56:DB:81:G:H2'    | 56:DB:82:U:H6     | 1.82                     | 0.45              |
| 26:DC:130:PRO:CD  | 26:DC:188:ARG:HG3 | 2.47                     | 0.45              |
| 24:DA:1799:G:OP1  | 26:DC:257:ARG:NH1 | 2.50                     | 0.45              |
| 28:DE:53:THR:OG1  | 28:DE:54:GLY:N    | 2.50                     | 0.45              |
| 31:DH:132:PHE:HB3 | 31:DH:140:ALA:HB3 | 1.98                     | 0.45              |
| 32:DI:20:SER:OG   | 32:DI:25:PRO:HG2  | 2.16                     | 0.45              |
| 33:DJ:4:PHE:CG    | 33:DJ:5:THR:N     | 2.85                     | 0.45              |
| 34:DK:61:VAL:HG13 | 34:DK:87:LEU:CD2  | 2.47                     | 0.45              |
| 40:DQ:64:ILE:HD12 | 40:DQ:95:ALA:HB1  | 1.99                     | 0.45              |
| 42:DS:47:VAL:O    | 42:DS:50:VAL:HB   | 2.15                     | 0.45              |
| 43:DT:45:ALA:HA   | 43:DT:48:GLN:HG2  | 1.99                     | 0.45              |
| 45:DV:21:ARG:HD3  | 45:DV:87:GLN:HG2  | 1.97                     | 0.45              |
| 47:DX:10:ARG:HB3  | 47:DX:11:PRO:HD2  | 1.99                     | 0.45              |
| 48:DY:58:ASN:C    | 48:DY:60:LYS:N    | 2.70                     | 0.45              |
| 21:AA:99:C:C2'    | 21:AA:100:G:OP2   | 2.65                     | 0.45              |
| 21:AA:1125:U:C2   | 21:AA:1127:G:C8   | 3.04                     | 0.45              |
| 21:AA:1137:C:H1'  | 21:AA:1138:G:N2   | 2.32                     | 0.45              |
| 21:AA:1185:G:C5   | 21:AA:1186:G:N7   | 2.85                     | 0.45              |
| 21:AA:1314:C:O2'  | 21:AA:1315:U:H5'  | 2.16                     | 0.45              |
| 21:AA:1403:C:H6   | 21:AA:1403:C:O5'  | 2.00                     | 0.45              |
| 21:AA:1418:A:N7   | 21:AA:1419:G:C1'  | 2.80                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:1453:G:HO2'  | 21:AA:1454:G:P     | 2.40                     | 0.45              |
| 21:AA:18:C:O2'     | 21:AA:19:A:H5'     | 2.17                     | 0.45              |
| 21:AA:409:U:H2'    | 21:AA:410:G:O4'    | 2.17                     | 0.45              |
| 21:AA:683:G:C6     | 21:AA:684:U:N3     | 2.85                     | 0.45              |
| 5:AF:53:LYS:HE2    | 5:AF:53:LYS:HB2    | 1.75                     | 0.45              |
| 6:AG:12:LEU:HD22   | 6:AG:12:LEU:N      | 2.32                     | 0.45              |
| 6:AG:86:VAL:CG1    | 6:AG:87:PRO:HD2    | 2.47                     | 0.45              |
| 7:AH:88:LYS:HB3    | 7:AH:120:LEU:O     | 2.16                     | 0.45              |
| 17:AR:70:THR:OG1   | 17:AR:72:ARG:HG2   | 2.17                     | 0.45              |
| 54:B4:4:ARG:HG3    | 54:B4:6:SER:O      | 2.16                     | 0.45              |
| 24:BA:1204:A:C8    | 24:BA:1206:G:C2    | 3.05                     | 0.45              |
| 24:BA:1247:A:C2    | 24:BA:1249:U:C6    | 3.05                     | 0.45              |
| 24:BA:1276:A:C2    | 24:BA:1277:G:C5    | 3.04                     | 0.45              |
| 24:BA:1425:G:H2'   | 24:BA:1426:G:C8    | 2.52                     | 0.45              |
| 24:BA:1606:C:H4'   | 24:BA:1607:C:H5'   | 1.98                     | 0.45              |
| 24:BA:161:A:C3'    | 24:BA:162:U:H5''   | 2.47                     | 0.45              |
| 24:BA:1665:A:H2'   | 24:BA:1666:G:H5'   | 1.97                     | 0.45              |
| 24:BA:1701:A:H2'   | 24:BA:1702:G:H5'   | 1.99                     | 0.45              |
| 24:BA:2448:A:H3'   | 24:BA:2449:U:H2'   | 1.97                     | 0.45              |
| 24:BA:2516:A:O2'   | 24:BA:2517:C:H5'   | 2.16                     | 0.45              |
| 24:BA:2520:C:C4    | 24:BA:2567:G:C8    | 3.05                     | 0.45              |
| 24:BA:2548:U:C2'   | 24:BA:2549:G:O5'   | 2.65                     | 0.45              |
| 24:BA:2650:U:H2'   | 24:BA:2651:C:H6    | 1.80                     | 0.45              |
| 24:BA:2662:A:N6    | 24:BA:2663:G:C2    | 2.85                     | 0.45              |
| 24:BA:374:A:H2'    | 24:BA:375:G:O4'    | 2.16                     | 0.45              |
| 24:BA:373:U:C5     | 24:BA:400:G:N2     | 2.85                     | 0.45              |
| 24:BA:681:G:H2'    | 24:BA:682:G:O5'    | 2.17                     | 0.45              |
| 24:BA:811:U:C2     | 24:BA:1251:C:H5    | 2.34                     | 0.45              |
| 25:BB:112:G:H2'    | 25:BB:113:C:C6     | 2.52                     | 0.45              |
| 26:BC:140:VAL:HA   | 26:BC:190:THR:O    | 2.16                     | 0.45              |
| 28:BE:75:SER:OG    | 28:BE:77:ILE:HG23  | 2.17                     | 0.45              |
| 28:BE:83:VAL:HG12  | 28:BE:83:VAL:O     | 2.16                     | 0.45              |
| 30:BG:84:LYS:CG    | 30:BG:85:LYS:H     | 2.29                     | 0.45              |
| 31:BH:134:VAL:HG23 | 31:BH:138:VAL:HG23 | 1.98                     | 0.45              |
| 31:BH:53:GLU:O     | 31:BH:53:GLU:HG2   | 2.17                     | 0.45              |
| 35:BL:82:LEU:HD23  | 35:BL:83:ALA:N     | 2.31                     | 0.45              |
| 37:BN:61:ALA:O     | 37:BN:64:ARG:HB2   | 2.17                     | 0.45              |
| 43:BT:52:GLU:CG    | 43:BT:52:GLU:O     | 2.61                     | 0.45              |
| 47:BX:19:HIS:C     | 47:BX:21:LEU:H     | 2.20                     | 0.45              |
| 47:BX:65:THR:O     | 47:BX:68:ALA:HB3   | 2.17                     | 0.45              |
| 49:BZ:40:THR:CG2   | 49:BZ:43:ILE:HG23  | 2.47                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:CA:1157:A:C2   | 55:CA:1181:G:C4    | 3.05                     | 0.45              |
| 55:CA:1297:G:C8   | 55:CA:1297:G:OP2   | 2.70                     | 0.45              |
| 55:CA:245:U:H5''  | 55:CA:245:U:H6     | 1.82                     | 0.45              |
| 55:CA:37:U:C2     | 55:CA:548:G:N1     | 2.84                     | 0.45              |
| 55:CA:89:U:O2'    | 55:CA:90:C:O4'     | 2.24                     | 0.45              |
| 55:CA:96:U:O2'    | 55:CA:97:G:C5'     | 2.65                     | 0.45              |
| 5:CF:25:TYR:HA    | 5:CF:28:ALA:HB3    | 1.98                     | 0.45              |
| 7:CH:12:ARG:HD2   | 7:CH:26:MET:HE2    | 1.99                     | 0.45              |
| 8:CI:9:GLY:CA     | 8:CI:16:ALA:HB3    | 2.39                     | 0.45              |
| 8:CI:58:GLU:HG3   | 8:CI:59:LYS:N      | 2.32                     | 0.45              |
| 15:CP:4:ILE:HD12  | 15:CP:4:ILE:N      | 2.32                     | 0.45              |
| 24:DA:1014:A:O2'  | 24:DA:1015:U:H5'   | 2.16                     | 0.45              |
| 24:DA:1130:U:O2'  | 24:DA:1131:G:N7    | 2.50                     | 0.45              |
| 24:DA:1545:A:H2'  | 24:DA:1546:G:O4'   | 2.16                     | 0.45              |
| 24:DA:1807:G:C2'  | 24:DA:1808:A:H5'   | 2.45                     | 0.45              |
| 24:DA:1816:C:O2'  | 24:DA:1817:G:P     | 2.74                     | 0.45              |
| 24:DA:1799:G:H22  | 24:DA:1818:U:H2'   | 1.82                     | 0.45              |
| 24:DA:1875:G:C8   | 24:DA:1875:G:OP2   | 2.70                     | 0.45              |
| 24:DA:1954:G:O2'  | 24:DA:1956:U:O4    | 2.25                     | 0.45              |
| 24:DA:2287:A:O2'  | 24:DA:2288:A:C3'   | 2.46                     | 0.45              |
| 24:DA:2332:C:H5'' | 46:DW:76:ARG:NH1   | 2.32                     | 0.45              |
| 24:DA:244:A:C2'   | 24:DA:245:G:O5'    | 2.65                     | 0.45              |
| 24:DA:2685:G:C2   | 24:DA:2725:A:C2    | 3.05                     | 0.45              |
| 24:DA:301:G:C5    | 24:DA:302:C:N4     | 2.85                     | 0.45              |
| 24:DA:350:G:H2'   | 24:DA:351:C:O4'    | 2.16                     | 0.45              |
| 24:DA:478:A:C2    | 24:DA:480:A:C8     | 3.04                     | 0.45              |
| 24:DA:52:A:N1     | 24:DA:178:G:O2'    | 2.47                     | 0.45              |
| 24:DA:567:U:C4    | 24:DA:568:U:C4     | 3.05                     | 0.45              |
| 24:DA:589:U:HO2'  | 24:DA:590:A:H8     | 0.67                     | 0.45              |
| 24:DA:604:G:O6    | 24:DA:625:G:C6     | 2.70                     | 0.45              |
| 24:DA:628:G:O2'   | 24:DA:629:G:H5'    | 2.17                     | 0.45              |
| 24:DA:630:G:OP1   | 53:D3:22:LYS:NZ    | 2.49                     | 0.45              |
| 24:DA:941:A:H2'   | 24:DA:942:G:H8     | 1.80                     | 0.45              |
| 56:DB:50:A:C5     | 56:DB:51:G:C8      | 3.05                     | 0.45              |
| 28:DE:133:LEU:C   | 28:DE:133:LEU:HD23 | 2.36                     | 0.45              |
| 31:DH:29:PHE:C    | 31:DH:32:PRO:HD2   | 2.37                     | 0.45              |
| 41:DR:51:VAL:HB   | 41:DR:52:PRO:CD    | 2.47                     | 0.45              |
| 43:DT:25:GLU:HA   | 43:DT:29:THR:O     | 2.17                     | 0.45              |
| 44:DU:54:PRO:CG   | 44:DU:55:GLY:H     | 2.23                     | 0.45              |
| 45:DV:4:ILE:HD11  | 45:DV:50:MET:CE    | 2.46                     | 0.45              |
| 21:AA:1061:G:C5   | 21:AA:1062:U:C4    | 3.05                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:1415:G:C6   | 21:AA:1486:G:C6    | 3.05                     | 0.45              |
| 21:AA:198:G:O2'   | 21:AA:199:A:C5'    | 2.65                     | 0.45              |
| 21:AA:245:U:O2'   | 21:AA:246:A:H5'    | 2.17                     | 0.45              |
| 21:AA:267:C:O2'   | 21:AA:268:U:C5'    | 2.65                     | 0.45              |
| 21:AA:914:A:O2'   | 21:AA:915:A:H5'    | 2.17                     | 0.45              |
| 1:AB:31:PHE:HB3   | 1:AB:40:ILE:O      | 2.17                     | 0.45              |
| 2:AC:16:PRO:HB2   | 2:AC:17:TRP:H      | 1.61                     | 0.45              |
| 4:AE:60:GLN:C     | 4:AE:62:ALA:H      | 2.19                     | 0.45              |
| 6:AG:77:ARG:NE    | 6:AG:77:ARG:HA     | 2.32                     | 0.45              |
| 8:AI:6:TYR:CG     | 8:AI:7:GLY:N       | 2.85                     | 0.45              |
| 13:AN:50:LEU:O    | 13:AN:51:PRO:C     | 2.55                     | 0.45              |
| 24:BA:1055:G:N2   | 24:BA:1105:U:O2    | 2.50                     | 0.45              |
| 24:BA:1166:G:C5   | 24:BA:1167:C:C5    | 3.05                     | 0.45              |
| 24:BA:1316:U:H2'  | 24:BA:1317:G:C8    | 2.52                     | 0.45              |
| 24:BA:1555:G:C6   | 24:BA:1556:C:C4    | 3.05                     | 0.45              |
| 24:BA:1727:C:H2'  | 24:BA:1728:C:O4'   | 2.16                     | 0.45              |
| 24:BA:1733:G:O2'  | 24:BA:1734:G:H5'   | 2.17                     | 0.45              |
| 24:BA:1880:U:H2'  | 24:BA:1881:C:C6    | 2.51                     | 0.45              |
| 24:BA:2025:C:H2'  | 24:BA:2026:U:H6    | 1.82                     | 0.45              |
| 24:BA:2147:A:H3'  | 24:BA:2148:G:C5'   | 2.46                     | 0.45              |
| 24:BA:239:C:C4    | 24:BA:240:C:N3     | 2.85                     | 0.45              |
| 24:BA:2660:A:H2'  | 24:BA:2661:G:O4'   | 2.16                     | 0.45              |
| 24:BA:2800:A:H5'' | 24:BA:2800:A:H8    | 1.82                     | 0.45              |
| 24:BA:216:A:C8    | 24:BA:432:A:C6     | 3.05                     | 0.45              |
| 24:BA:478:A:N6    | 24:BA:480:A:C6     | 2.85                     | 0.45              |
| 24:BA:484:C:H2'   | 24:BA:485:C:H6     | 1.81                     | 0.45              |
| 24:BA:515:A:H3'   | 24:BA:516:C:H6     | 1.82                     | 0.45              |
| 24:BA:658:U:C2'   | 24:BA:659:G:O5'    | 2.65                     | 0.45              |
| 24:BA:665:U:H2'   | 24:BA:666:A:C8     | 2.52                     | 0.45              |
| 24:BA:665:U:H2'   | 24:BA:666:A:H8     | 1.81                     | 0.45              |
| 24:BA:704:G:O2'   | 24:BA:705:A:P      | 2.75                     | 0.45              |
| 24:BA:829:A:O2'   | 24:BA:830:G:P      | 2.75                     | 0.45              |
| 24:BA:835:C:C2'   | 24:BA:836:G:H5'    | 2.47                     | 0.45              |
| 24:BA:854:C:H3'   | 24:BA:854:C:C6     | 2.52                     | 0.45              |
| 24:BA:969:G:C2    | 24:BA:970:U:C2     | 3.05                     | 0.45              |
| 25:BB:53:A:O2'    | 25:BB:54:G:C5'     | 2.60                     | 0.45              |
| 27:BD:8:LYS:HB2   | 27:BD:201:LEU:HD22 | 1.99                     | 0.45              |
| 29:BF:16:MET:O    | 29:BF:20:ASN:HA    | 2.17                     | 0.45              |
| 30:BG:154:GLU:OE2 | 30:BG:156:TYR:HB2  | 2.17                     | 0.45              |
| 32:BI:3:LYS:CD    | 32:BI:4:VAL:HG23   | 2.47                     | 0.45              |
| 33:BJ:42:ALA:O    | 33:BJ:44:TYR:O     | 2.35                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:BK:21:CYS:HB2  | 34:BK:39:ILE:HD13 | 1.98                     | 0.45              |
| 36:BM:71:LYS:HD3  | 36:BM:95:LEU:HD11 | 1.99                     | 0.45              |
| 40:BQ:45:ALA:O    | 40:BQ:46:TYR:C    | 2.54                     | 0.45              |
| 45:BV:1:MET:HG3   | 45:BV:2:PHE:N     | 2.31                     | 0.45              |
| 45:BV:68:LYS:O    | 45:BV:69:GLU:O    | 2.34                     | 0.45              |
| 46:BW:39:GLN:C    | 46:BW:41:GLY:N    | 2.68                     | 0.45              |
| 55:CA:1115:U:H2'  | 55:CA:1116:U:C6   | 2.52                     | 0.45              |
| 55:CA:1194:U:C4   | 55:CA:1195:C:N4   | 2.85                     | 0.45              |
| 55:CA:954:G:H1    | 55:CA:1228:C:N4   | 2.15                     | 0.45              |
| 55:CA:1238:A:OP1  | 55:CA:1336:C:H5   | 2.00                     | 0.45              |
| 55:CA:1422:G:H2'  | 55:CA:1423:G:H8   | 1.81                     | 0.45              |
| 55:CA:1495:U:O2'  | 55:CA:1496:C:H5'  | 2.17                     | 0.45              |
| 55:CA:609:A:N7    | 59:CA:1858:HOH:O  | 2.36                     | 0.45              |
| 55:CA:708:C:C5    | 55:CA:709:U:H5    | 2.34                     | 0.45              |
| 55:CA:929:G:C6    | 55:CA:930:C:C4    | 3.04                     | 0.45              |
| 1:CB:105:THR:HG22 | 1:CB:105:THR:O    | 2.16                     | 0.45              |
| 1:CB:158:ASP:O    | 1:CB:181:PRO:HD2  | 2.17                     | 0.45              |
| 1:CB:14:HIS:NE2   | 1:CB:42:LEU:HD21  | 2.32                     | 0.45              |
| 1:CB:44:LYS:O     | 1:CB:47:PRO:HD2   | 2.17                     | 0.45              |
| 2:CC:86:LEU:O     | 2:CC:90:VAL:HG22  | 2.17                     | 0.45              |
| 4:CE:131:ASN:C    | 4:CE:131:ASN:ND2  | 2.70                     | 0.45              |
| 5:CF:67:PRO:O     | 5:CF:68:GLN:C     | 2.56                     | 0.45              |
| 6:CG:134:VAL:HB   | 6:CG:137:ARG:NH2  | 2.32                     | 0.45              |
| 7:CH:3:GLN:HB3    | 55:CA:587:G:H4'   | 1.99                     | 0.45              |
| 11:CL:19:ASN:N    | 11:CL:19:ASN:ND2  | 2.65                     | 0.45              |
| 11:CL:6:LEU:HD13  | 16:CQ:33:TYR:HE2  | 1.82                     | 0.45              |
| 11:CL:86:VAL:CG1  | 11:CL:89:LEU:HD23 | 2.47                     | 0.45              |
| 12:CM:77:LYS:HA   | 12:CM:80:MET:HE2  | 1.99                     | 0.45              |
| 13:CN:27:LYS:HD2  | 13:CN:27:LYS:C    | 2.37                     | 0.45              |
| 15:CP:40:ASN:HA   | 15:CP:41:PRO:HD3  | 1.81                     | 0.45              |
| 15:CP:71:VAL:O    | 15:CP:75:ILE:HG13 | 2.16                     | 0.45              |
| 18:CS:50:VAL:HG21 | 18:CS:74:ALA:HB2  | 1.99                     | 0.45              |
| 24:DA:1021:A:C2   | 24:DA:1023:U:O2   | 2.69                     | 0.45              |
| 24:DA:1035:U:H5'' | 24:DA:1035:U:H6   | 1.82                     | 0.45              |
| 24:DA:1062:G:OP1  | 24:DA:1070:A:OP2  | 2.35                     | 0.45              |
| 24:DA:1229:C:H2'  | 24:DA:1230:A:O4'  | 2.16                     | 0.45              |
| 24:DA:1264:A:C5   | 24:DA:1265:A:C6   | 3.04                     | 0.45              |
| 24:DA:1438:U:O4   | 24:DA:1552:A:N1   | 2.50                     | 0.45              |
| 24:DA:1568:G:H8   | 24:DA:1568:G:H2'  | 1.53                     | 0.45              |
| 24:DA:1941:C:C6   | 24:DA:1965:C:C4   | 3.05                     | 0.45              |
| 24:DA:2137:U:O2   | 24:DA:2137:U:H2'  | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:2147:A:C4'  | 24:DA:2147:A:OP1  | 2.64                     | 0.45              |
| 24:DA:2144:G:H2'  | 24:DA:2147:A:OP2  | 2.17                     | 0.45              |
| 24:DA:232:G:C4'   | 24:DA:233:A:OP1   | 2.59                     | 0.45              |
| 24:DA:2520:C:O2'  | 24:DA:2521:C:H5'  | 2.17                     | 0.45              |
| 24:DA:2748:A:C4   | 24:DA:2757:A:C6   | 3.05                     | 0.45              |
| 24:DA:2886:A:N7   | 50:D0:39:ARG:CZ   | 2.80                     | 0.45              |
| 24:DA:5:A:C2      | 24:DA:2899:A:C2   | 3.05                     | 0.45              |
| 24:DA:377:G:C5    | 24:DA:378:C:C4    | 3.05                     | 0.45              |
| 24:DA:491:G:O2'   | 24:DA:492:A:H5'   | 2.17                     | 0.45              |
| 24:DA:746:U:C5'   | 24:DA:748:G:O4'   | 2.65                     | 0.45              |
| 56:DB:98:G:N1     | 45:DV:14:LYS:HB3  | 2.32                     | 0.45              |
| 27:DD:38:LYS:HD2  | 27:DD:45:TYR:CZ   | 2.52                     | 0.45              |
| 27:DD:76:GLY:O    | 27:DD:77:ARG:C    | 2.53                     | 0.45              |
| 28:DE:170:ARG:NH2 | 28:DE:176:ASP:OD2 | 2.50                     | 0.45              |
| 29:DF:107:VAL:N   | 29:DF:108:PRO:HD2 | 2.31                     | 0.45              |
| 29:DF:48:LEU:HB2  | 29:DF:149:ARG:NH2 | 2.31                     | 0.45              |
| 30:DG:22:VAL:HG12 | 30:DG:23:ILE:H    | 1.82                     | 0.45              |
| 30:DG:53:PRO:HB3  | 30:DG:61:TRP:H    | 1.81                     | 0.45              |
| 32:DI:52:LEU:HD11 | 32:DI:78:LEU:HD21 | 1.99                     | 0.45              |
| 35:DL:93:ASN:O    | 35:DL:95:LEU:N    | 2.44                     | 0.45              |
| 36:DM:136:MET:CE  | 45:DV:75:GLN:C    | 2.86                     | 0.45              |
| 24:DA:973:A:OP2   | 41:DR:81:LYS:HD2  | 2.17                     | 0.45              |
| 47:DX:31:ASN:ND2  | 47:DX:31:ASN:N    | 2.54                     | 0.45              |
| 21:AA:104:G:C2    | 21:AA:105:G:C8    | 3.04                     | 0.45              |
| 18:AS:76:THR:CG2  | 21:AA:1221:G:H4'  | 2.47                     | 0.45              |
| 21:AA:1253:G:C6   | 21:AA:1285:A:N6   | 2.85                     | 0.45              |
| 21:AA:1349:A:O2'  | 21:AA:1350:A:H5'  | 2.16                     | 0.45              |
| 21:AA:1504:G:C3'  | 21:AA:1505:G:H5'  | 2.48                     | 0.45              |
| 21:AA:325:A:H3'   | 21:AA:326:G:H8    | 1.82                     | 0.45              |
| 21:AA:65:A:C4     | 21:AA:381:C:C5    | 3.05                     | 0.45              |
| 21:AA:938:A:C6    | 21:AA:939:G:C5    | 3.05                     | 0.45              |
| 21:AA:993:G:N3    | 21:AA:993:G:H2'   | 2.32                     | 0.45              |
| 2:AC:10:ARG:O     | 2:AC:13:ILE:O     | 2.35                     | 0.45              |
| 4:AE:110:MET:SD   | 4:AE:139:THR:HG21 | 2.57                     | 0.45              |
| 6:AG:12:LEU:H     | 6:AG:12:LEU:HD22  | 1.82                     | 0.45              |
| 7:AH:33:VAL:O     | 7:AH:34:ALA:C     | 2.55                     | 0.45              |
| 8:AI:112:ARG:HG3  | 8:AI:112:ARG:O    | 2.17                     | 0.45              |
| 9:AJ:48:ARG:NH2   | 13:AN:100:TRP:CD2 | 2.84                     | 0.45              |
| 10:AK:12:ARG:O    | 10:AK:13:LYS:C    | 2.55                     | 0.45              |
| 22:AV:33:U:H3'    | 22:AV:35:A:OP2    | 2.17                     | 0.45              |
| 24:BA:1063:G:C5   | 24:BA:1064:C:C4   | 3.05                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:1289:C:H2'  | 24:BA:1290:C:H6    | 1.81                     | 0.45              |
| 24:BA:1300:G:C2   | 24:BA:1626:A:C6    | 3.05                     | 0.45              |
| 24:BA:1489:C:O2'  | 24:BA:1490:A:H5'   | 2.17                     | 0.45              |
| 24:BA:1906:G:H2'  | 24:BA:1907:G:O5'   | 2.16                     | 0.45              |
| 24:BA:1912:A:C2   | 24:BA:1919:A:C6    | 3.05                     | 0.45              |
| 24:BA:1965:C:H5'' | 24:BA:1966:A:H2'   | 1.99                     | 0.45              |
| 24:BA:2182:U:H2'  | 24:BA:2183:A:OP1   | 2.17                     | 0.45              |
| 24:BA:50:U:H6     | 24:BA:50:U:O5'     | 2.00                     | 0.45              |
| 26:BC:124:LYS:HB3 | 26:BC:127:ASN:HD22 | 1.81                     | 0.45              |
| 26:BC:236:GLY:O   | 59:BC:308:HOH:O    | 2.21                     | 0.45              |
| 29:BF:62:GLN:O    | 29:BF:64:PRO:HD3   | 2.17                     | 0.45              |
| 30:BG:37:ASN:OD1  | 30:BG:37:ASN:N     | 2.50                     | 0.45              |
| 33:BJ:30:THR:O    | 33:BJ:33:ALA:HB3   | 2.17                     | 0.45              |
| 34:BK:113:MET:O   | 34:BK:116:ILE:HG13 | 2.16                     | 0.45              |
| 34:BK:71:ARG:CB   | 34:BK:72:PRO:CD    | 2.93                     | 0.45              |
| 35:BL:90:VAL:HG13 | 35:BL:95:LEU:CD2   | 2.46                     | 0.45              |
| 35:BL:96:LYS:HD3  | 35:BL:103:ILE:HA   | 1.99                     | 0.45              |
| 36:BM:49:ALA:HB3  | 36:BM:103:TYR:OH   | 2.18                     | 0.45              |
| 37:BN:51:LEU:HD21 | 37:BN:70:THR:HG22  | 1.98                     | 0.45              |
| 39:BP:111:GLU:CD  | 39:BP:111:GLU:N    | 2.69                     | 0.45              |
| 40:BQ:63:ARG:HD2  | 40:BQ:64:ILE:HG13  | 1.99                     | 0.45              |
| 44:BU:12:VAL:O    | 44:BU:18:LYS:O     | 2.34                     | 0.45              |
| 44:BU:61:GLU:HG2  | 44:BU:61:GLU:H     | 1.54                     | 0.45              |
| 44:BU:98:ASN:C    | 44:BU:98:ASN:OD1   | 2.55                     | 0.45              |
| 47:BX:19:HIS:C    | 47:BX:21:LEU:N     | 2.71                     | 0.45              |
| 55:CA:1126:U:O2'  | 55:CA:1127:G:H8    | 2.00                     | 0.45              |
| 55:CA:1151:A:C2   | 55:CA:1152:A:C5    | 3.05                     | 0.45              |
| 55:CA:1252:A:H2'  | 55:CA:1253:G:O4'   | 2.17                     | 0.45              |
| 55:CA:1361:G:H2'  | 55:CA:1362:A:C5'   | 2.47                     | 0.45              |
| 6:CG:101:ARG:NH1  | 55:CA:1375:A:H4'   | 2.20                     | 0.45              |
| 55:CA:172:A:C5    | 55:CA:174:A:N7     | 2.85                     | 0.45              |
| 55:CA:518:C:H2'   | 55:CA:530:G:N3     | 2.31                     | 0.45              |
| 55:CA:665:A:C2    | 55:CA:732:C:C2     | 3.05                     | 0.45              |
| 55:CA:734:G:C4    | 55:CA:735:C:C5     | 3.05                     | 0.45              |
| 55:CA:783:C:C2'   | 55:CA:784:A:H5'    | 2.46                     | 0.45              |
| 55:CA:765:G:C4    | 55:CA:812:G:N1     | 2.85                     | 0.45              |
| 55:CA:953:G:H2'   | 55:CA:954:G:C8     | 2.52                     | 0.45              |
| 55:CA:994:A:C5    | 55:CA:1216:A:H4'   | 2.52                     | 0.45              |
| 6:CG:112:ASP:HB2  | 6:CG:118:ARG:HA    | 1.99                     | 0.45              |
| 9:CJ:5:ARG:N      | 9:CJ:6:ILE:HD12    | 2.32                     | 0.45              |
| 10:CK:86:LYS:HA   | 10:CK:113:THR:OG1  | 2.17                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:CL:20:VAL:O    | 11:CL:20:VAL:HG23  | 2.17                     | 0.45              |
| 12:CM:13:HIS:HD2  | 12:CM:14:ALA:H     | 1.64                     | 0.45              |
| 16:CQ:68:LYS:HG2  | 16:CQ:69:THR:HG23  | 1.98                     | 0.45              |
| 24:DA:1264:A:C5'  | 50:D0:15:ARG:HH22  | 2.30                     | 0.45              |
| 24:DA:125:A:OP2   | 52:D2:19:ARG:NH2   | 2.50                     | 0.45              |
| 52:D2:34:ARG:HB3  | 52:D2:42:LEU:CD1   | 2.45                     | 0.45              |
| 24:DA:104:A:O2'   | 24:DA:105:C:O4'    | 2.31                     | 0.45              |
| 24:DA:1423:G:C2   | 24:DA:1424:G:C4    | 3.05                     | 0.45              |
| 24:DA:1667:G:H1'  | 24:DA:1669:A:H62   | 1.81                     | 0.45              |
| 24:DA:1812:U:H2'  | 24:DA:1813:G:C8    | 2.52                     | 0.45              |
| 24:DA:1950:G:C2   | 24:DA:1954:G:C8    | 3.04                     | 0.45              |
| 24:DA:2245:U:H5'' | 24:DA:2246:G:H5'   | 1.99                     | 0.45              |
| 24:DA:2408:U:O2'  | 24:DA:2409:G:C5'   | 2.65                     | 0.45              |
| 24:DA:2443:C:C2'  | 24:DA:2444:G:H5'   | 2.46                     | 0.45              |
| 24:DA:2581:G:C6   | 24:DA:2610:C:O2    | 2.70                     | 0.45              |
| 24:DA:2662:A:H8   | 24:DA:2662:A:O5'   | 2.00                     | 0.45              |
| 24:DA:288:U:H2'   | 24:DA:289:G:O4'    | 2.17                     | 0.45              |
| 24:DA:303:G:C6    | 24:DA:315:G:C6     | 3.05                     | 0.45              |
| 24:DA:603:A:H4'   | 24:DA:604:G:C4'    | 2.46                     | 0.45              |
| 24:DA:769:U:HO2'  | 24:DA:1379:U:H6    | 1.63                     | 0.45              |
| 24:DA:464:U:C2    | 24:DA:788:A:C6     | 3.05                     | 0.45              |
| 56:DB:65:U:H3'    | 56:DB:108:A:N6     | 2.30                     | 0.45              |
| 26:DC:229:HIS:ND1 | 26:DC:230:PRO:HD2  | 2.32                     | 0.45              |
| 31:DH:15:LEU:HD22 | 31:DH:15:LEU:N     | 2.32                     | 0.45              |
| 31:DH:84:ALA:HB3  | 31:DH:148:ALA:CB   | 2.47                     | 0.45              |
| 32:DI:118:GLY:O   | 32:DI:123:ALA:HB3  | 2.17                     | 0.45              |
| 32:DI:132:ALA:HA  | 32:DI:137:LEU:HD12 | 1.98                     | 0.45              |
| 34:DK:35:VAL:HG23 | 34:DK:36:GLY:N     | 2.24                     | 0.45              |
| 34:DK:87:LEU:HA   | 34:DK:94:PRO:HA    | 1.98                     | 0.45              |
| 35:DL:122:VAL:O   | 35:DL:122:VAL:HG23 | 2.17                     | 0.45              |
| 36:DM:71:LYS:HA   | 36:DM:72:PRO:HD3   | 1.86                     | 0.45              |
| 37:DN:12:ARG:HA   | 37:DN:12:ARG:NE    | 2.32                     | 0.45              |
| 40:DQ:91:ARG:HG3  | 41:DR:11:GLN:CD    | 2.37                     | 0.45              |
| 42:DS:19:LEU:HG   | 50:D0:21:LEU:HG    | 1.99                     | 0.45              |
| 43:DT:74:ILE:HG13 | 43:DT:75:GLY:H     | 1.82                     | 0.45              |
| 24:DA:2269:G:O2'  | 46:DW:18:LYS:HG2   | 2.17                     | 0.45              |
| 21:AA:1020:G:H2'  | 21:AA:1021:A:C8    | 2.52                     | 0.44              |
| 21:AA:1073:U:O2'  | 21:AA:1074:G:H5'   | 2.17                     | 0.44              |
| 21:AA:332:G:O2'   | 21:AA:333:U:C5'    | 2.61                     | 0.44              |
| 21:AA:482:A:O2'   | 21:AA:483:C:H5'    | 2.18                     | 0.44              |
| 21:AA:556:C:O2    | 21:AA:556:C:H2'    | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:925:G:C4    | 21:AA:927:G:C8    | 3.04                     | 0.44              |
| 2:AC:55:VAL:O     | 2:AC:65:VAL:HA    | 2.17                     | 0.44              |
| 4:AE:83:PRO:HD3   | 4:AE:97:PRO:CG    | 2.47                     | 0.44              |
| 5:AF:79:ARG:NE    | 5:AF:79:ARG:HA    | 2.31                     | 0.44              |
| 8:AI:25:GLY:H     | 8:AI:58:GLU:HA    | 1.81                     | 0.44              |
| 8:AI:112:ARG:NH2  | 9:AJ:64:GLN:HE22  | 2.15                     | 0.44              |
| 13:AN:78:LEU:HB2  | 13:AN:83:VAL:HG22 | 1.99                     | 0.44              |
| 24:BA:2348:U:P    | 53:B3:37:THR:HG21 | 2.57                     | 0.44              |
| 24:BA:1094:U:H1'  | 24:BA:1098:A:C2   | 2.52                     | 0.44              |
| 24:BA:1212:G:C2   | 24:BA:1236:G:C5   | 3.05                     | 0.44              |
| 24:BA:1404:C:O2   | 24:BA:1405:U:C6   | 2.70                     | 0.44              |
| 24:BA:1698:A:H4'  | 24:BA:1699:G:O5'  | 2.16                     | 0.44              |
| 24:BA:528:A:C2    | 24:BA:2042:A:H2'  | 2.52                     | 0.44              |
| 24:BA:2058:A:O5'  | 24:BA:2058:A:H8   | 2.00                     | 0.44              |
| 24:BA:2197:U:H1'  | 24:BA:2198:A:C8   | 2.52                     | 0.44              |
| 24:BA:227:A:H4'   | 24:BA:229:C:N4    | 2.33                     | 0.44              |
| 24:BA:2331:G:O2'  | 24:BA:2336:A:N1   | 2.50                     | 0.44              |
| 24:BA:2478:A:H2'  | 24:BA:2479:U:O4'  | 2.17                     | 0.44              |
| 24:BA:2532:G:C4   | 24:BA:2533:U:C6   | 3.04                     | 0.44              |
| 24:BA:2539:C:O2'  | 24:BA:2540:C:H5'  | 2.17                     | 0.44              |
| 24:BA:2567:G:N2   | 24:BA:2568:U:C2   | 2.85                     | 0.44              |
| 24:BA:271:G:C4    | 24:BA:272:A:N7    | 2.85                     | 0.44              |
| 24:BA:2819:G:C5   | 24:BA:2821:A:C6   | 3.06                     | 0.44              |
| 24:BA:408:G:H2'   | 24:BA:409:G:O4'   | 2.17                     | 0.44              |
| 24:BA:463:G:C6    | 24:BA:467:G:O6    | 2.70                     | 0.44              |
| 24:BA:555:G:O2'   | 24:BA:556:A:P     | 2.74                     | 0.44              |
| 24:BA:867:C:C4    | 24:BA:868:U:C4    | 3.05                     | 0.44              |
| 24:BA:86:G:C2     | 24:BA:87:U:C5     | 3.05                     | 0.44              |
| 30:BG:174:LYS:C   | 30:BG:174:LYS:HD2 | 2.37                     | 0.44              |
| 30:BG:8:VAL:O     | 30:BG:9:VAL:O     | 2.34                     | 0.44              |
| 31:BH:9:VAL:O     | 31:BH:10:ALA:O    | 2.35                     | 0.44              |
| 33:BJ:88:THR:HG22 | 33:BJ:91:GLU:HG3  | 2.00                     | 0.44              |
| 35:BL:14:LYS:CG   | 35:BL:15:ALA:N    | 2.79                     | 0.44              |
| 49:BZ:35:VAL:HG22 | 49:BZ:36:GLU:N    | 2.32                     | 0.44              |
| 55:CA:1087:G:H2'  | 55:CA:1088:G:C8   | 2.51                     | 0.44              |
| 55:CA:113:G:C2    | 55:CA:315:A:C2    | 3.04                     | 0.44              |
| 55:CA:1142:G:C2   | 55:CA:1143:G:H1'  | 2.51                     | 0.44              |
| 55:CA:1160:G:O2'  | 55:CA:1161:C:H5'  | 2.17                     | 0.44              |
| 55:CA:1381:U:HO2' | 55:CA:1382:C:H6   | 1.64                     | 0.44              |
| 55:CA:1387:G:H2'  | 55:CA:1388:C:C6   | 2.52                     | 0.44              |
| 55:CA:1400:C:H4'  | 55:CA:1401:G:OP2  | 2.17                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:CA:368:U:H6    | 55:CA:368:U:H2'    | 1.44                     | 0.44              |
| 55:CA:866:C:C4    | 55:CA:867:G:H1'    | 2.52                     | 0.44              |
| 55:CA:91:U:C4     | 55:CA:92:U:C4      | 3.05                     | 0.44              |
| 55:CA:954:G:N7    | 55:CA:955:U:C4     | 2.85                     | 0.44              |
| 8:CI:129:ARG:O    | 55:CA:967:C:H5'    | 2.16                     | 0.44              |
| 1:CB:72:LYS:O     | 1:CB:76:SER:N      | 2.50                     | 0.44              |
| 2:CC:24:ASN:O     | 2:CC:28:PHE:HB2    | 2.17                     | 0.44              |
| 6:CG:78:ARG:HA    | 6:CG:84:TYR:HB2    | 1.99                     | 0.44              |
| 13:CN:13:VAL:O    | 13:CN:16:ALA:HB3   | 2.17                     | 0.44              |
| 16:CQ:46:HIS:HE2  | 16:CQ:48:GLU:HG2   | 1.81                     | 0.44              |
| 19:CT:66:ILE:HG13 | 19:CT:67:HIS:H     | 1.82                     | 0.44              |
| 19:CT:7:LYS:O     | 19:CT:10:ALA:HB3   | 2.18                     | 0.44              |
| 22:CV:35:A:C2     | 22:CV:36:A:N9      | 2.86                     | 0.44              |
| 54:D4:15:LYS:O    | 54:D4:16:ILE:HB    | 2.16                     | 0.44              |
| 24:DA:1343:G:O2'  | 24:DA:1344:U:C6    | 2.67                     | 0.44              |
| 24:DA:1953:A:N1   | 24:DA:2550:G:O4'   | 2.50                     | 0.44              |
| 24:DA:196:A:O2'   | 24:DA:197:A:OP1    | 2.34                     | 0.44              |
| 24:DA:1994:C:O2'  | 24:DA:1995:U:H5'   | 2.17                     | 0.44              |
| 24:DA:218:A:N6    | 24:DA:219:A:N6     | 2.65                     | 0.44              |
| 24:DA:223:A:C6    | 24:DA:422:A:C5     | 3.05                     | 0.44              |
| 24:DA:2489:U:C4   | 24:DA:2490:G:N1    | 2.85                     | 0.44              |
| 24:DA:2543:G:O6   | 24:DA:2765:A:C6    | 2.71                     | 0.44              |
| 24:DA:2625:G:C5   | 24:DA:2626:C:C4    | 3.05                     | 0.44              |
| 24:DA:2656:U:O2'  | 24:DA:2657:A:H8    | 2.00                     | 0.44              |
| 24:DA:2697:G:H2'  | 24:DA:2698:U:H6    | 1.82                     | 0.44              |
| 24:DA:2823:A:C2'  | 24:DA:2824:C:H5'   | 2.46                     | 0.44              |
| 24:DA:310:A:C2'   | 24:DA:312:G:N7     | 2.80                     | 0.44              |
| 24:DA:319:G:H2'   | 24:DA:320:A:C8     | 2.52                     | 0.44              |
| 24:DA:414:C:H2'   | 24:DA:415:A:C8     | 2.52                     | 0.44              |
| 24:DA:426:C:O2'   | 24:DA:427:U:H5'    | 2.18                     | 0.44              |
| 24:DA:493:G:H4'   | 42:DS:8:ARG:O      | 2.16                     | 0.44              |
| 24:DA:54:G:C5     | 24:DA:55:G:N7      | 2.85                     | 0.44              |
| 24:DA:464:U:H1'   | 24:DA:686:U:H5     | 1.81                     | 0.44              |
| 24:DA:792:A:C8    | 24:DA:2440:C:C2    | 3.05                     | 0.44              |
| 24:DA:1567:G:H5'' | 26:DC:84:PRO:CB    | 2.47                     | 0.44              |
| 24:DA:1993:U:H4'  | 27:DD:133:THR:HG22 | 1.98                     | 0.44              |
| 28:DE:28:VAL:O    | 28:DE:32:VAL:HG13  | 2.17                     | 0.44              |
| 29:DF:45:ASP:OD2  | 29:DF:47:LYS:HB2   | 2.17                     | 0.44              |
| 34:DK:7:MET:HA    | 34:DK:7:MET:HE2    | 2.00                     | 0.44              |
| 35:DL:85:VAL:O    | 35:DL:86:GLU:HB2   | 2.17                     | 0.44              |
| 37:DN:34:ILE:HD12 | 37:DN:44:LEU:HD21  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DO:74:VAL:HB    | 38:DO:106:LEU:HD11 | 1.99                     | 0.44              |
| 38:DO:82:ALA:HB3   | 38:DO:115:LEU:HD11 | 1.98                     | 0.44              |
| 27:DD:184:ARG:NH2  | 39:DP:6:GLN:HE21   | 2.06                     | 0.44              |
| 44:DU:96:LYS:O     | 44:DU:97:SER:HB3   | 2.17                     | 0.44              |
| 21:AA:1101:A:H4'   | 21:AA:1102:A:C5'   | 2.47                     | 0.44              |
| 21:AA:1346:A:C2    | 21:AA:1348:U:O4    | 2.70                     | 0.44              |
| 21:AA:366:A:O2'    | 21:AA:367:U:P      | 2.76                     | 0.44              |
| 21:AA:408:A:C2     | 21:AA:435:A:C2     | 3.05                     | 0.44              |
| 21:AA:428:G:C4     | 21:AA:430:A:N6     | 2.85                     | 0.44              |
| 21:AA:720:C:N3     | 21:AA:721:G:C6     | 2.85                     | 0.44              |
| 21:AA:961:U:OP2    | 21:AA:1223:C:H1'   | 2.17                     | 0.44              |
| 1:AB:136:ARG:O     | 1:AB:139:GLU:HB3   | 2.18                     | 0.44              |
| 1:AB:147:LEU:HD22  | 1:AB:150:ILE:HG21  | 1.99                     | 0.44              |
| 2:AC:159:ALA:C     | 2:AC:161:ILE:N     | 2.70                     | 0.44              |
| 2:AC:168:ARG:NH2   | 21:AA:1106:G:O2'   | 2.50                     | 0.44              |
| 3:AD:146:GLU:HA    | 3:AD:149:LYS:HE2   | 1.99                     | 0.44              |
| 6:AG:74:VAL:HA     | 6:AG:87:PRO:HA     | 1.98                     | 0.44              |
| 12:AM:70:ARG:CG    | 12:AM:71:GLU:N     | 2.77                     | 0.44              |
| 15:AP:19:VAL:HG22  | 15:AP:36:VAL:HG12  | 1.99                     | 0.44              |
| 24:BA:1057:A:N7    | 24:BA:1086:A:H2'   | 2.31                     | 0.44              |
| 24:BA:1085:A:H2'   | 24:BA:1086:A:N3    | 2.32                     | 0.44              |
| 24:BA:1383:A:C6    | 24:BA:1384:A:C6    | 3.04                     | 0.44              |
| 24:BA:1820:U:O2'   | 26:BC:157:ALA:HB3  | 2.17                     | 0.44              |
| 24:BA:206:U:O2'    | 24:BA:207:A:H5'    | 2.18                     | 0.44              |
| 24:BA:2478:A:H1'   | 24:BA:2529:G:C8    | 2.52                     | 0.44              |
| 24:BA:2762:C:C4    | 24:BA:2763:G:C5    | 3.05                     | 0.44              |
| 24:BA:28:A:C8      | 24:BA:513:A:N6     | 2.86                     | 0.44              |
| 24:BA:578:G:H21    | 24:BA:1252:G:N2    | 2.15                     | 0.44              |
| 24:BA:598:U:H2'    | 24:BA:599:A:C8     | 2.49                     | 0.44              |
| 24:BA:745:G:O2'    | 24:BA:748:G:H1'    | 2.18                     | 0.44              |
| 24:BA:932:U:H4'    | 24:BA:933:A:C5'    | 2.47                     | 0.44              |
| 26:BC:105:ALA:HA   | 26:BC:106:PRO:HD2  | 1.63                     | 0.44              |
| 27:BD:110:THR:OG1  | 27:BD:171:THR:HG22 | 2.17                     | 0.44              |
| 28:BE:117:ARG:HA   | 28:BE:185:LYS:CD   | 2.45                     | 0.44              |
| 28:BE:134:LEU:HD21 | 28:BE:161:ALA:HB2  | 1.98                     | 0.44              |
| 28:BE:5:LEU:HD23   | 28:BE:120:VAL:HG13 | 2.00                     | 0.44              |
| 29:BF:134:GLN:C    | 29:BF:136:ILE:N    | 2.70                     | 0.44              |
| 30:BG:29:ASN:CG    | 30:BG:30:GLY:H     | 2.20                     | 0.44              |
| 31:BH:137:GLU:HG3  | 31:BH:138:VAL:N    | 2.31                     | 0.44              |
| 36:BM:71:LYS:HA    | 36:BM:72:PRO:HD2   | 1.79                     | 0.44              |
| 27:BD:184:ARG:NH1  | 39:BP:6:GLN:OE1    | 2.37                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:BQ:3:VAL:HG12  | 40:BQ:3:VAL:O     | 2.16                     | 0.44              |
| 40:BQ:57:ARG:NH2  | 40:BQ:92:LYS:HE2  | 2.31                     | 0.44              |
| 41:BR:66:HIS:ND1  | 41:BR:94:THR:HG22 | 2.33                     | 0.44              |
| 42:BS:24:ILE:HD12 | 42:BS:32:ALA:CB   | 2.47                     | 0.44              |
| 43:BT:19:LYS:O    | 43:BT:23:ALA:N    | 2.37                     | 0.44              |
| 43:BT:40:LYS:N    | 43:BT:43:ILE:HG23 | 2.32                     | 0.44              |
| 55:CA:1064:G:C4   | 55:CA:1066:C:C4   | 3.05                     | 0.44              |
| 55:CA:1144:G:H21  | 55:CA:1146:A:H62  | 1.65                     | 0.44              |
| 20:CU:38:GLU:CG   | 55:CA:1526:G:OP1  | 2.62                     | 0.44              |
| 55:CA:180:U:O4    | 55:CA:181:A:N6    | 2.51                     | 0.44              |
| 55:CA:198:G:C4    | 55:CA:199:A:C8    | 3.06                     | 0.44              |
| 55:CA:251:G:C4    | 55:CA:266:G:C5    | 3.04                     | 0.44              |
| 55:CA:276:G:C2    | 55:CA:277:C:C2    | 3.05                     | 0.44              |
| 55:CA:293:G:O2'   | 55:CA:294:U:H5'   | 2.17                     | 0.44              |
| 55:CA:525:C:H2'   | 55:CA:526:C:H6    | 1.83                     | 0.44              |
| 55:CA:596:A:C2    | 55:CA:597:G:C8    | 3.05                     | 0.44              |
| 55:CA:815:A:H4'   | 55:CA:817:C:C4    | 2.52                     | 0.44              |
| 1:CB:125:PHE:H    | 1:CB:125:PHE:HD2  | 1.64                     | 0.44              |
| 1:CB:66:ILE:HB    | 1:CB:88:GLN:HB3   | 1.98                     | 0.44              |
| 2:CC:28:PHE:CE2   | 2:CC:32:LEU:HD11  | 2.52                     | 0.44              |
| 7:CH:124:ILE:HG22 | 7:CH:125:ILE:N    | 2.32                     | 0.44              |
| 9:CJ:35:GLN:NE2   | 9:CJ:78:GLU:H     | 2.16                     | 0.44              |
| 10:CK:21:HIS:HD2  | 10:CK:34:THR:CG2  | 2.28                     | 0.44              |
| 11:CL:93:ARG:HH21 | 55:CA:911:U:P     | 2.40                     | 0.44              |
| 11:CL:65:TYR:N    | 11:CL:94:TYR:O    | 2.45                     | 0.44              |
| 24:DA:2286:G:O6   | 51:D1:22:THR:HG21 | 2.17                     | 0.44              |
| 51:D1:38:PHE:CD2  | 51:D1:39:ASP:N    | 2.85                     | 0.44              |
| 24:DA:1146:C:H2'  | 24:DA:1147:A:C8   | 2.52                     | 0.44              |
| 24:DA:121:G:C2    | 24:DA:131:A:C4    | 3.05                     | 0.44              |
| 24:DA:1352:U:C5   | 24:DA:1377:G:C5   | 2.95                     | 0.44              |
| 24:DA:1517:G:N2   | 24:DA:1732:C:C5   | 2.85                     | 0.44              |
| 24:DA:180:G:H4'   | 24:DA:180:G:OP1   | 2.16                     | 0.44              |
| 24:DA:1839:G:O2'  | 24:DA:1840:G:C5'  | 2.65                     | 0.44              |
| 24:DA:188:G:C2    | 24:DA:209:C:N3    | 2.86                     | 0.44              |
| 24:DA:2148:G:O3'  | 24:DA:2149:U:O4'  | 2.35                     | 0.44              |
| 24:DA:2492:U:HO2' | 24:DA:2493:U:H5'  | 1.82                     | 0.44              |
| 24:DA:2861:U:H2'  | 24:DA:2862:G:C8   | 2.52                     | 0.44              |
| 24:DA:322:A:H3'   | 28:DE:163:ASN:ND2 | 2.32                     | 0.44              |
| 24:DA:347:A:O2'   | 24:DA:348:A:H5'   | 2.17                     | 0.44              |
| 24:DA:520:G:H5'   | 42:DS:73:LYS:NZ   | 2.31                     | 0.44              |
| 24:DA:638:G:C6    | 24:DA:651:G:C6    | 3.05                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:716:A:H3'   | 24:DA:717:C:H5''  | 1.98                     | 0.44              |
| 26:DC:245:THR:C   | 26:DC:247:TRP:N   | 2.70                     | 0.44              |
| 27:DD:12:THR:OG1  | 39:DP:4:ILE:HG23  | 2.17                     | 0.44              |
| 29:DF:48:LEU:O    | 29:DF:52:ALA:HB2  | 2.16                     | 0.44              |
| 30:DG:94:ARG:O    | 30:DG:95:ALA:HB2  | 2.17                     | 0.44              |
| 33:DJ:58:ASN:OD1  | 33:DJ:127:GLY:HA2 | 2.17                     | 0.44              |
| 33:DJ:80:HIS:O    | 33:DJ:81:ILE:O    | 2.34                     | 0.44              |
| 37:DN:16:HIS:O    | 37:DN:20:MET:N    | 2.51                     | 0.44              |
| 37:DN:1:MET:O     | 37:DN:2:ARG:HB2   | 2.17                     | 0.44              |
| 40:DQ:4:LYS:CD    | 40:DQ:7:VAL:HG22  | 2.46                     | 0.44              |
| 43:DT:68:LYS:HB3  | 43:DT:69:ARG:H    | 1.53                     | 0.44              |
| 44:DU:14:THR:HB   | 44:DU:68:ASN:CB   | 2.44                     | 0.44              |
| 45:DV:30:ILE:HG13 | 45:DV:40:ILE:HD11 | 1.98                     | 0.44              |
| 46:DW:9:THR:HG23  | 46:DW:10:ARG:N    | 2.32                     | 0.44              |
| 21:AA:1069:C:H4'  | 21:AA:1192:C:O2   | 2.17                     | 0.44              |
| 21:AA:1492:A:H2   | 23:AW:5:U:O2      | 1.99                     | 0.44              |
| 21:AA:227:G:C2'   | 21:AA:228:A:H5'   | 2.47                     | 0.44              |
| 21:AA:445:G:N2    | 21:AA:490:C:C2    | 2.86                     | 0.44              |
| 21:AA:66:A:H2'    | 21:AA:66:A:N3     | 2.31                     | 0.44              |
| 21:AA:695:A:C6    | 21:AA:696:A:C6    | 3.05                     | 0.44              |
| 21:AA:763:G:C4    | 21:AA:764:C:C6    | 3.05                     | 0.44              |
| 1:AB:101:THR:HG22 | 1:AB:174:GLU:OE1  | 2.17                     | 0.44              |
| 1:AB:26:MET:HA    | 1:AB:26:MET:HE3   | 1.98                     | 0.44              |
| 3:AD:117:VAL:HG22 | 3:AD:122:ILE:HD11 | 1.98                     | 0.44              |
| 4:AE:121:ASN:N    | 4:AE:121:ASN:HD22 | 2.14                     | 0.44              |
| 4:AE:15:ILE:HD11  | 4:AE:37:VAL:CG2   | 2.44                     | 0.44              |
| 4:AE:76:ASN:HD22  | 4:AE:81:GLN:HB3   | 1.82                     | 0.44              |
| 8:AI:44:ARG:H     | 8:AI:44:ARG:HG2   | 1.49                     | 0.44              |
| 8:AI:26:LYS:HG3   | 8:AI:61:ASP:OD1   | 2.17                     | 0.44              |
| 9:AJ:6:ILE:HD12   | 9:AJ:76:ILE:HB    | 1.98                     | 0.44              |
| 12:AM:113:LYS:HD3 | 12:AM:113:LYS:HA  | 1.59                     | 0.44              |
| 12:AM:13:HIS:NE2  | 21:AA:1296:C:H5'  | 2.32                     | 0.44              |
| 12:AM:88:LEU:O    | 12:AM:92:ARG:HG3  | 2.18                     | 0.44              |
| 15:AP:78:VAL:HG13 | 15:AP:78:VAL:O    | 2.17                     | 0.44              |
| 16:AQ:12:VAL:HG11 | 16:AQ:21:VAL:H    | 1.82                     | 0.44              |
| 16:AQ:30:HIS:HB2  | 16:AQ:37:ILE:HD11 | 1.99                     | 0.44              |
| 16:AQ:58:VAL:CG2  | 16:AQ:59:GLU:N    | 2.80                     | 0.44              |
| 24:BA:1707:G:O2'  | 24:BA:1708:C:H5'  | 2.18                     | 0.44              |
| 24:BA:1731:G:C2'  | 24:BA:1732:C:H5'' | 2.48                     | 0.44              |
| 24:BA:1816:C:C5   | 26:BC:61:TYR:CE1  | 3.05                     | 0.44              |
| 24:BA:1965:C:C6   | 24:BA:1965:C:C5'  | 2.90                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:2146:C:O4'  | 24:BA:2146:C:O2    | 2.35                     | 0.44              |
| 24:BA:2305:U:N3   | 24:BA:2306:C:C2    | 2.85                     | 0.44              |
| 24:BA:2533:U:H2'  | 24:BA:2534:A:H5'   | 1.99                     | 0.44              |
| 24:BA:106:C:O2'   | 24:BA:294:A:O2'    | 2.34                     | 0.44              |
| 24:BA:310:A:O2'   | 24:BA:311:A:P      | 2.75                     | 0.44              |
| 24:BA:545:U:C3'   | 24:BA:545:U:C6     | 3.00                     | 0.44              |
| 24:BA:827:U:H2'   | 24:BA:2068:U:C2    | 2.52                     | 0.44              |
| 24:BA:923:G:N3    | 46:BW:23:LYS:CE    | 2.80                     | 0.44              |
| 24:BA:92:U:H2'    | 24:BA:93:G:C8      | 2.53                     | 0.44              |
| 24:BA:946:C:O2'   | 24:BA:947:A:C5'    | 2.65                     | 0.44              |
| 26:BC:27:LYS:HE3  | 26:BC:27:LYS:N     | 2.31                     | 0.44              |
| 29:BF:146:ASP:O   | 29:BF:147:ARG:HB2  | 2.18                     | 0.44              |
| 29:BF:79:ARG:O    | 29:BF:82:TYR:HB2   | 2.17                     | 0.44              |
| 29:BF:82:TYR:HA   | 29:BF:83:PRO:HD2   | 1.79                     | 0.44              |
| 31:BH:4:ILE:HG23  | 31:BH:17:ASP:O     | 2.17                     | 0.44              |
| 32:BI:61:TYR:CD2  | 32:BI:61:TYR:N     | 2.85                     | 0.44              |
| 34:BK:102:PRO:HB3 | 34:BK:121:GLU:HB3  | 1.99                     | 0.44              |
| 35:BL:55:MET:HA   | 35:BL:56:PRO:HD3   | 1.53                     | 0.44              |
| 35:BL:67:THR:CG2  | 35:BL:68:SER:N     | 2.80                     | 0.44              |
| 38:BO:39:VAL:HG12 | 38:BO:39:VAL:O     | 2.17                     | 0.44              |
| 38:BO:58:ILE:HD11 | 38:BO:81:ARG:NH2   | 2.33                     | 0.44              |
| 39:BP:105:LYS:CA  | 39:BP:108:ARG:HH21 | 2.22                     | 0.44              |
| 40:BQ:91:ARG:HE   | 41:BR:11:GLN:HB2   | 1.82                     | 0.44              |
| 41:BR:51:VAL:HB   | 41:BR:52:PRO:HD3   | 1.99                     | 0.44              |
| 41:BR:72:VAL:HG13 | 41:BR:89:HIS:O     | 2.17                     | 0.44              |
| 42:BS:29:VAL:O    | 42:BS:33:LEU:CD2   | 2.65                     | 0.44              |
| 42:BS:40:ASN:O    | 42:BS:41:LYS:HG2   | 2.17                     | 0.44              |
| 43:BT:22:THR:O    | 43:BT:26:LYS:HG2   | 2.18                     | 0.44              |
| 45:BV:80:HIS:CD2  | 45:BV:83:LYS:N     | 2.72                     | 0.44              |
| 46:BW:14:ASP:O    | 46:BW:15:SER:CB    | 2.65                     | 0.44              |
| 46:BW:23:LYS:CG   | 46:BW:24:ARG:N     | 2.80                     | 0.44              |
| 55:CA:123:U:C5    | 55:CA:124:C:C5     | 3.06                     | 0.44              |
| 55:CA:1237:C:H4'  | 55:CA:1334:G:N2    | 2.32                     | 0.44              |
| 55:CA:1478:U:H2'  | 55:CA:1479:C:C6    | 2.52                     | 0.44              |
| 55:CA:328:C:O2    | 55:CA:328:C:H2'    | 2.17                     | 0.44              |
| 55:CA:329:A:C6    | 55:CA:332:G:C2     | 3.06                     | 0.44              |
| 55:CA:557:G:C5    | 55:CA:558:G:C6     | 3.05                     | 0.44              |
| 55:CA:571:U:H5''  | 55:CA:572:A:OP2    | 2.17                     | 0.44              |
| 55:CA:774:G:C5    | 55:CA:775:G:N7     | 2.85                     | 0.44              |
| 55:CA:80:A:C5     | 55:CA:81:A:H1'     | 2.51                     | 0.44              |
| 55:CA:885:G:O2'   | 55:CA:886:G:H8     | 2.01                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:CA:951:G:C6     | 55:CA:952:U:C4     | 3.06                     | 0.44              |
| 2:CC:113:LYS:HG3   | 2:CC:184:ASN:HD22  | 1.81                     | 0.44              |
| 11:CL:111:GLN:HE21 | 11:CL:111:GLN:HB2  | 1.60                     | 0.44              |
| 12:CM:13:HIS:HA    | 12:CM:43:LYS:HA    | 1.99                     | 0.44              |
| 12:CM:13:HIS:HD1   | 12:CM:43:LYS:HE2   | 1.81                     | 0.44              |
| 14:CO:28:VAL:HG13  | 14:CO:62:ARG:HG3   | 1.98                     | 0.44              |
| 15:CP:35:ARG:HH12  | 15:CP:38:PHE:HB3   | 1.82                     | 0.44              |
| 15:CP:52:LEU:O     | 15:CP:53:ASP:CB    | 2.64                     | 0.44              |
| 24:DA:1187:G:O5'   | 24:DA:1187:G:H8    | 2.00                     | 0.44              |
| 24:DA:125:A:H4'    | 24:DA:126:A:OP2    | 2.18                     | 0.44              |
| 24:DA:1495:A:H2'   | 24:DA:1496:A:C8    | 2.52                     | 0.44              |
| 24:DA:1667:G:C5'   | 34:DK:6:THR:H      | 2.31                     | 0.44              |
| 24:DA:1675:C:O2'   | 24:DA:1676:A:H5'   | 2.18                     | 0.44              |
| 24:DA:1923:U:H6    | 24:DA:1923:U:O5'   | 2.00                     | 0.44              |
| 24:DA:1946:U:H2'   | 24:DA:1947:C:C6    | 2.52                     | 0.44              |
| 24:DA:1956:U:O2    | 24:DA:1985:C:H4'   | 2.18                     | 0.44              |
| 24:DA:226:A:H5'    | 24:DA:257:C:O3'    | 2.16                     | 0.44              |
| 24:DA:2286:G:H4'   | 24:DA:2287:A:O4'   | 2.16                     | 0.44              |
| 24:DA:2345:G:C2    | 24:DA:2381:A:C5    | 3.05                     | 0.44              |
| 24:DA:241:A:N9     | 24:DA:243:U:C4     | 2.85                     | 0.44              |
| 24:DA:2459:A:C4    | 24:DA:2460:U:C5    | 3.06                     | 0.44              |
| 24:DA:608:A:C5     | 24:DA:621:A:C5     | 3.05                     | 0.44              |
| 24:DA:706:A:H2'    | 24:DA:707:G:O4'    | 2.18                     | 0.44              |
| 24:DA:725:G:C6     | 24:DA:726:G:C2     | 3.05                     | 0.44              |
| 26:DC:67:LYS:HB3   | 26:DC:150:GLY:HA2  | 1.99                     | 0.44              |
| 26:DC:70:LYS:HB2   | 26:DC:101:ARG:HH22 | 1.81                     | 0.44              |
| 28:DE:117:ARG:NH2  | 35:DL:2:ARG:HB3    | 2.32                     | 0.44              |
| 29:DF:11:VAL:C     | 29:DF:13:LYS:H     | 2.20                     | 0.44              |
| 34:DK:2:ILE:O      | 34:DK:3:GLN:HG2    | 2.17                     | 0.44              |
| 38:DO:17:LYS:O     | 38:DO:21:LEU:HG    | 2.17                     | 0.44              |
| 43:DT:17:SER:C     | 43:DT:18:GLU:HG2   | 2.37                     | 0.44              |
| 45:DV:14:LYS:CG    | 45:DV:18:ARG:HD2   | 2.46                     | 0.44              |
| 48:DY:11:VAL:HG12  | 48:DY:11:VAL:O     | 2.17                     | 0.44              |
| 21:AA:105:G:H2'    | 21:AA:106:C:C6     | 2.53                     | 0.44              |
| 21:AA:1084:G:H5'   | 21:AA:1102:A:OP2   | 2.17                     | 0.44              |
| 1:AB:142:LYS:HZ3   | 21:AA:1098:C:P     | 2.39                     | 0.44              |
| 21:AA:1279:G:N3    | 21:AA:1279:G:H2'   | 2.31                     | 0.44              |
| 12:AM:96:VAL:HB    | 21:AA:1308:U:H5'   | 2.00                     | 0.44              |
| 21:AA:1394:A:C8    | 21:AA:1501:C:O2'   | 2.68                     | 0.44              |
| 21:AA:1501:C:C6    | 21:AA:1504:G:N7    | 2.86                     | 0.44              |
| 21:AA:215:C:H2'    | 21:AA:216:U:C6     | 2.51                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:427:U:N3    | 21:AA:428:G:O6    | 2.50                     | 0.44              |
| 21:AA:471:U:C4    | 21:AA:472:U:C5    | 3.05                     | 0.44              |
| 21:AA:65:A:C5     | 21:AA:381:C:C4    | 3.05                     | 0.44              |
| 21:AA:71:A:N7     | 21:AA:100:G:C6    | 2.85                     | 0.44              |
| 21:AA:755:G:O2'   | 21:AA:756:C:H5'   | 2.17                     | 0.44              |
| 21:AA:806:C:H2'   | 21:AA:807:A:H8    | 1.79                     | 0.44              |
| 21:AA:943:U:H2'   | 21:AA:944:G:H8    | 1.82                     | 0.44              |
| 21:AA:993:G:C2'   | 21:AA:995:C:H41   | 2.30                     | 0.44              |
| 3:AD:96:ARG:HH21  | 3:AD:114:ARG:HH21 | 1.66                     | 0.44              |
| 3:AD:168:THR:HG22 | 3:AD:183:ARG:HH21 | 1.82                     | 0.44              |
| 3:AD:52:VAL:O     | 3:AD:56:GLU:HB2   | 2.17                     | 0.44              |
| 4:AE:32:PHE:CD2   | 4:AE:54:GLU:CA    | 2.92                     | 0.44              |
| 4:AE:36:THR:HG22  | 4:AE:59:ILE:HD12  | 1.98                     | 0.44              |
| 16:AQ:13:SER:O    | 16:AQ:16:MET:SD   | 2.75                     | 0.44              |
| 18:AS:17:LYS:HA   | 18:AS:20:LYS:NZ   | 2.33                     | 0.44              |
| 19:AT:14:GLU:O    | 19:AT:15:LYS:C    | 2.56                     | 0.44              |
| 19:AT:66:ILE:HD11 | 19:AT:70:LYS:HG2  | 1.99                     | 0.44              |
| 51:B1:47:ILE:CD1  | 51:B1:47:ILE:H    | 2.14                     | 0.44              |
| 24:BA:1096:A:N6   | 24:BA:1097:U:C4   | 2.86                     | 0.44              |
| 24:BA:1128:G:O2'  | 24:BA:1129:A:H5'' | 2.18                     | 0.44              |
| 24:BA:1343:G:N2   | 24:BA:1405:U:C6   | 2.85                     | 0.44              |
| 24:BA:1386:C:H5'  | 24:BA:1396:U:O2   | 2.17                     | 0.44              |
| 24:BA:1392:A:C6   | 24:BA:1393:A:C6   | 3.05                     | 0.44              |
| 24:BA:150:U:O2'   | 24:BA:151:C:H5'   | 2.17                     | 0.44              |
| 24:BA:1510:G:O2'  | 24:BA:1511:G:O5'  | 2.36                     | 0.44              |
| 24:BA:14:A:H3'    | 24:BA:15:G:C5'    | 2.47                     | 0.44              |
| 24:BA:1753:G:C2   | 24:BA:1756:G:C2   | 3.05                     | 0.44              |
| 24:BA:1808:A:C3'  | 24:BA:1809:A:H5'  | 2.48                     | 0.44              |
| 24:BA:1832:C:H2'  | 24:BA:1833:C:O5'  | 2.16                     | 0.44              |
| 24:BA:2495:G:O2'  | 24:BA:2496:C:H5'  | 2.17                     | 0.44              |
| 24:BA:254:G:H2'   | 24:BA:255:A:OP2   | 2.18                     | 0.44              |
| 24:BA:2592:G:C5   | 24:BA:2593:U:C4   | 3.06                     | 0.44              |
| 24:BA:2723:C:C4   | 24:BA:2724:U:C4   | 3.05                     | 0.44              |
| 24:BA:2813:A:C2   | 24:BA:2814:A:C5   | 3.06                     | 0.44              |
| 24:BA:285:G:N2    | 24:BA:286:U:C2    | 2.85                     | 0.44              |
| 24:BA:300:A:H2'   | 24:BA:334:C:H1'   | 1.98                     | 0.44              |
| 24:BA:336:C:O2'   | 24:BA:337:C:H5'   | 2.17                     | 0.44              |
| 24:BA:372:G:O2'   | 24:BA:373:U:P     | 2.75                     | 0.44              |
| 24:BA:513:A:C2    | 24:BA:514:A:C4    | 3.06                     | 0.44              |
| 24:BA:736:C:H2'   | 24:BA:737:C:C6    | 2.53                     | 0.44              |
| 24:BA:880:G:C8    | 24:BA:880:G:O5'   | 2.67                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:919:U:N3    | 24:BA:920:A:C5     | 2.86                     | 0.44              |
| 24:BA:985:C:C2'   | 24:BA:986:C:H5'    | 2.47                     | 0.44              |
| 24:BA:999:U:C2'   | 24:BA:1000:A:H5'   | 2.47                     | 0.44              |
| 25:BB:76:G:H5''   | 45:BV:17:SER:OG    | 2.17                     | 0.44              |
| 27:BD:151:THR:CB  | 27:BD:152:PRO:CD   | 2.95                     | 0.44              |
| 28:BE:46:GLN:CG   | 28:BE:87:ALA:H     | 2.29                     | 0.44              |
| 29:BF:43:ILE:HA   | 29:BF:82:TYR:CE1   | 2.52                     | 0.44              |
| 32:BI:109:ALA:CB  | 32:BI:128:ILE:HG13 | 2.47                     | 0.44              |
| 24:BA:1243:C:H1'  | 35:BL:4:ASN:O      | 2.17                     | 0.44              |
| 37:BN:32:GLU:OE1  | 37:BN:118:ARG:HA   | 2.17                     | 0.44              |
| 40:BQ:57:ARG:NH2  | 40:BQ:92:LYS:CD    | 2.79                     | 0.44              |
| 43:BT:57:VAL:O    | 43:BT:85:VAL:O     | 2.36                     | 0.44              |
| 45:BV:26:PHE:CZ   | 45:BV:42:LEU:HD12  | 2.52                     | 0.44              |
| 45:BV:89:ILE:HG21 | 45:BV:91:PHE:CZ    | 2.53                     | 0.44              |
| 47:BX:42:GLU:O    | 47:BX:43:LYS:C     | 2.55                     | 0.44              |
| 55:CA:1022:A:O2'  | 55:CA:1023:U:H5'   | 2.18                     | 0.44              |
| 55:CA:1039:G:H2'  | 55:CA:1040:U:O4'   | 2.16                     | 0.44              |
| 55:CA:1134:G:C4   | 55:CA:1135:U:H1'   | 2.53                     | 0.44              |
| 55:CA:1242:G:HO2' | 55:CA:1243:C:P     | 2.40                     | 0.44              |
| 55:CA:1423:G:H2'  | 55:CA:1424:U:C6    | 2.49                     | 0.44              |
| 55:CA:155:A:C6    | 55:CA:167:A:C6     | 3.05                     | 0.44              |
| 55:CA:250:A:H1'   | 55:CA:252:U:C2     | 2.52                     | 0.44              |
| 55:CA:301:G:C4    | 55:CA:302:G:C8     | 3.06                     | 0.44              |
| 55:CA:325:A:H2'   | 55:CA:326:G:O4'    | 2.17                     | 0.44              |
| 55:CA:471:U:H2'   | 55:CA:472:U:C6     | 2.52                     | 0.44              |
| 55:CA:491:G:O2'   | 55:CA:492:C:H5'    | 2.17                     | 0.44              |
| 55:CA:585:G:H2'   | 55:CA:586:C:O4'    | 2.17                     | 0.44              |
| 55:CA:887:G:C2'   | 55:CA:888:G:H5'    | 2.47                     | 0.44              |
| 2:CC:46:LEU:HD21  | 2:CC:86:LEU:HD11   | 1.98                     | 0.44              |
| 6:CG:142:ARG:C    | 6:CG:144:ALA:H     | 2.20                     | 0.44              |
| 14:CO:67:ASP:O    | 14:CO:71:ARG:HG3   | 2.17                     | 0.44              |
| 16:CQ:4:ILE:CG2   | 16:CQ:5:ARG:N      | 2.80                     | 0.44              |
| 16:CQ:71:SER:OG   | 55:CA:235:C:H5'    | 2.17                     | 0.44              |
| 18:CS:52:ASN:HD22 | 18:CS:52:ASN:H     | 1.64                     | 0.44              |
| 19:CT:4:LYS:HB3   | 19:CT:4:LYS:HE3    | 1.81                     | 0.44              |
| 24:DA:1210:G:N3   | 24:DA:1212:G:N2    | 2.66                     | 0.44              |
| 24:DA:1270:C:N3   | 24:DA:1648:U:C4    | 2.86                     | 0.44              |
| 24:DA:1399:C:H2'  | 24:DA:1400:U:C5    | 2.51                     | 0.44              |
| 24:DA:1440:U:O2   | 24:DA:1441:G:C8    | 2.71                     | 0.44              |
| 24:DA:1529:G:O6   | 24:DA:1543:G:N2    | 2.51                     | 0.44              |
| 24:DA:1796:U:O2   | 24:DA:1824:G:C2    | 2.70                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:530:G:N2     | 24:DA:2034:U:O3'   | 2.50                     | 0.44              |
| 24:DA:2135:A:H3'   | 24:DA:2136:G:C5'   | 2.43                     | 0.44              |
| 24:DA:2298:A:H2'   | 24:DA:2299:U:C6    | 2.52                     | 0.44              |
| 24:DA:2511:U:O5'   | 24:DA:2511:U:H6    | 2.00                     | 0.44              |
| 24:DA:325:G:O2'    | 24:DA:326:G:H5'    | 2.17                     | 0.44              |
| 24:DA:521:U:H2'    | 24:DA:522:A:H8     | 1.82                     | 0.44              |
| 24:DA:533:G:O2'    | 24:DA:534:U:H5'    | 2.18                     | 0.44              |
| 24:DA:593:U:C4     | 24:DA:594:U:O4     | 2.70                     | 0.44              |
| 24:DA:93:G:H2'     | 24:DA:94:A:H8      | 1.82                     | 0.44              |
| 56:DB:16:G:O6      | 56:DB:69:G:C6      | 2.70                     | 0.44              |
| 26:DC:244:VAL:HG12 | 26:DC:250:GLN:HA   | 1.98                     | 0.44              |
| 26:DC:43:ASN:CG    | 26:DC:44:ASN:N     | 2.71                     | 0.44              |
| 26:DC:93:VAL:HG12  | 26:DC:101:ARG:N    | 2.33                     | 0.44              |
| 28:DE:105:LEU:HD12 | 28:DE:200:LEU:HD21 | 2.00                     | 0.44              |
| 32:DI:5:GLN:OE1    | 32:DI:59:THR:HG21  | 2.18                     | 0.44              |
| 33:DJ:64:VAL:HG13  | 33:DJ:65:THR:N     | 2.32                     | 0.44              |
| 38:DO:30:ARG:HH22  | 38:DO:103:VAL:HG23 | 1.82                     | 0.44              |
| 39:DP:16:VAL:HG13  | 39:DP:19:PHE:HE2   | 1.82                     | 0.44              |
| 40:DQ:4:LYS:HG2    | 40:DQ:5:ARG:N      | 2.31                     | 0.44              |
| 41:DR:49:ILE:HG22  | 41:DR:54:VAL:H     | 1.81                     | 0.44              |
| 42:DS:6:LYS:NZ     | 42:DS:6:LYS:HB3    | 2.33                     | 0.44              |
| 43:DT:28:ASN:HB3   | 43:DT:91:GLN:HE22  | 1.83                     | 0.44              |
| 43:DT:40:LYS:HA    | 43:DT:43:ILE:CG2   | 2.47                     | 0.44              |
| 44:DU:52:ASN:CG    | 44:DU:54:PRO:HD3   | 2.37                     | 0.44              |
| 45:DV:61:LEU:HG    | 45:DV:72:VAL:O     | 2.17                     | 0.44              |
| 46:DW:43:LYS:HD3   | 46:DW:43:LYS:HA    | 1.64                     | 0.44              |
| 21:AA:1091:U:O2    | 21:AA:1095:U:C2    | 2.71                     | 0.44              |
| 21:AA:113:G:C1'    | 21:AA:354:G:H5'    | 2.48                     | 0.44              |
| 21:AA:113:G:C5     | 21:AA:114:U:C5     | 3.06                     | 0.44              |
| 13:AN:2:LYS:HE2    | 21:AA:1216:A:OP1   | 2.16                     | 0.44              |
| 21:AA:1281:C:O2'   | 21:AA:1282:C:H5'   | 2.17                     | 0.44              |
| 21:AA:1523:G:C6    | 21:AA:1524:C:C4    | 3.06                     | 0.44              |
| 21:AA:259:G:H2'    | 21:AA:260:G:C8     | 2.53                     | 0.44              |
| 21:AA:32:A:H2'     | 21:AA:33:A:H8      | 1.75                     | 0.44              |
| 21:AA:605:U:H2'    | 21:AA:606:G:H8     | 1.82                     | 0.44              |
| 21:AA:702:A:HO2'   | 21:AA:703:G:P      | 2.38                     | 0.44              |
| 21:AA:709:U:H2'    | 21:AA:710:G:C8     | 2.52                     | 0.44              |
| 21:AA:938:A:C2     | 21:AA:939:G:C4     | 3.06                     | 0.44              |
| 2:AC:38:VAL:O      | 2:AC:42:LEU:HB2    | 2.17                     | 0.44              |
| 4:AE:33:THR:HG22   | 4:AE:51:LYS:HB2    | 1.98                     | 0.44              |
| 15:AP:4:ILE:O      | 15:AP:67:ILE:HD12  | 2.18                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:AS:42:ASN:HD22 | 18:AS:43:MET:N     | 2.15                     | 0.44              |
| 20:AU:37:TYR:HB3  | 20:AU:38:GLU:H     | 1.67                     | 0.44              |
| 24:BA:1036:G:C6   | 24:BA:1120:G:C5    | 3.05                     | 0.44              |
| 24:BA:10:A:N7     | 24:BA:11:C:C5      | 2.86                     | 0.44              |
| 24:BA:1238:G:O2'  | 24:BA:1239:G:H5'   | 2.18                     | 0.44              |
| 24:BA:1660:G:N3   | 24:BA:1661:G:C8    | 2.85                     | 0.44              |
| 24:BA:1817:G:OP1  | 26:BC:86:ARG:NH2   | 2.45                     | 0.44              |
| 24:BA:1927:A:C2   | 24:BA:1928:A:C4    | 3.06                     | 0.44              |
| 24:BA:2093:G:C4   | 24:BA:2225:A:C5    | 3.05                     | 0.44              |
| 24:BA:2184:A:OP2  | 24:BA:2184:A:H8    | 2.00                     | 0.44              |
| 24:BA:2200:C:HO2' | 24:BA:2201:G:H8    | 1.65                     | 0.44              |
| 24:BA:2293:G:H2'  | 24:BA:2294:G:O4'   | 2.16                     | 0.44              |
| 24:BA:2297:A:N7   | 24:BA:2320:U:C4    | 2.85                     | 0.44              |
| 24:BA:2554:U:C4   | 24:BA:2555:U:O4    | 2.70                     | 0.44              |
| 24:BA:2612:C:H5'' | 24:BA:2613:U:OP1   | 2.18                     | 0.44              |
| 24:BA:2864:G:C2   | 24:BA:2865:U:C2    | 3.06                     | 0.44              |
| 24:BA:2720:U:C2   | 24:BA:2872:A:C6    | 3.05                     | 0.44              |
| 24:BA:3:U:H2'     | 24:BA:4:U:H6       | 1.83                     | 0.44              |
| 24:BA:466:A:O4'   | 24:BA:683:U:H4'    | 2.18                     | 0.44              |
| 24:BA:867:C:N4    | 24:BA:868:U:O4     | 2.51                     | 0.44              |
| 24:BA:89:A:N1     | 24:BA:90:U:C4      | 2.85                     | 0.44              |
| 25:BB:114:C:O4'   | 38:BO:47:VAL:CG2   | 2.66                     | 0.44              |
| 26:BC:109:LEU:CD2 | 26:BC:110:LYS:N    | 2.77                     | 0.44              |
| 27:BD:113:SER:O   | 27:BD:167:ASN:HA   | 2.18                     | 0.44              |
| 27:BD:64:GLU:O    | 27:BD:68:PHE:HD1   | 2.00                     | 0.44              |
| 28:BE:189:THR:O   | 28:BE:193:VAL:HG23 | 2.17                     | 0.44              |
| 59:BA:3241:HOH:O  | 28:BE:81:GLY:HA2   | 2.17                     | 0.44              |
| 29:BF:60:SER:O    | 29:BF:61:GLY:C     | 2.55                     | 0.44              |
| 30:BG:109:SER:O   | 30:BG:110:HIS:HB3  | 2.17                     | 0.44              |
| 35:BL:82:LEU:C    | 35:BL:84:LYS:N     | 2.71                     | 0.44              |
| 24:BA:1279:G:H5'  | 37:BN:34:ILE:HG22  | 1.98                     | 0.44              |
| 37:BN:72:ASP:OD1  | 37:BN:75:ILE:HG23  | 2.17                     | 0.44              |
| 40:BQ:3:VAL:O     | 40:BQ:4:LYS:C      | 2.55                     | 0.44              |
| 43:BT:28:ASN:OD1  | 43:BT:29:THR:HG22  | 2.17                     | 0.44              |
| 43:BT:51:PHE:O    | 43:BT:52:GLU:HG2   | 2.18                     | 0.44              |
| 45:BV:42:LEU:CD1  | 45:BV:47:VAL:HG21  | 2.48                     | 0.44              |
| 46:BW:66:VAL:HG12 | 46:BW:67:LYS:H     | 1.83                     | 0.44              |
| 48:BY:8:GLU:O     | 48:BY:12:GLU:HB2   | 2.17                     | 0.44              |
| 55:CA:1207:G:H2'  | 55:CA:1208:C:C6    | 2.46                     | 0.44              |
| 55:CA:1245:C:O2'  | 55:CA:1246:A:H5'   | 2.17                     | 0.44              |
| 55:CA:1435:G:H2'  | 55:CA:1436:U:C6    | 2.52                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:1533:C:C3'  | 55:CA:1534:A:H5'' | 2.48                     | 0.44              |
| 55:CA:184:G:H2'   | 55:CA:185:U:C6    | 2.53                     | 0.44              |
| 11:CL:119:LYS:HA  | 55:CA:36:C:O3'    | 2.18                     | 0.44              |
| 55:CA:528:C:H5'   | 55:CA:535:A:C6    | 2.52                     | 0.44              |
| 55:CA:55:A:H2'    | 55:CA:56:U:C5'    | 2.48                     | 0.44              |
| 55:CA:657:U:C4    | 55:CA:658:C:C5    | 3.06                     | 0.44              |
| 55:CA:582:C:C4    | 55:CA:760:G:C6    | 3.05                     | 0.44              |
| 11:CL:17:LYS:NZ   | 55:CA:910:C:OP2   | 2.43                     | 0.44              |
| 1:CB:101:THR:O    | 55:CA:1074:G:H4'  | 2.18                     | 0.44              |
| 8:CI:38:PHE:HZ    | 8:CI:74:GLN:HE21  | 1.65                     | 0.44              |
| 11:CL:72:ASN:ND2  | 11:CL:104:SER:OG  | 2.51                     | 0.44              |
| 14:CO:38:LEU:HD23 | 14:CO:55:LEU:HD13 | 1.99                     | 0.44              |
| 14:CO:57:ARG:NH1  | 55:CA:742:G:H5''  | 2.32                     | 0.44              |
| 24:DA:1268:A:O2'  | 24:DA:1269:A:H5'  | 2.18                     | 0.44              |
| 24:DA:1317:G:C2   | 24:DA:1336:A:C2   | 3.05                     | 0.44              |
| 24:DA:1397:U:H5'' | 24:DA:1398:C:C5   | 2.48                     | 0.44              |
| 24:DA:1462:C:HO2' | 24:DA:1463:C:H6   | 1.66                     | 0.44              |
| 24:DA:150:U:O2'   | 24:DA:151:C:H5'   | 2.18                     | 0.44              |
| 24:DA:1519:G:N1   | 24:DA:1520:U:C2   | 2.86                     | 0.44              |
| 24:DA:1555:G:H2'  | 24:DA:1556:C:C6   | 2.51                     | 0.44              |
| 24:DA:1869:G:H5'  | 24:DA:1870:C:OP2  | 2.18                     | 0.44              |
| 24:DA:1906:G:OP2  | 24:DA:1930:G:H8   | 2.01                     | 0.44              |
| 24:DA:860:U:C2    | 24:DA:2268:A:C8   | 3.05                     | 0.44              |
| 24:DA:2285:C:C2'  | 24:DA:2286:G:H5'' | 2.46                     | 0.44              |
| 24:DA:2323:G:N2   | 24:DA:2335:A:H2   | 2.15                     | 0.44              |
| 24:DA:2338:C:H6   | 24:DA:2338:C:H2'  | 1.43                     | 0.44              |
| 24:DA:2407:A:C2   | 24:DA:2408:U:N3   | 2.85                     | 0.44              |
| 24:DA:242:G:P     | 53:D3:2:LYS:HZ2   | 2.40                     | 0.44              |
| 24:DA:247:G:C6    | 24:DA:249:C:H1'   | 2.52                     | 0.44              |
| 24:DA:2511:U:C3'  | 24:DA:2511:U:C6   | 3.01                     | 0.44              |
| 24:DA:2782:G:N2   | 24:DA:2783:U:O2   | 2.50                     | 0.44              |
| 24:DA:26:G:C6     | 24:DA:27:G:C2     | 3.06                     | 0.44              |
| 24:DA:2875:C:H2'  | 24:DA:2876:G:H8   | 1.82                     | 0.44              |
| 24:DA:9:G:C6      | 24:DA:2895:G:O6   | 2.70                     | 0.44              |
| 24:DA:299:A:H2    | 24:DA:319:G:N3    | 2.15                     | 0.44              |
| 24:DA:335:C:H2'   | 24:DA:336:C:C6    | 2.52                     | 0.44              |
| 24:DA:372:G:P     | 47:DX:61:LYS:NZ   | 2.90                     | 0.44              |
| 24:DA:450:G:H2'   | 24:DA:451:U:H5''  | 1.99                     | 0.44              |
| 24:DA:509:C:H2'   | 24:DA:509:C:H6    | 1.30                     | 0.44              |
| 26:DC:144:GLU:CA  | 26:DC:151:GLY:HA2 | 2.30                     | 0.44              |
| 27:DD:78:GLY:O    | 27:DD:79:LEU:HD13 | 2.18                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DH:84:ALA:HB3  | 31:DH:148:ALA:HA   | 1.99                     | 0.44              |
| 24:DA:245:G:OP2   | 35:DL:67:THR:HG21  | 2.17                     | 0.44              |
| 40:DQ:18:LYS:C    | 40:DQ:18:LYS:HD2   | 2.38                     | 0.44              |
| 41:DR:39:LEU:HD23 | 41:DR:39:LEU:H     | 1.82                     | 0.44              |
| 41:DR:5:PHE:HB3   | 41:DR:59:ILE:HD12  | 1.99                     | 0.44              |
| 21:AA:1049:U:O2'  | 21:AA:1050:G:OP2   | 2.35                     | 0.44              |
| 21:AA:1275:A:N6   | 21:AA:1276:G:C6    | 2.85                     | 0.44              |
| 21:AA:212:G:O2'   | 21:AA:213:G:O5'    | 2.36                     | 0.44              |
| 21:AA:441:A:H2'   | 21:AA:441:A:N3     | 2.33                     | 0.44              |
| 21:AA:51:A:H4'    | 21:AA:52:C:C5'     | 2.47                     | 0.44              |
| 1:AB:13:VAL:HG23  | 1:AB:13:VAL:O      | 2.18                     | 0.44              |
| 6:AG:128:GLU:CD   | 6:AG:130:LYS:HE2   | 2.38                     | 0.44              |
| 8:AI:10:ARG:HA    | 8:AI:77:ALA:HB1    | 2.00                     | 0.44              |
| 10:AK:43:TRP:HE1  | 21:AA:686:U:C1'    | 2.30                     | 0.44              |
| 11:AL:58:ASN:ND2  | 11:AL:60:PHE:HD1   | 2.16                     | 0.44              |
| 19:AT:28:ARG:O    | 19:AT:32:LYS:HG2   | 2.18                     | 0.44              |
| 52:B2:12:ARG:HG2  | 52:B2:13:ASN:HD22  | 1.82                     | 0.44              |
| 52:B2:35:ARG:HG2  | 52:B2:42:LEU:HD11  | 1.99                     | 0.44              |
| 24:BA:1061:U:H3'  | 24:BA:1062:G:C5'   | 2.47                     | 0.44              |
| 24:BA:1401:G:H2'  | 24:BA:1402:U:O4'   | 2.17                     | 0.44              |
| 24:BA:1496:A:O3'  | 24:BA:1497:U:H6    | 2.01                     | 0.44              |
| 24:BA:1704:C:H2'  | 24:BA:1705:A:C8    | 2.52                     | 0.44              |
| 24:BA:1813:G:N3   | 26:BC:49:THR:HG22  | 2.32                     | 0.44              |
| 24:BA:1827:U:O2   | 24:BA:1827:U:H2'   | 2.18                     | 0.44              |
| 24:BA:1909:C:H2'  | 24:BA:1910:G:O4'   | 2.17                     | 0.44              |
| 24:BA:1993:U:H4'  | 27:BD:133:THR:HG22 | 1.96                     | 0.44              |
| 24:BA:2199:A:H5'  | 24:BA:2200:C:H5    | 1.82                     | 0.44              |
| 24:BA:319:G:O2'   | 24:BA:320:A:H5'    | 2.18                     | 0.44              |
| 24:BA:437:U:H2'   | 24:BA:438:G:C8     | 2.53                     | 0.44              |
| 24:BA:883:G:N2    | 24:BA:894:U:H1'    | 2.33                     | 0.44              |
| 30:BG:33:THR:HA   | 30:BG:34:ARG:NH1   | 2.19                     | 0.44              |
| 33:BJ:130:HIS:HD2 | 33:BJ:132:HIS:HB2  | 1.82                     | 0.44              |
| 34:BK:99:ILE:HG21 | 34:BK:119:ALA:HB2  | 1.98                     | 0.44              |
| 35:BL:28:GLY:C    | 35:BL:29:LYS:O     | 2.55                     | 0.44              |
| 35:BL:95:LEU:HB3  | 35:BL:100:ILE:CG1  | 2.48                     | 0.44              |
| 37:BN:8:ARG:HB3   | 37:BN:10:LEU:CD2   | 2.48                     | 0.44              |
| 46:BW:40:ARG:HD3  | 46:BW:45:HIS:HE1   | 1.81                     | 0.44              |
| 55:CA:1077:G:O6   | 55:CA:1081:A:N6    | 2.51                     | 0.44              |
| 4:CE:133:ILE:HD12 | 55:CA:1079:G:H5'   | 2.00                     | 0.44              |
| 55:CA:1053:G:C4   | 55:CA:1199:U:C5    | 3.05                     | 0.44              |
| 55:CA:1203:C:O5'  | 55:CA:1203:C:H6    | 2.01                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 55:CA:1255:G:C4  | 55:CA:1279:G:O6   | 2.71                     | 0.44              |
| 16:CQ:65:PRO:HD2 | 55:CA:130:A:N7    | 2.33                     | 0.44              |
| 55:CA:1316:G:N2  | 55:CA:1319:A:OP2  | 2.47                     | 0.44              |
| 55:CA:346:G:N3   | 55:CA:346:G:C2'   | 2.69                     | 0.44              |
| 55:CA:543:U:C2   | 55:CA:544:G:C8    | 3.06                     | 0.44              |
| 55:CA:723:U:H6   | 55:CA:723:U:H2'   | 1.23                     | 0.44              |
| 55:CA:881:G:C6   | 55:CA:882:C:C4    | 3.05                     | 0.44              |
| 55:CA:892:A:O2'  | 55:CA:893:C:H5'   | 2.17                     | 0.44              |
| 1:CB:9:LEU:CG    | 1:CB:10:LYS:H     | 2.13                     | 0.44              |
| 1:CB:68:PHE:HB2  | 1:CB:90:PHE:HB3   | 2.00                     | 0.44              |
| 2:CC:172:VAL:O   | 2:CC:174:LEU:HD23 | 2.18                     | 0.44              |
| 2:CC:69:THR:O    | 2:CC:105:VAL:HB   | 2.16                     | 0.44              |
| 5:CF:18:VAL:O    | 5:CF:22:ILE:HG12  | 2.17                     | 0.44              |
| 6:CG:132:THR:O   | 6:CG:133:ALA:CB   | 2.65                     | 0.44              |
| 7:CH:85:TYR:CE2  | 7:CH:123:GLU:HB2  | 2.53                     | 0.44              |
| 8:CI:46:VAL:O    | 8:CI:79:ARG:HB2   | 2.17                     | 0.44              |
| 9:CJ:31:ARG:HH12 | 9:CJ:32:THR:HB    | 1.83                     | 0.44              |
| 10:CK:21:HIS:CD2 | 55:CA:707:U:H4'   | 2.52                     | 0.44              |
| 12:CM:61:LYS:O   | 12:CM:62:PHE:HB2  | 2.18                     | 0.44              |
| 13:CN:71:GLY:O   | 13:CN:79:SER:HA   | 2.17                     | 0.44              |
| 15:CP:10:GLY:C   | 55:CA:624:C:H4'   | 2.38                     | 0.44              |
| 16:CQ:46:HIS:H   | 16:CQ:73:THR:HA   | 1.82                     | 0.44              |
| 20:CU:33:ARG:O   | 20:CU:34:ARG:O    | 2.35                     | 0.44              |
| 52:D2:30:VAL:C   | 52:D2:32:ALA:H    | 2.21                     | 0.44              |
| 24:DA:834:G:C5'  | 53:D3:56:LEU:HD11 | 2.48                     | 0.44              |
| 24:DA:1062:G:C2' | 24:DA:1063:G:H8   | 2.28                     | 0.44              |
| 24:DA:996:A:N6   | 24:DA:1160:G:C6   | 2.86                     | 0.44              |
| 24:DA:1189:A:H2' | 24:DA:1190:G:O4'  | 2.18                     | 0.44              |
| 24:DA:1191:G:C2  | 24:DA:1192:G:C4   | 3.05                     | 0.44              |
| 24:DA:1255:U:N3  | 24:DA:2060:A:H5'  | 2.33                     | 0.44              |
| 24:DA:1623:G:C5  | 24:DA:1624:U:C5   | 3.06                     | 0.44              |
| 24:DA:1782:U:H5' | 24:DA:2609:U:C2   | 2.53                     | 0.44              |
| 24:DA:182:A:C2   | 24:DA:183:C:C2    | 3.05                     | 0.44              |
| 24:DA:1947:C:H2' | 24:DA:1948:G:C8   | 2.43                     | 0.44              |
| 24:DA:2191:A:H3' | 24:DA:2192:U:C6   | 2.52                     | 0.44              |
| 24:DA:2666:C:O2  | 24:DA:2666:C:O4'  | 2.36                     | 0.44              |
| 24:DA:2750:A:O2' | 24:DA:2752:C:C5   | 2.70                     | 0.44              |
| 24:DA:2868:A:H2' | 24:DA:2869:G:H8   | 1.77                     | 0.44              |
| 24:DA:454:A:O2'  | 24:DA:455:C:OP1   | 2.33                     | 0.44              |
| 24:DA:49:A:C2    | 24:DA:118:A:N1    | 2.85                     | 0.44              |
| 24:DA:529:A:C4   | 24:DA:2023:C:C5   | 3.05                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:573:U:C4    | 24:DA:2030:A:H3'  | 2.53                     | 0.44              |
| 24:DA:581:C:N4    | 24:DA:582:A:N6    | 2.65                     | 0.44              |
| 24:DA:587:C:H1'   | 24:DA:671:C:H5'   | 2.00                     | 0.44              |
| 24:DA:712:G:N2    | 24:DA:720:U:H1'   | 2.32                     | 0.44              |
| 24:DA:716:A:C3'   | 24:DA:717:C:H5''  | 2.47                     | 0.44              |
| 24:DA:870:U:C2'   | 24:DA:871:U:H5'   | 2.48                     | 0.44              |
| 27:DD:131:ASP:N   | 27:DD:131:ASP:OD2 | 2.51                     | 0.44              |
| 28:DE:29:HIS:HA   | 28:DE:32:VAL:CG2  | 2.47                     | 0.44              |
| 28:DE:2:GLU:HA    | 28:DE:13:THR:HA   | 2.00                     | 0.44              |
| 24:DA:558:U:H5''  | 33:DJ:111:LYS:HD2 | 1.99                     | 0.44              |
| 34:DK:40:LYS:HZ2  | 34:DK:89:ASN:HD21 | 1.64                     | 0.44              |
| 35:DL:89:VAL:HG21 | 35:DL:123:ARG:NE  | 2.32                     | 0.44              |
| 36:DM:40:ARG:HB2  | 36:DM:93:VAL:CG2  | 2.47                     | 0.44              |
| 37:DN:70:THR:O    | 37:DN:70:THR:HG22 | 2.17                     | 0.44              |
| 44:DU:81:ARG:CB   | 44:DU:96:LYS:HD2  | 2.45                     | 0.44              |
| 46:DW:18:LYS:NZ   | 46:DW:18:LYS:HB2  | 2.33                     | 0.44              |
| 47:DX:20:ALA:O    | 47:DX:21:LEU:HB2  | 2.17                     | 0.44              |
| 47:DX:34:SER:O    | 47:DX:35:HIS:HB2  | 2.17                     | 0.44              |
| 21:AA:1023:U:H2'  | 21:AA:1024:G:H8   | 1.83                     | 0.44              |
| 21:AA:102:G:N3    | 21:AA:151:A:H2    | 2.15                     | 0.44              |
| 21:AA:1249:C:O2   | 21:AA:1249:C:H2'  | 2.18                     | 0.44              |
| 21:AA:948:C:H5'   | 21:AA:1306:A:O2'  | 2.17                     | 0.44              |
| 21:AA:1328:C:H2'  | 21:AA:1329:A:O4'  | 2.18                     | 0.44              |
| 21:AA:1366:C:H2'  | 21:AA:1367:C:C6   | 2.53                     | 0.44              |
| 21:AA:1512:U:H2'  | 21:AA:1513:A:H8   | 1.82                     | 0.44              |
| 21:AA:300:A:H2'   | 21:AA:301:G:O4'   | 2.17                     | 0.44              |
| 21:AA:423:G:C2'   | 21:AA:423:G:N3    | 2.70                     | 0.44              |
| 11:AL:69:GLU:HA   | 21:AA:521:G:OP1   | 2.18                     | 0.44              |
| 1:AB:93:HIS:O     | 1:AB:94:ARG:C     | 2.55                     | 0.44              |
| 5:AF:46:GLN:HB2   | 5:AF:56:LYS:HE2   | 2.00                     | 0.44              |
| 8:AI:27:ILE:N     | 8:AI:27:ILE:HD12  | 2.33                     | 0.44              |
| 8:AI:90:ASP:C     | 8:AI:92:SER:H     | 2.21                     | 0.44              |
| 9:AJ:35:GLN:HE21  | 9:AJ:35:GLN:CA    | 2.22                     | 0.44              |
| 10:AK:117:HIS:O   | 10:AK:118:ASN:HB2 | 2.18                     | 0.44              |
| 16:AQ:18:LYS:C    | 16:AQ:47:ASP:OD2  | 2.56                     | 0.44              |
| 22:AV:40:C:H2'    | 22:AV:41:C:H6     | 1.76                     | 0.44              |
| 24:BA:1097:U:C5   | 24:BA:1098:A:H1'  | 2.53                     | 0.44              |
| 24:BA:1181:U:O2'  | 24:BA:1182:G:P    | 2.75                     | 0.44              |
| 24:BA:1458:U:O4'  | 24:BA:1459:G:C2   | 2.71                     | 0.44              |
| 24:BA:1595:C:C6   | 24:BA:1595:C:H3'  | 2.52                     | 0.44              |
| 24:BA:1854:A:H2'  | 24:BA:1855:U:H5'  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:2430:A:H5'  | 24:BA:2431:U:OP2  | 2.18                     | 0.44              |
| 24:BA:2074:U:C6   | 24:BA:2436:G:N2   | 2.86                     | 0.44              |
| 24:BA:2734:A:H61  | 24:BA:2770:G:H1'  | 1.82                     | 0.44              |
| 24:BA:2805:C:C4   | 24:BA:2806:C:C5   | 3.05                     | 0.44              |
| 24:BA:77:G:C4     | 24:BA:78:U:C6     | 3.06                     | 0.44              |
| 25:BB:40:U:H1'    | 25:BB:45:A:N6     | 2.32                     | 0.44              |
| 26:BC:21:PRO:O    | 26:BC:23:LEU:N    | 2.50                     | 0.44              |
| 28:BE:31:VAL:O    | 28:BE:34:ALA:N    | 2.51                     | 0.44              |
| 30:BG:26:LYS:HB3  | 30:BG:32:LEU:CG   | 2.48                     | 0.44              |
| 30:BG:1:SER:O     | 30:BG:3:VAL:HG12  | 2.18                     | 0.44              |
| 33:BJ:141:ASP:HB3 | 33:BJ:142:ILE:H   | 1.47                     | 0.44              |
| 33:BJ:55:ILE:O    | 33:BJ:55:ILE:HG13 | 2.18                     | 0.44              |
| 41:BR:25:LEU:H    | 41:BR:94:THR:HG21 | 1.81                     | 0.44              |
| 43:BT:39:THR:CB   | 43:BT:42:GLU:HB2  | 2.36                     | 0.44              |
| 43:BT:55:VAL:O    | 43:BT:55:VAL:HG12 | 2.17                     | 0.44              |
| 45:BV:10:LYS:NZ   | 45:BV:10:LYS:HB2  | 2.33                     | 0.44              |
| 46:BW:39:GLN:HG2  | 46:BW:40:ARG:N    | 2.32                     | 0.44              |
| 55:CA:1279:G:O2'  | 55:CA:1282:C:N4   | 2.50                     | 0.44              |
| 55:CA:1359:C:H2'  | 55:CA:1361:G:OP2  | 2.18                     | 0.44              |
| 55:CA:17:U:H4'    | 55:CA:1080:A:O4'  | 2.18                     | 0.44              |
| 55:CA:18:C:C2     | 55:CA:19:A:C8     | 3.06                     | 0.44              |
| 55:CA:369:G:C6    | 55:CA:393:A:C6    | 3.04                     | 0.44              |
| 55:CA:438:U:C4    | 55:CA:494:G:C5    | 3.06                     | 0.44              |
| 55:CA:50:A:H1'    | 55:CA:52:C:C6     | 2.53                     | 0.44              |
| 55:CA:559:A:H4'   | 55:CA:560:A:O5'   | 2.18                     | 0.44              |
| 55:CA:644:U:H2'   | 55:CA:645:G:O4'   | 2.18                     | 0.44              |
| 55:CA:648:A:H2'   | 55:CA:649:A:C8    | 2.52                     | 0.44              |
| 55:CA:888:G:HO2'  | 55:CA:1488:G:HO2' | 1.66                     | 0.44              |
| 55:CA:892:A:H2'   | 55:CA:893:C:H6    | 1.79                     | 0.44              |
| 6:CG:2:ARG:NH1    | 55:CA:932:C:C4    | 2.82                     | 0.44              |
| 55:CA:994:A:N3    | 55:CA:995:C:C6    | 2.86                     | 0.44              |
| 1:CB:176:ASN:C    | 1:CB:178:LEU:H    | 2.21                     | 0.44              |
| 3:CD:10:LEU:HD12  | 3:CD:10:LEU:H     | 1.81                     | 0.44              |
| 4:CE:149:PRO:HA   | 4:CE:152:VAL:CG2  | 2.47                     | 0.44              |
| 4:CE:76:ASN:HA    | 4:CE:76:ASN:HD22  | 1.58                     | 0.44              |
| 8:CI:24:ASN:ND2   | 8:CI:26:LYS:HD2   | 2.29                     | 0.44              |
| 9:CJ:82:LYS:HA    | 9:CJ:86:ALA:CB    | 2.43                     | 0.44              |
| 11:CL:56:LEU:HG   | 11:CL:60:PHE:O    | 2.16                     | 0.44              |
| 13:CN:77:GLY:C    | 13:CN:78:LEU:HD12 | 2.38                     | 0.44              |
| 15:CP:54:LEU:N    | 15:CP:54:LEU:HD23 | 2.32                     | 0.44              |
| 24:DA:101:A:O2'   | 24:DA:102:U:P     | 2.76                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:1080:A:C6    | 24:DA:1081:U:C4    | 3.06                     | 0.44              |
| 24:DA:1311:G:O2'   | 24:DA:1312:U:H6    | 2.01                     | 0.44              |
| 24:DA:1338:G:C2'   | 24:DA:1339:G:H5'   | 2.48                     | 0.44              |
| 24:DA:1748:C:C2    | 24:DA:1749:A:C8    | 3.06                     | 0.44              |
| 24:DA:1773:A:H2'   | 24:DA:1774:C:C5'   | 2.48                     | 0.44              |
| 24:DA:740:C:C2     | 24:DA:1981:A:C2    | 3.06                     | 0.44              |
| 24:DA:2053:G:N2    | 24:DA:2054:A:N3    | 2.66                     | 0.44              |
| 24:DA:272:A:O2'    | 24:DA:273:G:O5'    | 2.35                     | 0.44              |
| 24:DA:2893:A:H5''  | 24:DA:2894:G:C5'   | 2.47                     | 0.44              |
| 24:DA:372:G:N2     | 24:DA:401:A:OP2    | 2.50                     | 0.44              |
| 24:DA:419:U:H2'    | 24:DA:420:C:C6     | 2.53                     | 0.44              |
| 24:DA:422:A:C2'    | 24:DA:423:A:C8     | 3.01                     | 0.44              |
| 24:DA:508:A:H3'    | 24:DA:509:C:H5'    | 2.00                     | 0.44              |
| 24:DA:523:C:O2'    | 24:DA:524:G:H5'    | 2.18                     | 0.44              |
| 24:DA:537:G:H21    | 24:DA:557:C:N4     | 2.13                     | 0.44              |
| 24:DA:574:A:H5''   | 24:DA:575:A:C5'    | 2.48                     | 0.44              |
| 24:DA:604:G:C2     | 24:DA:605:G:N7     | 2.85                     | 0.44              |
| 24:DA:633:A:H5''   | 35:DL:70:LYS:HD3   | 1.99                     | 0.44              |
| 24:DA:628:G:C5     | 24:DA:636:G:N2     | 2.86                     | 0.44              |
| 24:DA:670:A:HO2'   | 24:DA:671:C:P      | 2.33                     | 0.44              |
| 24:DA:705:A:C8     | 24:DA:705:A:O5'    | 2.71                     | 0.44              |
| 24:DA:763:G:H8     | 24:DA:763:G:H2'    | 1.47                     | 0.44              |
| 24:DA:974:G:H1'    | 24:DA:975:A:N7     | 2.32                     | 0.44              |
| 24:DA:988:A:H2'    | 49:DZ:13:ILE:HD11  | 2.00                     | 0.44              |
| 26:DC:152:GLN:HA   | 26:DC:155:ARG:HD3  | 2.00                     | 0.44              |
| 26:DC:212:TRP:O    | 26:DC:212:TRP:CD1  | 2.70                     | 0.44              |
| 27:DD:108:ASP:OD1  | 27:DD:207:VAL:HG23 | 2.18                     | 0.44              |
| 29:DF:27:VAL:O     | 29:DF:27:VAL:HG23  | 2.18                     | 0.44              |
| 30:DG:25:ILE:CG2   | 30:DG:78:VAL:HG21  | 2.48                     | 0.44              |
| 34:DK:62:VAL:HG11  | 34:DK:65:THR:HG23  | 2.00                     | 0.44              |
| 36:DM:72:PRO:HB2   | 36:DM:73:ILE:H     | 1.58                     | 0.44              |
| 37:DN:120:GLU:OE1  | 37:DN:120:GLU:HA   | 2.18                     | 0.44              |
| 40:DQ:9:ALA:C      | 40:DQ:11:ALA:H     | 2.21                     | 0.44              |
| 41:DR:49:ILE:HG13  | 41:DR:49:ILE:O     | 2.18                     | 0.44              |
| 42:DS:103:ILE:HD12 | 42:DS:103:ILE:N    | 2.32                     | 0.44              |
| 42:DS:51:LEU:HG    | 42:DS:55:ILE:CD1   | 2.48                     | 0.44              |
| 46:DW:20:LEU:HD11  | 46:DW:35:ILE:HG13  | 1.98                     | 0.44              |
| 46:DW:36:ILE:HG22  | 46:DW:37:VAL:O     | 2.17                     | 0.44              |
| 21:AA:1239:A:H4'   | 21:AA:1240:U:C5'   | 2.47                     | 0.44              |
| 21:AA:1512:U:H2'   | 21:AA:1513:A:C8    | 2.52                     | 0.44              |
| 21:AA:160:A:H4'    | 21:AA:344:A:N7     | 2.33                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:586:C:O2'    | 21:AA:587:G:H5'    | 2.17                     | 0.44              |
| 21:AA:625:U:O2     | 21:AA:626:G:N7     | 2.51                     | 0.44              |
| 21:AA:655:A:H2'    | 21:AA:656:G:H8     | 1.81                     | 0.44              |
| 21:AA:673:A:C4     | 21:AA:734:G:C2     | 3.06                     | 0.44              |
| 21:AA:987:G:C6     | 21:AA:988:G:N7     | 2.86                     | 0.44              |
| 4:AE:115:GLU:HA    | 4:AE:120:HIS:NE2   | 2.32                     | 0.44              |
| 5:AF:9:MET:HE2     | 5:AF:9:MET:HB3     | 1.84                     | 0.44              |
| 6:AG:3:ARG:CG      | 6:AG:4:ARG:H       | 2.17                     | 0.44              |
| 9:AJ:8:ILE:HD12    | 9:AJ:25:ILE:HG21   | 2.00                     | 0.44              |
| 13:AN:20:PHE:HA    | 13:AN:24:ALA:CB    | 2.32                     | 0.44              |
| 15:AP:70:ARG:HA    | 15:AP:70:ARG:HD2   | 1.82                     | 0.44              |
| 51:B1:22:THR:OG1   | 51:B1:23:THR:N     | 2.50                     | 0.44              |
| 24:BA:1062:G:C5    | 24:BA:1088:A:C8    | 3.06                     | 0.44              |
| 24:BA:1145:C:O2'   | 24:BA:1146:C:H5'   | 2.18                     | 0.44              |
| 24:BA:1647:U:OP2   | 24:BA:1647:U:H3'   | 2.18                     | 0.44              |
| 24:BA:1724:G:C6    | 24:BA:1725:U:N3    | 2.86                     | 0.44              |
| 24:BA:177:G:H3'    | 24:BA:178:G:H8     | 1.82                     | 0.44              |
| 24:BA:1854:A:H62   | 24:BA:1888:G:H1'   | 1.80                     | 0.44              |
| 24:BA:1973:G:C4    | 24:BA:1974:C:C5    | 3.06                     | 0.44              |
| 24:BA:2070:A:H2'   | 24:BA:2071:A:O4'   | 2.18                     | 0.44              |
| 24:BA:2290:G:O6    | 24:BA:2341:G:O6    | 2.35                     | 0.44              |
| 24:BA:2305:U:O4'   | 29:BF:130:GLY:HA3  | 2.17                     | 0.44              |
| 24:BA:2529:G:OP2   | 24:BA:2530:A:H5''  | 2.17                     | 0.44              |
| 24:BA:2682:A:H2'   | 24:BA:2683:C:H6    | 1.83                     | 0.44              |
| 24:BA:2813:A:N1    | 24:BA:2814:A:C6    | 2.85                     | 0.44              |
| 24:BA:359:G:H3'    | 24:BA:360:U:C6     | 2.52                     | 0.44              |
| 24:BA:643:A:H2'    | 24:BA:644:A:H8     | 1.83                     | 0.44              |
| 24:BA:68:G:H2'     | 24:BA:69:C:O4'     | 2.17                     | 0.44              |
| 24:BA:699:A:H2'    | 24:BA:700:G:O4'    | 2.18                     | 0.44              |
| 24:BA:738:G:N1     | 24:BA:739:A:C2     | 2.86                     | 0.44              |
| 24:BA:738:G:H2'    | 24:BA:739:A:O4'    | 2.18                     | 0.44              |
| 24:BA:763:G:C5     | 24:BA:765:C:C5     | 3.05                     | 0.44              |
| 24:BA:858:G:N2     | 24:BA:2269:G:OP2   | 2.51                     | 0.44              |
| 24:BA:975:A:C4     | 24:BA:976:G:C8     | 3.06                     | 0.44              |
| 25:BB:89:U:H6      | 25:BB:89:U:H2'     | 1.37                     | 0.44              |
| 26:BC:145:MET:HB2  | 26:BC:152:GLN:HE22 | 1.83                     | 0.44              |
| 26:BC:183:VAL:HG12 | 26:BC:184:GLU:N    | 2.33                     | 0.44              |
| 27:BD:108:ASP:O    | 27:BD:109:VAL:HB   | 2.18                     | 0.44              |
| 28:BE:83:VAL:HG11  | 28:BE:86:ALA:HA    | 1.99                     | 0.44              |
| 31:BH:33:GLN:HE21  | 31:BH:33:GLN:HB2   | 1.65                     | 0.44              |
| 31:BH:96:THR:C     | 31:BH:97:ARG:HG3   | 2.37                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:BJ:70:THR:C    | 33:BJ:71:ASP:OD2  | 2.56                     | 0.44              |
| 34:BK:12:ASP:HA   | 34:BK:98:ARG:O    | 2.17                     | 0.44              |
| 38:BO:34:HIS:HD2  | 38:BO:53:THR:O    | 2.00                     | 0.44              |
| 42:BS:69:LEU:HD12 | 42:BS:69:LEU:HA   | 1.65                     | 0.44              |
| 43:BT:29:THR:N    | 43:BT:91:GLN:NE2  | 2.61                     | 0.44              |
| 44:BU:73:ASN:HD22 | 44:BU:76:THR:N    | 2.12                     | 0.44              |
| 45:BV:40:ILE:CG2  | 45:BV:41:GLU:H    | 2.31                     | 0.44              |
| 46:BW:16:GLU:HA   | 46:BW:16:GLU:OE2  | 2.18                     | 0.44              |
| 24:BA:2230:G:O3'  | 47:BX:29:LEU:HD23 | 2.17                     | 0.44              |
| 49:BZ:9:THR:HG22  | 49:BZ:53:MET:C    | 2.38                     | 0.44              |
| 55:CA:1095:U:C5'  | 55:CA:1109:C:O2   | 2.65                     | 0.44              |
| 55:CA:1171:A:H2'  | 55:CA:1172:C:C6   | 2.52                     | 0.44              |
| 55:CA:1392:G:C2'  | 55:CA:1393:U:H5'  | 2.48                     | 0.44              |
| 55:CA:328:C:O2    | 55:CA:328:C:C2'   | 2.64                     | 0.44              |
| 55:CA:452:A:O2'   | 55:CA:453:G:O5'   | 2.35                     | 0.44              |
| 55:CA:586:C:O2'   | 55:CA:878:A:H4'   | 2.18                     | 0.44              |
| 55:CA:588:G:H2'   | 55:CA:589:U:C6    | 2.52                     | 0.44              |
| 55:CA:577:G:N9    | 55:CA:816:A:C2    | 2.86                     | 0.44              |
| 55:CA:81:A:H2     | 55:CA:89:U:O4     | 1.98                     | 0.44              |
| 1:CB:128:LEU:HB3  | 1:CB:131:LYS:HB3  | 1.99                     | 0.44              |
| 1:CB:78:ALA:O     | 1:CB:213:LEU:HD23 | 2.18                     | 0.44              |
| 3:CD:154:VAL:O    | 3:CD:157:ALA:HB3  | 2.18                     | 0.44              |
| 4:CE:135:VAL:O    | 4:CE:138:ALA:HB3  | 2.17                     | 0.44              |
| 5:CF:9:MET:HE1    | 17:CR:64:LEU:CA   | 2.45                     | 0.44              |
| 6:CG:137:ARG:CZ   | 6:CG:138:GLU:HG2  | 2.47                     | 0.44              |
| 9:CJ:5:ARG:HH21   | 9:CJ:77:VAL:HG13  | 1.83                     | 0.44              |
| 11:CL:27:PRO:HG3  | 55:CA:363:A:C2    | 2.52                     | 0.44              |
| 20:CU:19:LYS:N    | 20:CU:19:LYS:HZ3  | 2.15                     | 0.44              |
| 24:DA:1058:U:H2'  | 24:DA:1059:G:O4'  | 2.17                     | 0.44              |
| 24:DA:1180:U:C4   | 24:DA:1181:U:C4   | 3.05                     | 0.44              |
| 24:DA:1199:U:H2'  | 24:DA:1200:C:O4'  | 2.17                     | 0.44              |
| 24:DA:1278:C:H2'  | 24:DA:1279:G:C8   | 2.53                     | 0.44              |
| 24:DA:1439:A:C2   | 24:DA:1552:A:N1   | 2.83                     | 0.44              |
| 24:DA:1439:A:C3'  | 24:DA:1439:A:C8   | 3.01                     | 0.44              |
| 24:DA:1736:U:H2'  | 24:DA:1737:G:O4'  | 2.17                     | 0.44              |
| 24:DA:1886:U:O5'  | 24:DA:1886:U:H6   | 2.01                     | 0.44              |
| 24:DA:1924:C:H2'  | 24:DA:1925:C:O4'  | 2.17                     | 0.44              |
| 24:DA:1992:G:H22  | 24:DA:1996:C:C2'  | 2.28                     | 0.44              |
| 24:DA:2347:C:H4'  | 24:DA:2347:C:OP1  | 2.17                     | 0.44              |
| 24:DA:2547:A:H2   | 34:DK:23:LYS:HZ1  | 1.65                     | 0.44              |
| 24:DA:2625:G:C4   | 24:DA:2626:C:C5   | 3.06                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:DA:370:G:N1     | 24:DA:424:G:C5    | 2.85                     | 0.44              |
| 24:DA:482:A:HO2'   | 24:DA:483:A:P     | 2.41                     | 0.44              |
| 24:DA:562:U:C2     | 24:DA:572:A:C8    | 3.06                     | 0.44              |
| 24:DA:589:U:O2'    | 24:DA:590:A:C5'   | 2.64                     | 0.44              |
| 24:DA:593:U:N3     | 24:DA:594:U:C4    | 2.86                     | 0.44              |
| 24:DA:60:G:H21     | 24:DA:74:A:H2'    | 1.83                     | 0.44              |
| 24:DA:663:G:C6     | 24:DA:664:G:C5    | 3.05                     | 0.44              |
| 24:DA:85:G:C6      | 24:DA:98:G:C2     | 3.06                     | 0.44              |
| 56:DB:75:G:N1      | 56:DB:102:G:N2    | 2.58                     | 0.44              |
| 26:DC:24:HIS:N     | 26:DC:80:LEU:O    | 2.48                     | 0.44              |
| 27:DD:181:ASP:C    | 27:DD:183:GLU:N   | 2.70                     | 0.44              |
| 29:DF:103:ILE:HG12 | 29:DF:175:PRO:HD3 | 2.00                     | 0.44              |
| 29:DF:65:LEU:CD2   | 29:DF:65:LEU:H    | 2.29                     | 0.44              |
| 29:DF:67:THR:O     | 29:DF:84:ILE:HG22 | 2.18                     | 0.44              |
| 56:DB:31:C:H42     | 38:DO:32:PRO:HB3  | 1.83                     | 0.44              |
| 42:DS:2:GLU:OE2    | 42:DS:2:GLU:HA    | 2.18                     | 0.44              |
| 44:DU:84:PHE:HA    | 44:DU:92:VAL:O    | 2.18                     | 0.44              |
| 47:DX:77:TYR:C     | 47:DX:77:TYR:CD1  | 2.91                     | 0.44              |
| 48:DY:21:LEU:HA    | 48:DY:25:GLN:HB3  | 2.00                     | 0.44              |
| 21:AA:123:U:O2'    | 21:AA:124:C:H5'   | 2.18                     | 0.44              |
| 21:AA:1271:A:H2'   | 21:AA:1272:G:H8   | 1.82                     | 0.44              |
| 21:AA:1326:U:H2'   | 21:AA:1327:C:C6   | 2.52                     | 0.44              |
| 21:AA:290:C:H2'    | 21:AA:291:U:O4'   | 2.18                     | 0.44              |
| 21:AA:495:A:C2     | 21:AA:496:A:N6    | 2.86                     | 0.44              |
| 21:AA:82:G:H1      | 21:AA:88:U:H1'    | 1.83                     | 0.44              |
| 21:AA:961:U:C2     | 21:AA:983:A:C5    | 3.05                     | 0.44              |
| 21:AA:992:U:C4     | 21:AA:1045:C:C4   | 3.06                     | 0.44              |
| 1:AB:56:LEU:HD13   | 1:AB:56:LEU:C     | 2.38                     | 0.44              |
| 2:AC:13:ILE:H      | 2:AC:13:ILE:HD13  | 1.82                     | 0.44              |
| 2:AC:41:TYR:C      | 2:AC:41:TYR:CD1   | 2.91                     | 0.44              |
| 5:AF:90:MET:HB3    | 17:AR:60:ARG:NH2  | 2.32                     | 0.44              |
| 4:AE:155:LYS:HG3   | 7:AH:65:PHE:CD1   | 2.52                     | 0.44              |
| 8:AI:12:LYS:C      | 8:AI:14:SER:H     | 2.21                     | 0.44              |
| 8:AI:6:TYR:OH      | 21:AA:1148:U:H5'  | 2.18                     | 0.44              |
| 12:AM:9:PRO:O      | 12:AM:10:ASP:HB2  | 2.16                     | 0.44              |
| 53:B3:40:LYS:O     | 53:B3:41:ARG:C    | 2.55                     | 0.44              |
| 24:BA:1046:A:H3'   | 24:BA:1047:G:H5'  | 2.00                     | 0.44              |
| 24:BA:1049:C:O2'   | 24:BA:1050:A:H5'  | 2.17                     | 0.44              |
| 24:BA:1263:U:H2'   | 24:BA:1264:A:C8   | 2.53                     | 0.44              |
| 24:BA:169:G:C4     | 24:BA:170:U:C5    | 3.05                     | 0.44              |
| 24:BA:1759:A:O2'   | 24:BA:1760:C:C5'  | 2.60                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:1795:C:O2   | 24:BA:1795:C:H2'   | 2.17                     | 0.44              |
| 24:BA:1975:G:C6   | 24:BA:1976:U:C4    | 3.06                     | 0.44              |
| 24:BA:2064:C:H2'  | 24:BA:2065:C:C6    | 2.53                     | 0.44              |
| 24:BA:2346:A:C5   | 24:BA:2383:G:C2    | 3.06                     | 0.44              |
| 24:BA:2455:G:C2   | 24:BA:2456:C:C2    | 3.06                     | 0.44              |
| 24:BA:252:G:C2'   | 24:BA:253:C:H5'    | 2.48                     | 0.44              |
| 24:BA:2727:A:O2'  | 24:BA:2728:U:C5'   | 2.61                     | 0.44              |
| 24:BA:319:G:C5    | 24:BA:333:G:C2     | 3.05                     | 0.44              |
| 24:BA:503:A:C2    | 24:BA:505:A:C5     | 3.06                     | 0.44              |
| 24:BA:683:U:C2    | 24:BA:684:G:C8     | 3.05                     | 0.44              |
| 24:BA:745:G:H1'   | 24:BA:750:A:N6     | 2.32                     | 0.44              |
| 24:BA:823:C:C4    | 24:BA:824:U:C4     | 3.05                     | 0.44              |
| 24:BA:900:A:C4    | 24:BA:901:C:C6     | 3.06                     | 0.44              |
| 24:BA:89:A:C2     | 24:BA:90:U:C2      | 3.05                     | 0.44              |
| 26:BC:246:PRO:HG2 | 26:BC:247:TRP:CH2  | 2.53                     | 0.44              |
| 27:BD:142:VAL:HB  | 27:BD:143:PRO:CD   | 2.48                     | 0.44              |
| 29:BF:3:LEU:HD12  | 29:BF:172:PHE:CE2  | 2.52                     | 0.44              |
| 30:BG:51:PHE:N    | 30:BG:51:PHE:CD2   | 2.86                     | 0.44              |
| 30:BG:61:TRP:O    | 30:BG:64:ALA:HB3   | 2.18                     | 0.44              |
| 31:BH:100:ALA:O   | 31:BH:101:ASP:C    | 2.56                     | 0.44              |
| 34:BK:52:VAL:HG23 | 34:BK:53:LYS:N     | 2.33                     | 0.44              |
| 34:BK:91:SER:O    | 34:BK:93:GLN:HB2   | 2.18                     | 0.44              |
| 34:BK:97:THR:O    | 34:BK:118:LEU:HD21 | 2.18                     | 0.44              |
| 40:BQ:85:ALA:O    | 40:BQ:87:VAL:C     | 2.56                     | 0.44              |
| 44:BU:3:LYS:NZ    | 44:BU:83:GLY:H     | 2.14                     | 0.44              |
| 48:BY:23:ARG:O    | 48:BY:24:GLU:C     | 2.57                     | 0.44              |
| 55:CA:1061:G:C5   | 55:CA:1062:U:C5    | 3.06                     | 0.44              |
| 55:CA:1064:G:N3   | 55:CA:1066:C:N4    | 2.66                     | 0.44              |
| 55:CA:1426:G:C6   | 55:CA:1427:C:C4    | 3.06                     | 0.44              |
| 55:CA:1456:A:H2'  | 55:CA:1457:G:O4'   | 2.17                     | 0.44              |
| 55:CA:16:A:C5     | 55:CA:17:U:C5      | 3.06                     | 0.44              |
| 55:CA:286:C:H2'   | 55:CA:287:U:C6     | 2.53                     | 0.44              |
| 55:CA:312:C:C2    | 55:CA:313:A:C8     | 3.06                     | 0.44              |
| 55:CA:426:U:H2'   | 55:CA:427:U:C6     | 2.52                     | 0.44              |
| 55:CA:488:C:H2'   | 55:CA:489:C:H6     | 1.83                     | 0.44              |
| 55:CA:496:A:C2'   | 55:CA:496:A:N3     | 2.71                     | 0.44              |
| 55:CA:501:C:H2'   | 55:CA:502:A:H8     | 1.81                     | 0.44              |
| 55:CA:519:C:H2'   | 55:CA:520:A:N7     | 2.32                     | 0.44              |
| 55:CA:860:A:C6    | 55:CA:861:G:C4     | 3.06                     | 0.44              |
| 55:CA:954:G:C6    | 55:CA:955:U:C2     | 3.06                     | 0.44              |
| 1:CB:61:SER:HA    | 1:CB:224:ARG:HA    | 2.00                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:CC:70:ALA:O      | 2:CC:72:PRO:HD2   | 2.17                     | 0.44              |
| 3:CD:167:PRO:HB3   | 3:CD:169:TRP:CZ3  | 2.52                     | 0.44              |
| 3:CD:172:VAL:HA    | 3:CD:179:GLY:HA2  | 2.00                     | 0.44              |
| 8:CI:126:PHE:N     | 8:CI:126:PHE:CD2  | 2.86                     | 0.44              |
| 8:CI:83:THR:HG21   | 8:CI:102:PHE:HB3  | 2.00                     | 0.44              |
| 10:CK:15:VAL:HG21  | 10:CK:35:ASP:HB3  | 1.99                     | 0.44              |
| 12:CM:64:VAL:CG1   | 12:CM:65:GLU:HG3  | 2.48                     | 0.44              |
| 13:CN:2:LYS:O      | 13:CN:5:MET:HB2   | 2.18                     | 0.44              |
| 13:CN:80:ARG:C     | 13:CN:82:LYS:H    | 2.21                     | 0.44              |
| 17:CR:41:SER:HB3   | 17:CR:51:GLN:NE2  | 2.33                     | 0.44              |
| 18:CS:19:GLU:HA    | 18:CS:22:VAL:HG23 | 2.00                     | 0.44              |
| 24:DA:1022:G:C6    | 24:DA:1140:C:C5   | 3.06                     | 0.44              |
| 24:DA:1202:G:C5    | 24:DA:1203:U:C5   | 3.05                     | 0.44              |
| 24:DA:1385:A:C6    | 24:DA:1403:A:C5   | 3.05                     | 0.44              |
| 24:DA:1415:U:O3'   | 24:DA:1416:G:H4'  | 2.17                     | 0.44              |
| 24:DA:1651:G:C2    | 24:DA:2007:U:N3   | 2.86                     | 0.44              |
| 24:DA:1839:G:O2'   | 24:DA:1840:G:H5'  | 2.17                     | 0.44              |
| 24:DA:1908:C:H2'   | 24:DA:1909:C:C6   | 2.53                     | 0.44              |
| 24:DA:217:A:H2'    | 24:DA:218:A:O4'   | 2.18                     | 0.44              |
| 24:DA:227:A:H4'    | 24:DA:228:C:OP1   | 2.17                     | 0.44              |
| 24:DA:243:U:O2'    | 24:DA:244:A:C5'   | 2.64                     | 0.44              |
| 24:DA:2470:G:C2    | 24:DA:2481:G:H1'  | 2.52                     | 0.44              |
| 24:DA:2509:G:C6    | 24:DA:2510:C:C5   | 3.05                     | 0.44              |
| 24:DA:2517:C:HO2'  | 24:DA:2518:A:P    | 2.41                     | 0.44              |
| 24:DA:2585:U:HO2'  | 24:DA:2586:U:P    | 2.41                     | 0.44              |
| 24:DA:2723:C:H5'   | 37:DN:3:HIS:HB2   | 2.00                     | 0.44              |
| 24:DA:82:U:H5''    | 24:DA:296:U:H5''  | 2.00                     | 0.44              |
| 24:DA:273:G:N2     | 24:DA:365:U:C2    | 2.85                     | 0.44              |
| 24:DA:513:A:O5'    | 24:DA:513:A:H8    | 2.01                     | 0.44              |
| 24:DA:524:G:O2'    | 24:DA:525:U:H5'   | 2.18                     | 0.44              |
| 24:DA:548:G:C5'    | 24:DA:549:G:H5'   | 2.48                     | 0.44              |
| 24:DA:55:G:H2'     | 24:DA:55:G:N3     | 2.33                     | 0.44              |
| 24:DA:568:U:OP1    | 35:DL:36:LYS:HD3  | 2.17                     | 0.44              |
| 24:DA:601:C:H4'    | 28:DE:99:LYS:HE2  | 2.00                     | 0.44              |
| 24:DA:659:G:C6     | 24:DA:660:C:C4    | 3.06                     | 0.44              |
| 24:DA:745:G:H5''   | 24:DA:746:U:OP2   | 2.18                     | 0.44              |
| 24:DA:776:G:N7     | 24:DA:793:A:C4    | 2.86                     | 0.44              |
| 24:DA:976:G:H2'    | 24:DA:977:G:C8    | 2.53                     | 0.44              |
| 56:DB:58:A:O2'     | 56:DB:59:A:C5'    | 2.66                     | 0.44              |
| 28:DE:105:LEU:HD13 | 28:DE:105:LEU:O   | 2.17                     | 0.44              |
| 29:DF:103:ILE:HG21 | 29:DF:173:ASP:O   | 2.17                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:DJ:97:PRO:C     | 33:DJ:99:ARG:H    | 2.22                     | 0.44              |
| 35:DL:105:ILE:HG22 | 35:DL:106:GLU:N   | 2.33                     | 0.44              |
| 24:DA:670:A:OP1    | 35:DL:43:GLY:HA3  | 2.17                     | 0.44              |
| 35:DL:3:LEU:HG     | 35:DL:4:ASN:N     | 2.33                     | 0.44              |
| 36:DM:68:PHE:CD1   | 36:DM:69:PRO:HD2  | 2.53                     | 0.44              |
| 36:DM:96:ILE:O     | 36:DM:96:ILE:HG13 | 2.06                     | 0.44              |
| 37:DN:21:PHE:N     | 37:DN:21:PHE:CD1  | 2.86                     | 0.44              |
| 42:DS:35:ILE:HA    | 50:D0:24:VAL:HG21 | 2.00                     | 0.44              |
| 46:DW:37:VAL:HG23  | 46:DW:38:ARG:HD2  | 1.99                     | 0.44              |
| 48:DY:25:GLN:HA    | 48:DY:28:LEU:HB3  | 1.99                     | 0.44              |
| 21:AA:1078:U:H3'   | 21:AA:1079:G:H8   | 1.83                     | 0.43              |
| 21:AA:1324:A:C5    | 21:AA:1325:C:C4   | 3.06                     | 0.43              |
| 21:AA:1474:U:H2'   | 21:AA:1475:G:O4'  | 2.18                     | 0.43              |
| 21:AA:1504:G:H5'   | 21:AA:1505:G:C2   | 2.53                     | 0.43              |
| 21:AA:1405:G:O4'   | 21:AA:1519:A:H4'  | 2.18                     | 0.43              |
| 21:AA:146:G:C2     | 21:AA:177:G:N7    | 2.86                     | 0.43              |
| 21:AA:451:A:N6     | 21:AA:481:G:N9    | 2.66                     | 0.43              |
| 21:AA:914:A:N3     | 21:AA:915:A:C8    | 2.86                     | 0.43              |
| 21:AA:961:U:O2     | 21:AA:983:A:C4    | 2.71                     | 0.43              |
| 21:AA:986:U:H2'    | 21:AA:987:G:O4'   | 2.17                     | 0.43              |
| 1:AB:110:ILE:HD13  | 1:AB:150:ILE:HD13 | 1.99                     | 0.43              |
| 2:AC:9:ILE:HA      | 2:AC:9:ILE:HD12   | 1.86                     | 0.43              |
| 3:AD:151:GLN:H     | 3:AD:154:VAL:CG1  | 2.31                     | 0.43              |
| 5:AF:21:MET:HE2    | 5:AF:25:TYR:HE1   | 1.83                     | 0.43              |
| 8:AI:20:ILE:CG2    | 8:AI:60:LEU:HD12  | 2.47                     | 0.43              |
| 9:AJ:26:VAL:HG12   | 9:AJ:30:LYS:CE    | 2.47                     | 0.43              |
| 9:AJ:53:ILE:O      | 9:AJ:53:ILE:HG12  | 2.17                     | 0.43              |
| 11:AL:33:CYS:H     | 11:AL:54:VAL:HG13 | 1.82                     | 0.43              |
| 11:AL:72:ASN:O     | 11:AL:73:LEU:O    | 2.36                     | 0.43              |
| 12:AM:44:ILE:N     | 12:AM:44:ILE:CD1  | 2.81                     | 0.43              |
| 13:AN:29:ILE:O     | 13:AN:34:ASN:ND2  | 2.51                     | 0.43              |
| 13:AN:19:TYR:HD2   | 13:AN:50:LEU:HD13 | 1.83                     | 0.43              |
| 15:AP:5:ARG:HD2    | 21:AA:376:G:H5''  | 2.00                     | 0.43              |
| 16:AQ:11:VAL:CG1   | 16:AQ:12:VAL:H    | 2.28                     | 0.43              |
| 16:AQ:16:MET:HG3   | 16:AQ:20:ILE:CA   | 2.45                     | 0.43              |
| 17:AR:63:TYR:CE1   | 21:AA:673:A:H1'   | 2.53                     | 0.43              |
| 52:B2:18:PHE:HA    | 52:B2:43:THR:HG21 | 2.00                     | 0.43              |
| 24:BA:1048:A:C5    | 24:BA:1049:C:C5   | 3.06                     | 0.43              |
| 24:BA:1071:G:N7    | 24:BA:1089:A:N6   | 2.66                     | 0.43              |
| 24:BA:1099:G:H2'   | 24:BA:1100:C:C6   | 2.53                     | 0.43              |
| 24:BA:1436:G:C2    | 24:BA:1557:C:C2   | 3.06                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:1652:A:N6   | 24:BA:1653:G:N2    | 2.66                     | 0.43              |
| 24:BA:1833:C:C2   | 24:BA:1834:U:C5    | 3.06                     | 0.43              |
| 24:BA:1842:G:C5   | 24:BA:1843:C:C5    | 3.06                     | 0.43              |
| 24:BA:1897:G:O2'  | 24:BA:1898:U:H5'   | 2.17                     | 0.43              |
| 24:BA:1914:C:O2'  | 24:BA:1915:U:C5'   | 2.66                     | 0.43              |
| 24:BA:1972:G:C2   | 24:BA:1973:G:N7    | 2.86                     | 0.43              |
| 24:BA:2064:C:H1'  | 24:BA:2450:A:C6    | 2.52                     | 0.43              |
| 24:BA:2786:U:H2'  | 24:BA:2787:C:H6    | 1.84                     | 0.43              |
| 24:BA:2785:C:H2'  | 24:BA:2786:U:O4'   | 2.17                     | 0.43              |
| 24:BA:308:G:C8    | 24:BA:501:A:O4'    | 2.71                     | 0.43              |
| 24:BA:804:A:H5''  | 24:BA:805:G:OP1    | 2.18                     | 0.43              |
| 24:BA:820:A:N1    | 24:BA:821:A:C2     | 2.86                     | 0.43              |
| 24:BA:959:A:H62   | 36:BM:82:MET:HE3   | 1.83                     | 0.43              |
| 27:BD:149:ASN:CG  | 27:BD:150:GLN:N    | 2.70                     | 0.43              |
| 27:BD:91:THR:C    | 27:BD:93:GLY:N     | 2.71                     | 0.43              |
| 28:BE:172:ALA:O   | 28:BE:175:ILE:CG2  | 2.66                     | 0.43              |
| 29:BF:84:ILE:CG1  | 29:BF:84:ILE:O     | 2.66                     | 0.43              |
| 32:BI:56:VAL:HG22 | 32:BI:57:VAL:N     | 2.33                     | 0.43              |
| 33:BJ:38:GLY:C    | 33:BJ:40:HIS:N     | 2.69                     | 0.43              |
| 36:BM:53:MET:HE2  | 36:BM:53:MET:HB2   | 1.73                     | 0.43              |
| 38:BO:28:VAL:HG21 | 38:BO:103:VAL:HG12 | 2.00                     | 0.43              |
| 40:BQ:79:ILE:O    | 40:BQ:80:ASN:C     | 2.57                     | 0.43              |
| 44:BU:73:ASN:C    | 44:BU:75:ALA:N     | 2.70                     | 0.43              |
| 49:BZ:30:ARG:HE   | 49:BZ:30:ARG:HB2   | 1.57                     | 0.43              |
| 55:CA:1008:U:H2'  | 55:CA:1009:U:C6    | 2.53                     | 0.43              |
| 55:CA:117:G:H2'   | 55:CA:118:U:C6     | 2.53                     | 0.43              |
| 55:CA:1069:C:H4'  | 55:CA:1192:C:O2    | 2.18                     | 0.43              |
| 55:CA:1308:U:C2   | 55:CA:1330:U:N3    | 2.86                     | 0.43              |
| 55:CA:32:A:OP2    | 55:CA:398:U:O2'    | 2.28                     | 0.43              |
| 55:CA:562:U:H2'   | 55:CA:562:U:OP2    | 2.18                     | 0.43              |
| 55:CA:695:A:N1    | 55:CA:696:A:C2     | 2.86                     | 0.43              |
| 55:CA:786:G:C2    | 55:CA:797:C:C2     | 3.06                     | 0.43              |
| 55:CA:842:U:H3'   | 55:CA:842:U:OP1    | 2.18                     | 0.43              |
| 55:CA:878:A:O2'   | 55:CA:879:C:H5'    | 2.18                     | 0.43              |
| 55:CA:757:U:O2'   | 55:CA:879:C:H1'    | 2.17                     | 0.43              |
| 1:CB:127:LYS:HG3  | 1:CB:132:GLU:HG3   | 2.00                     | 0.43              |
| 1:CB:170:ILE:HD12 | 55:CA:1101:A:C8    | 2.53                     | 0.43              |
| 1:CB:30:ILE:HG21  | 1:CB:38:HIS:CG     | 2.52                     | 0.43              |
| 1:CB:67:LEU:CD1   | 1:CB:157:PRO:HG3   | 2.48                     | 0.43              |
| 1:CB:79:VAL:HA    | 1:CB:213:LEU:CD2   | 2.36                     | 0.43              |
| 2:CC:159:ALA:HB1  | 2:CC:161:ILE:HD13  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CC:178:ARG:O    | 2:CC:205:GLU:O     | 2.36                     | 0.43              |
| 2:CC:84:GLU:C     | 2:CC:86:LEU:H      | 2.19                     | 0.43              |
| 7:CH:26:MET:O     | 7:CH:58:LEU:N      | 2.51                     | 0.43              |
| 9:CJ:28:THR:HG23  | 9:CJ:29:ALA:N      | 2.33                     | 0.43              |
| 10:CK:127:ARG:HG2 | 10:CK:127:ARG:O    | 2.17                     | 0.43              |
| 12:CM:68:LEU:HB3  | 12:CM:69:ARG:HD2   | 2.00                     | 0.43              |
| 15:CP:48:GLU:CD   | 15:CP:51:ARG:HB2   | 2.39                     | 0.43              |
| 24:DA:1083:U:H1'  | 24:DA:1086:A:C2    | 2.53                     | 0.43              |
| 24:DA:1456:G:C6   | 24:DA:1457:U:C4    | 3.06                     | 0.43              |
| 24:DA:1700:A:H2'  | 24:DA:1701:A:C5'   | 2.43                     | 0.43              |
| 24:DA:1721:G:HO2' | 24:DA:1722:A:P     | 2.41                     | 0.43              |
| 24:DA:171:U:H2'   | 24:DA:172:A:C8     | 2.52                     | 0.43              |
| 24:DA:1950:G:H1   | 24:DA:1954:G:H2'   | 1.83                     | 0.43              |
| 24:DA:2072:C:H6   | 24:DA:2072:C:OP2   | 2.01                     | 0.43              |
| 24:DA:2229:U:H2'  | 24:DA:2230:G:C8    | 2.52                     | 0.43              |
| 24:DA:2460:U:O2'  | 24:DA:2461:A:C5'   | 2.66                     | 0.43              |
| 24:DA:2517:C:O2'  | 24:DA:2518:A:C3'   | 2.48                     | 0.43              |
| 24:DA:2522:U:C2'  | 24:DA:2523:G:H5'   | 2.48                     | 0.43              |
| 24:DA:2548:U:C4   | 24:DA:2549:G:N7    | 2.86                     | 0.43              |
| 24:DA:2635:A:C2   | 24:DA:2784:U:C2    | 3.06                     | 0.43              |
| 24:DA:2:G:C6      | 24:DA:3:U:C4       | 3.05                     | 0.43              |
| 24:DA:531:C:C5    | 24:DA:2035:G:C2    | 3.06                     | 0.43              |
| 24:DA:675:A:C6    | 24:DA:676:A:C6     | 3.06                     | 0.43              |
| 24:DA:739:A:O2'   | 24:DA:740:C:C6     | 2.71                     | 0.43              |
| 56:DB:30:C:C2'    | 56:DB:31:C:H5'     | 2.45                     | 0.43              |
| 56:DB:90:C:H5'    | 36:DM:18:ARG:HD2   | 1.99                     | 0.43              |
| 27:DD:114:LYS:HD2 | 27:DD:116:LYS:NZ   | 2.33                     | 0.43              |
| 27:DD:62:LYS:HE3  | 27:DD:62:LYS:HA    | 1.99                     | 0.43              |
| 30:DG:6:ALA:HA    | 30:DG:7:PRO:HD3    | 1.66                     | 0.43              |
| 31:DH:25:TYR:CD1  | 31:DH:30:LEU:HG    | 2.53                     | 0.43              |
| 32:DI:112:LYS:NZ  | 32:DI:128:ILE:HD12 | 2.33                     | 0.43              |
| 24:DA:1061:U:H6   | 32:DI:9:LYS:HD3    | 1.83                     | 0.43              |
| 34:DK:21:CYS:HA   | 34:DK:41:ILE:HD12  | 2.00                     | 0.43              |
| 36:DM:42:THR:HB   | 36:DM:45:GLN:CG    | 2.47                     | 0.43              |
| 39:DP:9:GLN:HA    | 39:DP:12:MET:HG3   | 1.98                     | 0.43              |
| 40:DQ:74:SER:O    | 40:DQ:78:PHE:HB2   | 2.18                     | 0.43              |
| 42:DS:88:ARG:NH2  | 42:DS:88:ARG:CG    | 2.77                     | 0.43              |
| 44:DU:54:PRO:HG2  | 44:DU:55:GLY:N     | 2.22                     | 0.43              |
| 46:DW:44:PHE:HE2  | 46:DW:76:ARG:NE    | 2.16                     | 0.43              |
| 48:DY:1:MET:N     | 48:DY:1:MET:CE     | 2.78                     | 0.43              |
| 21:AA:996:A:N1    | 21:AA:1045:C:O2'   | 2.49                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:1084:G:C6   | 21:AA:1085:U:C4   | 3.06                     | 0.43              |
| 21:AA:1158:C:H5'' | 21:AA:1158:C:O2   | 2.18                     | 0.43              |
| 21:AA:1321:U:C5   | 21:AA:1322:C:C5   | 3.07                     | 0.43              |
| 21:AA:198:G:O2'   | 21:AA:199:A:O5'   | 2.36                     | 0.43              |
| 21:AA:340:U:O2'   | 21:AA:341:C:H5'   | 2.18                     | 0.43              |
| 14:AO:53:ARG:NH1  | 21:AA:579:A:O2'   | 2.51                     | 0.43              |
| 21:AA:903:G:C4    | 21:AA:904:U:C5    | 3.05                     | 0.43              |
| 21:AA:953:G:C2    | 21:AA:1229:A:C2   | 3.07                     | 0.43              |
| 1:AB:27:LYS:N     | 1:AB:28:PRO:CD    | 2.81                     | 0.43              |
| 1:AB:38:HIS:CD2   | 1:AB:38:HIS:O     | 2.71                     | 0.43              |
| 1:AB:49:PHE:HB2   | 1:AB:53:LEU:HD23  | 1.99                     | 0.43              |
| 2:AC:119:ILE:O    | 2:AC:123:LEU:HG   | 2.16                     | 0.43              |
| 3:AD:104:MET:HE2  | 3:AD:170:LEU:HB2  | 2.00                     | 0.43              |
| 3:AD:96:ARG:HH21  | 3:AD:114:ARG:NH2  | 2.16                     | 0.43              |
| 4:AE:151:MET:O    | 4:AE:153:ALA:N    | 2.52                     | 0.43              |
| 6:AG:148:LYS:C    | 6:AG:150:PHE:N    | 2.71                     | 0.43              |
| 4:AE:155:LYS:HB3  | 7:AH:64:TYR:O     | 2.18                     | 0.43              |
| 8:AI:8:THR:O      | 8:AI:16:ALA:O     | 2.36                     | 0.43              |
| 12:AM:90:HIS:HA   | 12:AM:108:ARG:NH2 | 2.33                     | 0.43              |
| 20:AU:36:PHE:CD1  | 20:AU:39:LYS:HG2  | 2.53                     | 0.43              |
| 24:BA:1588:G:C2   | 24:BA:1589:U:C6   | 3.07                     | 0.43              |
| 24:BA:1769:U:N3   | 24:BA:1984:G:C6   | 2.87                     | 0.43              |
| 24:BA:1950:G:C8   | 24:BA:1951:U:C5   | 3.06                     | 0.43              |
| 24:BA:2079:U:O2'  | 47:BX:22:ASN:ND2  | 2.51                     | 0.43              |
| 24:BA:2250:G:OP1  | 24:BA:2275:C:H2'  | 2.17                     | 0.43              |
| 24:BA:2465:C:O2   | 24:BA:2465:C:H2'  | 2.18                     | 0.43              |
| 24:BA:2576:G:C8   | 24:BA:2580:U:O4   | 2.71                     | 0.43              |
| 24:BA:2631:G:H2'  | 24:BA:2632:A:O4'  | 2.17                     | 0.43              |
| 24:BA:279:A:H2'   | 24:BA:280:U:C6    | 2.44                     | 0.43              |
| 24:BA:2894:G:H2'  | 24:BA:2894:G:H8   | 1.36                     | 0.43              |
| 24:BA:301:G:C6    | 24:BA:317:G:C6    | 3.06                     | 0.43              |
| 24:BA:378:C:O2'   | 24:BA:379:G:H5'   | 2.18                     | 0.43              |
| 24:BA:491:G:H2'   | 24:BA:492:A:C8    | 2.53                     | 0.43              |
| 24:BA:59:U:H1'    | 24:BA:73:A:O2'    | 2.18                     | 0.43              |
| 24:BA:60:G:HO2'   | 24:BA:61:C:P      | 2.38                     | 0.43              |
| 24:BA:611:C:H2'   | 24:BA:612:G:O4'   | 2.19                     | 0.43              |
| 24:BA:919:U:C3'   | 24:BA:919:U:C6    | 3.00                     | 0.43              |
| 24:BA:941:A:H2'   | 24:BA:942:G:C8    | 2.53                     | 0.43              |
| 25:BB:33:G:O2'    | 25:BB:34:A:H5'    | 2.18                     | 0.43              |
| 25:BB:33:G:N3     | 25:BB:50:A:C2     | 2.86                     | 0.43              |
| 26:BC:141:HIS:NE2 | 26:BC:194:VAL:HA  | 2.33                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BD:58:ASN:OD1   | 27:BD:59:ARG:HG2   | 2.18                     | 0.43              |
| 29:BF:3:LEU:HD13   | 29:BF:3:LEU:HA     | 1.69                     | 0.43              |
| 29:BF:42:ALA:HA    | 29:BF:45:ASP:O     | 2.18                     | 0.43              |
| 30:BG:120:ILE:HG21 | 30:BG:143:VAL:HG21 | 1.99                     | 0.43              |
| 30:BG:84:LYS:CB    | 30:BG:132:LEU:H    | 2.31                     | 0.43              |
| 30:BG:41:GLU:O     | 30:BG:41:GLU:HG3   | 2.17                     | 0.43              |
| 30:BG:83:THR:O     | 30:BG:84:LYS:HB3   | 2.17                     | 0.43              |
| 31:BH:89:LYS:CG    | 31:BH:90:LEU:H     | 2.25                     | 0.43              |
| 35:BL:132:ARG:HG3  | 35:BL:142:ILE:HD12 | 1.99                     | 0.43              |
| 38:BO:7:ARG:HD2    | 38:BO:97:PHE:CZ    | 2.52                     | 0.43              |
| 39:BP:17:PRO:HG3   | 39:BP:83:ILE:O     | 2.18                     | 0.43              |
| 40:BQ:40:LYS:HG2   | 40:BQ:44:TYR:CE1   | 2.53                     | 0.43              |
| 40:BQ:94:LEU:C     | 40:BQ:96:ASP:H     | 2.21                     | 0.43              |
| 45:BV:5:ASN:N      | 45:BV:5:ASN:ND2    | 2.66                     | 0.43              |
| 47:BX:19:HIS:O     | 47:BX:21:LEU:N     | 2.51                     | 0.43              |
| 55:CA:1130:A:C5    | 55:CA:1146:A:C6    | 3.06                     | 0.43              |
| 55:CA:1182:G:C4'   | 55:CA:1183:U:H5'   | 2.49                     | 0.43              |
| 55:CA:1265:C:C2'   | 55:CA:1266:G:H5'   | 2.48                     | 0.43              |
| 55:CA:978:A:C6     | 55:CA:1318:A:C6    | 3.05                     | 0.43              |
| 55:CA:298:A:N6     | 55:CA:299:G:N1     | 2.67                     | 0.43              |
| 55:CA:391:G:C6     | 55:CA:392:C:C2     | 3.07                     | 0.43              |
| 55:CA:570:G:C6     | 55:CA:873:A:C2     | 3.06                     | 0.43              |
| 55:CA:936:C:O2'    | 55:CA:937:A:H5'    | 2.18                     | 0.43              |
| 1:CB:185:ILE:HA    | 1:CB:199:ILE:HG13  | 2.00                     | 0.43              |
| 6:CG:86:VAL:HA     | 6:CG:87:PRO:HD2    | 1.83                     | 0.43              |
| 8:CI:49:GLN:O      | 8:CI:52:GLU:HG2    | 2.17                     | 0.43              |
| 9:CJ:25:ILE:HD11   | 9:CJ:93:ALA:CB     | 2.48                     | 0.43              |
| 11:CL:98:ARG:HD3   | 11:CL:103:CYS:SG   | 2.57                     | 0.43              |
| 11:CL:28:GLN:HE21  | 11:CL:28:GLN:HB3   | 1.61                     | 0.43              |
| 12:CM:1:ALA:H3     | 12:CM:2:ARG:HD2    | 1.82                     | 0.43              |
| 15:CP:77:GLU:C     | 15:CP:79:ASN:H     | 2.21                     | 0.43              |
| 52:D2:10:LEU:O     | 52:D2:10:LEU:HD23  | 2.18                     | 0.43              |
| 24:DA:1122:G:N3    | 24:DA:1122:G:H2'   | 2.33                     | 0.43              |
| 24:DA:1286:A:C4    | 24:DA:1289:C:N4    | 2.87                     | 0.43              |
| 24:DA:142:A:H5''   | 24:DA:142:A:C8     | 2.53                     | 0.43              |
| 24:DA:142:A:O2'    | 24:DA:143:C:H5'    | 2.18                     | 0.43              |
| 24:DA:122:G:P      | 24:DA:149:A:H4'    | 2.58                     | 0.43              |
| 24:DA:1668:A:N3    | 24:DA:1670:C:C4    | 2.86                     | 0.43              |
| 24:DA:1771:C:N4    | 24:DA:1772:A:H62   | 2.16                     | 0.43              |
| 24:DA:1774:C:H5''  | 24:DA:1775:U:OP2   | 2.18                     | 0.43              |
| 24:DA:1828:G:H8    | 24:DA:1828:G:OP2   | 2.01                     | 0.43              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 24:DA:1973:G:C6    | 24:DA:1974:C:C4  | 3.07                     | 0.43              |
| 24:DA:2066:C:H2'   | 24:DA:2067:G:C8  | 2.47                     | 0.43              |
| 24:DA:2080:A:C2    | 24:DA:2081:U:H1' | 2.54                     | 0.43              |
| 24:DA:2093:G:C5    | 24:DA:2225:A:N7  | 2.86                     | 0.43              |
| 24:DA:2675:A:C2    | 24:DA:2676:C:C2  | 3.06                     | 0.43              |
| 24:DA:2716:C:C2    | 24:DA:2717:C:C5  | 3.07                     | 0.43              |
| 24:DA:2835:A:C6    | 24:DA:2879:A:C4  | 3.06                     | 0.43              |
| 24:DA:409:G:O2'    | 24:DA:410:G:H5'  | 2.17                     | 0.43              |
| 24:DA:529:A:H4'    | 24:DA:530:G:OP1  | 2.18                     | 0.43              |
| 24:DA:464:U:H1'    | 24:DA:686:U:C5   | 2.53                     | 0.43              |
| 24:DA:713:G:N2     | 24:DA:718:A:H2   | 2.10                     | 0.43              |
| 24:DA:921:C:O5'    | 24:DA:921:C:H6   | 2.01                     | 0.43              |
| 24:DA:973:A:OP1    | 24:DA:973:A:C8   | 2.63                     | 0.43              |
| 56:DB:104:A:C2     | 56:DB:105:G:H1'  | 2.53                     | 0.43              |
| 56:DB:11:C:H5      | 56:DB:12:C:C5    | 2.33                     | 0.43              |
| 26:DC:188:ARG:HD3  | 26:DC:188:ARG:H  | 1.82                     | 0.43              |
| 26:DC:244:VAL:HB   | 26:DC:249:VAL:H  | 1.83                     | 0.43              |
| 31:DH:68:ARG:CD    | 31:DH:71:LYS:HB2 | 2.48                     | 0.43              |
| 32:DI:74:PRO:O     | 32:DI:78:LEU:HG  | 2.18                     | 0.43              |
| 33:DJ:35:ARG:HA    | 33:DJ:40:HIS:HD2 | 1.84                     | 0.43              |
| 35:DL:116:VAL:HG13 | 35:DL:117:THR:H  | 1.83                     | 0.43              |
| 39:DP:4:ILE:O      | 39:DP:4:ILE:HG22 | 2.18                     | 0.43              |
| 39:DP:75:THR:HG23  | 39:DP:76:HIS:CD2 | 2.54                     | 0.43              |
| 39:DP:9:GLN:HB3    | 39:DP:12:MET:HE3 | 2.00                     | 0.43              |
| 41:DR:49:ILE:HG22  | 41:DR:54:VAL:N   | 2.33                     | 0.43              |
| 41:DR:81:LYS:O     | 41:DR:82:HIS:C   | 2.57                     | 0.43              |
| 43:DT:29:THR:OG1   | 43:DT:85:VAL:HB  | 2.17                     | 0.43              |
| 44:DU:35:VAL:CG1   | 44:DU:36:GLU:H   | 2.24                     | 0.43              |
| 44:DU:3:LYS:O      | 44:DU:4:ILE:C    | 2.56                     | 0.43              |
| 47:DX:52:ALA:C     | 47:DX:54:GLY:H   | 2.21                     | 0.43              |
| 21:AA:1523:G:C6    | 21:AA:1524:C:N4  | 2.86                     | 0.43              |
| 21:AA:161:A:H2'    | 21:AA:162:A:H8   | 1.83                     | 0.43              |
| 21:AA:169:C:C5     | 21:AA:170:U:C5   | 3.06                     | 0.43              |
| 21:AA:49:U:C4      | 21:AA:364:A:C6   | 3.06                     | 0.43              |
| 21:AA:680:C:C2     | 21:AA:711:G:C2   | 3.06                     | 0.43              |
| 21:AA:845:A:H8     | 21:AA:846:G:H4'  | 1.83                     | 0.43              |
| 21:AA:977:A:H8     | 21:AA:1223:C:C2  | 2.37                     | 0.43              |
| 5:AF:9:MET:HE1     | 5:AF:59:TYR:CE2  | 2.53                     | 0.43              |
| 10:AK:59:PRO:HD3   | 10:AK:90:PRO:HB3 | 2.01                     | 0.43              |
| 12:AM:94:LEU:CD1   | 21:AA:1226:C:H5' | 2.48                     | 0.43              |
| 16:AQ:25:GLU:OE1   | 16:AQ:25:GLU:HA  | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:B3:7:ARG:O     | 53:B3:11:LYS:HG3  | 2.18                     | 0.43              |
| 24:BA:1145:C:H2'  | 24:BA:1146:C:H6   | 1.83                     | 0.43              |
| 24:BA:1295:C:H2'  | 24:BA:1296:G:H8   | 1.84                     | 0.43              |
| 24:BA:1464:G:H2'  | 24:BA:1465:G:C8   | 2.51                     | 0.43              |
| 24:BA:1797:G:H1'  | 24:BA:1823:G:N2   | 2.32                     | 0.43              |
| 24:BA:1857:G:O2'  | 24:BA:1858:A:OP2  | 2.29                     | 0.43              |
| 24:BA:1865:U:HO2' | 24:BA:1866:A:H8   | 1.63                     | 0.43              |
| 24:BA:195:A:C5    | 59:BA:3767:HOH:O  | 2.70                     | 0.43              |
| 24:BA:747:U:O2    | 24:BA:2014:A:H1'  | 2.18                     | 0.43              |
| 24:BA:2286:G:O6   | 51:B1:22:THR:CG2  | 2.66                     | 0.43              |
| 24:BA:2339:C:H2'  | 24:BA:2340:A:H8   | 1.84                     | 0.43              |
| 24:BA:2410:G:C6   | 24:BA:2411:A:C4   | 3.07                     | 0.43              |
| 24:BA:243:U:OP2   | 53:B3:7:ARG:NE    | 2.47                     | 0.43              |
| 24:BA:2520:C:O2'  | 24:BA:2521:C:H5'  | 2.18                     | 0.43              |
| 24:BA:2578:G:H1'  | 27:BD:144:GLY:HA2 | 2.00                     | 0.43              |
| 24:BA:2580:U:H3'  | 24:BA:2581:G:C2   | 2.53                     | 0.43              |
| 24:BA:2587:A:H2'  | 24:BA:2588:G:H5'  | 2.00                     | 0.43              |
| 24:BA:2747:G:N1   | 24:BA:2754:U:C2   | 2.87                     | 0.43              |
| 24:BA:399:U:H2'   | 24:BA:400:G:H5'   | 2.00                     | 0.43              |
| 24:BA:482:A:C6    | 24:BA:506:G:C4    | 3.06                     | 0.43              |
| 24:BA:986:C:H2'   | 24:BA:987:C:H5'   | 1.99                     | 0.43              |
| 24:BA:986:C:O2'   | 24:BA:987:C:H5'   | 2.17                     | 0.43              |
| 25:BB:27:C:C5     | 25:BB:28:C:C5     | 3.05                     | 0.43              |
| 26:BC:225:ASN:O   | 26:BC:227:VAL:N   | 2.51                     | 0.43              |
| 26:BC:245:THR:HG1 | 26:BC:249:VAL:HB  | 1.80                     | 0.43              |
| 26:BC:269:ARG:HA  | 26:BC:269:ARG:HD3 | 1.81                     | 0.43              |
| 27:BD:121:THR:O   | 27:BD:122:VAL:CB  | 2.66                     | 0.43              |
| 27:BD:16:THR:O    | 27:BD:19:GLY:N    | 2.40                     | 0.43              |
| 28:BE:19:PHE:HE2  | 28:BE:197:GLU:OE1 | 2.01                     | 0.43              |
| 28:BE:72:SER:C    | 28:BE:74:LYS:N    | 2.72                     | 0.43              |
| 30:BG:83:THR:C    | 30:BG:84:LYS:HD3  | 2.38                     | 0.43              |
| 24:BA:558:U:H5''  | 33:BJ:111:LYS:HE3 | 2.00                     | 0.43              |
| 24:BA:587:C:OP2   | 35:BL:21:ARG:NH1  | 2.51                     | 0.43              |
| 37:BN:93:GLY:C    | 37:BN:95:THR:N    | 2.71                     | 0.43              |
| 24:BA:1154:G:OP1  | 40:BQ:57:ARG:HD3  | 2.18                     | 0.43              |
| 41:BR:72:VAL:O    | 41:BR:72:VAL:HG22 | 2.17                     | 0.43              |
| 42:BS:50:VAL:O    | 42:BS:51:LEU:C    | 2.57                     | 0.43              |
| 42:BS:59:GLU:HA   | 42:BS:64:ALA:HA   | 2.00                     | 0.43              |
| 59:BB:315:HOH:O   | 45:BV:14:LYS:HD2  | 2.18                     | 0.43              |
| 45:BV:62:THR:HA   | 45:BV:71:LYS:HA   | 1.98                     | 0.43              |
| 46:BW:22:VAL:HG13 | 46:BW:25:PHE:CD2  | 2.52                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:BW:75:ASN:O    | 46:BW:76:ARG:CB    | 2.66                     | 0.43              |
| 48:BY:24:GLU:O    | 48:BY:28:LEU:HB2   | 2.17                     | 0.43              |
| 55:CA:1050:G:N2   | 55:CA:1051:C:C2    | 2.86                     | 0.43              |
| 55:CA:1129:C:O2'  | 55:CA:1130:A:H8    | 1.94                     | 0.43              |
| 55:CA:1163:A:N1   | 55:CA:1174:G:C6    | 2.86                     | 0.43              |
| 55:CA:1349:A:H2'  | 55:CA:1350:A:H8    | 1.82                     | 0.43              |
| 6:CG:101:ARG:NH2  | 55:CA:1375:A:O2'   | 2.51                     | 0.43              |
| 55:CA:1394:A:N6   | 55:CA:1501:C:H4'   | 2.33                     | 0.43              |
| 55:CA:181:A:N6    | 55:CA:195:A:OP2    | 2.51                     | 0.43              |
| 55:CA:355:C:C4    | 55:CA:356:A:N7     | 2.86                     | 0.43              |
| 55:CA:452:A:HO2'  | 55:CA:453:G:C4'    | 2.30                     | 0.43              |
| 3:CD:68:GLU:HB2   | 55:CA:545:C:H5'    | 2.00                     | 0.43              |
| 55:CA:614:C:H2'   | 55:CA:615:G:O4'    | 2.18                     | 0.43              |
| 55:CA:760:G:N7    | 55:CA:761:G:C8     | 2.85                     | 0.43              |
| 55:CA:821:G:C2    | 55:CA:822:U:C2     | 3.06                     | 0.43              |
| 55:CA:823:C:O2'   | 55:CA:824:G:H5'    | 2.17                     | 0.43              |
| 1:CB:164:ASP:OD1  | 1:CB:203:ASP:CB    | 2.66                     | 0.43              |
| 2:CC:13:ILE:HG22  | 2:CC:14:VAL:HG23   | 2.00                     | 0.43              |
| 4:CE:38:VAL:O     | 4:CE:45:VAL:HG23   | 2.18                     | 0.43              |
| 8:CI:53:LEU:HD21  | 8:CI:96:GLU:HB3    | 2.00                     | 0.43              |
| 11:CL:50:LYS:HD2  | 11:CL:50:LYS:N     | 2.33                     | 0.43              |
| 14:CO:44:GLU:HG2  | 14:CO:45:HIS:CD2   | 2.53                     | 0.43              |
| 18:CS:38:THR:OG1  | 18:CS:39:ILE:N     | 2.51                     | 0.43              |
| 51:D1:16:THR:CG2  | 51:D1:42:VAL:HG23  | 2.48                     | 0.43              |
| 24:DA:1045:C:O4'  | 24:DA:1111:A:N6    | 2.51                     | 0.43              |
| 24:DA:1048:A:O2'  | 24:DA:1049:C:C6    | 2.71                     | 0.43              |
| 24:DA:1054:A:C2   | 24:DA:1055:G:H1'   | 2.53                     | 0.43              |
| 24:DA:1262:A:H2   | 50:D0:6:LYS:HD2    | 1.83                     | 0.43              |
| 24:DA:1315:C:C2   | 24:DA:1338:G:C2    | 3.06                     | 0.43              |
| 24:DA:142:A:C2'   | 24:DA:143:C:H6     | 2.25                     | 0.43              |
| 24:DA:1803:A:H3'  | 24:DA:1804:C:H6    | 1.82                     | 0.43              |
| 24:DA:1816:C:HO2' | 24:DA:1817:G:P     | 2.40                     | 0.43              |
| 24:DA:1825:U:O3'  | 26:DC:231:HIS:CE1  | 2.71                     | 0.43              |
| 24:DA:2373:G:C6   | 24:DA:2381:A:N1    | 2.86                     | 0.43              |
| 24:DA:2581:G:H4'  | 24:DA:2582:G:C8    | 2.53                     | 0.43              |
| 24:DA:303:G:N1    | 24:DA:315:G:C6     | 2.86                     | 0.43              |
| 24:DA:353:C:N4    | 24:DA:354:A:H62    | 2.15                     | 0.43              |
| 24:DA:471:A:H5''  | 28:DE:79:ARG:NH1   | 2.31                     | 0.43              |
| 24:DA:972:A:H3'   | 24:DA:973:A:H5''   | 1.99                     | 0.43              |
| 24:DA:1797:G:H4'  | 26:DC:254:LYS:O    | 2.18                     | 0.43              |
| 26:DC:255:LYS:O   | 26:DC:256:THR:HG23 | 2.18                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:DQ:84:LYS:C    | 40:DQ:86:SER:H     | 2.22                     | 0.43              |
| 46:DW:31:LEU:C    | 46:DW:33:GLY:N     | 2.71                     | 0.43              |
| 24:DA:2232:C:P    | 47:DX:26:ARG:NH1   | 2.91                     | 0.43              |
| 48:DY:58:ASN:C    | 48:DY:60:LYS:H     | 2.22                     | 0.43              |
| 21:AA:104:G:N1    | 21:AA:105:G:C5     | 2.86                     | 0.43              |
| 21:AA:119:A:N7    | 21:AA:240:G:C5     | 2.86                     | 0.43              |
| 21:AA:71:A:HO2'   | 21:AA:72:A:C5'     | 2.30                     | 0.43              |
| 21:AA:724:G:H2'   | 21:AA:725:G:C8     | 2.53                     | 0.43              |
| 1:AB:14:HIS:CD2   | 1:AB:202:ASN:H     | 2.36                     | 0.43              |
| 1:AB:219:THR:HG23 | 1:AB:220:VAL:N     | 2.33                     | 0.43              |
| 1:AB:66:ILE:O     | 1:AB:160:LEU:HD12  | 2.18                     | 0.43              |
| 2:AC:194:VAL:O    | 2:AC:194:VAL:HG12  | 2.18                     | 0.43              |
| 7:AH:41:GLU:OE1   | 7:AH:41:GLU:HA     | 2.18                     | 0.43              |
| 9:AJ:41:PRO:O     | 9:AJ:42:LEU:HB2    | 2.19                     | 0.43              |
| 14:AO:50:HIS:ND1  | 21:AA:667:G:H4'    | 2.33                     | 0.43              |
| 16:AQ:58:VAL:CG2  | 16:AQ:59:GLU:H     | 2.30                     | 0.43              |
| 20:AU:19:LYS:C    | 20:AU:21:SER:N     | 2.71                     | 0.43              |
| 24:BA:1048:A:N7   | 24:BA:1111:A:C6    | 2.85                     | 0.43              |
| 24:BA:1137:G:H2'  | 24:BA:1138:G:O4'   | 2.18                     | 0.43              |
| 24:BA:1170:C:H2'  | 24:BA:1171:G:O4'   | 2.18                     | 0.43              |
| 24:BA:1277:G:C4'  | 37:BN:20:MET:HE2   | 2.48                     | 0.43              |
| 24:BA:1295:C:H2'  | 24:BA:1296:G:O4'   | 2.17                     | 0.43              |
| 24:BA:1399:C:H2'  | 24:BA:1400:U:C6    | 2.44                     | 0.43              |
| 24:BA:1654:A:H4'  | 27:BD:118:PHE:CE1  | 2.52                     | 0.43              |
| 24:BA:1721:G:H1'  | 24:BA:1739:A:N6    | 2.33                     | 0.43              |
| 24:BA:1926:U:H2'  | 24:BA:1928:A:N7    | 2.34                     | 0.43              |
| 24:BA:2287:A:C6   | 24:BA:2289:G:C4    | 3.07                     | 0.43              |
| 24:BA:2287:A:C4   | 24:BA:2289:G:N7    | 2.87                     | 0.43              |
| 24:BA:2305:U:O2'  | 29:BF:132:ARG:HG2  | 2.18                     | 0.43              |
| 24:BA:2297:A:H61  | 24:BA:2319:G:H1'   | 1.84                     | 0.43              |
| 24:BA:2365:G:C2'  | 24:BA:2366:A:C8    | 3.02                     | 0.43              |
| 24:BA:2656:U:O2'  | 24:BA:2657:A:H5'   | 2.18                     | 0.43              |
| 24:BA:2832:U:C2   | 24:BA:2834:G:C2    | 3.06                     | 0.43              |
| 24:BA:336:C:C2'   | 24:BA:337:C:H5'    | 2.48                     | 0.43              |
| 24:BA:601:C:O2    | 24:BA:605:G:H4'    | 2.19                     | 0.43              |
| 24:BA:636:G:OP2   | 35:BL:128:THR:HG22 | 2.17                     | 0.43              |
| 24:BA:696:G:C2    | 24:BA:697:G:C8     | 3.06                     | 0.43              |
| 24:BA:987:C:C4    | 24:BA:988:A:C5     | 3.06                     | 0.43              |
| 26:BC:142:ASN:CG  | 26:BC:142:ASN:O    | 2.56                     | 0.43              |
| 27:BD:22:ILE:HA   | 27:BD:23:PRO:HD3   | 1.79                     | 0.43              |
| 29:BF:35:LEU:CD1  | 29:BF:56:LEU:HD22  | 2.41                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:BG:61:TRP:O    | 30:BG:64:ALA:N     | 2.51                     | 0.43              |
| 33:BJ:114:LEU:O   | 33:BJ:117:ALA:HB3  | 2.19                     | 0.43              |
| 34:BK:65:THR:O    | 34:BK:79:PHE:HB2   | 2.18                     | 0.43              |
| 24:BA:825:A:C2'   | 35:BL:54:GLN:HE21  | 2.32                     | 0.43              |
| 37:BN:94:TYR:O    | 37:BN:116:VAL:HG12 | 2.18                     | 0.43              |
| 40:BQ:63:ARG:HH22 | 40:BQ:96:ASP:CA    | 2.31                     | 0.43              |
| 41:BR:35:PHE:HB2  | 41:BR:59:ILE:HB    | 2.00                     | 0.43              |
| 46:BW:24:ARG:HD3  | 46:BW:65:LYS:CD    | 2.48                     | 0.43              |
| 46:BW:70:VAL:C    | 46:BW:71:LYS:HD2   | 2.37                     | 0.43              |
| 31:BH:27:ARG:HG3  | 47:BX:59:ASP:CG    | 2.38                     | 0.43              |
| 55:CA:1000:A:H2'  | 55:CA:1001:C:C6    | 2.53                     | 0.43              |
| 55:CA:17:U:H1'    | 55:CA:1080:A:N3    | 2.34                     | 0.43              |
| 55:CA:1163:A:N3   | 55:CA:1174:G:C2    | 2.87                     | 0.43              |
| 55:CA:122:G:O2'   | 55:CA:123:U:H5'    | 2.17                     | 0.43              |
| 55:CA:1266:G:C2   | 55:CA:1270:G:C6    | 3.07                     | 0.43              |
| 55:CA:1301:U:H2'  | 55:CA:1301:U:O2    | 2.17                     | 0.43              |
| 55:CA:1349:A:C2'  | 55:CA:1350:A:H8    | 2.31                     | 0.43              |
| 55:CA:1415:G:N2   | 55:CA:1486:G:N9    | 2.66                     | 0.43              |
| 55:CA:268:U:N3    | 55:CA:269:C:C4     | 2.86                     | 0.43              |
| 55:CA:331:G:O2'   | 55:CA:332:G:P      | 2.77                     | 0.43              |
| 55:CA:484:G:O2'   | 55:CA:485:U:O5'    | 2.32                     | 0.43              |
| 13:CN:12:ARG:NH2  | 55:CA:980:C:O3'    | 2.49                     | 0.43              |
| 4:CE:71:ILE:HG12  | 4:CE:144:GLU:CG    | 2.48                     | 0.43              |
| 8:CI:60:LEU:O     | 8:CI:60:LEU:HD12   | 2.18                     | 0.43              |
| 13:CN:25:GLU:O    | 13:CN:28:ALA:HB3   | 2.18                     | 0.43              |
| 15:CP:46:LYS:HB2  | 15:CP:47:GLU:H     | 1.64                     | 0.43              |
| 15:CP:70:ARG:O    | 15:CP:74:LEU:HG    | 2.18                     | 0.43              |
| 16:CQ:22:VAL:HG21 | 16:CQ:58:VAL:HG21  | 1.99                     | 0.43              |
| 20:CU:17:ARG:H    | 20:CU:17:ARG:HD3   | 1.83                     | 0.43              |
| 22:CV:28:G:O2'    | 22:CV:29:G:H5'     | 2.18                     | 0.43              |
| 22:CV:33:U:C5'    | 22:CV:34:G:OP2     | 2.66                     | 0.43              |
| 53:D3:24:LYS:O    | 53:D3:25:HIS:CD2   | 2.71                     | 0.43              |
| 24:DA:1050:A:H2'  | 24:DA:1051:G:H8    | 1.81                     | 0.43              |
| 24:DA:1077:A:H2'  | 24:DA:1078:U:O4'   | 2.19                     | 0.43              |
| 24:DA:121:G:N2    | 24:DA:131:A:N9     | 2.66                     | 0.43              |
| 24:DA:1371:G:O2'  | 24:DA:1372:U:H5'   | 2.18                     | 0.43              |
| 24:DA:1677:A:H2'  | 24:DA:1678:A:C8    | 2.52                     | 0.43              |
| 24:DA:16:C:O2'    | 24:DA:17:G:H5'     | 2.18                     | 0.43              |
| 24:DA:1787:A:H2'  | 24:DA:1788:C:C5    | 2.53                     | 0.43              |
| 24:DA:1815:A:H1'  | 24:DA:1817:G:N7    | 2.33                     | 0.43              |
| 24:DA:1906:G:H8   | 24:DA:1929:G:H2'   | 1.82                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:DA:2208:C:C2    | 24:DA:2217:G:N2   | 2.86                     | 0.43              |
| 24:DA:197:A:N7     | 24:DA:2430:A:C4   | 2.86                     | 0.43              |
| 24:DA:2483:C:C5    | 24:DA:2484:G:C8   | 3.06                     | 0.43              |
| 24:DA:2781:A:H3'   | 24:DA:2782:G:H5'  | 2.00                     | 0.43              |
| 24:DA:2882:A:H5''  | 37:DN:96:ARG:HD3  | 1.99                     | 0.43              |
| 24:DA:579:G:C2     | 24:DA:1262:A:C5   | 3.06                     | 0.43              |
| 24:DA:66:C:N4      | 24:DA:67:U:N3     | 2.67                     | 0.43              |
| 24:DA:761:A:OP2    | 59:DA:3304:HOH:O  | 2.21                     | 0.43              |
| 24:DA:762:U:C2     | 24:DA:1431:A:H5'' | 2.53                     | 0.43              |
| 24:DA:83:A:H61     | 24:DA:101:A:C5'   | 2.20                     | 0.43              |
| 24:DA:94:A:C2      | 24:DA:95:A:C4     | 3.07                     | 0.43              |
| 56:DB:35:C:H3'     | 56:DB:36:C:H5''   | 2.01                     | 0.43              |
| 56:DB:98:G:O6      | 45:DV:14:LYS:N    | 2.51                     | 0.43              |
| 26:DC:130:PRO:HD3  | 26:DC:188:ARG:HG3 | 1.99                     | 0.43              |
| 28:DE:134:LEU:HA   | 28:DE:137:LYS:HB2 | 2.00                     | 0.43              |
| 29:DF:102:LEU:HD22 | 29:DF:102:LEU:N   | 2.34                     | 0.43              |
| 29:DF:41:GLU:O     | 29:DF:43:ILE:N    | 2.51                     | 0.43              |
| 29:DF:4:HIS:CE1    | 29:DF:96:TRP:CZ2  | 3.06                     | 0.43              |
| 34:DK:103:VAL:HG23 | 34:DK:122:VAL:O   | 2.17                     | 0.43              |
| 39:DP:105:LYS:HA   | 39:DP:108:ARG:CZ  | 2.49                     | 0.43              |
| 41:DR:30:GLY:HA2   | 41:DR:63:VAL:O    | 2.18                     | 0.43              |
| 44:DU:73:ASN:HB3   | 44:DU:95:PHE:CE2  | 2.53                     | 0.43              |
| 45:DV:75:GLN:HG3   | 45:DV:92:VAL:CG1  | 2.48                     | 0.43              |
| 47:DX:1:SER:C      | 47:DX:3:VAL:N     | 2.72                     | 0.43              |
| 47:DX:48:LEU:O     | 47:DX:50:VAL:HG13 | 2.18                     | 0.43              |
| 49:DZ:43:ILE:HD12  | 49:DZ:44:ARG:N    | 2.34                     | 0.43              |
| 21:AA:1068:G:H2'   | 21:AA:1068:G:N3   | 2.33                     | 0.43              |
| 21:AA:1098:C:H2'   | 21:AA:1099:G:O4'  | 2.19                     | 0.43              |
| 21:AA:1074:G:N3    | 21:AA:1101:A:C2   | 2.86                     | 0.43              |
| 8:AI:123:ARG:O     | 21:AA:1343:G:H4'  | 2.19                     | 0.43              |
| 21:AA:1428:A:C6    | 21:AA:1429:A:N7   | 2.87                     | 0.43              |
| 21:AA:172:A:C5     | 21:AA:174:A:N7    | 2.87                     | 0.43              |
| 21:AA:243:A:C4'    | 21:AA:244:U:H5''  | 2.42                     | 0.43              |
| 21:AA:596:A:N6     | 21:AA:645:G:C5    | 2.85                     | 0.43              |
| 21:AA:828:U:O4     | 21:AA:859:G:C8    | 2.72                     | 0.43              |
| 1:AB:113:LEU:HD11  | 1:AB:144:GLU:OE1  | 2.19                     | 0.43              |
| 2:AC:17:TRP:O      | 2:AC:19:SER:N     | 2.52                     | 0.43              |
| 3:AD:92:LEU:HA     | 3:AD:135:GLN:NE2  | 2.33                     | 0.43              |
| 4:AE:14:LEU:HD13   | 4:AE:14:LEU:O     | 2.17                     | 0.43              |
| 8:AI:25:GLY:HA2    | 8:AI:60:LEU:O     | 2.19                     | 0.43              |
| 8:AI:51:LEU:HB3    | 8:AI:56:MET:HG2   | 2.01                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AL:29:LYS:HD3   | 11:AL:58:ASN:HB3   | 2.01                     | 0.43              |
| 11:AL:64:SER:OG    | 11:AL:96:THR:HG23  | 2.19                     | 0.43              |
| 14:AO:36:ASN:N     | 14:AO:36:ASN:HD22  | 2.16                     | 0.43              |
| 5:AF:90:MET:CB     | 17:AR:60:ARG:HH21  | 2.31                     | 0.43              |
| 20:AU:7:GLU:HB2    | 20:AU:11:PHE:CZ    | 2.54                     | 0.43              |
| 20:AU:36:PHE:CD1   | 20:AU:39:LYS:HB3   | 2.52                     | 0.43              |
| 51:B1:9:LYS:N      | 51:B1:9:LYS:HD3    | 2.33                     | 0.43              |
| 53:B3:56:LEU:N     | 53:B3:56:LEU:HD22  | 2.28                     | 0.43              |
| 24:BA:110:G:N3     | 24:BA:110:G:H2'    | 2.33                     | 0.43              |
| 24:BA:1189:A:OP1   | 41:BR:82:HIS:HD2   | 2.01                     | 0.43              |
| 24:BA:1216:G:C2    | 24:BA:1234:U:O2    | 2.71                     | 0.43              |
| 24:BA:1277:G:C6    | 24:BA:1278:C:N4    | 2.86                     | 0.43              |
| 24:BA:1282:U:H2'   | 24:BA:1283:G:O4'   | 2.18                     | 0.43              |
| 24:BA:1712:U:C4    | 24:BA:1713:A:C6    | 3.06                     | 0.43              |
| 24:BA:24:G:C6      | 24:BA:25:U:N3      | 2.86                     | 0.43              |
| 24:BA:313:G:C4     | 24:BA:314:C:C5     | 3.07                     | 0.43              |
| 24:BA:324:A:N6     | 24:BA:339:U:H5'    | 2.33                     | 0.43              |
| 24:BA:640:C:H2'    | 24:BA:641:U:H6     | 1.83                     | 0.43              |
| 24:BA:728:G:O2'    | 24:BA:730:A:H8     | 2.01                     | 0.43              |
| 24:BA:78:U:H2'     | 24:BA:79:C:H6      | 1.82                     | 0.43              |
| 24:BA:963:U:O2'    | 24:BA:964:C:H5'    | 2.17                     | 0.43              |
| 25:BB:75:G:H1      | 25:BB:102:G:N2     | 2.16                     | 0.43              |
| 26:BC:15:VAL:HG12  | 26:BC:16:VAL:N     | 2.33                     | 0.43              |
| 26:BC:200:MET:HB3  | 26:BC:201:LEU:HD13 | 1.99                     | 0.43              |
| 27:BD:72:GLY:O     | 27:BD:73:VAL:O     | 2.37                     | 0.43              |
| 28:BE:119:ILE:HD11 | 28:BE:187:VAL:HG22 | 2.00                     | 0.43              |
| 33:BJ:99:ARG:NH1   | 33:BJ:103:ILE:HG22 | 2.34                     | 0.43              |
| 33:BJ:105:VAL:HG22 | 33:BJ:106:LYS:N    | 2.33                     | 0.43              |
| 34:BK:22:ILE:HG23  | 34:BK:42:THR:HG22  | 2.01                     | 0.43              |
| 34:BK:92:GLU:O     | 34:BK:93:GLN:O     | 2.37                     | 0.43              |
| 34:BK:95:ILE:O     | 34:BK:95:ILE:HD12  | 2.18                     | 0.43              |
| 38:BO:53:THR:HB    | 38:BO:65:THR:HG22  | 2.00                     | 0.43              |
| 40:BQ:59:LEU:O     | 40:BQ:62:ALA:N     | 2.52                     | 0.43              |
| 47:BX:77:TYR:CG    | 47:BX:77:TYR:O     | 2.71                     | 0.43              |
| 48:BY:61:ALA:C     | 48:BY:63:ALA:H     | 2.22                     | 0.43              |
| 55:CA:1270:G:O2'   | 55:CA:1314:C:H5'   | 2.18                     | 0.43              |
| 19:CT:26:MET:CG    | 55:CA:1457:G:O2'   | 2.64                     | 0.43              |
| 55:CA:1484:C:H2'   | 55:CA:1485:U:C6    | 2.54                     | 0.43              |
| 55:CA:247:G:C5     | 55:CA:278:G:N2     | 2.86                     | 0.43              |
| 55:CA:518:C:H4'    | 55:CA:519:C:C5'    | 2.41                     | 0.43              |
| 55:CA:683:G:C2     | 55:CA:684:U:C2     | 3.07                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:CA:868:C:C2'   | 55:CA:869:G:H5'    | 2.49                     | 0.43              |
| 55:CA:562:U:C4    | 55:CA:884:U:C6     | 3.07                     | 0.43              |
| 55:CA:947:G:H2'   | 55:CA:948:C:O4'    | 2.18                     | 0.43              |
| 2:CC:125:ARG:HB2  | 2:CC:127:VAL:CG1   | 2.48                     | 0.43              |
| 2:CC:131:ARG:HA   | 2:CC:134:LYS:HB3   | 1.99                     | 0.43              |
| 3:CD:19:PHE:C     | 3:CD:20:LEU:O      | 2.55                     | 0.43              |
| 3:CD:81:LEU:HB2   | 3:CD:88:ASN:HD22   | 1.83                     | 0.43              |
| 4:CE:80:LEU:O     | 4:CE:97:PRO:HG3    | 2.18                     | 0.43              |
| 7:CH:94:VAL:CG2   | 7:CH:101:ALA:HB2   | 2.49                     | 0.43              |
| 12:CM:113:LYS:HD3 | 12:CM:113:LYS:H    | 1.83                     | 0.43              |
| 12:CM:13:HIS:CD2  | 12:CM:14:ALA:H     | 2.37                     | 0.43              |
| 16:CQ:4:ILE:CG2   | 16:CQ:5:ARG:H      | 2.32                     | 0.43              |
| 19:CT:2:ASN:N     | 19:CT:7:LYS:NZ     | 2.59                     | 0.43              |
| 52:D2:23:ALA:O    | 52:D2:24:THR:HB    | 2.18                     | 0.43              |
| 52:D2:43:THR:O    | 52:D2:44:VAL:C     | 2.57                     | 0.43              |
| 24:DA:101:A:HO2'  | 24:DA:102:U:P      | 2.41                     | 0.43              |
| 24:DA:1265:A:C8   | 24:DA:1267:U:C2    | 3.06                     | 0.43              |
| 24:DA:1287:A:H5'  | 37:DN:103:ARG:NH1  | 2.34                     | 0.43              |
| 24:DA:1333:G:O2'  | 24:DA:1334:G:C5'   | 2.65                     | 0.43              |
| 24:DA:1496:A:H4'  | 24:DA:1497:U:H5    | 1.84                     | 0.43              |
| 24:DA:2060:A:C8   | 28:DE:63:LYS:NZ    | 2.87                     | 0.43              |
| 24:DA:2077:A:N1   | 24:DA:2078:C:C4    | 2.87                     | 0.43              |
| 24:DA:2209:G:C2   | 24:DA:2210:U:O4    | 2.71                     | 0.43              |
| 24:DA:1127:A:H61  | 24:DA:2463:C:H1'   | 1.84                     | 0.43              |
| 24:DA:2711:A:N6   | 24:DA:2714:G:N7    | 2.66                     | 0.43              |
| 24:DA:2721:A:H2'  | 24:DA:2722:G:C8    | 2.54                     | 0.43              |
| 24:DA:2746:U:C2'  | 24:DA:2747:G:H5'   | 2.48                     | 0.43              |
| 24:DA:2800:A:N3   | 24:DA:2801:G:H1'   | 2.34                     | 0.43              |
| 24:DA:352:A:N3    | 24:DA:353:C:H1'    | 2.34                     | 0.43              |
| 24:DA:3:U:C5      | 24:DA:4:U:C5       | 3.06                     | 0.43              |
| 24:DA:771:G:O2'   | 24:DA:772:C:H5'    | 2.18                     | 0.43              |
| 24:DA:838:C:C4    | 24:DA:839:U:C4     | 3.07                     | 0.43              |
| 24:DA:2052:A:C8   | 27:DD:146:ILE:HD11 | 2.53                     | 0.43              |
| 28:DE:128:ALA:O   | 28:DE:130:LYS:HG2  | 2.19                     | 0.43              |
| 29:DF:2:LYS:H     | 29:DF:2:LYS:HD3    | 1.82                     | 0.43              |
| 29:DF:5:ASP:C     | 29:DF:7:TYR:N      | 2.70                     | 0.43              |
| 32:DI:20:SER:N    | 32:DI:21:PRO:CD    | 2.81                     | 0.43              |
| 33:DJ:49:ASP:HB2  | 33:DJ:121:LYS:HZ1  | 1.83                     | 0.43              |
| 24:DA:636:G:O5'   | 35:DL:128:THR:HG23 | 2.19                     | 0.43              |
| 37:DN:96:ARG:O    | 37:DN:113:ILE:HA   | 2.18                     | 0.43              |
| 38:DO:115:LEU:H   | 38:DO:115:LEU:CD1  | 2.15                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:DR:79:ARG:O    | 41:DR:80:ARG:CB    | 2.67                     | 0.43              |
| 24:DA:1614:A:N6   | 42:DS:91:GLY:HA2   | 2.34                     | 0.43              |
| 45:DV:35:GLU:HB2  | 45:DV:93:ARG:NH1   | 2.33                     | 0.43              |
| 21:AA:1053:G:O5'  | 21:AA:1054:C:H3'   | 2.18                     | 0.43              |
| 21:AA:1095:U:P    | 21:AA:1108:G:H22   | 2.41                     | 0.43              |
| 21:AA:112:G:C5    | 21:AA:330:C:N4     | 2.86                     | 0.43              |
| 21:AA:1389:C:H2'  | 21:AA:1390:U:O4'   | 2.19                     | 0.43              |
| 21:AA:1462:C:C2   | 21:AA:1463:U:C6    | 3.07                     | 0.43              |
| 21:AA:191:G:C6    | 21:AA:192:A:C6     | 3.07                     | 0.43              |
| 21:AA:355:C:N3    | 21:AA:356:A:N7     | 2.66                     | 0.43              |
| 21:AA:786:G:C2    | 21:AA:797:C:C2     | 3.05                     | 0.43              |
| 21:AA:833:G:C2'   | 21:AA:834:U:H5'    | 2.49                     | 0.43              |
| 21:AA:900:A:C6    | 21:AA:901:A:C2     | 3.06                     | 0.43              |
| 21:AA:930:C:C4    | 21:AA:931:C:C5     | 3.07                     | 0.43              |
| 1:AB:191:ASP:HA   | 1:AB:192:PRO:HD2   | 1.80                     | 0.43              |
| 2:AC:91:ALA:C     | 2:AC:93:ILE:N      | 2.71                     | 0.43              |
| 3:AD:88:ASN:O     | 3:AD:92:LEU:HD23   | 2.18                     | 0.43              |
| 4:AE:45:VAL:HG23  | 4:AE:73:VAL:HG23   | 1.99                     | 0.43              |
| 5:AF:32:ALA:HB1   | 5:AF:67:PRO:HG3    | 2.00                     | 0.43              |
| 8:AI:51:LEU:CD1   | 8:AI:56:MET:HG2    | 2.44                     | 0.43              |
| 10:AK:22:ILE:HD13 | 10:AK:95:THR:HG21  | 1.98                     | 0.43              |
| 14:AO:32:THR:OG1  | 14:AO:84:LEU:HD21  | 2.18                     | 0.43              |
| 17:AR:44:THR:C    | 17:AR:46:THR:H     | 2.22                     | 0.43              |
| 53:B3:35:LYS:O    | 53:B3:40:LYS:HE2   | 2.19                     | 0.43              |
| 24:BA:1027:A:C2'  | 24:BA:1027:A:N3    | 2.78                     | 0.43              |
| 24:BA:1238:G:O2'  | 24:BA:1239:G:C5'   | 2.66                     | 0.43              |
| 24:BA:1495:A:O2'  | 24:BA:1496:A:O5'   | 2.37                     | 0.43              |
| 24:BA:16:C:H4'    | 50:B0:10:SER:OG    | 2.19                     | 0.43              |
| 24:BA:1731:G:C4   | 24:BA:1733:G:C8    | 3.06                     | 0.43              |
| 24:BA:1776:G:C6   | 24:BA:1777:U:C4    | 3.06                     | 0.43              |
| 24:BA:1997:C:H6   | 24:BA:1997:C:C5'   | 2.32                     | 0.43              |
| 24:BA:2282:G:C6   | 24:BA:2425:A:C2    | 3.07                     | 0.43              |
| 24:BA:2297:A:C2   | 24:BA:2321:U:H5    | 2.36                     | 0.43              |
| 24:BA:2340:A:H2'  | 24:BA:2341:G:H8    | 1.83                     | 0.43              |
| 24:BA:2706:A:H8   | 24:BA:2706:A:O5'   | 2.02                     | 0.43              |
| 24:BA:313:G:C5    | 24:BA:314:C:C5     | 3.07                     | 0.43              |
| 24:BA:960:A:H5''  | 24:BA:961:C:OP2    | 2.18                     | 0.43              |
| 25:BB:27:C:C6     | 25:BB:28:C:C5      | 3.06                     | 0.43              |
| 26:BC:140:VAL:CG1 | 26:BC:189:ALA:HB1  | 2.48                     | 0.43              |
| 26:BC:250:GLN:N   | 26:BC:250:GLN:HE21 | 2.17                     | 0.43              |
| 28:BE:117:ARG:CA  | 28:BE:185:LYS:HD3  | 2.43                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:BF:113:PHE:HE1 | 29:BF:116:LEU:HD22 | 1.82                     | 0.43              |
| 30:BG:82:PHE:CZ   | 30:BG:137:LYS:HD2  | 2.54                     | 0.43              |
| 32:BI:59:THR:HG22 | 32:BI:61:TYR:CE2   | 2.52                     | 0.43              |
| 33:BJ:18:VAL:HG12 | 33:BJ:19:ASP:N     | 2.33                     | 0.43              |
| 34:BK:105:ARG:HD3 | 34:BK:105:ARG:H    | 1.83                     | 0.43              |
| 36:BM:71:LYS:HB3  | 36:BM:93:VAL:O     | 2.19                     | 0.43              |
| 42:BS:73:LYS:CB   | 42:BS:106:VAL:HB   | 2.46                     | 0.43              |
| 42:BS:24:ILE:HD12 | 42:BS:32:ALA:HA    | 2.01                     | 0.43              |
| 46:BW:22:VAL:O    | 46:BW:23:LYS:C     | 2.57                     | 0.43              |
| 46:BW:43:LYS:CG   | 46:BW:79:ILE:HD11  | 2.48                     | 0.43              |
| 47:BX:39:VAL:O    | 47:BX:41:SER:N     | 2.46                     | 0.43              |
| 48:BY:42:LEU:HD12 | 48:BY:42:LEU:HA    | 1.75                     | 0.43              |
| 49:BZ:8:GLN:O     | 49:BZ:10:ARG:N     | 2.45                     | 0.43              |
| 55:CA:1266:G:C4   | 55:CA:1268:G:OP2   | 2.72                     | 0.43              |
| 55:CA:1392:G:O2'  | 55:CA:1393:U:H5'   | 2.19                     | 0.43              |
| 55:CA:1487:G:C6   | 55:CA:1488:G:N7    | 2.87                     | 0.43              |
| 55:CA:272:C:C4    | 55:CA:273:U:C5     | 3.06                     | 0.43              |
| 55:CA:275:G:C2    | 55:CA:276:G:C8     | 3.06                     | 0.43              |
| 55:CA:495:A:C2    | 55:CA:496:A:C6     | 3.06                     | 0.43              |
| 55:CA:570:G:O6    | 55:CA:873:A:C2     | 2.71                     | 0.43              |
| 1:CB:139:GLU:O    | 1:CB:140:LEU:C     | 2.57                     | 0.43              |
| 4:CE:111:ARG:C    | 4:CE:113:VAL:N     | 2.72                     | 0.43              |
| 4:CE:46:GLY:HA3   | 4:CE:70:MET:HA     | 2.00                     | 0.43              |
| 5:CF:44:ARG:HA    | 5:CF:58:HIS:HA     | 2.00                     | 0.43              |
| 5:CF:5:GLU:HA     | 5:CF:63:ASN:HA     | 2.00                     | 0.43              |
| 6:CG:31:VAL:HG12  | 55:CA:1240:U:C2    | 2.53                     | 0.43              |
| 7:CH:46:GLU:N     | 7:CH:63:LYS:HG3    | 2.33                     | 0.43              |
| 8:CI:63:TYR:C     | 8:CI:63:TYR:CD1    | 2.92                     | 0.43              |
| 10:CK:19:VAL:O    | 10:CK:33:ILE:HA    | 2.19                     | 0.43              |
| 12:CM:85:TYR:HB3  | 18:CS:72:GLU:OE2   | 2.18                     | 0.43              |
| 20:CU:3:ILE:HG12  | 20:CU:18:PHE:CD1   | 2.54                     | 0.43              |
| 24:DA:2344:U:OP1  | 51:D1:36:LYS:HD2   | 2.18                     | 0.43              |
| 53:D3:29:ARG:HH21 | 53:D3:29:ARG:HG2   | 1.84                     | 0.43              |
| 24:DA:1149:G:H2'  | 24:DA:1150:C:C6    | 2.54                     | 0.43              |
| 24:DA:1202:G:C6   | 24:DA:1203:U:C4    | 3.06                     | 0.43              |
| 24:DA:1345:C:H5'  | 24:DA:1396:U:O4    | 2.18                     | 0.43              |
| 24:DA:1647:U:H3'  | 24:DA:1647:U:OP2   | 2.19                     | 0.43              |
| 24:DA:1800:C:C2   | 24:DA:1818:U:O2    | 2.71                     | 0.43              |
| 24:DA:1829:A:C8   | 24:DA:1830:C:C5    | 3.07                     | 0.43              |
| 24:DA:1858:A:H62  | 24:DA:1884:G:H21   | 1.66                     | 0.43              |
| 24:DA:1907:G:C2   | 24:DA:1924:C:C2    | 3.07                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:1914:C:C4   | 24:DA:1915:U:C4    | 3.07                     | 0.43              |
| 24:DA:1938:A:O2'  | 24:DA:1939:U:H5''  | 2.17                     | 0.43              |
| 24:DA:202:U:H2'   | 24:DA:203:A:C8     | 2.54                     | 0.43              |
| 24:DA:2282:G:O2'  | 24:DA:2283:C:OP2   | 2.37                     | 0.43              |
| 24:DA:2294:G:H5'' | 38:DO:10:ARG:HD3   | 1.99                     | 0.43              |
| 24:DA:230:G:HO2'  | 24:DA:231:A:C5'    | 2.31                     | 0.43              |
| 24:DA:2422:C:N4   | 24:DA:2424:C:C4    | 2.86                     | 0.43              |
| 24:DA:2590:A:O2'  | 24:DA:2591:C:H5'   | 2.19                     | 0.43              |
| 24:DA:2601:C:H4'  | 24:DA:2602:A:OP2   | 2.18                     | 0.43              |
| 24:DA:2848:G:H1'  | 24:DA:2868:A:N6    | 2.33                     | 0.43              |
| 24:DA:300:A:N6    | 59:DA:3596:HOH:O   | 2.51                     | 0.43              |
| 24:DA:545:U:C4    | 24:DA:547:A:H4'    | 2.54                     | 0.43              |
| 24:DA:585:G:H2'   | 24:DA:1254:A:H61   | 1.83                     | 0.43              |
| 24:DA:686:U:N3    | 52:D2:12:ARG:HG3   | 2.34                     | 0.43              |
| 24:DA:771:G:H2'   | 24:DA:772:C:H6     | 1.82                     | 0.43              |
| 24:DA:958:U:H2'   | 24:DA:958:U:H6     | 1.29                     | 0.43              |
| 24:DA:996:A:N3    | 24:DA:997:G:C8     | 2.86                     | 0.43              |
| 26:DC:135:PRO:HG2 | 26:DC:138:SER:OG   | 2.18                     | 0.43              |
| 27:DD:110:THR:OG1 | 27:DD:171:THR:HG22 | 2.18                     | 0.43              |
| 28:DE:34:ALA:HB1  | 28:DE:94:GLN:HB2   | 2.01                     | 0.43              |
| 29:DF:97:GLU:HG2  | 29:DF:97:GLU:O     | 2.16                     | 0.43              |
| 31:DH:71:LYS:N    | 31:DH:71:LYS:CD    | 2.82                     | 0.43              |
| 32:DI:139:VAL:O   | 32:DI:140:GLU:HB2  | 2.19                     | 0.43              |
| 32:DI:89:SER:HB3  | 32:DI:97:VAL:HG11  | 1.99                     | 0.43              |
| 33:DJ:24:THR:O    | 33:DJ:25:LEU:HB3   | 2.19                     | 0.43              |
| 33:DJ:25:LEU:C    | 33:DJ:25:LEU:HD22  | 2.38                     | 0.43              |
| 34:DK:41:ILE:O    | 34:DK:57:VAL:HA    | 2.19                     | 0.43              |
| 37:DN:31:HIS:C    | 37:DN:33:ILE:H     | 2.21                     | 0.43              |
| 39:DP:26:GLU:HB2  | 39:DP:86:LYS:HD3   | 2.01                     | 0.43              |
| 40:DQ:4:LYS:HD3   | 40:DQ:7:VAL:H      | 1.83                     | 0.43              |
| 24:DA:996:A:C5'   | 40:DQ:91:ARG:NH1   | 2.80                     | 0.43              |
| 45:DV:44:HIS:NE2  | 45:DV:86:LEU:O     | 2.52                     | 0.43              |
| 47:DX:1:SER:O     | 47:DX:3:VAL:HG13   | 2.18                     | 0.43              |
| 21:AA:1152:A:H2'  | 21:AA:1153:G:H8    | 1.84                     | 0.43              |
| 21:AA:124:C:O2'   | 21:AA:125:U:H5'    | 2.19                     | 0.43              |
| 21:AA:16:A:C2'    | 21:AA:17:U:H5'     | 2.48                     | 0.43              |
| 21:AA:596:A:H2'   | 21:AA:597:G:C8     | 2.39                     | 0.43              |
| 21:AA:597:G:N7    | 21:AA:598:U:C5     | 2.87                     | 0.43              |
| 21:AA:644:U:H2'   | 21:AA:645:G:O4'    | 2.19                     | 0.43              |
| 1:AB:61:SER:HA    | 1:AB:224:ARG:N     | 2.33                     | 0.43              |
| 2:AC:21:TRP:O     | 13:AN:93:PRO:HB3   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:AE:49:TYR:O     | 4:AE:62:ALA:HA    | 2.18                     | 0.43              |
| 5:AF:66:ALA:HB1   | 5:AF:67:PRO:HD2   | 2.00                     | 0.43              |
| 7:AH:26:MET:O     | 7:AH:58:LEU:N     | 2.50                     | 0.43              |
| 7:AH:85:TYR:C     | 7:AH:86:LYS:HD2   | 2.39                     | 0.43              |
| 8:AI:21:LYS:NZ    | 8:AI:61:ASP:HB3   | 2.34                     | 0.43              |
| 9:AJ:29:ALA:C     | 9:AJ:31:ARG:H     | 2.22                     | 0.43              |
| 10:AK:88:PRO:HD3  | 20:AU:28:LEU:HD13 | 2.01                     | 0.43              |
| 11:AL:62:VAL:CG2  | 11:AL:94:TYR:HE2  | 2.23                     | 0.43              |
| 13:AN:92:ILE:HA   | 13:AN:93:PRO:HD3  | 1.84                     | 0.43              |
| 16:AQ:13:SER:HB3  | 16:AQ:16:MET:HE1  | 2.00                     | 0.43              |
| 16:AQ:37:ILE:N    | 16:AQ:37:ILE:HD12 | 2.34                     | 0.43              |
| 16:AQ:66:LEU:CB   | 16:AQ:70:LYS:HE2  | 2.48                     | 0.43              |
| 18:AS:62:THR:CG2  | 18:AS:63:ASP:H    | 2.27                     | 0.43              |
| 19:AT:57:VAL:HG12 | 19:AT:71:ALA:HB1  | 2.01                     | 0.43              |
| 19:AT:75:LYS:HD2  | 21:AA:185:U:O2'   | 2.18                     | 0.43              |
| 24:BA:1052:C:C4   | 24:BA:1053:C:H5   | 2.37                     | 0.43              |
| 24:BA:1070:A:HO2' | 24:BA:1071:G:P    | 2.41                     | 0.43              |
| 24:BA:1151:A:C6   | 24:BA:1152:C:C4   | 3.07                     | 0.43              |
| 24:BA:1312:U:C4'  | 24:BA:1313:U:O2   | 2.67                     | 0.43              |
| 24:BA:159:G:N2    | 24:BA:166:U:C5    | 2.87                     | 0.43              |
| 24:BA:1790:C:H2'  | 24:BA:1791:A:N7   | 2.34                     | 0.43              |
| 24:BA:1816:C:H5   | 26:BC:61:TYR:CE1  | 2.36                     | 0.43              |
| 24:BA:1992:G:H4'  | 24:BA:1993:U:OP1  | 2.14                     | 0.43              |
| 24:BA:222:A:C5    | 24:BA:224:U:C2    | 3.07                     | 0.43              |
| 24:BA:2472:G:C5   | 24:BA:2475:C:C4   | 3.06                     | 0.43              |
| 24:BA:2482:A:C5   | 24:BA:2483:C:C5   | 3.07                     | 0.43              |
| 24:BA:2821:A:H2'  | 24:BA:2822:G:H8   | 1.83                     | 0.43              |
| 24:BA:301:G:N1    | 24:BA:317:G:C5    | 2.87                     | 0.43              |
| 24:BA:857:G:H1'   | 46:BW:19:ARG:HD2  | 2.01                     | 0.43              |
| 24:BA:95:A:O2'    | 48:BY:41:HIS:CD2  | 2.71                     | 0.43              |
| 25:BB:33:G:N2     | 25:BB:50:A:C4     | 2.87                     | 0.43              |
| 25:BB:9:G:O2'     | 25:BB:10:G:H5'    | 2.19                     | 0.43              |
| 26:BC:120:ASP:O   | 26:BC:121:ALA:O   | 2.37                     | 0.43              |
| 26:BC:229:HIS:CE1 | 26:BC:230:PRO:HD2 | 2.54                     | 0.43              |
| 28:BE:29:HIS:O    | 28:BE:32:VAL:HG22 | 2.19                     | 0.43              |
| 29:BF:132:ARG:O   | 29:BF:133:GLU:CB  | 2.57                     | 0.43              |
| 33:BJ:21:THR:C    | 33:BJ:23:LYS:H    | 2.22                     | 0.43              |
| 39:BP:37:LYS:O    | 39:BP:37:LYS:CG   | 2.66                     | 0.43              |
| 39:BP:44:GLY:HA3  | 39:BP:61:ARG:O    | 2.18                     | 0.43              |
| 40:BQ:69:ARG:CG   | 40:BQ:69:ARG:HH21 | 2.32                     | 0.43              |
| 40:BQ:88:GLU:C    | 40:BQ:88:GLU:OE1  | 2.57                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:BR:43:ASN:HD22 | 41:BR:43:ASN:HA   | 1.57                     | 0.43              |
| 45:BV:38:LEU:HD12 | 45:BV:38:LEU:HA   | 1.70                     | 0.43              |
| 48:BY:40:SER:O    | 48:BY:42:LEU:N    | 2.52                     | 0.43              |
| 55:CA:1409:C:H2'  | 55:CA:1410:A:C8   | 2.54                     | 0.43              |
| 55:CA:1442:G:N2   | 55:CA:1443:C:C2   | 2.87                     | 0.43              |
| 55:CA:1448:C:O2'  | 55:CA:1449:C:C6   | 2.67                     | 0.43              |
| 55:CA:1494:G:H4'  | 24:DA:1913:A:C8   | 2.53                     | 0.43              |
| 55:CA:191:G:H2'   | 55:CA:192:A:C8    | 2.54                     | 0.43              |
| 55:CA:302:G:N3    | 55:CA:303:A:C8    | 2.87                     | 0.43              |
| 55:CA:397:A:C6    | 55:CA:548:G:N7    | 2.87                     | 0.43              |
| 55:CA:491:G:C2'   | 55:CA:492:C:H5'   | 2.48                     | 0.43              |
| 55:CA:293:G:H5'   | 55:CA:610:U:C5    | 2.54                     | 0.43              |
| 55:CA:752:G:H1'   | 55:CA:754:C:H41   | 1.84                     | 0.43              |
| 55:CA:759:A:C8    | 55:CA:760:G:C8    | 3.06                     | 0.43              |
| 55:CA:774:G:C2    | 55:CA:806:C:C2    | 3.07                     | 0.43              |
| 55:CA:810:C:H2'   | 55:CA:811:C:O4'   | 2.19                     | 0.43              |
| 55:CA:926:G:H2'   | 55:CA:1505:G:C2   | 2.54                     | 0.43              |
| 55:CA:946:A:H2'   | 55:CA:947:G:C8    | 2.54                     | 0.43              |
| 55:CA:95:C:C6     | 55:CA:95:C:H5''   | 2.53                     | 0.43              |
| 1:CB:112:ARG:HA   | 1:CB:115:ASP:OD2  | 2.19                     | 0.43              |
| 1:CB:53:LEU:O     | 1:CB:57:ASN:HB2   | 2.19                     | 0.43              |
| 2:CC:168:ARG:HG2  | 2:CC:168:ARG:HH11 | 1.82                     | 0.43              |
| 2:CC:149:LYS:HD2  | 2:CC:200:TRP:CE3  | 2.54                     | 0.43              |
| 3:CD:10:LEU:O     | 3:CD:11:SER:C     | 2.57                     | 0.43              |
| 3:CD:27:ILE:HG22  | 3:CD:27:ILE:O     | 2.19                     | 0.43              |
| 3:CD:39:GLN:C     | 3:CD:41:GLY:H     | 2.21                     | 0.43              |
| 4:CE:38:VAL:HG21  | 4:CE:66:ALA:C     | 2.39                     | 0.43              |
| 5:CF:68:GLN:HG2   | 5:CF:69:GLU:HG3   | 2.01                     | 0.43              |
| 6:CG:134:VAL:CB   | 6:CG:137:ARG:HH21 | 2.31                     | 0.43              |
| 6:CG:59:GLU:OE2   | 6:CG:63:VAL:HG23  | 2.18                     | 0.43              |
| 6:CG:9:ARG:C      | 6:CG:10:LYS:HG3   | 2.39                     | 0.43              |
| 7:CH:38:VAL:O     | 7:CH:41:GLU:HB2   | 2.18                     | 0.43              |
| 12:CM:47:LEU:HD23 | 12:CM:47:LEU:C    | 2.39                     | 0.43              |
| 12:CM:95:PRO:HG3  | 12:CM:99:GLN:HE21 | 1.83                     | 0.43              |
| 18:CS:18:VAL:CG2  | 18:CS:42:ASN:HB3  | 2.48                     | 0.43              |
| 18:CS:52:ASN:N    | 18:CS:52:ASN:HD22 | 2.16                     | 0.43              |
| 20:CU:24:LYS:NZ   | 20:CU:25:ALA:HB2  | 2.34                     | 0.43              |
| 51:D1:8:ILE:HG22  | 51:D1:9:LYS:N     | 2.34                     | 0.43              |
| 24:DA:1022:G:O6   | 33:DJ:68:LYS:HD3  | 2.19                     | 0.43              |
| 24:DA:1693:U:H2'  | 26:DC:13:ARG:HH21 | 1.84                     | 0.43              |
| 24:DA:1746:A:H2'  | 24:DA:1747:U:H6   | 1.81                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:1774:C:C5   | 24:DA:1775:U:H5    | 2.37                     | 0.43              |
| 24:DA:1817:G:H3'  | 26:DC:155:ARG:HH21 | 1.83                     | 0.43              |
| 24:DA:2072:C:H2'  | 24:DA:2073:C:H5'   | 1.99                     | 0.43              |
| 24:DA:2148:G:O2'  | 24:DA:2149:U:N1    | 2.50                     | 0.43              |
| 24:DA:2304:G:N2   | 24:DA:2312:U:H3    | 2.16                     | 0.43              |
| 24:DA:2869:G:C6   | 24:DA:2870:C:N3    | 2.87                     | 0.43              |
| 24:DA:460:A:N3    | 24:DA:470:A:C6     | 2.87                     | 0.43              |
| 24:DA:639:U:H2'   | 24:DA:640:C:C6     | 2.53                     | 0.43              |
| 24:DA:807:U:H1'   | 24:DA:2445:G:H5'   | 2.01                     | 0.43              |
| 56:DB:49:C:OP1    | 38:DO:102:ARG:N    | 2.44                     | 0.43              |
| 56:DB:56:G:H21    | 56:DB:59:A:H2      | 1.66                     | 0.43              |
| 24:DA:2636:C:H4'  | 27:DD:81:GLU:CD    | 2.39                     | 0.43              |
| 24:DA:320:A:H62   | 28:DE:132:LYS:HG3  | 1.82                     | 0.43              |
| 31:DH:70:GLU:HB2  | 31:DH:71:LYS:HD2   | 1.99                     | 0.43              |
| 33:DJ:45:THR:OG1  | 33:DJ:48:VAL:HB    | 2.19                     | 0.43              |
| 34:DK:14:SER:HG   | 34:DK:51:LYS:H     | 1.65                     | 0.43              |
| 35:DL:40:SER:O    | 35:DL:41:ARG:C     | 2.56                     | 0.43              |
| 35:DL:93:ASN:CG   | 35:DL:94:THR:N     | 2.72                     | 0.43              |
| 36:DM:100:LYS:HD3 | 36:DM:100:LYS:HA   | 1.88                     | 0.43              |
| 36:DM:62:LYS:C    | 36:DM:63:ILE:HD12  | 2.38                     | 0.43              |
| 40:DQ:87:VAL:HG11 | 41:DR:52:PRO:CG    | 2.42                     | 0.43              |
| 46:DW:8:SER:O     | 46:DW:9:THR:CB     | 2.66                     | 0.43              |
| 21:AA:71:A:C8     | 21:AA:100:G:C6     | 3.07                     | 0.43              |
| 21:AA:1143:G:H2'  | 21:AA:1144:G:C8    | 2.53                     | 0.43              |
| 21:AA:1234:C:O4'  | 21:AA:1364:U:H1'   | 2.19                     | 0.43              |
| 21:AA:1363:A:O2'  | 21:AA:1364:U:H5''  | 2.18                     | 0.43              |
| 21:AA:1363:A:C8   | 21:AA:1365:G:C5    | 3.07                     | 0.43              |
| 21:AA:1402:C:H2'  | 21:AA:1403:C:O4'   | 2.17                     | 0.43              |
| 21:AA:165:G:C2    | 21:AA:166:U:C2     | 3.07                     | 0.43              |
| 21:AA:183:C:H2'   | 21:AA:183:C:H6     | 1.47                     | 0.43              |
| 21:AA:383:A:C5    | 21:AA:384:G:H1'    | 2.54                     | 0.43              |
| 21:AA:551:U:O2'   | 21:AA:552:U:H5'    | 2.19                     | 0.43              |
| 21:AA:688:G:C2    | 21:AA:689:C:C6     | 3.06                     | 0.43              |
| 1:AB:9:LEU:HD21   | 1:AB:11:ALA:O      | 2.18                     | 0.43              |
| 2:AC:5:HIS:HA     | 2:AC:6:PRO:HD2     | 1.87                     | 0.43              |
| 3:AD:190:LEU:O    | 3:AD:190:LEU:HD12  | 2.17                     | 0.43              |
| 4:AE:149:PRO:HA   | 4:AE:152:VAL:CG1   | 2.47                     | 0.43              |
| 4:AE:155:LYS:HD3  | 7:AH:70:VAL:CG2    | 2.48                     | 0.43              |
| 17:AR:66:LEU:O    | 17:AR:67:LEU:HD23  | 2.19                     | 0.43              |
| 13:AN:46:LYS:O    | 18:AS:12:LEU:HD11  | 2.18                     | 0.43              |
| 24:BA:1015:U:O2'  | 24:BA:1016:G:H5'   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:1206:G:C2   | 24:BA:1207:C:C2   | 3.07                     | 0.43              |
| 24:BA:141:G:H3'   | 24:BA:142:A:O4'   | 2.18                     | 0.43              |
| 24:BA:1456:G:H2'  | 24:BA:1457:U:H5'  | 2.00                     | 0.43              |
| 24:BA:1810:A:O2'  | 24:BA:1811:G:H5'  | 2.19                     | 0.43              |
| 24:BA:1885:A:H2'  | 24:BA:1886:U:O4'  | 2.19                     | 0.43              |
| 24:BA:2086:U:H2'  | 24:BA:2087:G:O4'  | 2.18                     | 0.43              |
| 24:BA:2215:C:O5'  | 24:BA:2215:C:H6   | 2.02                     | 0.43              |
| 24:BA:2674:G:C4   | 24:BA:2675:A:C8   | 3.06                     | 0.43              |
| 24:BA:2748:A:C6   | 24:BA:2749:A:C5   | 3.06                     | 0.43              |
| 24:BA:2819:G:H5'' | 59:BA:3813:HOH:O  | 2.19                     | 0.43              |
| 24:BA:2824:C:C4   | 24:BA:2825:G:C5   | 3.07                     | 0.43              |
| 24:BA:2864:G:H2'  | 24:BA:2865:U:C6   | 2.54                     | 0.43              |
| 24:BA:2842:G:C2   | 24:BA:2876:G:C2   | 3.07                     | 0.43              |
| 24:BA:416:U:C4    | 24:BA:417:C:C4    | 3.07                     | 0.43              |
| 24:BA:536:G:O6    | 24:BA:537:G:C2    | 2.71                     | 0.43              |
| 24:BA:558:U:OP1   | 33:BJ:113:PRO:HB2 | 2.18                     | 0.43              |
| 25:BB:20:G:N2     | 25:BB:64:G:N3     | 2.66                     | 0.43              |
| 26:BC:145:MET:HB2 | 26:BC:152:GLN:NE2 | 2.34                     | 0.43              |
| 28:BE:121:VAL:O   | 28:BE:189:THR:HA  | 2.18                     | 0.43              |
| 29:BF:28:PRO:HB3  | 29:BF:159:ALA:HB2 | 2.00                     | 0.43              |
| 31:BH:21:VAL:CG2  | 31:BH:25:TYR:HD2  | 2.29                     | 0.43              |
| 31:BH:97:ARG:HE   | 31:BH:97:ARG:HB2  | 1.65                     | 0.43              |
| 35:BL:40:SER:O    | 35:BL:41:ARG:HB2  | 2.18                     | 0.43              |
| 36:BM:52:ALA:O    | 36:BM:53:MET:C    | 2.57                     | 0.43              |
| 38:BO:116:GLN:O   | 38:BO:117:PHE:HB3 | 2.19                     | 0.43              |
| 40:BQ:88:GLU:CD   | 40:BQ:88:GLU:C    | 2.78                     | 0.43              |
| 24:BA:1266:G:H5'' | 42:BS:15:GLN:HE22 | 1.84                     | 0.43              |
| 46:BW:22:VAL:CG1  | 46:BW:25:PHE:CE2  | 3.01                     | 0.43              |
| 55:CA:1269:A:C2   | 55:CA:1313:U:H1'  | 2.54                     | 0.43              |
| 55:CA:1528:U:H5'  | 55:CA:1529:G:OP1  | 2.19                     | 0.43              |
| 55:CA:444:G:C2    | 55:CA:445:G:C8    | 3.06                     | 0.43              |
| 55:CA:496:A:O2'   | 55:CA:497:G:C8    | 2.66                     | 0.43              |
| 55:CA:536:C:O2'   | 55:CA:537:G:H5'   | 2.19                     | 0.43              |
| 55:CA:595:A:N6    | 55:CA:641:U:C6    | 2.87                     | 0.43              |
| 55:CA:67:C:O2'    | 55:CA:68:G:H8     | 2.01                     | 0.43              |
| 55:CA:694:A:H3'   | 55:CA:695:A:H5''  | 2.01                     | 0.43              |
| 55:CA:741:G:C5    | 55:CA:742:G:N7    | 2.87                     | 0.43              |
| 55:CA:994:A:O2'   | 55:CA:995:C:C5'   | 2.66                     | 0.43              |
| 1:CB:10:LYS:HA    | 1:CB:10:LYS:HE3   | 2.00                     | 0.43              |
| 2:CC:9:ILE:CG2    | 2:CC:10:ARG:N     | 2.82                     | 0.43              |
| 3:CD:90:LEU:HD13  | 3:CD:90:LEU:HA    | 1.80                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:CF:7:VAL:O      | 5:CF:7:VAL:HG22    | 2.19                     | 0.43              |
| 5:CF:38:ARG:HB3   | 5:CF:97:THR:HA     | 2.00                     | 0.43              |
| 7:CH:6:ILE:HB     | 7:CH:76:ARG:NH1    | 2.33                     | 0.43              |
| 7:CH:95:MET:HE1   | 7:CH:98:LEU:HB2    | 2.01                     | 0.43              |
| 10:CK:47:GLY:CA   | 10:CK:56:LYS:HE3   | 2.49                     | 0.43              |
| 12:CM:16:ILE:CD1  | 12:CM:16:ILE:H     | 2.26                     | 0.43              |
| 15:CP:48:GLU:CG   | 15:CP:51:ARG:HH21  | 2.25                     | 0.43              |
| 19:CT:22:SER:HB3  | 55:CA:1458:G:O2'   | 2.17                     | 0.43              |
| 19:CT:60:GLN:HB3  | 19:CT:65:LEU:HD12  | 2.01                     | 0.43              |
| 50:D0:42:ILE:HD13 | 50:D0:42:ILE:HA    | 1.76                     | 0.43              |
| 24:DA:117:G:C2    | 24:DA:119:A:N6     | 2.87                     | 0.43              |
| 24:DA:1386:C:O2'  | 24:DA:1387:A:O5'   | 2.28                     | 0.43              |
| 24:DA:143:C:H3'   | 24:DA:144:A:H8     | 1.84                     | 0.43              |
| 24:DA:1528:A:H2'  | 24:DA:1529:G:O4'   | 2.19                     | 0.43              |
| 24:DA:1638:C:H5'' | 24:DA:2710:C:O2'   | 2.18                     | 0.43              |
| 24:DA:1867:G:O6   | 24:DA:1875:G:N2    | 2.52                     | 0.43              |
| 24:DA:2078:C:C4   | 24:DA:2079:U:C4    | 3.06                     | 0.43              |
| 24:DA:2262:U:H4'  | 24:DA:2328:A:H2    | 1.79                     | 0.43              |
| 24:DA:2266:A:H4'  | 24:DA:2267:A:O5'   | 2.18                     | 0.43              |
| 24:DA:2361:G:H2'  | 24:DA:2362:C:H6    | 1.83                     | 0.43              |
| 24:DA:2547:A:C8   | 24:DA:2566:A:C8    | 3.07                     | 0.43              |
| 24:DA:2811:G:OP1  | 27:DD:61:THR:HB    | 2.18                     | 0.43              |
| 24:DA:294:A:C2'   | 24:DA:295:G:O5'    | 2.67                     | 0.43              |
| 24:DA:324:A:N7    | 24:DA:339:U:H4'    | 2.34                     | 0.43              |
| 24:DA:352:A:H2'   | 24:DA:353:C:C4'    | 2.49                     | 0.43              |
| 24:DA:467:G:H2'   | 24:DA:468:G:C8     | 2.53                     | 0.43              |
| 24:DA:527:C:O2'   | 24:DA:528:A:N7     | 2.51                     | 0.43              |
| 24:DA:528:A:H8    | 24:DA:528:A:H2'    | 1.63                     | 0.43              |
| 24:DA:67:U:H2'    | 24:DA:68:G:C8      | 2.44                     | 0.43              |
| 24:DA:739:A:O2'   | 24:DA:740:C:H5     | 2.02                     | 0.43              |
| 56:DB:16:G:C6     | 56:DB:69:G:C4      | 3.07                     | 0.43              |
| 26:DC:16:VAL:N    | 26:DC:203:VAL:HG12 | 2.33                     | 0.43              |
| 27:DD:115:GLY:O   | 37:DN:3:HIS:CE1    | 2.72                     | 0.43              |
| 27:DD:76:GLY:O    | 27:DD:78:GLY:N     | 2.52                     | 0.43              |
| 27:DD:47:ALA:HB2  | 27:DD:83:ARG:HD2   | 2.00                     | 0.43              |
| 27:DD:37:VAL:HB   | 27:DD:91:THR:HA    | 2.00                     | 0.43              |
| 32:DI:127:SER:O   | 32:DI:131:THR:HG23 | 2.19                     | 0.43              |
| 33:DJ:69:ARG:CZ   | 33:DJ:89:PHE:HE1   | 2.32                     | 0.43              |
| 33:DJ:84:ILE:HG23 | 33:DJ:84:ILE:O     | 2.19                     | 0.43              |
| 24:DA:1245:G:OP1  | 35:DL:8:PRO:HG3    | 2.19                     | 0.43              |
| 38:DO:18:LEU:HD13 | 38:DO:25:ARG:HD2   | 2.00                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:DO:58:ILE:O     | 38:DO:62:LEU:HB2  | 2.19                     | 0.43              |
| 39:DP:91:VAL:HG11  | 39:DP:96:LEU:CG   | 2.49                     | 0.43              |
| 40:DQ:87:VAL:HG12  | 40:DQ:88:GLU:N    | 2.33                     | 0.43              |
| 41:DR:55:ASP:CG    | 41:DR:56:GLY:N    | 2.72                     | 0.43              |
| 43:DT:14:PRO:O     | 43:DT:32:LEU:HA   | 2.18                     | 0.43              |
| 49:DZ:8:GLN:OE1    | 49:DZ:30:ARG:O    | 2.37                     | 0.43              |
| 21:AA:1074:G:N2    | 21:AA:1102:A:C5   | 2.87                     | 0.43              |
| 21:AA:1139:G:C2    | 21:AA:1141:C:N4   | 2.87                     | 0.43              |
| 18:AS:9:PHE:CE1    | 21:AA:1318:A:H4'  | 2.54                     | 0.43              |
| 21:AA:1390:U:H2'   | 21:AA:1391:U:H6   | 1.84                     | 0.43              |
| 21:AA:49:U:O4      | 21:AA:365:U:C5    | 2.69                     | 0.43              |
| 21:AA:792:A:C4     | 21:AA:794:A:C6    | 3.07                     | 0.43              |
| 1:AB:38:HIS:HD2    | 1:AB:38:HIS:O     | 2.02                     | 0.43              |
| 2:AC:179:ALA:HB1   | 2:AC:202:PHE:HE1  | 1.83                     | 0.43              |
| 2:AC:78:LYS:HG2    | 2:AC:79:LYS:HD2   | 2.01                     | 0.43              |
| 3:AD:100:VAL:O     | 3:AD:100:VAL:HG12 | 2.17                     | 0.43              |
| 3:AD:88:ASN:O      | 3:AD:91:ALA:HB3   | 2.19                     | 0.43              |
| 4:AE:83:PRO:CG     | 4:AE:97:PRO:HD3   | 2.48                     | 0.43              |
| 10:AK:94:SER:HA    | 10:AK:97:ARG:HG2  | 2.01                     | 0.43              |
| 15:AP:22:ALA:CB    | 15:AP:32:PHE:HA   | 2.49                     | 0.43              |
| 50:B0:45:ASP:O     | 50:B0:52:LYS:HE3  | 2.18                     | 0.43              |
| 24:BA:1643:G:H2'   | 24:BA:1644:C:O4'  | 2.18                     | 0.43              |
| 24:BA:1857:G:HO2'  | 24:BA:1858:A:P    | 2.41                     | 0.43              |
| 24:BA:1858:A:H2'   | 24:BA:1859:U:H6   | 1.83                     | 0.43              |
| 24:BA:1860:G:C2    | 24:BA:1861:G:C8   | 3.07                     | 0.43              |
| 24:BA:2026:U:C2    | 24:BA:2027:G:C8   | 3.06                     | 0.43              |
| 24:BA:2040:G:H2'   | 24:BA:2041:U:C6   | 2.53                     | 0.43              |
| 24:BA:2503:A:O2'   | 24:BA:2505:G:OP2  | 2.26                     | 0.43              |
| 24:BA:2548:U:O2    | 34:BK:23:LYS:NZ   | 2.38                     | 0.43              |
| 24:BA:2611:C:H2'   | 24:BA:2612:C:H6   | 1.84                     | 0.43              |
| 24:BA:2617:U:O2'   | 24:BA:2618:G:H5'  | 2.18                     | 0.43              |
| 24:BA:527:C:H4'    | 24:BA:528:A:O5'   | 2.19                     | 0.43              |
| 24:BA:57:C:H2'     | 24:BA:58:G:O4'    | 2.19                     | 0.43              |
| 24:BA:613:A:C8     | 24:BA:616:A:N1    | 2.86                     | 0.43              |
| 24:BA:954:G:C6     | 24:BA:955:U:C4    | 3.06                     | 0.43              |
| 28:BE:178:VAL:HG22 | 28:BE:179:SER:N   | 2.33                     | 0.43              |
| 31:BH:37:VAL:HG23  | 31:BH:38:PRO:HD2  | 2.00                     | 0.43              |
| 31:BH:62:LEU:C     | 31:BH:62:LEU:HD12 | 2.39                     | 0.43              |
| 36:BM:49:ALA:HB1   | 36:BM:120:ALA:HB1 | 2.01                     | 0.43              |
| 38:BO:94:ARG:O     | 38:BO:95:SER:C    | 2.57                     | 0.43              |
| 24:BA:994:C:O2     | 41:BR:10:LYS:HE2  | 2.19                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 44:BU:17:ASP:HB3   | 44:BU:20:LYS:HD3  | 2.01                     | 0.43              |
| 47:BX:20:ALA:O     | 47:BX:21:LEU:HB2  | 2.19                     | 0.43              |
| 49:BZ:26:LEU:HA    | 49:BZ:26:LEU:HD23 | 1.79                     | 0.43              |
| 55:CA:1064:G:C2    | 55:CA:1066:C:N4   | 2.87                     | 0.43              |
| 55:CA:10:A:H2'     | 55:CA:11:G:H8     | 1.84                     | 0.43              |
| 55:CA:1106:G:C4    | 55:CA:1107:C:C5   | 3.07                     | 0.43              |
| 55:CA:1264:U:C2    | 55:CA:1272:G:N2   | 2.87                     | 0.43              |
| 55:CA:1303:C:O2    | 55:CA:1303:C:H2'  | 2.18                     | 0.43              |
| 55:CA:1386:G:N3    | 55:CA:1387:G:C8   | 2.87                     | 0.43              |
| 55:CA:533:A:C2     | 55:CA:536:C:C6    | 3.06                     | 0.43              |
| 55:CA:680:C:C2     | 55:CA:711:G:N2    | 2.87                     | 0.43              |
| 55:CA:774:G:C6     | 55:CA:775:G:C5    | 3.07                     | 0.43              |
| 55:CA:790:A:N6     | 55:CA:791:G:C6    | 2.86                     | 0.43              |
| 55:CA:818:G:C3'    | 55:CA:819:A:C5'   | 2.97                     | 0.43              |
| 55:CA:906:A:N6     | 59:CA:1760:HOH:O  | 2.51                     | 0.43              |
| 1:CB:46:VAL:N      | 1:CB:47:PRO:HD2   | 2.33                     | 0.43              |
| 3:CD:125:ASN:HB2   | 3:CD:141:VAL:H    | 1.82                     | 0.43              |
| 6:CG:9:ARG:HH12    | 55:CA:1346:A:H62  | 1.64                     | 0.43              |
| 7:CH:10:LEU:HD13   | 7:CH:75:GLN:O     | 2.19                     | 0.43              |
| 8:CI:80:HIS:CD2    | 8:CI:84:ARG:HG3   | 2.53                     | 0.43              |
| 10:CK:127:ARG:HH21 | 55:CA:795:C:C5'   | 2.28                     | 0.43              |
| 11:CL:59:GLY:O     | 11:CL:60:PHE:C    | 2.57                     | 0.43              |
| 16:CQ:11:VAL:HG23  | 16:CQ:56:ASP:O    | 2.19                     | 0.43              |
| 16:CQ:62:GLU:HB2   | 16:CQ:72:TRP:CH2  | 2.54                     | 0.43              |
| 24:DA:1348:C:C5    | 24:DA:1349:C:C2   | 3.06                     | 0.43              |
| 24:DA:1407:G:H2'   | 24:DA:1408:G:C8   | 2.53                     | 0.43              |
| 24:DA:1413:A:C5    | 24:DA:1414:C:N4   | 2.87                     | 0.43              |
| 24:DA:1462:C:O2'   | 24:DA:1463:C:C5'  | 2.66                     | 0.43              |
| 24:DA:1695:G:C2'   | 24:DA:1695:G:N3   | 2.82                     | 0.43              |
| 24:DA:1766:G:C4    | 24:DA:1987:A:C2   | 3.06                     | 0.43              |
| 24:DA:1936:A:C4    | 24:DA:1940:U:C5   | 3.07                     | 0.43              |
| 24:DA:1945:G:N2    | 24:DA:1946:U:C2   | 2.87                     | 0.43              |
| 24:DA:2389:G:O5'   | 24:DA:2390:U:H5'  | 2.19                     | 0.43              |
| 24:DA:2458:G:C4    | 24:DA:2490:G:C6   | 3.07                     | 0.43              |
| 24:DA:252:G:H2'    | 24:DA:253:C:H6    | 1.80                     | 0.43              |
| 24:DA:2542:A:C2    | 24:DA:2567:G:O6   | 2.72                     | 0.43              |
| 24:DA:2654:A:N3    | 24:DA:2656:U:C4   | 2.87                     | 0.43              |
| 24:DA:2683:C:H2'   | 24:DA:2684:U:H6   | 1.84                     | 0.43              |
| 24:DA:2686:G:H2'   | 24:DA:2687:U:C6   | 2.54                     | 0.43              |
| 24:DA:2869:G:C5    | 24:DA:2870:C:C4   | 3.06                     | 0.43              |
| 24:DA:308:G:C2     | 24:DA:309:A:C2    | 3.06                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:478:A:N1     | 24:DA:480:A:C4     | 2.87                     | 0.43              |
| 24:DA:486:C:O5'    | 24:DA:486:C:H6     | 2.01                     | 0.43              |
| 24:DA:3:U:H2'      | 24:DA:4:U:O4'      | 2.18                     | 0.43              |
| 24:DA:763:G:C5     | 24:DA:765:C:C4     | 3.07                     | 0.43              |
| 26:DC:250:GLN:HG2  | 26:DC:250:GLN:H    | 1.51                     | 0.43              |
| 27:DD:119:ALA:O    | 27:DD:120:GLY:O    | 2.37                     | 0.43              |
| 27:DD:98:VAL:O     | 27:DD:99:GLU:C     | 2.58                     | 0.43              |
| 28:DE:149:ILE:CD1  | 28:DE:188:MET:HG3  | 2.49                     | 0.43              |
| 28:DE:178:VAL:HG13 | 28:DE:179:SER:H    | 1.83                     | 0.43              |
| 29:DF:72:SER:H     | 29:DF:78:ILE:HG21  | 1.84                     | 0.43              |
| 30:DG:116:LEU:HD13 | 30:DG:120:ILE:O    | 2.19                     | 0.43              |
| 30:DG:132:LEU:N    | 30:DG:132:LEU:HD12 | 2.34                     | 0.43              |
| 31:DH:84:ALA:HB3   | 31:DH:148:ALA:HB2  | 2.01                     | 0.43              |
| 31:DH:90:LEU:HB3   | 31:DH:123:ARG:HD2  | 2.00                     | 0.43              |
| 33:DJ:110:PRO:O    | 33:DJ:115:GLY:HA3  | 2.19                     | 0.43              |
| 33:DJ:17:VAL:HG23  | 33:DJ:137:PRO:CB   | 2.44                     | 0.43              |
| 35:DL:79:LEU:CB    | 35:DL:113:ALA:H    | 2.23                     | 0.43              |
| 39:DP:85:VAL:O     | 39:DP:85:VAL:HG13  | 2.18                     | 0.43              |
| 24:DA:533:G:N2     | 40:DQ:44:TYR:CD1   | 2.82                     | 0.43              |
| 41:DR:16:GLU:HG3   | 41:DR:16:GLU:O     | 2.19                     | 0.43              |
| 43:DT:39:THR:C     | 43:DT:41:ALA:H     | 2.22                     | 0.43              |
| 44:DU:58:VAL:HG12  | 44:DU:59:GLU:N     | 2.34                     | 0.43              |
| 24:DA:2355:G:H5''  | 46:DW:20:LEU:HD22  | 2.00                     | 0.43              |
| 48:DY:31:GLN:C     | 48:DY:33:ALA:N     | 2.72                     | 0.43              |
| 21:AA:1059:C:O2'   | 21:AA:1060:U:H5'   | 2.19                     | 0.43              |
| 21:AA:1124:G:C2    | 21:AA:1150:A:C2    | 3.07                     | 0.43              |
| 2:AC:3:LYS:HE3     | 21:AA:1191:A:H5''  | 2.00                     | 0.43              |
| 21:AA:1498:U:H2'   | 23:AW:2:U:OP1      | 2.18                     | 0.43              |
| 21:AA:329:A:H2'    | 21:AA:332:G:N7     | 2.34                     | 0.43              |
| 21:AA:782:A:H2'    | 21:AA:783:C:O4'    | 2.19                     | 0.43              |
| 21:AA:987:G:H2'    | 21:AA:988:G:H8     | 1.84                     | 0.43              |
| 1:AB:89:PHE:O      | 1:AB:90:PHE:HB3    | 2.19                     | 0.43              |
| 4:AE:93:VAL:HG12   | 4:AE:94:PHE:N      | 2.33                     | 0.43              |
| 10:AK:39:ASN:O     | 21:AA:684:U:O2'    | 2.36                     | 0.43              |
| 11:AL:22:ALA:O     | 11:AL:23:LEU:O     | 2.37                     | 0.43              |
| 12:AM:5:GLY:O      | 12:AM:7:ASN:N      | 2.51                     | 0.43              |
| 14:AO:31:LEU:CD1   | 14:AO:62:ARG:HB2   | 2.48                     | 0.43              |
| 20:AU:19:LYS:CE    | 20:AU:19:LYS:HA    | 2.48                     | 0.43              |
| 50:B0:33:SER:OG    | 50:B0:35:GLU:HG3   | 2.19                     | 0.43              |
| 24:BA:1006:C:H1'   | 33:BJ:108:MET:HB3  | 2.00                     | 0.43              |
| 24:BA:1032:A:O2'   | 24:BA:1033:U:H5'   | 2.19                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 24:BA:1034:G:C6  | 24:BA:1035:U:N3   | 2.87                     | 0.43              |
| 24:BA:1056:G:O2' | 24:BA:1086:A:H1'  | 2.19                     | 0.43              |
| 24:BA:149:A:H2'  | 24:BA:150:U:H6    | 1.84                     | 0.43              |
| 24:BA:1569:A:C6  | 24:BA:1570:A:C2   | 3.07                     | 0.43              |
| 24:BA:1342:A:OP2 | 24:BA:1602:U:O4   | 2.36                     | 0.43              |
| 24:BA:1719:G:H2' | 24:BA:1720:U:H6   | 1.84                     | 0.43              |
| 24:BA:176:A:C5   | 24:BA:177:G:C5    | 3.07                     | 0.43              |
| 24:BA:1849:G:H2' | 24:BA:1850:G:C8   | 2.53                     | 0.43              |
| 24:BA:1866:A:H61 | 24:BA:1875:G:C2'  | 2.32                     | 0.43              |
| 24:BA:1967:C:C2  | 24:BA:1968:G:C8   | 3.07                     | 0.43              |
| 24:BA:2298:A:H2' | 24:BA:2299:U:C6   | 2.54                     | 0.43              |
| 24:BA:247:G:P    | 24:BA:388:G:H21   | 2.41                     | 0.43              |
| 24:BA:541:A:C5   | 24:BA:542:C:C5    | 3.07                     | 0.43              |
| 24:BA:825:A:C2   | 24:BA:833:A:C2    | 3.06                     | 0.43              |
| 24:BA:857:G:C2'  | 24:BA:858:G:H5'   | 2.49                     | 0.43              |
| 31:BH:24:GLY:O   | 31:BH:26:ALA:N    | 2.52                     | 0.43              |
| 33:BJ:44:TYR:C   | 33:BJ:44:TYR:HD1  | 2.22                     | 0.43              |
| 33:BJ:44:TYR:CD2 | 40:BQ:63:ARG:HG2  | 2.54                     | 0.43              |
| 34:BK:43:ILE:CG1 | 34:BK:56:ASP:HB2  | 2.48                     | 0.43              |
| 39:BP:105:LYS:HA | 39:BP:108:ARG:NH2 | 2.25                     | 0.43              |
| 40:BQ:40:LYS:HA  | 40:BQ:43:GLN:HB2  | 2.00                     | 0.43              |
| 40:BQ:91:ARG:NE  | 41:BR:11:GLN:HB2  | 2.34                     | 0.43              |
| 47:BX:12:VAL:CG2 | 47:BX:28:PHE:HB2  | 2.48                     | 0.43              |
| 47:BX:32:LEU:HA  | 47:BX:51:SER:HA   | 2.00                     | 0.43              |
| 47:BX:51:SER:O   | 47:BX:52:ALA:C    | 2.55                     | 0.43              |
| 55:CA:110:C:O2'  | 55:CA:111:G:H5'   | 2.19                     | 0.43              |
| 55:CA:1175:G:H2' | 55:CA:1176:A:O4'  | 2.19                     | 0.43              |
| 55:CA:181:A:H4'  | 55:CA:182:A:O5'   | 2.18                     | 0.43              |
| 55:CA:251:G:C8   | 55:CA:266:G:C8    | 3.06                     | 0.43              |
| 55:CA:727:G:N1   | 55:CA:731:G:C6    | 2.86                     | 0.43              |
| 55:CA:959:A:N3   | 55:CA:985:C:H1'   | 2.34                     | 0.43              |
| 1:CB:74:ALA:C    | 1:CB:76:SER:H     | 2.22                     | 0.43              |
| 4:CE:107:GLY:O   | 4:CE:108:GLY:C    | 2.56                     | 0.43              |
| 6:CG:104:VAL:HA  | 6:CG:107:ALA:CB   | 2.48                     | 0.43              |
| 12:CM:77:LYS:HE3 | 12:CM:77:LYS:C    | 2.38                     | 0.43              |
| 20:CU:24:LYS:HA  | 20:CU:24:LYS:HD2  | 1.87                     | 0.43              |
| 24:DA:1108:U:H2' | 24:DA:1109:C:O4'  | 2.18                     | 0.43              |
| 24:DA:1142:A:C8  | 24:DA:1144:A:C5   | 3.07                     | 0.43              |
| 24:DA:1765:U:O2' | 24:DA:1766:G:H5'  | 2.19                     | 0.43              |
| 24:DA:2312:U:P   | 29:DF:70:ARG:HB3  | 2.59                     | 0.43              |
| 24:DA:2428:G:O5' | 24:DA:2428:G:H8   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:2584:U:H5   | 59:DA:3697:HOH:O   | 2.02                     | 0.43              |
| 24:DA:281:C:H2'   | 24:DA:282:A:C8     | 2.51                     | 0.43              |
| 24:DA:2854:G:H2'  | 24:DA:2855:C:C6    | 2.53                     | 0.43              |
| 24:DA:422:A:N1    | 24:DA:423:A:C6     | 2.87                     | 0.43              |
| 24:DA:430:A:OP2   | 24:DA:431:U:H5     | 2.02                     | 0.43              |
| 24:DA:695:G:C2    | 24:DA:768:G:C2     | 3.07                     | 0.43              |
| 24:DA:94:A:C6     | 24:DA:95:A:C6      | 3.06                     | 0.43              |
| 24:DA:962:G:O2'   | 24:DA:963:U:C5'    | 2.65                     | 0.43              |
| 28:DE:134:LEU:O   | 28:DE:138:LEU:HG   | 2.18                     | 0.43              |
| 24:DA:674:G:H5''  | 28:DE:71:GLY:CA    | 2.49                     | 0.43              |
| 28:DE:75:SER:O    | 28:DE:78:TRP:HB2   | 2.19                     | 0.43              |
| 29:DF:160:LYS:HB2 | 29:DF:160:LYS:HE2  | 1.87                     | 0.43              |
| 30:DG:78:VAL:HG23 | 30:DG:79:THR:HG23  | 2.01                     | 0.43              |
| 35:DL:132:ARG:HA  | 35:DL:135:ILE:HG22 | 2.00                     | 0.43              |
| 35:DL:50:PHE:CE2  | 35:DL:53:GLY:N     | 2.86                     | 0.43              |
| 37:DN:16:HIS:C    | 37:DN:18:GLN:H     | 2.22                     | 0.43              |
| 38:DO:7:ARG:HA    | 38:DO:10:ARG:NH2   | 2.34                     | 0.43              |
| 38:DO:89:ASP:O    | 38:DO:90:VAL:HG13  | 2.18                     | 0.43              |
| 41:DR:23:GLU:O    | 41:DR:25:LEU:HD22  | 2.19                     | 0.43              |
| 42:DS:7:HIS:HB2   | 42:DS:50:VAL:CG2   | 2.49                     | 0.43              |
| 45:DV:2:PHE:HD1   | 45:DV:50:MET:HE3   | 1.83                     | 0.43              |
| 46:DW:14:ASP:C    | 46:DW:16:GLU:H     | 2.23                     | 0.43              |
| 49:DZ:40:THR:C    | 49:DZ:42:ALA:N     | 2.71                     | 0.43              |
| 21:AA:1134:G:C2   | 21:AA:1141:C:C2    | 3.07                     | 0.42              |
| 21:AA:1145:A:HO2' | 21:AA:1146:A:H8    | 1.62                     | 0.42              |
| 16:AQ:44:HIS:CE1  | 21:AA:276:G:O3'    | 2.66                     | 0.42              |
| 21:AA:308:C:H2'   | 21:AA:309:A:C8     | 2.51                     | 0.42              |
| 21:AA:350:G:N1    | 21:AA:351:G:O6     | 2.52                     | 0.42              |
| 21:AA:374:A:H5''  | 21:AA:452:A:C2     | 2.54                     | 0.42              |
| 21:AA:497:G:O2'   | 21:AA:498:A:H8     | 1.91                     | 0.42              |
| 21:AA:569:C:O5'   | 21:AA:569:C:H6     | 2.01                     | 0.42              |
| 21:AA:843:U:H2'   | 21:AA:844:G:H5'    | 2.01                     | 0.42              |
| 21:AA:910:C:H2'   | 21:AA:911:U:H6     | 1.84                     | 0.42              |
| 1:AB:9:LEU:HD12   | 1:AB:42:LEU:HD11   | 1.99                     | 0.42              |
| 3:AD:62:ARG:HA    | 3:AD:62:ARG:CZ     | 2.49                     | 0.42              |
| 7:AH:21:LYS:HE2   | 7:AH:21:LYS:CA     | 2.48                     | 0.42              |
| 8:AI:52:GLU:C     | 8:AI:54:VAL:H      | 2.23                     | 0.42              |
| 10:AK:121:ARG:HA  | 10:AK:122:PRO:HD2  | 1.89                     | 0.42              |
| 11:AL:24:GLU:HB3  | 11:AL:26:CYS:SG    | 2.59                     | 0.42              |
| 13:AN:19:TYR:HB2  | 13:AN:54:SER:OG    | 2.19                     | 0.42              |
| 13:AN:20:PHE:O    | 13:AN:22:LYS:N     | 2.52                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:AO:55:LEU:O    | 14:AO:59:VAL:HG23 | 2.19                     | 0.42              |
| 17:AR:29:LYS:HG3  | 17:AR:30:ASN:ND2  | 2.34                     | 0.42              |
| 24:BA:1017:G:C5   | 24:BA:1018:U:H5   | 2.35                     | 0.42              |
| 24:BA:1140:C:P    | 33:BJ:68:LYS:NZ   | 2.83                     | 0.42              |
| 24:BA:1252:G:N3   | 40:BQ:32:ARG:CG   | 2.82                     | 0.42              |
| 24:BA:1281:G:H2'  | 24:BA:1282:U:C6   | 2.53                     | 0.42              |
| 24:BA:1444:G:C6   | 24:BA:1445:G:C6   | 3.07                     | 0.42              |
| 24:BA:1652:A:H2   | 24:BA:2006:C:C2   | 2.37                     | 0.42              |
| 24:BA:1812:U:H2'  | 24:BA:1813:G:C8   | 2.53                     | 0.42              |
| 24:BA:2154:A:H5'  | 24:BA:2155:U:OP2  | 2.18                     | 0.42              |
| 24:BA:2209:G:C6   | 24:BA:2210:U:N3   | 2.87                     | 0.42              |
| 24:BA:2688:G:H1'  | 24:BA:2721:A:N6   | 2.34                     | 0.42              |
| 24:BA:281:C:H2'   | 24:BA:282:A:H8    | 1.82                     | 0.42              |
| 24:BA:464:U:O2'   | 24:BA:465:G:H5'   | 2.19                     | 0.42              |
| 24:BA:541:A:C2    | 24:BA:553:G:N3    | 2.87                     | 0.42              |
| 24:BA:638:G:C6    | 24:BA:651:G:C2    | 3.07                     | 0.42              |
| 24:BA:652:U:H4'   | 24:BA:653:U:OP2   | 2.19                     | 0.42              |
| 24:BA:947:A:O2'   | 24:BA:984:A:H2    | 2.02                     | 0.42              |
| 24:BA:992:C:O2    | 24:BA:993:G:C8    | 2.72                     | 0.42              |
| 25:BB:46:A:C5     | 25:BB:47:C:C5     | 3.07                     | 0.42              |
| 25:BB:73:A:C5     | 25:BB:104:A:C2    | 3.07                     | 0.42              |
| 26:BC:68:ARG:HD3  | 26:BC:103:ILE:CD1 | 2.17                     | 0.42              |
| 26:BC:80:LEU:HD11 | 26:BC:109:LEU:CG  | 2.41                     | 0.42              |
| 27:BD:113:SER:HB2 | 27:BD:114:LYS:CE  | 2.49                     | 0.42              |
| 24:BA:1654:A:C4'  | 27:BD:118:PHE:CE1 | 3.02                     | 0.42              |
| 28:BE:77:ILE:C    | 28:BE:78:TRP:O    | 2.57                     | 0.42              |
| 29:BF:127:TYR:O   | 29:BF:128:SER:HB2 | 2.19                     | 0.42              |
| 33:BJ:36:LEU:HD12 | 33:BJ:36:LEU:HA   | 1.70                     | 0.42              |
| 33:BJ:35:ARG:O    | 33:BJ:37:ARG:N    | 2.52                     | 0.42              |
| 35:BL:62:PRO:HB2  | 53:B3:29:ARG:NH2  | 2.34                     | 0.42              |
| 36:BM:61:GLY:HA2  | 36:BM:107:GLY:CA  | 2.49                     | 0.42              |
| 37:BN:73:ASN:O    | 37:BN:74:GLU:C    | 2.56                     | 0.42              |
| 38:BO:57:ALA:O    | 38:BO:59:ALA:N    | 2.52                     | 0.42              |
| 39:BP:24:THR:O    | 39:BP:24:THR:HG23 | 2.19                     | 0.42              |
| 40:BQ:67:ALA:O    | 40:BQ:68:ALA:C    | 2.57                     | 0.42              |
| 41:BR:60:LYS:H    | 41:BR:100:GLY:HA3 | 1.85                     | 0.42              |
| 41:BR:37:GLU:O    | 41:BR:37:GLU:OE1  | 2.36                     | 0.42              |
| 41:BR:43:ASN:HB3  | 41:BR:44:GLY:H    | 1.56                     | 0.42              |
| 42:BS:54:ALA:O    | 42:BS:57:ASN:HB2  | 2.19                     | 0.42              |
| 49:BZ:3:THR:C     | 49:BZ:4:ILE:CG2   | 2.87                     | 0.42              |
| 55:CA:1231:G:C6   | 55:CA:1232:U:C4   | 3.07                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 16:CQ:17:GLU:O     | 55:CA:254:G:O2'   | 2.37                     | 0.42              |
| 55:CA:266:G:O2'    | 55:CA:267:C:H3'   | 2.19                     | 0.42              |
| 55:CA:324:G:N2     | 55:CA:327:A:C8    | 2.87                     | 0.42              |
| 55:CA:550:G:H2'    | 55:CA:551:U:C6    | 2.54                     | 0.42              |
| 55:CA:610:U:O4'    | 55:CA:610:U:O2    | 2.36                     | 0.42              |
| 55:CA:692:U:H5'    | 55:CA:797:C:H4'   | 2.01                     | 0.42              |
| 1:CB:20:ARG:CG     | 55:CA:831:A:OP1   | 2.67                     | 0.42              |
| 55:CA:855:U:O2'    | 55:CA:856:C:H5'   | 2.19                     | 0.42              |
| 55:CA:90:C:O2'     | 55:CA:91:U:O4'    | 2.37                     | 0.42              |
| 3:CD:187:ARG:CZ    | 3:CD:191:SER:OG   | 2.67                     | 0.42              |
| 5:CF:57:ALA:O      | 5:CF:59:TYR:CD1   | 2.70                     | 0.42              |
| 5:CF:3:HIS:CD2     | 5:CF:65:GLU:HG3   | 2.53                     | 0.42              |
| 8:CI:35:GLU:O      | 8:CI:36:GLN:C     | 2.57                     | 0.42              |
| 10:CK:44:ALA:HB1   | 10:CK:68:ARG:NH2  | 2.34                     | 0.42              |
| 11:CL:22:ALA:CB    | 11:CL:94:TYR:OH   | 2.67                     | 0.42              |
| 12:CM:107:THR:HG21 | 55:CA:1307:U:H1'  | 2.00                     | 0.42              |
| 16:CQ:9:GLY:O      | 16:CQ:57:VAL:HG13 | 2.19                     | 0.42              |
| 18:CS:11:ASP:OD1   | 18:CS:14:LEU:HD21 | 2.19                     | 0.42              |
| 18:CS:4:LEU:HB3    | 18:CS:5:LYS:H     | 1.56                     | 0.42              |
| 24:DA:1328:A:H2'   | 24:DA:1330:C:N4   | 2.33                     | 0.42              |
| 24:DA:1593:A:C6    | 24:DA:1594:U:C4   | 3.07                     | 0.42              |
| 24:DA:1598:A:H2'   | 24:DA:1599:U:O4'  | 2.19                     | 0.42              |
| 24:DA:1889:A:C2    | 24:DA:2086:U:H1'  | 2.53                     | 0.42              |
| 24:DA:2019:A:H4'   | 40:DQ:33:VAL:CG2  | 2.49                     | 0.42              |
| 24:DA:531:C:C6     | 24:DA:2035:G:C2   | 3.07                     | 0.42              |
| 24:DA:2183:A:H2'   | 24:DA:2184:A:C8   | 2.54                     | 0.42              |
| 24:DA:2391:G:O2'   | 24:DA:2392:A:H8   | 2.02                     | 0.42              |
| 24:DA:2425:A:H5''  | 24:DA:2426:A:H2'  | 2.01                     | 0.42              |
| 24:DA:242:G:P      | 53:D3:2:LYS:NZ    | 2.92                     | 0.42              |
| 24:DA:2438:U:O2'   | 24:DA:2439:A:H5'' | 2.19                     | 0.42              |
| 24:DA:2467:C:H2'   | 24:DA:2468:A:O4'  | 2.19                     | 0.42              |
| 24:DA:2492:U:H6    | 24:DA:2492:U:O5'  | 2.01                     | 0.42              |
| 24:DA:2522:U:O2'   | 24:DA:2523:G:H5'  | 2.19                     | 0.42              |
| 24:DA:2624:G:C2    | 24:DA:2625:G:H1'  | 2.54                     | 0.42              |
| 24:DA:2654:A:C4    | 24:DA:2656:U:C4   | 3.07                     | 0.42              |
| 24:DA:2693:G:C2    | 24:DA:2694:G:N7   | 2.87                     | 0.42              |
| 24:DA:2746:U:N3    | 24:DA:2759:G:N1   | 2.67                     | 0.42              |
| 24:DA:617:G:C4     | 24:DA:618:G:C8    | 3.07                     | 0.42              |
| 24:DA:831:G:O2'    | 24:DA:832:U:C5'   | 2.67                     | 0.42              |
| 56:DB:16:G:H2'     | 56:DB:17:C:H6     | 1.84                     | 0.42              |
| 26:DC:171:VAL:HG12 | 26:DC:173:LEU:CD1 | 2.49                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:2620:C:O4'  | 27:DD:161:MET:HG3  | 2.18                     | 0.42              |
| 27:DD:196:ALA:O   | 27:DD:197:THR:C    | 2.57                     | 0.42              |
| 30:DG:120:ILE:CG1 | 30:DG:140:ILE:HG22 | 2.41                     | 0.42              |
| 30:DG:175:LYS:HD3 | 30:DG:175:LYS:C    | 2.40                     | 0.42              |
| 32:DI:29:GLN:O    | 32:DI:30:GLN:HB3   | 2.19                     | 0.42              |
| 34:DK:19:VAL:HG12 | 34:DK:41:ILE:CG1   | 2.49                     | 0.42              |
| 36:DM:41:LEU:HD23 | 36:DM:46:ILE:CG2   | 2.44                     | 0.42              |
| 24:DA:1650:A:O2'  | 37:DN:108:ALA:HB1  | 2.19                     | 0.42              |
| 37:DN:82:GLU:O    | 37:DN:85:PRO:HD2   | 2.19                     | 0.42              |
| 38:DO:108:ASP:C   | 38:DO:110:ALA:H    | 2.22                     | 0.42              |
| 39:DP:61:ARG:NH1  | 39:DP:63:ILE:HD11  | 2.34                     | 0.42              |
| 39:DP:86:LYS:N    | 39:DP:86:LYS:HZ3   | 2.16                     | 0.42              |
| 40:DQ:61:ILE:HD12 | 40:DQ:61:ILE:N     | 2.34                     | 0.42              |
| 40:DQ:4:LYS:CD    | 40:DQ:7:VAL:H      | 2.32                     | 0.42              |
| 45:DV:26:PHE:HE2  | 45:DV:42:LEU:HD12  | 1.84                     | 0.42              |
| 45:DV:4:ILE:HD11  | 45:DV:50:MET:HE2   | 2.00                     | 0.42              |
| 46:DW:27:GLY:HA3  | 46:DW:31:LEU:HD11  | 1.95                     | 0.42              |
| 21:AA:1021:A:C3'  | 21:AA:1022:A:H5''  | 2.49                     | 0.42              |
| 21:AA:1087:G:N2   | 21:AA:1088:G:C5    | 2.87                     | 0.42              |
| 21:AA:1091:U:N3   | 21:AA:1094:G:OP2   | 2.38                     | 0.42              |
| 21:AA:1118:U:H1'  | 21:AA:1179:A:C4    | 2.54                     | 0.42              |
| 21:AA:1206:G:H2'  | 21:AA:1207:G:O4'   | 2.19                     | 0.42              |
| 21:AA:1320:C:O2'  | 21:AA:1321:U:O5'   | 2.37                     | 0.42              |
| 13:AN:74:ARG:CG   | 21:AA:1358:U:OP1   | 2.67                     | 0.42              |
| 21:AA:1251:A:H1'  | 21:AA:1369:C:O2'   | 2.19                     | 0.42              |
| 21:AA:1449:C:C2   | 21:AA:1455:G:C2    | 3.07                     | 0.42              |
| 21:AA:564:C:C4    | 21:AA:565:U:C4     | 3.07                     | 0.42              |
| 21:AA:692:U:O2    | 21:AA:694:A:C8     | 2.72                     | 0.42              |
| 2:AC:171:ARG:HG2  | 2:AC:173:PRO:HD3   | 2.00                     | 0.42              |
| 4:AE:37:VAL:CG2   | 4:AE:113:VAL:HG12  | 2.40                     | 0.42              |
| 4:AE:83:PRO:HD3   | 4:AE:97:PRO:CD     | 2.49                     | 0.42              |
| 7:AH:11:THR:HA    | 7:AH:14:ARG:HB3    | 2.01                     | 0.42              |
| 8:AI:61:ASP:CG    | 8:AI:62:LEU:N      | 2.72                     | 0.42              |
| 8:AI:62:LEU:HD23  | 8:AI:62:LEU:N      | 2.34                     | 0.42              |
| 13:AN:56:PRO:HA   | 13:AN:59:GLN:OE1   | 2.19                     | 0.42              |
| 17:AR:32:ILE:HG13 | 17:AR:32:ILE:O     | 2.18                     | 0.42              |
| 19:AT:3:ILE:HA    | 19:AT:7:LYS:HD3    | 2.01                     | 0.42              |
| 20:AU:44:ARG:HD2  | 20:AU:44:ARG:N     | 2.35                     | 0.42              |
| 22:AV:33:U:H2'    | 22:AV:35:A:N7      | 2.34                     | 0.42              |
| 52:B2:12:ARG:O    | 52:B2:12:ARG:HG3   | 2.18                     | 0.42              |
| 24:BA:1060:U:C6   | 24:BA:1060:U:OP1   | 2.68                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:991:C:C2    | 24:BA:1185:G:C6    | 3.08                     | 0.42              |
| 24:BA:1677:A:C6   | 24:BA:1678:A:C6    | 3.07                     | 0.42              |
| 24:BA:1734:G:O2'  | 24:BA:1735:A:H5'   | 2.19                     | 0.42              |
| 24:BA:184:C:H2'   | 24:BA:185:G:C8     | 2.53                     | 0.42              |
| 24:BA:1967:C:H2'  | 24:BA:1968:G:C8    | 2.54                     | 0.42              |
| 24:BA:1659:G:C2   | 24:BA:2002:G:N3    | 2.87                     | 0.42              |
| 24:BA:2074:U:N3   | 24:BA:2075:U:C4    | 2.87                     | 0.42              |
| 24:BA:2231:U:H2'  | 24:BA:2232:C:H6    | 1.83                     | 0.42              |
| 24:BA:858:G:C5    | 24:BA:2268:A:C2    | 3.07                     | 0.42              |
| 24:BA:2555:U:C5   | 24:BA:2556:C:C2    | 3.07                     | 0.42              |
| 24:BA:2845:U:H2'  | 24:BA:2846:G:O4'   | 2.19                     | 0.42              |
| 24:BA:388:G:H8    | 24:BA:388:G:H2'    | 1.70                     | 0.42              |
| 24:BA:447:A:N1    | 24:BA:454:A:H2'    | 2.34                     | 0.42              |
| 24:BA:55:G:H2'    | 24:BA:56:A:H8      | 1.84                     | 0.42              |
| 24:BA:683:U:C2'   | 24:BA:684:G:O5'    | 2.67                     | 0.42              |
| 24:BA:714:U:H2'   | 24:BA:716:A:N7     | 2.34                     | 0.42              |
| 24:BA:776:G:H4'   | 24:BA:777:G:H5''   | 2.01                     | 0.42              |
| 24:BA:84:A:H1'    | 24:BA:85:G:O4'     | 2.19                     | 0.42              |
| 24:BA:988:A:C2    | 24:BA:989:G:C2     | 3.07                     | 0.42              |
| 24:BA:85:G:C5     | 24:BA:98:G:C2      | 3.07                     | 0.42              |
| 26:BC:104:LEU:HA  | 26:BC:104:LEU:HD12 | 1.68                     | 0.42              |
| 26:BC:209:ALA:HA  | 26:BC:212:TRP:CE2  | 2.54                     | 0.42              |
| 27:BD:103:ASP:CG  | 27:BD:104:VAL:N    | 2.72                     | 0.42              |
| 24:BA:1654:A:C4'  | 27:BD:118:PHE:CZ   | 2.98                     | 0.42              |
| 27:BD:151:THR:HB  | 27:BD:152:PRO:CD   | 2.46                     | 0.42              |
| 29:BF:100:GLU:C   | 29:BF:102:LEU:N    | 2.73                     | 0.42              |
| 32:BI:126:ARG:HD3 | 32:BI:126:ARG:H    | 1.84                     | 0.42              |
| 32:BI:40:ALA:HB3  | 32:BI:68:PHE:CE1   | 2.54                     | 0.42              |
| 33:BJ:72:LYS:HB2  | 33:BJ:89:PHE:HB2   | 2.01                     | 0.42              |
| 34:BK:117:SER:C   | 34:BK:118:LEU:O    | 2.58                     | 0.42              |
| 34:BK:18:ARG:HD2  | 34:BK:18:ARG:HA    | 1.78                     | 0.42              |
| 24:BA:1996:C:C5   | 34:BK:32:TYR:OH    | 2.72                     | 0.42              |
| 35:BL:82:LEU:HD23 | 35:BL:82:LEU:C     | 2.40                     | 0.42              |
| 36:BM:109:PRO:O   | 36:BM:110:GLU:C    | 2.57                     | 0.42              |
| 36:BM:69:PRO:CA   | 36:BM:94:ALA:HB2   | 2.49                     | 0.42              |
| 37:BN:96:ARG:NH2  | 37:BN:116:VAL:HG23 | 2.34                     | 0.42              |
| 40:BQ:93:ILE:HG12 | 40:BQ:93:ILE:O     | 2.16                     | 0.42              |
| 41:BR:24:LYS:HE2  | 41:BR:24:LYS:HB3   | 1.73                     | 0.42              |
| 43:BT:68:LYS:HG2  | 43:BT:69:ARG:H     | 1.84                     | 0.42              |
| 46:BW:26:GLY:O    | 46:BW:27:GLY:C     | 2.58                     | 0.42              |
| 47:BX:44:ARG:HG2  | 47:BX:45:PHE:N     | 2.35                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:BY:18:LEU:O    | 48:BY:22:LEU:CB   | 2.66                     | 0.42              |
| 8:CI:125:GLN:HE22 | 55:CA:1232:U:H5'' | 1.82                     | 0.42              |
| 55:CA:1320:C:N3   | 55:CA:1321:U:C2   | 2.87                     | 0.42              |
| 55:CA:1408:A:N6   | 55:CA:1409:C:N4   | 2.67                     | 0.42              |
| 55:CA:1463:U:H2'  | 55:CA:1464:U:C6   | 2.54                     | 0.42              |
| 55:CA:276:G:O2'   | 55:CA:277:C:O4'   | 2.37                     | 0.42              |
| 55:CA:369:G:C5    | 55:CA:393:A:C2    | 3.07                     | 0.42              |
| 55:CA:451:A:C5    | 55:CA:481:G:C5    | 3.07                     | 0.42              |
| 11:CL:110:LYS:N   | 55:CA:538:G:OP1   | 2.41                     | 0.42              |
| 55:CA:629:A:H2'   | 55:CA:630:A:O4'   | 2.19                     | 0.42              |
| 55:CA:944:G:C2    | 55:CA:1340:A:C6   | 3.07                     | 0.42              |
| 5:CF:39:LEU:HD12  | 5:CF:40:GLU:H     | 1.83                     | 0.42              |
| 7:CH:114:ALA:O    | 7:CH:117:GLN:HB3  | 2.19                     | 0.42              |
| 8:CI:44:ARG:C     | 8:CI:46:VAL:N     | 2.71                     | 0.42              |
| 9:CJ:47:GLU:HB2   | 9:CJ:67:ILE:CG1   | 2.42                     | 0.42              |
| 11:CL:5:GLN:HE21  | 55:CA:882:C:H41   | 1.66                     | 0.42              |
| 14:CO:57:ARG:O    | 14:CO:61:GLN:HG2  | 2.18                     | 0.42              |
| 16:CQ:22:VAL:HG21 | 16:CQ:58:VAL:CG2  | 2.49                     | 0.42              |
| 20:CU:22:CYS:HB2  | 20:CU:23:GLU:H    | 1.51                     | 0.42              |
| 50:D0:31:LYS:H    | 50:D0:31:LYS:HG3  | 1.61                     | 0.42              |
| 52:D2:28:ARG:O    | 52:D2:31:LEU:N    | 2.50                     | 0.42              |
| 24:DA:1010:A:C2'  | 24:DA:1011:G:H5'' | 2.48                     | 0.42              |
| 24:DA:1031:G:N2   | 24:DA:1124:G:C4   | 2.87                     | 0.42              |
| 24:DA:1223:G:O6   | 41:DR:71:LYS:NZ   | 2.51                     | 0.42              |
| 24:DA:1455:G:C2   | 24:DA:1456:G:C4   | 3.07                     | 0.42              |
| 24:DA:1496:A:H2'  | 24:DA:1498:C:C4   | 2.53                     | 0.42              |
| 24:DA:1611:C:O2'  | 24:DA:1612:C:H5'  | 2.19                     | 0.42              |
| 24:DA:1647:U:H5'' | 24:DA:1648:U:OP1  | 2.19                     | 0.42              |
| 24:DA:1824:G:H2'  | 24:DA:1825:U:O4'  | 2.18                     | 0.42              |
| 24:DA:1838:C:N4   | 24:DA:1898:U:H2'  | 2.34                     | 0.42              |
| 24:DA:2023:C:O2'  | 24:DA:2024:G:O5'  | 2.35                     | 0.42              |
| 24:DA:2303:G:H5'  | 29:DF:121:PHE:CZ  | 2.53                     | 0.42              |
| 24:DA:2315:G:C6   | 24:DA:2316:G:C5   | 3.08                     | 0.42              |
| 24:DA:2459:A:C5   | 24:DA:2460:U:C5   | 3.07                     | 0.42              |
| 24:DA:2472:G:H1'  | 24:DA:2478:A:N6   | 2.34                     | 0.42              |
| 24:DA:289:G:H2'   | 24:DA:290:U:O4'   | 2.19                     | 0.42              |
| 24:DA:389:G:C6    | 24:DA:2413:G:O2'  | 2.71                     | 0.42              |
| 24:DA:615:U:H3'   | 24:DA:616:A:H5'   | 2.01                     | 0.42              |
| 24:DA:699:A:H5'   | 24:DA:699:A:H8    | 1.84                     | 0.42              |
| 24:DA:755:U:H2'   | 24:DA:756:A:C8    | 2.54                     | 0.42              |
| 24:DA:820:A:H2'   | 24:DA:821:A:O4'   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:DC:213:ARG:HB3 | 26:DC:214:GLY:H    | 1.47                     | 0.42              |
| 26:DC:63:ILE:O    | 26:DC:64:VAL:HB    | 2.19                     | 0.42              |
| 27:DD:19:GLY:O    | 34:DK:72:PRO:HB2   | 2.18                     | 0.42              |
| 27:DD:4:LEU:HD12  | 27:DD:32:ASN:OD1   | 2.19                     | 0.42              |
| 27:DD:45:TYR:CE2  | 27:DD:47:ALA:HB3   | 2.51                     | 0.42              |
| 24:DA:2060:A:H2'  | 28:DE:63:LYS:HZ3   | 1.83                     | 0.42              |
| 29:DF:41:GLU:O    | 29:DF:43:ILE:HG22  | 2.20                     | 0.42              |
| 32:DI:51:GLY:O    | 32:DI:52:LEU:CB    | 2.66                     | 0.42              |
| 36:DM:4:PRO:HD3   | 36:DM:68:PHE:HE2   | 1.83                     | 0.42              |
| 39:DP:102:ARG:O   | 39:DP:103:THR:CB   | 2.67                     | 0.42              |
| 24:DA:18:U:H5''   | 40:DQ:23:TYR:O     | 2.19                     | 0.42              |
| 41:DR:7:SER:HB2   | 41:DR:22:LEU:HB2   | 2.01                     | 0.42              |
| 24:DA:1342:A:OP1  | 43:DT:59:ASN:HB3   | 2.18                     | 0.42              |
| 47:DX:32:LEU:HD22 | 47:DX:32:LEU:N     | 2.34                     | 0.42              |
| 49:DZ:28:LEU:CD2  | 49:DZ:28:LEU:N     | 2.82                     | 0.42              |
| 21:AA:1054:C:O2   | 21:AA:1054:C:O4'   | 2.37                     | 0.42              |
| 21:AA:1262:C:N4   | 21:AA:1274:A:C2    | 2.88                     | 0.42              |
| 21:AA:1446:A:H2'  | 21:AA:1447:A:H5'   | 2.01                     | 0.42              |
| 21:AA:1468:A:C3'  | 21:AA:1469:C:H5''  | 2.49                     | 0.42              |
| 21:AA:138:G:C6    | 21:AA:226:G:C6     | 3.08                     | 0.42              |
| 21:AA:320:A:H2'   | 21:AA:321:A:C8     | 2.54                     | 0.42              |
| 21:AA:356:A:C2    | 21:AA:368:U:O2     | 2.72                     | 0.42              |
| 21:AA:373:A:O2'   | 21:AA:374:A:C5'    | 2.67                     | 0.42              |
| 21:AA:573:A:O2'   | 21:AA:574:A:H5'    | 2.19                     | 0.42              |
| 5:AF:53:LYS:HZ2   | 21:AA:710:G:H5''   | 1.79                     | 0.42              |
| 21:AA:578:C:O2    | 21:AA:728:A:H2     | 2.02                     | 0.42              |
| 21:AA:717:U:H3'   | 21:AA:734:G:OP2    | 2.20                     | 0.42              |
| 21:AA:984:C:O2'   | 21:AA:985:C:C5'    | 2.67                     | 0.42              |
| 1:AB:128:LEU:O    | 1:AB:129:THR:HG23  | 2.18                     | 0.42              |
| 1:AB:159:ALA:HB1  | 1:AB:181:PRO:O     | 2.18                     | 0.42              |
| 1:AB:63:LYS:NZ    | 1:AB:87:ASP:HB3    | 2.34                     | 0.42              |
| 2:AC:153:SER:HA   | 2:AC:156:LEU:HD11  | 2.02                     | 0.42              |
| 10:AK:89:GLY:O    | 10:AK:92:ARG:HB3   | 2.19                     | 0.42              |
| 12:AM:95:PRO:HG2  | 12:AM:101:THR:HG22 | 2.01                     | 0.42              |
| 14:AO:86:LEU:HD23 | 14:AO:86:LEU:N     | 2.34                     | 0.42              |
| 24:BA:1295:C:H2'  | 24:BA:1296:G:C8    | 2.54                     | 0.42              |
| 24:BA:1331:G:C5   | 24:BA:1333:G:N7    | 2.87                     | 0.42              |
| 24:BA:2231:U:OP1  | 47:BX:29:LEU:HD23  | 2.19                     | 0.42              |
| 24:BA:2287:A:C5   | 24:BA:2289:G:C5    | 3.07                     | 0.42              |
| 24:BA:2737:G:H2'  | 24:BA:2738:A:O4'   | 2.19                     | 0.42              |
| 24:BA:2854:G:C6   | 24:BA:2864:G:C6    | 3.07                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:606:U:OP1   | 28:BE:99:LYS:HD2   | 2.19                     | 0.42              |
| 24:BA:638:G:O2'   | 24:BA:639:U:O4'    | 2.23                     | 0.42              |
| 24:BA:715:A:N6    | 24:BA:716:A:C6     | 2.87                     | 0.42              |
| 24:BA:68:G:N3     | 24:BA:74:A:C8      | 2.87                     | 0.42              |
| 24:BA:78:U:H2'    | 24:BA:79:C:C6      | 2.55                     | 0.42              |
| 24:BA:860:U:C6    | 24:BA:2268:A:O4'   | 2.73                     | 0.42              |
| 25:BB:34:A:N6     | 25:BB:44:G:O2'     | 2.52                     | 0.42              |
| 26:BC:151:GLY:O   | 26:BC:152:GLN:HG3  | 2.19                     | 0.42              |
| 26:BC:18:VAL:O    | 26:BC:18:VAL:HG22  | 2.19                     | 0.42              |
| 26:BC:141:HIS:CB  | 26:BC:190:THR:HB   | 2.44                     | 0.42              |
| 26:BC:44:ASN:C    | 26:BC:44:ASN:OD1   | 2.57                     | 0.42              |
| 26:BC:83:ASP:OD1  | 26:BC:85:ASN:OD1   | 2.36                     | 0.42              |
| 27:BD:94:GLN:O    | 27:BD:95:SER:HB2   | 2.17                     | 0.42              |
| 28:BE:175:ILE:CG1 | 28:BE:180:LEU:HD11 | 2.49                     | 0.42              |
| 28:BE:48:THR:O    | 28:BE:52:VAL:HG23  | 2.19                     | 0.42              |
| 30:BG:8:VAL:CG1   | 30:BG:49:LEU:H     | 2.29                     | 0.42              |
| 33:BJ:35:ARG:C    | 33:BJ:37:ARG:N     | 2.72                     | 0.42              |
| 33:BJ:78:THR:OG1  | 33:BJ:80:HIS:HB2   | 2.19                     | 0.42              |
| 34:BK:119:ALA:HA  | 34:BK:120:PRO:HD2  | 1.67                     | 0.42              |
| 35:BL:66:PHE:CD1  | 35:BL:66:PHE:C     | 2.91                     | 0.42              |
| 38:BO:2:ASP:OD1   | 38:BO:3:LYS:HG2    | 2.19                     | 0.42              |
| 38:BO:59:ALA:HA   | 38:BO:62:LEU:HD12  | 2.01                     | 0.42              |
| 41:BR:49:ILE:HG21 | 41:BR:53:PHE:H     | 1.84                     | 0.42              |
| 43:BT:28:ASN:HA   | 43:BT:91:GLN:CD    | 2.40                     | 0.42              |
| 43:BT:29:THR:H    | 43:BT:91:GLN:NE2   | 2.17                     | 0.42              |
| 55:CA:1006:G:H2'  | 55:CA:1006:G:N3    | 2.34                     | 0.42              |
| 55:CA:1215:G:H2'  | 55:CA:1216:A:H8    | 1.84                     | 0.42              |
| 55:CA:1352:C:H2'  | 55:CA:1353:G:C8    | 2.54                     | 0.42              |
| 55:CA:1444:U:H2'  | 55:CA:1445:U:C6    | 2.54                     | 0.42              |
| 55:CA:190:A:H2'   | 55:CA:191:G:O4'    | 2.19                     | 0.42              |
| 55:CA:22:G:H5''   | 55:CA:561:U:N3     | 2.34                     | 0.42              |
| 55:CA:255:G:C2    | 55:CA:272:C:O2     | 2.72                     | 0.42              |
| 55:CA:41:G:N2     | 55:CA:402:G:C4     | 2.87                     | 0.42              |
| 55:CA:459:A:C2'   | 55:CA:460:A:H5'    | 2.48                     | 0.42              |
| 55:CA:487:A:H2'   | 55:CA:488:C:O4'    | 2.19                     | 0.42              |
| 55:CA:66:A:H8     | 55:CA:66:A:OP1     | 2.03                     | 0.42              |
| 55:CA:696:A:H1'   | 55:CA:786:G:O2'    | 2.20                     | 0.42              |
| 55:CA:764:C:C4    | 55:CA:812:G:O6     | 2.73                     | 0.42              |
| 55:CA:662:U:O2'   | 55:CA:836:G:OP1    | 2.35                     | 0.42              |
| 1:CB:218:ALA:O    | 1:CB:222:GLU:HB2   | 2.18                     | 0.42              |
| 1:CB:46:VAL:HA    | 1:CB:49:PHE:CZ     | 2.54                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:CC:129:PHE:CD2   | 2:CC:130:ARG:N     | 2.88                     | 0.42              |
| 2:CC:18:ASN:ND2    | 2:CC:53:ARG:HD3    | 2.34                     | 0.42              |
| 3:CD:61:ARG:NH2    | 3:CD:67:LEU:HA     | 2.34                     | 0.42              |
| 4:CE:22:LYS:HE3    | 55:CA:1082:A:OP2   | 2.19                     | 0.42              |
| 4:CE:80:LEU:HB3    | 4:CE:97:PRO:CA     | 2.49                     | 0.42              |
| 6:CG:70:PRO:HD2    | 6:CG:95:ARG:O      | 2.20                     | 0.42              |
| 8:CI:53:LEU:HD13   | 8:CI:53:LEU:O      | 2.19                     | 0.42              |
| 9:CJ:81:GLU:C      | 9:CJ:83:THR:H      | 2.23                     | 0.42              |
| 10:CK:27:ASN:ND2   | 10:CK:27:ASN:N     | 2.68                     | 0.42              |
| 17:CR:49:LYS:HE2   | 17:CR:50:TYR:CE2   | 2.54                     | 0.42              |
| 50:D0:21:LEU:HB3   | 50:D0:22:THR:H     | 1.55                     | 0.42              |
| 51:D1:34:GLU:HG3   | 51:D1:49:LYS:CB    | 2.48                     | 0.42              |
| 24:DA:1171:G:C4    | 24:DA:1179:G:N2    | 2.87                     | 0.42              |
| 24:DA:1208:C:N3    | 24:DA:1209:U:C5    | 2.87                     | 0.42              |
| 24:DA:1289:C:O2'   | 24:DA:1290:C:C6    | 2.70                     | 0.42              |
| 24:DA:1315:C:O2'   | 24:DA:1316:U:H5'   | 2.19                     | 0.42              |
| 24:DA:1471:G:C6    | 24:DA:1472:C:C4    | 3.07                     | 0.42              |
| 24:DA:1582:C:H2'   | 24:DA:1585:C:H42   | 1.83                     | 0.42              |
| 24:DA:1653:G:OP2   | 24:DA:1653:G:H8    | 2.01                     | 0.42              |
| 24:DA:1654:A:N3    | 24:DA:1655:A:C8    | 2.87                     | 0.42              |
| 24:DA:2056:G:N2    | 50:D0:1:ALA:H1     | 2.16                     | 0.42              |
| 24:DA:2307:G:C8    | 24:DA:2312:U:C5    | 3.07                     | 0.42              |
| 24:DA:244:A:O2'    | 24:DA:245:G:O4'    | 2.36                     | 0.42              |
| 24:DA:2625:G:C6    | 24:DA:2626:C:C4    | 3.07                     | 0.42              |
| 24:DA:2800:A:O2'   | 24:DA:2801:G:C4'   | 2.65                     | 0.42              |
| 24:DA:310:A:C2     | 24:DA:330:A:C4     | 3.06                     | 0.42              |
| 24:DA:455:C:C3'    | 24:DA:456:C:H5'    | 2.50                     | 0.42              |
| 24:DA:510:C:O5'    | 24:DA:510:C:H6     | 2.02                     | 0.42              |
| 24:DA:64:A:OP1     | 43:DT:77:ARG:HA    | 2.19                     | 0.42              |
| 24:DA:765:C:O2'    | 24:DA:766:U:O4'    | 2.37                     | 0.42              |
| 24:DA:862:G:C2     | 24:DA:863:A:H1'    | 2.54                     | 0.42              |
| 24:DA:61:C:C4      | 24:DA:94:A:N1      | 2.87                     | 0.42              |
| 28:DE:31:VAL:HG11  | 28:DE:100:MET:O    | 2.20                     | 0.42              |
| 28:DE:146:VAL:HG13 | 28:DE:187:VAL:HG23 | 2.02                     | 0.42              |
| 29:DF:37:MET:HE3   | 29:DF:56:LEU:HB2   | 2.00                     | 0.42              |
| 30:DG:122:ALA:O    | 30:DG:123:GLU:HB2  | 2.19                     | 0.42              |
| 33:DJ:43:GLU:HG2   | 33:DJ:43:GLU:O     | 2.20                     | 0.42              |
| 36:DM:23:GLY:O     | 36:DM:101:VAL:HG12 | 2.19                     | 0.42              |
| 37:DN:5:LYS:CG     | 37:DN:6:SER:H      | 2.28                     | 0.42              |
| 24:DA:2848:G:OP2   | 39:DP:94:ALA:CB    | 2.68                     | 0.42              |
| 24:DA:446:G:OP1    | 40:DQ:2:ARG:HD3    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:DQ:79:ILE:C    | 40:DQ:79:ILE:HD13  | 2.39                     | 0.42              |
| 41:DR:10:LYS:N    | 41:DR:10:LYS:HD2   | 2.33                     | 0.42              |
| 41:DR:43:ASN:HD22 | 41:DR:44:GLY:H     | 1.67                     | 0.42              |
| 42:DS:6:LYS:HD2   | 42:DS:8:ARG:HD2    | 2.01                     | 0.42              |
| 44:DU:39:ASN:O    | 44:DU:40:LEU:C     | 2.57                     | 0.42              |
| 46:DW:16:GLU:OE2  | 46:DW:16:GLU:HA    | 2.20                     | 0.42              |
| 46:DW:28:GLU:HG3  | 46:DW:29:SER:H     | 1.84                     | 0.42              |
| 21:AA:1008:U:C4   | 21:AA:1022:A:C6    | 3.07                     | 0.42              |
| 21:AA:1145:A:O2'  | 21:AA:1146:A:H5''  | 2.20                     | 0.42              |
| 21:AA:780:A:N7    | 21:AA:800:G:C6     | 2.87                     | 0.42              |
| 21:AA:91:U:C5     | 21:AA:92:U:N3      | 2.88                     | 0.42              |
| 21:AA:977:A:H3'   | 21:AA:1362:A:N6    | 2.32                     | 0.42              |
| 1:AB:88:GLN:HE21  | 1:AB:88:GLN:C      | 2.22                     | 0.42              |
| 2:AC:51:VAL:HG22  | 2:AC:52:SER:N      | 2.33                     | 0.42              |
| 2:AC:55:VAL:HG12  | 2:AC:56:ILE:H      | 1.84                     | 0.42              |
| 3:AD:149:LYS:NZ   | 3:AD:177:MET:HB2   | 2.34                     | 0.42              |
| 4:AE:121:ASN:N    | 4:AE:121:ASN:ND2   | 2.67                     | 0.42              |
| 6:AG:68:VAL:HB    | 6:AG:99:ALA:HB1    | 2.02                     | 0.42              |
| 7:AH:9:MET:HG2    | 7:AH:10:LEU:N      | 2.34                     | 0.42              |
| 14:AO:34:GLN:O    | 14:AO:35:ILE:C     | 2.57                     | 0.42              |
| 17:AR:40:PRO:CB   | 17:AR:42:ARG:HG2   | 2.49                     | 0.42              |
| 24:BA:1177:G:H2'  | 24:BA:1178:C:O4'   | 2.20                     | 0.42              |
| 24:BA:1204:A:C1'  | 24:BA:1206:G:C5    | 3.01                     | 0.42              |
| 24:BA:1205:A:C6   | 28:BE:165:HIS:HB2  | 2.55                     | 0.42              |
| 24:BA:1392:A:H62  | 43:BT:19:LYS:HD2   | 1.84                     | 0.42              |
| 24:BA:1437:C:C4   | 24:BA:1438:U:C4    | 3.07                     | 0.42              |
| 24:BA:1346:G:N2   | 24:BA:1601:G:C4    | 2.88                     | 0.42              |
| 24:BA:749:A:N7    | 24:BA:1618:A:C6    | 2.87                     | 0.42              |
| 24:BA:1670:C:N4   | 24:BA:1674:G:O5'   | 2.51                     | 0.42              |
| 24:BA:1808:A:C5'  | 24:BA:1809:A:OP2   | 2.68                     | 0.42              |
| 24:BA:2052:A:N7   | 27:BD:146:ILE:HD11 | 2.34                     | 0.42              |
| 24:BA:2075:U:C4   | 24:BA:2238:G:C6    | 3.07                     | 0.42              |
| 24:BA:2357:G:C2   | 24:BA:2361:G:C6    | 3.07                     | 0.42              |
| 24:BA:2366:A:C2   | 24:BA:2367:G:H1'   | 2.54                     | 0.42              |
| 24:BA:2661:G:C2'  | 24:BA:2662:A:H5'   | 2.50                     | 0.42              |
| 24:BA:296:U:H2'   | 24:BA:297:G:H8     | 1.84                     | 0.42              |
| 24:BA:30:G:C6     | 24:BA:31:C:C4      | 3.07                     | 0.42              |
| 24:BA:319:G:C5    | 24:BA:333:G:N2     | 2.88                     | 0.42              |
| 24:BA:555:G:C2'   | 24:BA:556:A:OP2    | 2.67                     | 0.42              |
| 24:BA:915:C:O2    | 25:BB:100:G:H4'    | 2.20                     | 0.42              |
| 24:BA:941:A:H2'   | 24:BA:942:G:O4'    | 2.18                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:987:C:H2'   | 24:BA:988:A:C5'    | 2.48                     | 0.42              |
| 26:BC:108:GLY:C   | 26:BC:109:LEU:HD22 | 2.39                     | 0.42              |
| 27:BD:172:VAL:O   | 27:BD:173:GLN:HB2  | 2.19                     | 0.42              |
| 28:BE:31:VAL:HG21 | 28:BE:104:ALA:HB2  | 2.02                     | 0.42              |
| 29:BF:80:GLN:OE1  | 29:BF:81:GLY:N     | 2.53                     | 0.42              |
| 30:BG:10:VAL:HB   | 30:BG:14:VAL:HG21  | 2.02                     | 0.42              |
| 31:BH:12:LEU:HD12 | 31:BH:19:VAL:HG11  | 2.02                     | 0.42              |
| 31:BH:27:ARG:NH1  | 47:BX:59:ASP:O     | 2.52                     | 0.42              |
| 31:BH:30:LEU:HA   | 31:BH:30:LEU:HD23  | 1.82                     | 0.42              |
| 31:BH:57:LYS:O    | 31:BH:61:VAL:HG23  | 2.20                     | 0.42              |
| 31:BH:66:ASN:O    | 31:BH:68:ARG:N     | 2.53                     | 0.42              |
| 31:BH:94:ILE:HG23 | 31:BH:98:ASP:HB3   | 2.02                     | 0.42              |
| 32:BI:115:ASP:C   | 32:BI:115:ASP:OD1  | 2.58                     | 0.42              |
| 32:BI:56:VAL:CG2  | 32:BI:68:PHE:HB2   | 2.49                     | 0.42              |
| 34:BK:88:ASN:C    | 34:BK:88:ASN:ND2   | 2.73                     | 0.42              |
| 35:BL:94:THR:HG22 | 35:BL:95:LEU:N     | 2.35                     | 0.42              |
| 37:BN:17:ARG:HH21 | 37:BN:17:ARG:HG3   | 1.85                     | 0.42              |
| 40:BQ:93:ILE:CG2  | 40:BQ:94:LEU:N     | 2.83                     | 0.42              |
| 41:BR:27:ILE:HG13 | 41:BR:33:VAL:CG1   | 2.49                     | 0.42              |
| 41:BR:38:VAL:HG12 | 41:BR:59:ILE:HG13  | 2.01                     | 0.42              |
| 24:BA:923:G:C5'   | 46:BW:25:PHE:CZ    | 3.01                     | 0.42              |
| 46:BW:30:VAL:HG23 | 46:BW:59:PHE:HD1   | 1.84                     | 0.42              |
| 46:BW:18:LYS:CA   | 46:BW:36:ILE:HG12  | 2.50                     | 0.42              |
| 55:CA:1091:U:O2   | 55:CA:1093:A:OP2   | 2.37                     | 0.42              |
| 55:CA:1282:C:C2   | 55:CA:1283:U:C4    | 3.08                     | 0.42              |
| 55:CA:1319:A:N6   | 55:CA:1323:G:N3    | 2.68                     | 0.42              |
| 55:CA:1433:A:C5   | 55:CA:1468:A:C2    | 3.08                     | 0.42              |
| 55:CA:1454:G:HO2' | 55:CA:1455:G:P     | 2.42                     | 0.42              |
| 19:CT:22:SER:CB   | 55:CA:1458:G:H4'   | 2.48                     | 0.42              |
| 55:CA:1473:G:H2'  | 55:CA:1474:U:O4'   | 2.19                     | 0.42              |
| 55:CA:218:U:H2'   | 55:CA:219:U:O4'    | 2.19                     | 0.42              |
| 55:CA:251:G:C5    | 55:CA:266:G:C5     | 3.06                     | 0.42              |
| 55:CA:348:G:O2'   | 55:CA:349:A:H5'    | 2.20                     | 0.42              |
| 55:CA:438:U:O2'   | 55:CA:439:U:C5     | 2.72                     | 0.42              |
| 55:CA:51:A:H4'    | 55:CA:52:C:C5'     | 2.49                     | 0.42              |
| 55:CA:499:A:N1    | 55:CA:546:A:H2'    | 2.35                     | 0.42              |
| 55:CA:631:C:O3'   | 55:CA:632:U:H6     | 2.02                     | 0.42              |
| 55:CA:654:G:C5    | 55:CA:753:A:C6     | 3.07                     | 0.42              |
| 11:CL:93:ARG:NH2  | 55:CA:911:U:OP2    | 2.53                     | 0.42              |
| 1:CB:104:LYS:H    | 1:CB:104:LYS:CD    | 2.11                     | 0.42              |
| 1:CB:137:THR:O    | 1:CB:140:LEU:HB3   | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CB:139:GLU:HG3  | 1:CB:140:LEU:H    | 1.84                     | 0.42              |
| 2:CC:113:LYS:O    | 2:CC:117:ASP:OD1  | 2.38                     | 0.42              |
| 3:CD:196:GLU:O    | 3:CD:199:ILE:HG12 | 2.20                     | 0.42              |
| 3:CD:98:ASP:OD1   | 3:CD:99:ASN:N     | 2.53                     | 0.42              |
| 5:CF:39:LEU:HD12  | 5:CF:61:LEU:O     | 2.19                     | 0.42              |
| 6:CG:104:VAL:O    | 6:CG:107:ALA:N    | 2.48                     | 0.42              |
| 6:CG:12:LEU:HB2   | 6:CG:13:PRO:HD2   | 2.01                     | 0.42              |
| 6:CG:78:ARG:HG3   | 6:CG:82:SER:O     | 2.19                     | 0.42              |
| 10:CK:109:ILE:O   | 20:CU:5:VAL:HB    | 2.20                     | 0.42              |
| 10:CK:16:SER:HA   | 10:CK:77:GLY:O    | 2.19                     | 0.42              |
| 10:CK:34:THR:HA   | 10:CK:41:LEU:HG   | 2.01                     | 0.42              |
| 12:CM:22:TYR:C    | 12:CM:65:GLU:HG2  | 2.40                     | 0.42              |
| 20:CU:7:GLU:HB3   | 20:CU:11:PHE:CE1  | 2.54                     | 0.42              |
| 54:D4:7:VAL:O     | 54:D4:8:LYS:O     | 2.37                     | 0.42              |
| 24:DA:1358:G:H1'  | 24:DA:1374:G:N2   | 2.34                     | 0.42              |
| 24:DA:1773:A:C8   | 24:DA:1829:A:C8   | 3.08                     | 0.42              |
| 24:DA:1906:G:H5'' | 24:DA:1929:G:O2'  | 2.20                     | 0.42              |
| 24:DA:1910:G:N1   | 24:DA:1921:G:C5   | 2.87                     | 0.42              |
| 24:DA:2030:A:C2   | 24:DA:2499:C:OP1  | 2.72                     | 0.42              |
| 24:DA:2074:U:C2   | 24:DA:2436:G:C2   | 3.07                     | 0.42              |
| 24:DA:2083:G:O2'  | 24:DA:2084:C:H5'  | 2.19                     | 0.42              |
| 24:DA:230:G:C2    | 24:DA:231:A:N7    | 2.87                     | 0.42              |
| 24:DA:2459:A:O2'  | 24:DA:2460:U:C5'  | 2.65                     | 0.42              |
| 24:DA:2520:C:C4   | 24:DA:2567:G:C5   | 3.07                     | 0.42              |
| 24:DA:255:A:H2'   | 24:DA:256:A:O4'   | 2.19                     | 0.42              |
| 24:DA:2733:A:C2   | 24:DA:2734:A:C4   | 3.08                     | 0.42              |
| 24:DA:2810:A:H2'  | 24:DA:2811:G:O4'  | 2.19                     | 0.42              |
| 24:DA:340:A:H2'   | 24:DA:341:C:H5'   | 2.01                     | 0.42              |
| 24:DA:38:A:N6     | 24:DA:39:G:C5     | 2.88                     | 0.42              |
| 24:DA:503:A:C2    | 24:DA:505:A:C2    | 3.07                     | 0.42              |
| 24:DA:540:C:O2'   | 24:DA:541:A:H5'   | 2.19                     | 0.42              |
| 24:DA:668:A:N7    | 24:DA:670:A:N7    | 2.67                     | 0.42              |
| 24:DA:781:A:N1    | 24:DA:1776:G:O2'  | 2.44                     | 0.42              |
| 24:DA:783:A:HO2'  | 24:DA:784:G:H4'   | 1.81                     | 0.42              |
| 24:DA:956:G:C2    | 24:DA:962:G:O6    | 2.72                     | 0.42              |
| 24:DA:976:G:O6    | 24:DA:988:A:C2    | 2.73                     | 0.42              |
| 56:DB:17:C:O2'    | 56:DB:18:G:H5'    | 2.18                     | 0.42              |
| 26:DC:30:ALA:C    | 26:DC:32:LEU:H    | 2.22                     | 0.42              |
| 26:DC:82:TYR:O    | 26:DC:84:PRO:CD   | 2.64                     | 0.42              |
| 24:DA:443:A:N6    | 28:DE:36:ALA:HB1  | 2.34                     | 0.42              |
| 24:DA:615:U:O4    | 28:DE:39:ALA:HB2  | 2.19                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:DF:11:VAL:CG1  | 29:DF:12:VAL:N     | 2.83                     | 0.42              |
| 29:DF:136:ILE:CG2 | 29:DF:142:TYR:HB2  | 2.49                     | 0.42              |
| 31:DH:40:THR:O    | 31:DH:42:LYS:N     | 2.45                     | 0.42              |
| 32:DI:42:ASN:HA   | 32:DI:45:THR:HB    | 2.01                     | 0.42              |
| 32:DI:7:TYR:HD1   | 32:DI:9:LYS:NZ     | 2.17                     | 0.42              |
| 32:DI:78:LEU:O    | 32:DI:81:LYS:HG2   | 2.18                     | 0.42              |
| 36:DM:19:GLY:O    | 36:DM:20:LEU:HB2   | 2.19                     | 0.42              |
| 36:DM:34:LYS:HB3  | 36:DM:129:THR:HG22 | 2.01                     | 0.42              |
| 40:DQ:10:ARG:HB2  | 40:DQ:10:ARG:NH1   | 2.34                     | 0.42              |
| 43:DT:48:GLN:HA   | 43:DT:48:GLN:NE2   | 2.33                     | 0.42              |
| 45:DV:63:ILE:HG22 | 45:DV:63:ILE:O     | 2.20                     | 0.42              |
| 46:DW:77:LYS:O    | 46:DW:78:PHE:CB    | 2.67                     | 0.42              |
| 21:AA:113:G:C4    | 21:AA:114:U:C5     | 3.07                     | 0.42              |
| 21:AA:1360:A:C4   | 21:AA:1361:G:C8    | 3.08                     | 0.42              |
| 21:AA:1346:A:N1   | 21:AA:1374:A:H5''  | 2.34                     | 0.42              |
| 21:AA:154:U:C2    | 21:AA:168:G:N2     | 2.88                     | 0.42              |
| 21:AA:216:U:H2'   | 21:AA:217:C:C6     | 2.54                     | 0.42              |
| 21:AA:320:A:C2    | 21:AA:334:C:C2     | 3.07                     | 0.42              |
| 21:AA:420:U:O2    | 21:AA:424:G:C2     | 2.73                     | 0.42              |
| 21:AA:373:A:H1'   | 21:AA:481:G:N3     | 2.34                     | 0.42              |
| 11:AL:11:ARG:HB3  | 21:AA:562:U:H1'    | 2.02                     | 0.42              |
| 14:AO:64:LYS:HD2  | 21:AA:755:G:OP2    | 2.19                     | 0.42              |
| 21:AA:841:C:H5'   | 21:AA:843:U:OP2    | 2.20                     | 0.42              |
| 21:AA:925:G:C5    | 21:AA:927:G:N7     | 2.88                     | 0.42              |
| 1:AB:67:LEU:HB3   | 1:AB:160:LEU:CD1   | 2.48                     | 0.42              |
| 6:AG:88:VAL:HG22  | 6:AG:89:GLU:N      | 2.25                     | 0.42              |
| 8:AI:27:ILE:HG22  | 8:AI:28:VAL:N      | 2.34                     | 0.42              |
| 10:AK:86:LYS:CG   | 10:AK:114:PRO:HD3  | 2.49                     | 0.42              |
| 9:AJ:52:LEU:HB2   | 13:AN:80:ARG:HD2   | 2.01                     | 0.42              |
| 14:AO:84:LEU:HB3  | 14:AO:86:LEU:CD2   | 2.50                     | 0.42              |
| 18:AS:20:LYS:HB3  | 18:AS:20:LYS:HZ2   | 1.85                     | 0.42              |
| 19:AT:24:ARG:HG2  | 19:AT:28:ARG:HH12  | 1.82                     | 0.42              |
| 20:AU:36:PHE:HB3  | 20:AU:40:PRO:HD3   | 2.02                     | 0.42              |
| 22:AX:38:A:C6     | 22:AX:39:U:C4      | 3.07                     | 0.42              |
| 51:B1:12:SER:HB2  | 51:B1:48:TYR:CE1   | 2.54                     | 0.42              |
| 24:BA:1006:C:C5   | 24:BA:1138:G:N2    | 2.87                     | 0.42              |
| 24:BA:1408:G:N1   | 24:BA:1595:C:C2    | 2.87                     | 0.42              |
| 24:BA:1496:A:H2'  | 24:BA:1498:C:C4    | 2.53                     | 0.42              |
| 24:BA:1532:A:C6   | 24:BA:1540:G:C6    | 3.08                     | 0.42              |
| 24:BA:1565:C:O2'  | 24:BA:1566:A:O5'   | 2.34                     | 0.42              |
| 24:BA:2310:C:H6   | 24:BA:2310:C:O5'   | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:2417:C:O2'  | 24:BA:2418:A:H5'  | 2.19                     | 0.42              |
| 24:BA:238:C:O2    | 24:BA:260:G:C2    | 2.73                     | 0.42              |
| 24:BA:9:G:H2'     | 24:BA:2629:U:O4   | 2.19                     | 0.42              |
| 24:BA:2648:G:H2'  | 24:BA:2649:C:C6   | 2.54                     | 0.42              |
| 24:BA:2830:C:O3'  | 27:BD:56:LYS:NZ   | 2.53                     | 0.42              |
| 24:BA:2850:A:H2'  | 24:BA:2851:A:H8   | 1.82                     | 0.42              |
| 24:BA:32:C:OP1    | 24:BA:1238:G:H5'' | 2.20                     | 0.42              |
| 24:BA:364:C:H2'   | 24:BA:365:U:C6    | 2.55                     | 0.42              |
| 24:BA:455:C:H42   | 24:BA:472:A:H2'   | 1.85                     | 0.42              |
| 24:BA:634:C:H6    | 24:BA:634:C:O5'   | 2.02                     | 0.42              |
| 24:BA:7:G:C6      | 24:BA:8:C:N4      | 2.87                     | 0.42              |
| 26:BC:139:THR:O   | 26:BC:161:VAL:O   | 2.38                     | 0.42              |
| 26:BC:69:ASN:O    | 26:BC:70:LYS:C    | 2.56                     | 0.42              |
| 24:BA:2530:A:H3'  | 30:BG:156:TYR:OH  | 2.19                     | 0.42              |
| 31:BH:66:ASN:C    | 31:BH:68:ARG:N    | 2.72                     | 0.42              |
| 31:BH:67:ALA:C    | 31:BH:69:ALA:N    | 2.73                     | 0.42              |
| 32:BI:123:ALA:HA  | 32:BI:126:ARG:CZ  | 2.48                     | 0.42              |
| 32:BI:37:PHE:HD1  | 32:BI:37:PHE:O    | 2.02                     | 0.42              |
| 32:BI:56:VAL:HG22 | 32:BI:68:PHE:HB2  | 2.01                     | 0.42              |
| 32:BI:31:GLY:HA3  | 32:BI:60:VAL:HG11 | 2.01                     | 0.42              |
| 33:BJ:93:ILE:O    | 33:BJ:97:PRO:HG3  | 2.19                     | 0.42              |
| 34:BK:121:GLU:O   | 34:BK:122:VAL:C   | 2.58                     | 0.42              |
| 35:BL:74:THR:CG2  | 35:BL:107:PHE:HB2 | 2.21                     | 0.42              |
| 35:BL:120:VAL:CG1 | 35:BL:121:THR:N   | 2.82                     | 0.42              |
| 35:BL:19:LEU:HA   | 35:BL:27:LEU:O    | 2.20                     | 0.42              |
| 40:BQ:86:SER:HB3  | 41:BR:51:VAL:CG1  | 2.50                     | 0.42              |
| 55:CA:1102:A:O2'  | 55:CA:1103:C:C5'  | 2.68                     | 0.42              |
| 55:CA:1124:G:C4'  | 55:CA:1125:U:OP1  | 2.65                     | 0.42              |
| 55:CA:1349:A:H3'  | 55:CA:1350:A:H8   | 1.84                     | 0.42              |
| 55:CA:1380:U:H5'  | 55:CA:1381:U:OP1  | 2.19                     | 0.42              |
| 55:CA:1480:A:N1   | 55:CA:1481:U:C2   | 2.88                     | 0.42              |
| 55:CA:1499:A:C8   | 55:CA:1499:A:O5'  | 2.72                     | 0.42              |
| 55:CA:178:C:H2'   | 55:CA:179:A:O4'   | 2.18                     | 0.42              |
| 55:CA:261:U:C2    | 55:CA:263:A:OP2   | 2.72                     | 0.42              |
| 55:CA:253:A:C6    | 55:CA:274:A:C2    | 3.07                     | 0.42              |
| 55:CA:28:A:C5     | 55:CA:29:U:C6     | 3.07                     | 0.42              |
| 55:CA:380:G:N2    | 55:CA:382:A:H2'   | 2.34                     | 0.42              |
| 55:CA:532:A:N6    | 55:CA:1206:G:O2'  | 2.52                     | 0.42              |
| 55:CA:695:A:H61   | 55:CA:797:C:C1'   | 2.29                     | 0.42              |
| 55:CA:760:G:C5    | 55:CA:761:G:C8    | 3.07                     | 0.42              |
| 55:CA:83:C:O2     | 55:CA:83:C:C2'    | 2.67                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CB:103:TRP:HA    | 1:CB:106:VAL:CB   | 2.44                     | 0.42              |
| 1:CB:30:ILE:HD11   | 1:CB:188:THR:HG22 | 2.02                     | 0.42              |
| 2:CC:122:GLN:O     | 2:CC:127:VAL:HG22 | 2.19                     | 0.42              |
| 6:CG:70:PRO:HG2    | 6:CG:94:ARG:O     | 2.18                     | 0.42              |
| 7:CH:95:MET:HE2    | 7:CH:95:MET:HB3   | 1.85                     | 0.42              |
| 9:CJ:20:GLN:O      | 9:CJ:23:ALA:HB3   | 2.19                     | 0.42              |
| 13:CN:80:ARG:C     | 13:CN:82:LYS:N    | 2.72                     | 0.42              |
| 19:CT:23:ARG:HE    | 19:CT:23:ARG:HA   | 1.85                     | 0.42              |
| 20:CU:53:LYS:HB2   | 20:CU:53:LYS:HZ2  | 1.85                     | 0.42              |
| 54:D4:9:LYS:HD3    | 54:D4:9:LYS:C     | 2.40                     | 0.42              |
| 24:DA:1008:A:C4'   | 24:DA:1009:A:OP1  | 2.66                     | 0.42              |
| 24:DA:1139:G:O2'   | 24:DA:1140:C:H5'  | 2.18                     | 0.42              |
| 24:DA:1247:A:N7    | 24:DA:1249:U:O4   | 2.53                     | 0.42              |
| 24:DA:1281:G:O2'   | 24:DA:1282:U:H5'  | 2.19                     | 0.42              |
| 24:DA:1307:A:C6    | 24:DA:1308:A:C5   | 3.08                     | 0.42              |
| 24:DA:1422:G:H1'   | 24:DA:1495:A:H61  | 1.85                     | 0.42              |
| 24:DA:1505:A:C2    | 24:DA:1506:U:C2   | 3.08                     | 0.42              |
| 24:DA:1566:A:N3    | 26:DC:212:TRP:HB2 | 2.34                     | 0.42              |
| 24:DA:1870:C:H5''  | 24:DA:1871:A:C2   | 2.55                     | 0.42              |
| 24:DA:2040:G:C6    | 24:DA:2041:U:C4   | 3.08                     | 0.42              |
| 24:DA:216:A:N3     | 24:DA:217:A:C8    | 2.88                     | 0.42              |
| 24:DA:2229:U:C2    | 24:DA:2230:G:C8   | 3.08                     | 0.42              |
| 24:DA:2297:A:O2'   | 24:DA:2298:A:C5'  | 2.67                     | 0.42              |
| 24:DA:2323:G:N2    | 24:DA:2335:A:C2   | 2.88                     | 0.42              |
| 24:DA:2454:G:C2    | 24:DA:2499:C:N3   | 2.87                     | 0.42              |
| 24:DA:347:A:H2'    | 24:DA:348:A:C8    | 2.55                     | 0.42              |
| 24:DA:642:U:H4'    | 24:DA:2349:G:O2'  | 2.19                     | 0.42              |
| 24:DA:743:A:H2'    | 24:DA:744:U:O4'   | 2.19                     | 0.42              |
| 24:DA:75:G:O2'     | 24:DA:76:C:O5'    | 2.38                     | 0.42              |
| 24:DA:846:U:H4'    | 24:DA:847:U:O2    | 2.19                     | 0.42              |
| 24:DA:89:A:C6      | 24:DA:90:U:C4     | 3.08                     | 0.42              |
| 26:DC:28:PRO:HB3   | 26:DC:62:ARG:NH2  | 2.34                     | 0.42              |
| 27:DD:115:GLY:O    | 37:DN:3:HIS:HE1   | 2.03                     | 0.42              |
| 27:DD:124:ARG:CD   | 27:DD:125:TRP:CD1 | 2.82                     | 0.42              |
| 28:DE:132:LYS:HG2  | 28:DE:132:LYS:O   | 2.20                     | 0.42              |
| 31:DH:9:VAL:HG12   | 31:DH:10:ALA:N    | 2.34                     | 0.42              |
| 31:DH:2:GLN:HB3    | 31:DH:18:GLN:CD   | 2.40                     | 0.42              |
| 31:DH:68:ARG:CG    | 31:DH:71:LYS:HD3  | 2.49                     | 0.42              |
| 35:DL:128:THR:HG22 | 35:DL:130:GLY:H   | 1.84                     | 0.42              |
| 36:DM:57:VAL:O     | 36:DM:58:LYS:HB2  | 2.20                     | 0.42              |
| 24:DA:962:G:N2     | 36:DM:82:MET:CE   | 2.82                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:DQ:21:LYS:HA   | 40:DQ:21:LYS:HD2  | 1.83                     | 0.42              |
| 41:DR:27:ILE:CG2  | 41:DR:28:ALA:H    | 2.15                     | 0.42              |
| 42:DS:36:LEU:C    | 42:DS:38:TYR:N    | 2.72                     | 0.42              |
| 42:DS:74:ILE:HG12 | 42:DS:74:ILE:O    | 2.17                     | 0.42              |
| 24:DA:456:C:HO2'  | 43:DT:73:ARG:HG3  | 1.80                     | 0.42              |
| 46:DW:43:LYS:HD2  | 46:DW:79:ILE:HD11 | 2.01                     | 0.42              |
| 49:DZ:51:SER:C    | 49:DZ:53:MET:N    | 2.72                     | 0.42              |
| 21:AA:1074:G:C2   | 21:AA:1102:A:C6   | 3.08                     | 0.42              |
| 6:AG:32:ASP:O     | 21:AA:1351:U:H1'  | 2.19                     | 0.42              |
| 21:AA:215:C:O2'   | 21:AA:216:U:H5'   | 2.19                     | 0.42              |
| 21:AA:39:G:N2     | 21:AA:40:C:C2     | 2.88                     | 0.42              |
| 21:AA:488:C:O2'   | 21:AA:489:C:H5'   | 2.20                     | 0.42              |
| 21:AA:678:U:O2'   | 21:AA:679:C:H5'   | 2.20                     | 0.42              |
| 21:AA:687:A:C2    | 21:AA:704:A:C6    | 3.07                     | 0.42              |
| 21:AA:724:G:H2'   | 21:AA:725:G:H8    | 1.84                     | 0.42              |
| 10:AK:125:LYS:HG3 | 21:AA:797:C:OP2   | 2.17                     | 0.42              |
| 1:AB:102:ASN:C    | 1:AB:104:LYS:H    | 2.22                     | 0.42              |
| 1:AB:104:LYS:HB3  | 1:AB:104:LYS:HE2  | 1.89                     | 0.42              |
| 1:AB:110:ILE:CG1  | 1:AB:147:LEU:HD13 | 2.49                     | 0.42              |
| 2:AC:139:ASN:HD22 | 2:AC:139:ASN:H    | 1.66                     | 0.42              |
| 3:AD:149:LYS:HZ3  | 3:AD:177:MET:HB2  | 1.84                     | 0.42              |
| 4:AE:48:GLY:HA3   | 4:AE:65:LYS:C     | 2.40                     | 0.42              |
| 6:AG:76:SER:HA    | 6:AG:85:GLN:CB    | 2.48                     | 0.42              |
| 9:AJ:45:ARG:HD3   | 9:AJ:45:ARG:HA    | 1.88                     | 0.42              |
| 9:AJ:50:THR:HG22  | 9:AJ:64:GLN:CG    | 2.49                     | 0.42              |
| 10:AK:125:LYS:HG3 | 21:AA:797:C:P     | 2.59                     | 0.42              |
| 11:AL:9:LYS:NZ    | 11:AL:9:LYS:HB2   | 2.34                     | 0.42              |
| 12:AM:44:ILE:C    | 12:AM:46:GLU:H    | 2.23                     | 0.42              |
| 15:AP:35:ARG:HH21 | 15:AP:51:ARG:CZ   | 2.32                     | 0.42              |
| 20:AU:13:VAL:HG13 | 20:AU:15:LEU:CG   | 2.50                     | 0.42              |
| 20:AU:46:ARG:HG3  | 20:AU:49:ALA:HB3  | 2.00                     | 0.42              |
| 52:B2:24:THR:HG23 | 52:B2:27:GLY:N    | 2.31                     | 0.42              |
| 24:BA:1064:C:C1'  | 32:BI:89:SER:HB2  | 2.50                     | 0.42              |
| 24:BA:1177:G:C5   | 24:BA:1178:C:C5   | 3.08                     | 0.42              |
| 24:BA:117:G:C6    | 24:BA:119:A:C6    | 3.08                     | 0.42              |
| 24:BA:1530:G:C2   | 24:BA:1542:U:O2   | 2.72                     | 0.42              |
| 24:BA:1781:U:O2'  | 24:BA:1782:U:OP2  | 2.37                     | 0.42              |
| 24:BA:2027:G:H2'  | 24:BA:2028:U:C6   | 2.54                     | 0.42              |
| 24:BA:2180:U:H2'  | 24:BA:2181:U:C6   | 2.55                     | 0.42              |
| 24:BA:2253:G:C4   | 24:BA:2254:C:C5   | 3.07                     | 0.42              |
| 24:BA:2552:U:C2   | 24:BA:2554:U:C5'  | 3.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:10:A:C5     | 24:BA:2800:A:N6   | 2.87                     | 0.42              |
| 24:BA:312:G:O2'   | 24:BA:313:G:H5'   | 2.19                     | 0.42              |
| 24:BA:357:C:H2'   | 24:BA:358:U:C6    | 2.54                     | 0.42              |
| 24:BA:42:A:C2     | 24:BA:438:G:C5    | 3.08                     | 0.42              |
| 24:BA:529:A:H2'   | 24:BA:2023:C:N4   | 2.33                     | 0.42              |
| 24:BA:556:A:H3'   | 24:BA:557:C:H6    | 1.84                     | 0.42              |
| 24:BA:633:A:C5'   | 24:BA:633:A:H8    | 2.31                     | 0.42              |
| 24:BA:753:A:O2'   | 24:BA:754:U:C5'   | 2.68                     | 0.42              |
| 25:BB:13:G:O2'    | 25:BB:14:U:H5''   | 2.20                     | 0.42              |
| 26:BC:259:ASN:O   | 26:BC:260:LYS:CB  | 2.65                     | 0.42              |
| 27:BD:176:ASP:OD2 | 27:BD:176:ASP:N   | 2.53                     | 0.42              |
| 27:BD:42:ASN:O    | 27:BD:43:ASP:O    | 2.38                     | 0.42              |
| 28:BE:37:ALA:C    | 28:BE:39:ALA:N    | 2.69                     | 0.42              |
| 30:BG:7:PRO:HB2   | 30:BG:8:VAL:H     | 1.71                     | 0.42              |
| 32:BI:9:LYS:HB2   | 32:BI:55:PRO:CB   | 2.50                     | 0.42              |
| 33:BJ:121:LYS:HE3 | 33:BJ:121:LYS:HB2 | 1.67                     | 0.42              |
| 34:BK:2:ILE:O     | 34:BK:3:GLN:O     | 2.38                     | 0.42              |
| 37:BN:100:CYS:SG  | 37:BN:111:ALA:HA  | 2.60                     | 0.42              |
| 37:BN:85:PRO:HA   | 37:BN:88:ALA:HB2  | 2.00                     | 0.42              |
| 55:CA:1002:G:N2   | 55:CA:1039:G:C4   | 2.88                     | 0.42              |
| 55:CA:1040:U:O2'  | 55:CA:1041:G:H5'  | 2.20                     | 0.42              |
| 8:CI:125:GLN:HB3  | 55:CA:1342:C:H4'  | 2.02                     | 0.42              |
| 55:CA:1363:A:H2'  | 55:CA:1365:G:N7   | 2.35                     | 0.42              |
| 55:CA:1448:C:HO2' | 55:CA:1449:C:H6   | 1.56                     | 0.42              |
| 55:CA:1449:C:C2   | 55:CA:1455:G:C2   | 3.08                     | 0.42              |
| 55:CA:16:A:C2     | 55:CA:17:U:C6     | 3.07                     | 0.42              |
| 55:CA:174:A:OP1   | 55:CA:174:A:H3'   | 2.19                     | 0.42              |
| 55:CA:202:G:H2'   | 55:CA:203:G:H8    | 1.78                     | 0.42              |
| 55:CA:386:C:H2'   | 55:CA:387:U:H5'   | 2.01                     | 0.42              |
| 55:CA:724:G:O2'   | 55:CA:725:G:C5'   | 2.67                     | 0.42              |
| 55:CA:878:A:C5    | 55:CA:879:C:C5    | 3.07                     | 0.42              |
| 55:CA:957:U:N3    | 55:CA:960:U:C2    | 2.87                     | 0.42              |
| 2:CC:129:PHE:CG   | 2:CC:130:ARG:N    | 2.87                     | 0.42              |
| 2:CC:190:THR:CG2  | 2:CC:191:THR:N    | 2.83                     | 0.42              |
| 2:CC:199:VAL:HG23 | 2:CC:199:VAL:O    | 2.20                     | 0.42              |
| 3:CD:2:ARG:NH2    | 3:CD:114:ARG:HD3  | 2.27                     | 0.42              |
| 4:CE:25:LYS:HB2   | 4:CE:25:LYS:HZ2   | 1.84                     | 0.42              |
| 5:CF:43:GLY:HA2   | 5:CF:58:HIS:HE1   | 1.84                     | 0.42              |
| 6:CG:64:ALA:HB2   | 6:CG:126:ALA:CB   | 2.48                     | 0.42              |
| 8:CI:54:VAL:HG23  | 8:CI:59:LYS:HZ3   | 1.84                     | 0.42              |
| 9:CJ:49:PHE:CD1   | 9:CJ:67:ILE:HD11  | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:CK:51:PHE:CE2  | 10:CK:64:VAL:HG21 | 2.51                     | 0.42              |
| 14:CO:88:ARG:HD2  | 24:DA:716:A:OP1   | 2.19                     | 0.42              |
| 18:CS:27:LYS:HE3  | 18:CS:30:LEU:HD11 | 2.02                     | 0.42              |
| 19:CT:17:ARG:HD2  | 19:CT:17:ARG:O    | 2.20                     | 0.42              |
| 20:CU:14:ALA:O    | 20:CU:15:LEU:O    | 2.38                     | 0.42              |
| 50:D0:53:VAL:O    | 50:D0:54:ILE:O    | 2.37                     | 0.42              |
| 24:DA:1127:A:HO2' | 24:DA:1128:G:H5'  | 1.82                     | 0.42              |
| 24:DA:1130:U:O2'  | 24:DA:1131:G:C8   | 2.66                     | 0.42              |
| 24:DA:1208:C:H2'  | 24:DA:1209:U:H5'  | 2.02                     | 0.42              |
| 24:DA:579:G:N2    | 24:DA:1262:A:C4   | 2.88                     | 0.42              |
| 24:DA:1304:A:C6   | 24:DA:1305:C:C4   | 3.07                     | 0.42              |
| 24:DA:1534:U:C2'  | 24:DA:1534:U:O2   | 2.67                     | 0.42              |
| 24:DA:1394:U:H4'  | 24:DA:1603:A:H4'  | 2.02                     | 0.42              |
| 24:DA:1710:G:C2   | 24:DA:1749:A:C2   | 3.07                     | 0.42              |
| 24:DA:1815:A:C4   | 24:DA:1817:G:C6   | 3.07                     | 0.42              |
| 24:DA:1819:A:C1'  | 24:DA:1821:A:C6   | 2.95                     | 0.42              |
| 24:DA:2093:G:C5   | 24:DA:2225:A:C8   | 3.08                     | 0.42              |
| 24:DA:2489:U:C5   | 24:DA:2490:G:C6   | 3.08                     | 0.42              |
| 24:DA:2811:G:H2'  | 24:DA:2812:G:C8   | 2.55                     | 0.42              |
| 24:DA:360:U:H2'   | 24:DA:361:G:O4'   | 2.19                     | 0.42              |
| 24:DA:406:G:H2'   | 24:DA:407:G:H8    | 1.85                     | 0.42              |
| 24:DA:522:A:C4    | 24:DA:523:C:C5    | 3.08                     | 0.42              |
| 24:DA:597:G:C6    | 24:DA:598:U:C2    | 3.07                     | 0.42              |
| 24:DA:605:G:H21   | 24:DA:658:U:H5''  | 1.85                     | 0.42              |
| 24:DA:668:A:N3    | 24:DA:670:A:N6    | 2.68                     | 0.42              |
| 24:DA:705:A:H61   | 24:DA:726:G:H1'   | 1.83                     | 0.42              |
| 24:DA:705:A:C2    | 24:DA:727:A:O4'   | 2.72                     | 0.42              |
| 24:DA:736:C:H2'   | 24:DA:737:C:H6    | 1.84                     | 0.42              |
| 24:DA:759:G:C2    | 24:DA:760:G:C4    | 3.08                     | 0.42              |
| 24:DA:975:A:C8    | 24:DA:990:A:N6    | 2.85                     | 0.42              |
| 56:DB:58:A:O2'    | 56:DB:59:A:H5'    | 2.20                     | 0.42              |
| 26:DC:79:ARG:CG   | 26:DC:92:LEU:HB2  | 2.49                     | 0.42              |
| 29:DF:31:GLU:HG3  | 29:DF:32:LYS:N    | 2.35                     | 0.42              |
| 29:DF:43:ILE:HG23 | 29:DF:44:ALA:N    | 2.26                     | 0.42              |
| 31:DH:45:GLU:C    | 31:DH:47:PHE:H    | 2.21                     | 0.42              |
| 32:DI:57:VAL:HG12 | 32:DI:58:ILE:N    | 2.28                     | 0.42              |
| 42:DS:29:VAL:O    | 42:DS:33:LEU:HB2  | 2.20                     | 0.42              |
| 48:DY:22:LEU:HG   | 48:DY:23:ARG:H    | 1.84                     | 0.42              |
| 49:DZ:6:ILE:HG22  | 49:DZ:7:THR:N     | 2.35                     | 0.42              |
| 21:AA:1110:A:N6   | 21:AA:1111:A:C6   | 2.87                     | 0.42              |
| 21:AA:1202:U:O2'  | 21:AA:1203:C:H5'  | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:1343:G:C2   | 21:AA:1344:C:C2   | 3.08                     | 0.42              |
| 21:AA:1367:C:H2'  | 21:AA:1368:A:O4'  | 2.20                     | 0.42              |
| 21:AA:1441:A:H62  | 21:AA:1461:G:H21  | 1.68                     | 0.42              |
| 21:AA:223:A:C4    | 21:AA:224:U:C5    | 3.07                     | 0.42              |
| 21:AA:428:G:C1'   | 21:AA:430:A:C8    | 3.03                     | 0.42              |
| 21:AA:645:G:C2'   | 21:AA:646:G:H5'   | 2.50                     | 0.42              |
| 21:AA:852:G:N1    | 21:AA:853:C:C2    | 2.87                     | 0.42              |
| 1:AB:186:VAL:CG2  | 1:AB:198:VAL:HG23 | 2.49                     | 0.42              |
| 2:AC:122:GLN:O    | 2:AC:127:VAL:HG22 | 2.19                     | 0.42              |
| 2:AC:15:LYS:CD    | 2:AC:16:PRO:HD2   | 2.48                     | 0.42              |
| 2:AC:5:HIS:NE2    | 2:AC:183:TYR:CE2  | 2.87                     | 0.42              |
| 7:AH:21:LYS:N     | 7:AH:64:TYR:OH    | 2.50                     | 0.42              |
| 7:AH:95:MET:SD    | 7:AH:129:ALA:HB1  | 2.59                     | 0.42              |
| 8:AI:61:ASP:CG    | 8:AI:62:LEU:H     | 2.22                     | 0.42              |
| 8:AI:99:LYS:HE3   | 8:AI:99:LYS:HB3   | 1.85                     | 0.42              |
| 12:AM:47:LEU:HD22 | 12:AM:52:ILE:HB   | 2.02                     | 0.42              |
| 18:AS:5:LYS:HD3   | 21:AA:1314:C:C6   | 2.55                     | 0.42              |
| 20:AU:38:GLU:HA   | 20:AU:38:GLU:OE1  | 2.20                     | 0.42              |
| 24:BA:1055:G:H2'  | 24:BA:1056:G:O4'  | 2.19                     | 0.42              |
| 24:BA:1107:G:H2'  | 24:BA:1108:U:C6   | 2.55                     | 0.42              |
| 24:BA:1360:G:H5'  | 24:BA:1361:G:OP2  | 2.19                     | 0.42              |
| 24:BA:1511:G:C2'  | 24:BA:1512:C:OP2  | 2.65                     | 0.42              |
| 24:BA:1608:A:O2'  | 24:BA:1610:A:OP1  | 2.36                     | 0.42              |
| 24:BA:1831:G:C5   | 24:BA:1832:C:C5   | 3.07                     | 0.42              |
| 24:BA:2024:G:C6   | 24:BA:2025:C:N3   | 2.88                     | 0.42              |
| 24:BA:2197:U:O2'  | 24:BA:2198:A:P    | 2.78                     | 0.42              |
| 24:BA:2345:G:N3   | 24:BA:2381:A:H2'  | 2.34                     | 0.42              |
| 24:BA:2414:G:C2   | 24:BA:2415:G:C8   | 3.08                     | 0.42              |
| 24:BA:2820:A:H2'  | 27:BD:196:ALA:HB2 | 2.00                     | 0.42              |
| 24:BA:392:U:H2'   | 24:BA:393:C:H6    | 1.85                     | 0.42              |
| 24:BA:559:G:H2'   | 24:BA:560:C:O4'   | 2.19                     | 0.42              |
| 24:BA:833:A:H2'   | 24:BA:834:G:H8    | 1.78                     | 0.42              |
| 24:BA:904:G:H2'   | 24:BA:905:A:O4'   | 2.19                     | 0.42              |
| 24:BA:569:U:OP1   | 24:BA:945:A:C4    | 2.73                     | 0.42              |
| 26:BC:171:VAL:O   | 26:BC:182:LYS:HA  | 2.20                     | 0.42              |
| 27:BD:73:VAL:HG23 | 27:BD:74:GLU:H    | 1.84                     | 0.42              |
| 28:BE:154:ASP:C   | 28:BE:154:ASP:OD2 | 2.58                     | 0.42              |
| 28:BE:193:VAL:O   | 28:BE:197:GLU:HB2 | 2.19                     | 0.42              |
| 29:BF:27:VAL:O    | 29:BF:27:VAL:CG1  | 2.67                     | 0.42              |
| 30:BG:115:GLN:O   | 30:BG:116:LEU:C   | 2.57                     | 0.42              |
| 30:BG:159:LYS:HE2 | 30:BG:159:LYS:HB3 | 1.78                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:BI:27:LEU:HD12 | 32:BI:27:LEU:C    | 2.40                     | 0.42              |
| 36:BM:76:LYS:O    | 36:BM:77:PRO:O    | 2.37                     | 0.42              |
| 37:BN:24:MET:CE   | 37:BN:44:LEU:HD22 | 2.50                     | 0.42              |
| 38:BO:31:THR:HG23 | 38:BO:33:ARG:N    | 2.32                     | 0.42              |
| 43:BT:23:ALA:C    | 43:BT:25:GLU:H    | 2.23                     | 0.42              |
| 46:BW:71:LYS:HB3  | 46:BW:72:GLY:H    | 1.73                     | 0.42              |
| 31:BH:27:ARG:HG3  | 47:BX:59:ASP:OD1  | 2.19                     | 0.42              |
| 55:CA:1054:C:OP2  | 55:CA:1197:A:OP2  | 2.38                     | 0.42              |
| 55:CA:1134:G:N1   | 55:CA:1141:C:C4   | 2.87                     | 0.42              |
| 55:CA:1171:A:O2'  | 55:CA:1172:C:H5'  | 2.20                     | 0.42              |
| 55:CA:1387:G:C6   | 55:CA:1388:C:C4   | 3.08                     | 0.42              |
| 55:CA:152:A:N6    | 55:CA:170:U:C2    | 2.87                     | 0.42              |
| 55:CA:206:C:C6    | 55:CA:206:C:C3'   | 3.02                     | 0.42              |
| 55:CA:25:C:H2'    | 55:CA:26:A:H8     | 1.80                     | 0.42              |
| 55:CA:257:G:C2    | 55:CA:270:A:N1    | 2.87                     | 0.42              |
| 55:CA:320:A:H2'   | 55:CA:321:A:O4'   | 2.19                     | 0.42              |
| 55:CA:404:G:C4    | 55:CA:405:U:C6    | 3.08                     | 0.42              |
| 55:CA:414:A:C2    | 55:CA:415:A:N9    | 2.87                     | 0.42              |
| 55:CA:45:G:H5''   | 55:CA:307:C:O2'   | 2.19                     | 0.42              |
| 55:CA:506:G:H2'   | 55:CA:507:C:H6    | 1.85                     | 0.42              |
| 55:CA:49:U:O2'    | 55:CA:50:A:H2'    | 2.19                     | 0.42              |
| 55:CA:596:A:N6    | 55:CA:645:G:N1    | 2.67                     | 0.42              |
| 55:CA:86:G:HO2'   | 55:CA:87:C:P      | 2.41                     | 0.42              |
| 55:CA:999:C:N4    | 55:CA:1000:A:N7   | 2.67                     | 0.42              |
| 1:CB:125:PHE:N    | 1:CB:125:PHE:CD2  | 2.88                     | 0.42              |
| 2:CC:133:MET:HE3  | 2:CC:152:VAL:HG13 | 2.02                     | 0.42              |
| 3:CD:112:GLU:HB2  | 55:CA:407:U:O2'   | 2.20                     | 0.42              |
| 4:CE:156:ARG:NH1  | 7:CH:63:LYS:NZ    | 2.68                     | 0.42              |
| 7:CH:98:LEU:HB2   | 7:CH:99:GLY:H     | 1.74                     | 0.42              |
| 8:CI:23:GLY:H     | 8:CI:60:LEU:HA    | 1.84                     | 0.42              |
| 8:CI:30:ASN:HD21  | 8:CI:66:VAL:N     | 2.04                     | 0.42              |
| 10:CK:74:LYS:HD2  | 10:CK:104:PHE:CZ  | 2.55                     | 0.42              |
| 10:CK:95:THR:HG23 | 10:CK:96:ILE:H    | 1.83                     | 0.42              |
| 11:CL:8:ARG:HB3   | 11:CL:9:LYS:HD3   | 2.01                     | 0.42              |
| 12:CM:16:ILE:HD12 | 12:CM:16:ILE:N    | 2.29                     | 0.42              |
| 13:CN:30:ILE:C    | 13:CN:40:ARG:HA   | 2.40                     | 0.42              |
| 18:CS:60:PHE:HE2  | 18:CS:62:THR:HG1  | 1.65                     | 0.42              |
| 54:D4:16:ILE:O    | 54:D4:17:VAL:HG13 | 2.20                     | 0.42              |
| 24:DA:100:U:H1'   | 24:DA:101:A:C5    | 2.55                     | 0.42              |
| 24:DA:100:U:H3'   | 24:DA:100:U:P     | 2.60                     | 0.42              |
| 24:DA:1013:C:H2'  | 24:DA:1014:A:C8   | 2.55                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:100:U:O2'   | 24:DA:101:A:H5''   | 2.18                     | 0.42              |
| 24:DA:1056:G:H3'  | 24:DA:1056:G:OP2   | 2.19                     | 0.42              |
| 24:DA:1218:G:H2'  | 24:DA:1219:U:O4'   | 2.19                     | 0.42              |
| 24:DA:1222:U:H2'  | 24:DA:1223:G:C8    | 2.55                     | 0.42              |
| 24:DA:1437:C:HO2' | 24:DA:1516:G:HO2'  | 1.62                     | 0.42              |
| 24:DA:1636:U:H2'  | 24:DA:1637:A:C8    | 2.55                     | 0.42              |
| 24:DA:1680:U:H2'  | 24:DA:1681:G:O4'   | 2.18                     | 0.42              |
| 24:DA:1717:A:C2'  | 24:DA:1718:G:O4'   | 2.68                     | 0.42              |
| 24:DA:1788:C:H2'  | 24:DA:1789:A:C8    | 2.51                     | 0.42              |
| 24:DA:1808:A:O3'  | 24:DA:1809:A:H8    | 2.03                     | 0.42              |
| 24:DA:1848:A:H2'  | 24:DA:1849:G:C8    | 2.55                     | 0.42              |
| 24:DA:223:A:N6    | 24:DA:422:A:N6     | 2.67                     | 0.42              |
| 24:DA:2467:C:N4   | 24:DA:2468:A:N1    | 2.67                     | 0.42              |
| 24:DA:2513:A:H2'  | 24:DA:2514:U:H6    | 1.85                     | 0.42              |
| 24:DA:265:A:H5'   | 24:DA:428:A:C2     | 2.54                     | 0.42              |
| 24:DA:2710:C:H2'  | 24:DA:2711:A:C8    | 2.55                     | 0.42              |
| 24:DA:2638:G:H1'  | 24:DA:2778:A:H61   | 1.83                     | 0.42              |
| 24:DA:2847:U:H2'  | 24:DA:2848:G:C5'   | 2.48                     | 0.42              |
| 24:DA:743:A:C6    | 24:DA:744:U:C4     | 3.07                     | 0.42              |
| 56:DB:75:G:N2     | 56:DB:102:G:N2     | 2.68                     | 0.42              |
| 26:DC:141:HIS:HB3 | 26:DC:142:ASN:H    | 1.58                     | 0.42              |
| 26:DC:76:VAL:O    | 26:DC:76:VAL:HG23  | 2.19                     | 0.42              |
| 27:DD:148:GLN:CD  | 27:DD:152:PRO:HG2  | 2.39                     | 0.42              |
| 29:DF:11:VAL:O    | 29:DF:13:LYS:HD2   | 2.19                     | 0.42              |
| 29:DF:139:GLU:CB  | 29:DF:142:TYR:HB3  | 2.49                     | 0.42              |
| 29:DF:74:ALA:CB   | 29:DF:78:ILE:CD1   | 2.98                     | 0.42              |
| 30:DG:11:PRO:HD2  | 30:DG:14:VAL:HG11  | 2.00                     | 0.42              |
| 34:DK:28:SER:O    | 34:DK:29:HIS:HB3   | 2.19                     | 0.42              |
| 34:DK:63:VAL:HG12 | 34:DK:64:ARG:HG3   | 2.02                     | 0.42              |
| 38:DO:38:GLN:HA   | 38:DO:50:ALA:HA    | 2.00                     | 0.42              |
| 40:DQ:77:LYS:CE   | 40:DQ:116:LEU:HD11 | 2.49                     | 0.42              |
| 46:DW:20:LEU:HD11 | 46:DW:35:ILE:CG1   | 2.50                     | 0.42              |
| 24:DA:2336:A:N7   | 46:DW:40:ARG:NE    | 2.67                     | 0.42              |
| 46:DW:51:GLY:HA3  | 46:DW:59:PHE:HB3   | 2.02                     | 0.42              |
| 21:AA:1213:A:C4   | 21:AA:1215:G:C8    | 3.07                     | 0.42              |
| 12:AM:85:TYR:CE1  | 21:AA:1321:U:H4'   | 2.55                     | 0.42              |
| 21:AA:261:U:N1    | 21:AA:263:A:OP2    | 2.52                     | 0.42              |
| 21:AA:579:A:H2'   | 21:AA:580:C:H6     | 1.85                     | 0.42              |
| 7:AH:106:SER:HA   | 21:AA:642:A:N7     | 2.34                     | 0.42              |
| 21:AA:683:G:C2    | 21:AA:684:U:C2     | 3.08                     | 0.42              |
| 21:AA:791:G:C6    | 21:AA:792:A:N6     | 2.84                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AB:22:TRP:CD1    | 1:AB:38:HIS:HE1   | 2.37                     | 0.42              |
| 1:AB:65:LYS:HE2    | 1:AB:153:MET:HG2  | 2.02                     | 0.42              |
| 2:AC:107:LYS:HA    | 2:AC:108:PRO:HD2  | 1.88                     | 0.42              |
| 2:AC:26:LYS:HB3    | 2:AC:26:LYS:NZ    | 2.34                     | 0.42              |
| 3:AD:166:LYS:HB3   | 3:AD:166:LYS:HZ2  | 1.80                     | 0.42              |
| 4:AE:131:ASN:HA    | 4:AE:132:PRO:HD2  | 1.61                     | 0.42              |
| 12:AM:84:CYS:SG    | 12:AM:85:TYR:N    | 2.92                     | 0.42              |
| 13:AN:54:SER:O     | 13:AN:55:SER:HB2  | 2.20                     | 0.42              |
| 15:AP:8:ARG:NH2    | 15:AP:11:ALA:O    | 2.52                     | 0.42              |
| 16:AQ:16:MET:O     | 16:AQ:18:LYS:N    | 2.53                     | 0.42              |
| 19:AT:54:GLN:N     | 19:AT:55:PRO:HD2  | 2.34                     | 0.42              |
| 22:AV:35:A:C2      | 22:AV:36:A:N9     | 2.87                     | 0.42              |
| 24:BA:1031:G:H4'   | 54:B4:6:SER:HB2   | 2.01                     | 0.42              |
| 24:BA:1063:G:N2    | 24:BA:1076:C:C2   | 2.88                     | 0.42              |
| 24:BA:1110:G:O2'   | 24:BA:1111:A:C8   | 2.72                     | 0.42              |
| 24:BA:1002:G:N2    | 24:BA:1154:G:H1'  | 2.35                     | 0.42              |
| 24:BA:1328:A:H4'   | 24:BA:1329:U:C5   | 2.55                     | 0.42              |
| 24:BA:1595:C:H2'   | 24:BA:1596:A:O4'  | 2.19                     | 0.42              |
| 24:BA:1655:A:H3'   | 24:BA:1656:C:H6   | 1.85                     | 0.42              |
| 24:BA:1681:G:HO2'  | 24:BA:1762:A:C2'  | 2.31                     | 0.42              |
| 24:BA:183:C:O2     | 24:BA:432:A:H2    | 2.03                     | 0.42              |
| 24:BA:1959:G:N1    | 24:BA:1960:A:C4   | 2.88                     | 0.42              |
| 24:BA:2017:U:H4'   | 50:B0:4:GLN:O     | 2.19                     | 0.42              |
| 24:BA:2225:A:H5'   | 24:BA:2226:C:H5'  | 2.02                     | 0.42              |
| 24:BA:2297:A:N6    | 24:BA:2319:G:H1'  | 2.35                     | 0.42              |
| 24:BA:2418:A:C4    | 24:BA:2419:U:C6   | 3.06                     | 0.42              |
| 24:BA:2259:U:C2    | 24:BA:2427:C:C4   | 3.08                     | 0.42              |
| 24:BA:251:A:H2'    | 24:BA:252:G:O4'   | 2.18                     | 0.42              |
| 24:BA:2549:G:C2    | 24:BA:2560:A:C5   | 3.08                     | 0.42              |
| 24:BA:2630:G:H2'   | 24:BA:2631:G:H8   | 1.85                     | 0.42              |
| 24:BA:227:A:N6     | 24:BA:410:G:H1'   | 2.35                     | 0.42              |
| 24:BA:64:A:O2'     | 43:BT:70:HIS:CE1  | 2.73                     | 0.42              |
| 24:BA:813:U:H4'    | 24:BA:1225:G:O2'  | 2.18                     | 0.42              |
| 24:BA:98:G:N1      | 24:BA:99:U:C4     | 2.87                     | 0.42              |
| 26:BC:170:TYR:HD2  | 26:BC:183:VAL:C   | 2.23                     | 0.42              |
| 26:BC:255:LYS:O    | 26:BC:257:ARG:N   | 2.53                     | 0.42              |
| 28:BE:119:ILE:HD13 | 28:BE:119:ILE:H   | 1.85                     | 0.42              |
| 28:BE:88:ARG:O     | 28:BE:89:PRO:C    | 2.56                     | 0.42              |
| 24:BA:2305:U:C6    | 29:BF:152:ASP:HB3 | 2.55                     | 0.42              |
| 30:BG:112:VAL:HG23 | 30:BG:113:ASP:N   | 2.34                     | 0.42              |
| 32:BI:90:GLY:O     | 32:BI:92:PRO:HD3  | 2.20                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:BJ:41:LYS:N    | 40:BQ:66:ALA:HB1   | 2.35                     | 0.42              |
| 24:BA:2684:U:H4'  | 34:BK:76:VAL:HG21  | 2.01                     | 0.42              |
| 38:BO:3:LYS:HG3   | 38:BO:4:LYS:H      | 1.83                     | 0.42              |
| 38:BO:67:ASN:O    | 38:BO:67:ASN:CG    | 2.58                     | 0.42              |
| 41:BR:100:GLY:C   | 41:BR:101:ILE:HG12 | 2.40                     | 0.42              |
| 44:BU:60:LYS:HA   | 44:BU:60:LYS:HD2   | 1.77                     | 0.42              |
| 46:BW:24:ARG:O    | 46:BW:25:PHE:CB    | 2.63                     | 0.42              |
| 46:BW:37:VAL:HG13 | 46:BW:55:ASP:C     | 2.40                     | 0.42              |
| 55:CA:100:G:O6    | 55:CA:101:A:C6     | 2.72                     | 0.42              |
| 55:CA:1114:C:H2'  | 55:CA:1115:U:C6    | 2.55                     | 0.42              |
| 55:CA:1216:A:O2'  | 55:CA:1217:C:O4'   | 2.37                     | 0.42              |
| 55:CA:1308:U:N3   | 55:CA:1330:U:N3    | 2.67                     | 0.42              |
| 55:CA:1365:G:H2'  | 55:CA:1366:C:C6    | 2.54                     | 0.42              |
| 55:CA:1494:G:C2   | 55:CA:1495:U:C5    | 3.08                     | 0.42              |
| 55:CA:192:A:H8    | 55:CA:192:A:O5'    | 2.02                     | 0.42              |
| 55:CA:316:C:N4    | 55:CA:351:G:C6     | 2.88                     | 0.42              |
| 55:CA:402:G:C6    | 55:CA:403:C:C4     | 3.08                     | 0.42              |
| 55:CA:519:C:C2'   | 55:CA:520:A:H8     | 2.31                     | 0.42              |
| 55:CA:688:G:C6    | 55:CA:700:G:C5     | 3.07                     | 0.42              |
| 55:CA:774:G:C4    | 55:CA:775:G:C8     | 3.07                     | 0.42              |
| 55:CA:878:A:C2'   | 55:CA:879:C:H5'    | 2.49                     | 0.42              |
| 55:CA:935:A:C2    | 55:CA:936:C:C2     | 3.07                     | 0.42              |
| 5:CF:36:ILE:HG22  | 5:CF:38:ARG:O      | 2.20                     | 0.42              |
| 6:CG:149:ALA:C    | 6:CG:150:PHE:CG    | 2.93                     | 0.42              |
| 6:CG:47:GLU:OE1   | 6:CG:47:GLU:HA     | 2.20                     | 0.42              |
| 7:CH:17:GLN:OE1   | 7:CH:64:TYR:CZ     | 2.73                     | 0.42              |
| 9:CJ:6:ILE:HD12   | 9:CJ:6:ILE:N       | 2.34                     | 0.42              |
| 12:CM:67:ASP:O    | 12:CM:70:ARG:HB3   | 2.20                     | 0.42              |
| 13:CN:22:LYS:O    | 13:CN:26:LEU:N     | 2.53                     | 0.42              |
| 13:CN:76:PHE:HE2  | 13:CN:92:ILE:HG21  | 1.85                     | 0.42              |
| 14:CO:28:VAL:HG21 | 14:CO:66:LEU:HD23  | 2.01                     | 0.42              |
| 15:CP:6:LEU:HB3   | 15:CP:19:VAL:HA    | 2.02                     | 0.42              |
| 19:CT:24:ARG:HD3  | 19:CT:28:ARG:NH2   | 2.25                     | 0.42              |
| 54:D4:2:LYS:HZ3   | 54:D4:2:LYS:HA     | 1.83                     | 0.42              |
| 24:DA:1008:A:N6   | 24:DA:1136:G:N1    | 2.67                     | 0.42              |
| 24:DA:1232:G:C6   | 24:DA:1233:C:C4    | 3.08                     | 0.42              |
| 24:DA:1585:C:C2'  | 24:DA:1586:A:O5'   | 2.68                     | 0.42              |
| 24:DA:1731:G:C2   | 24:DA:1733:G:N7    | 2.88                     | 0.42              |
| 24:DA:1859:U:H2'  | 24:DA:1860:G:C8    | 2.55                     | 0.42              |
| 24:DA:1917:U:C2'  | 24:DA:1918:A:H5'   | 2.50                     | 0.42              |
| 24:DA:1920:C:C2   | 24:DA:1921:G:C8    | 3.07                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:1963:U:O2'  | 24:DA:1964:G:H5''  | 2.19                     | 0.42              |
| 24:DA:2077:A:C2   | 24:DA:2078:C:C2    | 3.08                     | 0.42              |
| 24:DA:2077:A:C5   | 24:DA:2435:A:C6    | 3.08                     | 0.42              |
| 24:DA:220:G:H1    | 24:DA:427:U:H2'    | 1.85                     | 0.42              |
| 24:DA:2342:C:O2'  | 24:DA:2374:C:H5''  | 2.20                     | 0.42              |
| 24:DA:2406:A:C2   | 35:DL:69:ARG:NH2   | 2.87                     | 0.42              |
| 24:DA:2441:U:O2'  | 24:DA:2442:C:C5'   | 2.65                     | 0.42              |
| 24:DA:2485:G:C2'  | 24:DA:2486:C:H5'   | 2.50                     | 0.42              |
| 24:DA:2635:A:H5'  | 27:DD:79:LEU:HB2   | 2.02                     | 0.42              |
| 24:DA:2835:A:H4'  | 24:DA:2836:U:OP1   | 2.20                     | 0.42              |
| 24:DA:571:U:H1'   | 24:DA:573:U:C6     | 2.54                     | 0.42              |
| 24:DA:572:A:H5''  | 41:DR:79:ARG:NH2   | 2.34                     | 0.42              |
| 24:DA:637:A:O5'   | 35:DL:112:LEU:HD21 | 2.19                     | 0.42              |
| 24:DA:650:C:O4'   | 53:D3:22:LYS:NZ    | 2.53                     | 0.42              |
| 24:DA:770:G:H1'   | 24:DA:1379:U:O4    | 2.19                     | 0.42              |
| 26:DC:67:LYS:HG2  | 26:DC:150:GLY:HA2  | 2.01                     | 0.42              |
| 24:DA:1816:C:H3'  | 26:DC:61:TYR:CE2   | 2.55                     | 0.42              |
| 27:DD:98:VAL:O    | 27:DD:100:LEU:N    | 2.52                     | 0.42              |
| 27:DD:127:PHE:HZ  | 27:DD:160:LYS:HD2  | 1.84                     | 0.42              |
| 27:DD:110:THR:HA  | 27:DD:171:THR:HA   | 2.01                     | 0.42              |
| 28:DE:85:PHE:O    | 28:DE:86:ALA:C     | 2.58                     | 0.42              |
| 28:DE:9:GLN:HG3   | 28:DE:9:GLN:O      | 2.20                     | 0.42              |
| 34:DK:28:SER:O    | 34:DK:29:HIS:CB    | 2.68                     | 0.42              |
| 35:DL:29:LYS:O    | 35:DL:30:THR:OG1   | 2.33                     | 0.42              |
| 36:DM:29:GLY:CA   | 36:DM:64:TRP:HZ3   | 2.33                     | 0.42              |
| 36:DM:36:VAL:HG22 | 45:DV:82:TYR:CD1   | 2.55                     | 0.42              |
| 36:DM:57:VAL:HA   | 36:DM:112:LEU:HD11 | 2.01                     | 0.42              |
| 36:DM:69:PRO:O    | 36:DM:70:ASP:HB3   | 2.20                     | 0.42              |
| 38:DO:79:ALA:HB1  | 38:DO:114:GLY:CA   | 2.48                     | 0.42              |
| 43:DT:19:LYS:O    | 43:DT:20:ALA:HB2   | 2.20                     | 0.42              |
| 24:DA:309:A:H4'   | 44:DU:16:LYS:H     | 1.83                     | 0.42              |
| 44:DU:20:LYS:HD2  | 44:DU:38:ILE:CD1   | 2.50                     | 0.42              |
| 21:AA:1210:C:C4   | 21:AA:1211:U:C5    | 3.07                     | 0.42              |
| 21:AA:960:U:N3    | 21:AA:1225:A:C5    | 2.88                     | 0.42              |
| 21:AA:1246:A:H2'  | 21:AA:1247:U:O4'   | 2.20                     | 0.42              |
| 21:AA:1353:G:C2   | 21:AA:1370:G:N2    | 2.88                     | 0.42              |
| 21:AA:1425:U:O2   | 21:AA:1476:A:C2    | 2.73                     | 0.42              |
| 21:AA:1496:C:H2'  | 21:AA:1497:G:O4'   | 2.19                     | 0.42              |
| 21:AA:15:G:N7     | 21:AA:1396:A:N1    | 2.68                     | 0.42              |
| 21:AA:502:A:H2'   | 21:AA:503:C:C6     | 2.55                     | 0.42              |
| 21:AA:587:G:O2'   | 21:AA:588:G:C5'    | 2.68                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:594:U:C2'    | 21:AA:595:A:H5'    | 2.50                     | 0.42              |
| 21:AA:587:G:N2     | 21:AA:755:G:C5     | 2.88                     | 0.42              |
| 21:AA:76:G:C2      | 21:AA:95:C:C4      | 3.07                     | 0.42              |
| 1:AB:143:LEU:HB2   | 1:AB:147:LEU:CD1   | 2.47                     | 0.42              |
| 1:AB:185:ILE:HD11  | 1:AB:203:ASP:HA    | 2.01                     | 0.42              |
| 1:AB:209:VAL:O     | 1:AB:212:TYR:N     | 2.52                     | 0.42              |
| 2:AC:6:PRO:HB3     | 2:AC:174:LEU:CD1   | 2.50                     | 0.42              |
| 4:AE:100:GLU:HB3   | 4:AE:121:ASN:CA    | 2.47                     | 0.42              |
| 4:AE:123:LEU:O     | 4:AE:124:ALA:CB    | 2.66                     | 0.42              |
| 4:AE:155:LYS:H     | 4:AE:155:LYS:HG3   | 1.59                     | 0.42              |
| 4:AE:84:VAL:O      | 4:AE:95:MET:HG2    | 2.20                     | 0.42              |
| 6:AG:106:ALA:HB1   | 6:AG:132:THR:HB    | 2.00                     | 0.42              |
| 7:AH:34:ALA:HB1    | 7:AH:109:VAL:CB    | 2.50                     | 0.42              |
| 10:AK:23:HIS:HB3   | 10:AK:30:ILE:CG1   | 2.49                     | 0.42              |
| 16:AQ:79:GLU:O     | 16:AQ:80:LYS:HD3   | 2.19                     | 0.42              |
| 18:AS:17:LYS:HB3   | 18:AS:30:LEU:HD23  | 2.02                     | 0.42              |
| 53:B3:6:VAL:HG23   | 53:B3:60:CYS:O     | 2.20                     | 0.42              |
| 24:BA:1035:U:H2'   | 24:BA:1036:G:H8    | 1.85                     | 0.42              |
| 24:BA:1076:C:H2'   | 24:BA:1077:A:O4'   | 2.20                     | 0.42              |
| 24:BA:999:U:C5     | 24:BA:1154:G:C5    | 3.08                     | 0.42              |
| 24:BA:1805:A:C6    | 24:BA:1806:C:C5    | 3.07                     | 0.42              |
| 24:BA:1815:A:C4    | 24:BA:1817:G:C5    | 3.07                     | 0.42              |
| 24:BA:1876:A:H2'   | 24:BA:1877:A:C8    | 2.52                     | 0.42              |
| 24:BA:1931:U:O2'   | 24:BA:1932:A:C5'   | 2.66                     | 0.42              |
| 24:BA:2373:G:C6    | 24:BA:2381:A:N1    | 2.88                     | 0.42              |
| 24:BA:2425:A:H5'   | 24:BA:2426:A:H3'   | 2.01                     | 0.42              |
| 24:BA:2602:A:C4'   | 24:BA:2603:G:OP2   | 2.56                     | 0.42              |
| 24:BA:2720:U:H5''  | 39:BP:52:ARG:HH22  | 1.85                     | 0.42              |
| 24:BA:2743:U:H2'   | 24:BA:2744:G:O4'   | 2.19                     | 0.42              |
| 24:BA:324:A:H61    | 24:BA:338:G:C2'    | 2.32                     | 0.42              |
| 24:BA:37:C:O2'     | 28:BE:45:ALA:HA    | 2.20                     | 0.42              |
| 24:BA:740:C:C6     | 24:BA:740:C:O5'    | 2.73                     | 0.42              |
| 26:BC:115:ILE:HD12 | 26:BC:115:ILE:HA   | 1.67                     | 0.42              |
| 24:BA:1789:A:OP1   | 26:BC:219:VAL:HA   | 2.20                     | 0.42              |
| 24:BA:1798:U:OP1   | 26:BC:255:LYS:O    | 2.38                     | 0.42              |
| 27:BD:169:ARG:C    | 27:BD:170:VAL:HG13 | 2.39                     | 0.42              |
| 29:BF:116:LEU:HB3  | 29:BF:127:TYR:OH   | 2.20                     | 0.42              |
| 29:BF:39:VAL:HG13  | 29:BF:40:GLY:N     | 2.35                     | 0.42              |
| 31:BH:30:LEU:C     | 31:BH:31:VAL:O     | 2.58                     | 0.42              |
| 32:BI:58:ILE:HG23  | 32:BI:66:PHE:CD1   | 2.55                     | 0.42              |
| 33:BJ:118:MET:HA   | 33:BJ:121:LYS:HE2  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:BL:77:ILE:N    | 35:BL:77:ILE:HD12 | 2.35                     | 0.42              |
| 38:BO:21:LEU:O    | 38:BO:22:GLY:O    | 2.38                     | 0.42              |
| 40:BQ:85:ALA:O    | 40:BQ:87:VAL:O    | 2.37                     | 0.42              |
| 43:BT:27:SER:O    | 43:BT:28:ASN:CG   | 2.58                     | 0.42              |
| 44:BU:66:VAL:C    | 44:BU:68:ASN:H    | 2.23                     | 0.42              |
| 55:CA:1093:A:C4   | 55:CA:1095:U:O4'  | 2.73                     | 0.42              |
| 55:CA:1279:G:H8   | 55:CA:1282:C:N3   | 2.16                     | 0.42              |
| 55:CA:1310:G:N2   | 55:CA:1328:C:C2   | 2.88                     | 0.42              |
| 55:CA:144:G:C6    | 55:CA:145:G:C5    | 3.07                     | 0.42              |
| 55:CA:1460:C:H2'  | 55:CA:1461:G:O4'  | 2.20                     | 0.42              |
| 55:CA:169:C:C5    | 55:CA:170:U:C5    | 3.08                     | 0.42              |
| 55:CA:181:A:O2'   | 55:CA:182:A:H2    | 1.76                     | 0.42              |
| 55:CA:182:A:H5''  | 55:CA:182:A:N3    | 2.34                     | 0.42              |
| 55:CA:203:G:O2'   | 55:CA:204:G:H8    | 2.03                     | 0.42              |
| 55:CA:243:A:O2'   | 55:CA:244:U:P     | 2.78                     | 0.42              |
| 55:CA:363:A:H2'   | 55:CA:364:A:O4'   | 2.19                     | 0.42              |
| 55:CA:369:G:O2'   | 55:CA:370:C:C5'   | 2.68                     | 0.42              |
| 55:CA:397:A:N7    | 55:CA:548:G:C8    | 2.88                     | 0.42              |
| 55:CA:39:G:N2     | 55:CA:40:C:C2     | 2.88                     | 0.42              |
| 3:CD:30:LYS:HA    | 55:CA:413:G:O6    | 2.20                     | 0.42              |
| 55:CA:484:G:O2'   | 55:CA:485:U:P     | 2.78                     | 0.42              |
| 55:CA:709:U:C2    | 55:CA:710:G:C8    | 3.07                     | 0.42              |
| 55:CA:734:G:C6    | 55:CA:735:C:C4    | 3.07                     | 0.42              |
| 55:CA:82:G:C6     | 55:CA:89:U:C5     | 3.08                     | 0.42              |
| 55:CA:845:A:N3    | 55:CA:845:A:H2'   | 2.35                     | 0.42              |
| 3:CD:170:LEU:HD12 | 3:CD:170:LEU:O    | 2.20                     | 0.42              |
| 3:CD:57:LYS:HA    | 3:CD:199:ILE:CG2  | 2.49                     | 0.42              |
| 5:CF:81:ASN:O     | 5:CF:84:VAL:HG12  | 2.20                     | 0.42              |
| 6:CG:29:LEU:O     | 6:CG:30:MET:O     | 2.38                     | 0.42              |
| 9:CJ:45:ARG:O     | 9:CJ:46:LYS:C     | 2.58                     | 0.42              |
| 9:CJ:66:GLU:OE2   | 9:CJ:68:ARG:NE    | 2.52                     | 0.42              |
| 11:CL:2:THR:HG22  | 11:CL:4:ASN:N     | 2.35                     | 0.42              |
| 12:CM:85:TYR:O    | 12:CM:88:LEU:HB2  | 2.19                     | 0.42              |
| 18:CS:43:MET:O    | 18:CS:61:VAL:HG11 | 2.20                     | 0.42              |
| 20:CU:19:LYS:HA   | 20:CU:19:LYS:HD3  | 1.80                     | 0.42              |
| 20:CU:32:ARG:HD3  | 20:CU:33:ARG:HB2  | 2.02                     | 0.42              |
| 50:D0:37:HIS:HB2  | 50:D0:41:HIS:CE1  | 2.55                     | 0.42              |
| 50:D0:54:ILE:O    | 50:D0:55:ALA:HB2  | 2.19                     | 0.42              |
| 24:DA:1155:A:C4   | 24:DA:1157:G:C8   | 3.07                     | 0.42              |
| 24:DA:1306:C:H41  | 24:DA:1606:C:H2'  | 1.85                     | 0.42              |
| 24:DA:1341:G:H4'  | 24:DA:1342:A:OP2  | 2.19                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:DA:1366:A:H2'   | 24:DA:1367:A:O4'  | 2.20                     | 0.42              |
| 24:DA:1941:C:C5    | 24:DA:1942:C:N4   | 2.87                     | 0.42              |
| 24:DA:2061:G:C2    | 24:DA:2063:C:C4   | 3.07                     | 0.42              |
| 24:DA:241:A:C4     | 24:DA:243:U:O4    | 2.72                     | 0.42              |
| 24:DA:2645:G:H4'   | 24:DA:2732:G:H2'  | 2.02                     | 0.42              |
| 24:DA:280:U:O2     | 24:DA:280:U:O4'   | 2.37                     | 0.42              |
| 24:DA:364:C:C2'    | 24:DA:365:U:C6    | 2.91                     | 0.42              |
| 24:DA:605:G:H2'    | 24:DA:606:U:C6    | 2.54                     | 0.42              |
| 24:DA:646:U:H6     | 24:DA:646:U:OP2   | 2.03                     | 0.42              |
| 24:DA:77:G:C4      | 24:DA:110:G:C2    | 3.08                     | 0.42              |
| 24:DA:950:G:H2'    | 24:DA:951:C:C6    | 2.55                     | 0.42              |
| 26:DC:123:ILE:HD12 | 26:DC:123:ILE:HA  | 1.89                     | 0.42              |
| 27:DD:184:ARG:HH22 | 39:DP:6:GLN:NE2   | 2.06                     | 0.42              |
| 28:DE:5:LEU:CD1    | 28:DE:10:SER:HB2  | 2.50                     | 0.42              |
| 28:DE:108:ILE:CD1  | 28:DE:181:ILE:HB  | 2.41                     | 0.42              |
| 24:DA:2307:G:O6    | 29:DF:84:ILE:HD11 | 2.20                     | 0.42              |
| 30:DG:39:ALA:O     | 30:DG:40:VAL:HG13 | 2.20                     | 0.42              |
| 31:DH:58:LEU:HA    | 31:DH:61:VAL:HG12 | 2.01                     | 0.42              |
| 33:DJ:105:VAL:HA   | 33:DJ:108:MET:HG3 | 2.01                     | 0.42              |
| 35:DL:56:PRO:HB3   | 35:DL:58:TYR:CE2  | 2.55                     | 0.42              |
| 35:DL:79:LEU:C     | 35:DL:82:LEU:HD11 | 2.39                     | 0.42              |
| 36:DM:45:GLN:OE1   | 36:DM:125:PRO:HG3 | 2.20                     | 0.42              |
| 38:DO:69:ASP:O     | 38:DO:70:ALA:C    | 2.57                     | 0.42              |
| 39:DP:52:ARG:HG2   | 39:DP:52:ARG:NH1  | 2.35                     | 0.42              |
| 40:DQ:69:ARG:HH21  | 40:DQ:69:ARG:CB   | 2.28                     | 0.42              |
| 42:DS:88:ARG:HG3   | 42:DS:88:ARG:NH2  | 2.33                     | 0.42              |
| 45:DV:44:HIS:CE1   | 45:DV:85:LYS:HD3  | 2.55                     | 0.42              |
| 21:AA:66:A:N6      | 21:AA:104:G:C2    | 2.87                     | 0.42              |
| 21:AA:1163:A:H2'   | 21:AA:1164:G:H8   | 1.83                     | 0.42              |
| 21:AA:355:C:C2     | 21:AA:356:A:C8    | 3.08                     | 0.42              |
| 21:AA:445:G:C2     | 21:AA:490:C:C2    | 3.08                     | 0.42              |
| 21:AA:693:G:O2'    | 21:AA:694:A:H5'   | 2.20                     | 0.42              |
| 21:AA:918:A:N6     | 21:AA:919:A:N1    | 2.68                     | 0.42              |
| 1:AB:110:ILE:O     | 1:AB:114:LYS:N    | 2.53                     | 0.42              |
| 1:AB:133:ALA:O     | 1:AB:137:THR:HG23 | 2.20                     | 0.42              |
| 1:AB:205:ALA:HB3   | 1:AB:208:ALA:CB   | 2.48                     | 0.42              |
| 2:AC:19:SER:HB2    | 2:AC:39:ARG:NH2   | 2.34                     | 0.42              |
| 2:AC:51:VAL:CG2    | 2:AC:52:SER:N     | 2.82                     | 0.42              |
| 4:AE:90:GLY:O      | 4:AE:129:SER:N    | 2.38                     | 0.42              |
| 11:AL:23:LEU:C     | 11:AL:25:ALA:N    | 2.71                     | 0.42              |
| 12:AM:89:ARG:HH11  | 12:AM:94:LEU:HB3  | 1.84                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:AN:56:PRO:O     | 13:AN:59:GLN:HB2  | 2.19                     | 0.42              |
| 13:AN:83:VAL:HG12  | 13:AN:84:ARG:N    | 2.34                     | 0.42              |
| 19:AT:73:ARG:O     | 19:AT:77:ASN:ND2  | 2.53                     | 0.42              |
| 54:B4:16:ILE:HA    | 54:B4:24:ARG:O    | 2.19                     | 0.42              |
| 24:BA:1001:A:C2'   | 24:BA:1002:G:H5'  | 2.50                     | 0.42              |
| 24:BA:1068:G:N3    | 24:BA:1068:G:H2'  | 2.35                     | 0.42              |
| 24:BA:1423:G:C2    | 24:BA:1424:G:N9   | 2.88                     | 0.42              |
| 24:BA:1510:G:O2'   | 24:BA:1511:G:C5'  | 2.67                     | 0.42              |
| 24:BA:1923:U:H2'   | 24:BA:1924:C:C6   | 2.55                     | 0.42              |
| 24:BA:200:U:HO2'   | 24:BA:201:C:H5'   | 1.85                     | 0.42              |
| 24:BA:2073:C:H2'   | 24:BA:2074:U:H6   | 1.84                     | 0.42              |
| 24:BA:2095:A:C2    | 24:BA:2195:U:O2   | 2.73                     | 0.42              |
| 24:BA:2209:G:C6    | 24:BA:2210:U:O4   | 2.72                     | 0.42              |
| 24:BA:2379:G:H4'   | 38:BO:21:LEU:HD11 | 2.02                     | 0.42              |
| 24:BA:2478:A:N9    | 24:BA:2529:G:N7   | 2.66                     | 0.42              |
| 24:BA:2531:A:OP1   | 30:BG:174:LYS:CG  | 2.65                     | 0.42              |
| 24:BA:25:U:C5      | 24:BA:26:G:C6     | 3.08                     | 0.42              |
| 24:BA:2688:G:H1'   | 24:BA:2721:A:H61  | 1.83                     | 0.42              |
| 24:BA:2828:G:N2    | 24:BA:2829:A:C4   | 2.88                     | 0.42              |
| 24:BA:2856:A:C2'   | 24:BA:2857:G:H5'  | 2.49                     | 0.42              |
| 24:BA:2837:A:N1    | 24:BA:2882:A:C6   | 2.88                     | 0.42              |
| 24:BA:489:G:H2'    | 24:BA:491:G:C8    | 2.55                     | 0.42              |
| 24:BA:584:C:C2'    | 24:BA:585:G:H5'   | 2.50                     | 0.42              |
| 24:BA:608:A:C6     | 24:BA:609:A:C6    | 3.08                     | 0.42              |
| 24:BA:632:A:H1'    | 35:BL:66:PHE:HE2  | 1.84                     | 0.42              |
| 24:BA:699:A:HO2'   | 24:BA:1634:A:H8   | 1.64                     | 0.42              |
| 24:BA:729:G:H2'    | 24:BA:1775:U:H1'  | 2.01                     | 0.42              |
| 24:BA:846:U:O4     | 24:BA:927:A:OP2   | 2.38                     | 0.42              |
| 24:BA:919:U:C2     | 24:BA:920:A:C5    | 3.08                     | 0.42              |
| 24:BA:933:A:H2'    | 24:BA:933:A:N3    | 2.35                     | 0.42              |
| 26:BC:229:HIS:CG   | 26:BC:230:PRO:CD  | 3.02                     | 0.42              |
| 24:BA:1654:A:O3'   | 27:BD:118:PHE:CE2 | 2.73                     | 0.42              |
| 27:BD:133:THR:HG23 | 27:BD:134:HIS:CD2 | 2.55                     | 0.42              |
| 29:BF:123:GLY:HA2  | 29:BF:162:ASP:OD2 | 2.20                     | 0.42              |
| 30:BG:38:ASP:H     | 30:BG:40:VAL:HG13 | 1.85                     | 0.42              |
| 33:BJ:70:THR:HA    | 33:BJ:90:GLU:HG2  | 2.02                     | 0.42              |
| 35:BL:68:SER:O     | 35:BL:69:ARG:HB2  | 2.20                     | 0.42              |
| 37:BN:10:LEU:HA    | 37:BN:10:LEU:HD13 | 1.79                     | 0.42              |
| 24:BA:2708:G:H1'   | 37:BN:71:ARG:CZ   | 2.49                     | 0.42              |
| 55:CA:1140:C:O2'   | 55:CA:1141:C:H6   | 2.01                     | 0.42              |
| 55:CA:937:A:C2     | 55:CA:1379:G:C6   | 3.08                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:253:A:C4    | 55:CA:254:G:N7    | 2.88                     | 0.42              |
| 55:CA:359:G:C6    | 55:CA:360:G:C5    | 3.08                     | 0.42              |
| 55:CA:9:G:C2      | 55:CA:10:A:C5     | 3.08                     | 0.42              |
| 2:CC:54:ILE:HG13  | 2:CC:67:ILE:HD13  | 2.01                     | 0.42              |
| 3:CD:197:HIS:O    | 3:CD:201:GLU:HG3  | 2.20                     | 0.42              |
| 6:CG:94:ARG:HA    | 6:CG:98:LEU:HG    | 2.01                     | 0.42              |
| 11:CL:49:ARG:HG2  | 11:CL:49:ARG:HH11 | 1.84                     | 0.42              |
| 13:CN:20:PHE:CA   | 13:CN:24:ALA:HB2  | 2.50                     | 0.42              |
| 18:CS:6:LYS:H     | 18:CS:6:LYS:HD2   | 1.85                     | 0.42              |
| 19:CT:17:ARG:HD2  | 19:CT:17:ARG:C    | 2.40                     | 0.42              |
| 24:DA:987:C:O2    | 24:DA:1000:A:H2   | 2.03                     | 0.42              |
| 24:DA:1045:C:O5'  | 24:DA:1046:A:H5'' | 2.19                     | 0.42              |
| 24:DA:1295:C:H1'  | 37:DN:23:ASN:HD21 | 1.85                     | 0.42              |
| 24:DA:1332:G:H4'  | 24:DA:1333:G:OP2  | 2.19                     | 0.42              |
| 24:DA:1345:C:H5'  | 24:DA:1396:U:C4   | 2.55                     | 0.42              |
| 24:DA:1440:U:H2'  | 24:DA:1441:G:C8   | 2.50                     | 0.42              |
| 24:DA:1446:C:N4   | 24:DA:1447:C:N4   | 2.67                     | 0.42              |
| 24:DA:1480:C:H2'  | 24:DA:1481:U:O4'  | 2.20                     | 0.42              |
| 24:DA:1438:U:C4   | 24:DA:1555:G:N1   | 2.88                     | 0.42              |
| 24:DA:1585:C:H2'  | 24:DA:1586:A:O5'  | 2.19                     | 0.42              |
| 24:DA:1787:A:N3   | 24:DA:1788:C:C5   | 2.88                     | 0.42              |
| 24:DA:1948:G:O2'  | 24:DA:1949:G:H5'  | 2.19                     | 0.42              |
| 24:DA:2016:U:C4   | 24:DA:2017:U:O4   | 2.73                     | 0.42              |
| 24:DA:2415:G:H4'  | 35:DL:66:PHE:CB   | 2.38                     | 0.42              |
| 24:DA:2251:G:C8   | 24:DA:2450:A:H4'  | 2.54                     | 0.42              |
| 24:DA:2657:A:H2'  | 24:DA:2658:C:C6   | 2.55                     | 0.42              |
| 24:DA:2710:C:H2'  | 24:DA:2711:A:H8   | 1.84                     | 0.42              |
| 24:DA:2738:A:H2   | 24:DA:2766:A:N6   | 2.11                     | 0.42              |
| 24:DA:2750:A:HO2' | 24:DA:2752:C:H41  | 1.66                     | 0.42              |
| 24:DA:2800:A:C2   | 24:DA:2801:G:N3   | 2.87                     | 0.42              |
| 24:DA:2816:G:H4'  | 50:D0:40:HIS:HB3  | 2.02                     | 0.42              |
| 24:DA:303:G:C6    | 24:DA:315:G:O6    | 2.73                     | 0.42              |
| 24:DA:422:A:C2    | 24:DA:423:A:C5    | 3.07                     | 0.42              |
| 24:DA:436:C:HO2'  | 24:DA:437:U:H6    | 1.67                     | 0.42              |
| 24:DA:629:G:O2'   | 24:DA:630:G:H5'   | 2.20                     | 0.42              |
| 24:DA:670:A:O2'   | 24:DA:671:C:P     | 2.78                     | 0.42              |
| 24:DA:805:G:OP2   | 35:DL:41:ARG:HB3  | 2.20                     | 0.42              |
| 24:DA:834:G:H5''  | 53:D3:56:LEU:HD11 | 2.02                     | 0.42              |
| 24:DA:991:C:C4    | 24:DA:1185:G:C6   | 3.08                     | 0.42              |
| 26:DC:79:ARG:HD2  | 26:DC:92:LEU:HD22 | 2.02                     | 0.42              |
| 27:DD:62:LYS:CA   | 27:DD:62:LYS:HE3  | 2.50                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:DD:73:VAL:O     | 27:DD:74:GLU:HB2   | 2.20                     | 0.42              |
| 28:DE:129:PRO:HG3  | 28:DE:159:LEU:HB3  | 2.01                     | 0.42              |
| 29:DF:105:ILE:HG22 | 29:DF:105:ILE:O    | 2.20                     | 0.42              |
| 29:DF:155:ILE:HD12 | 29:DF:155:ILE:N    | 2.34                     | 0.42              |
| 29:DF:19:PHE:HB3   | 29:DF:21:TYR:CE2   | 2.55                     | 0.42              |
| 32:DI:32:VAL:HG13  | 32:DI:58:ILE:HD12  | 2.01                     | 0.42              |
| 33:DJ:41:LYS:C     | 33:DJ:43:GLU:N     | 2.73                     | 0.42              |
| 34:DK:118:LEU:N    | 34:DK:118:LEU:HD23 | 2.35                     | 0.42              |
| 35:DL:65:GLY:O     | 35:DL:66:PHE:HB2   | 2.20                     | 0.42              |
| 36:DM:126:ILE:O    | 36:DM:128:THR:HG23 | 2.19                     | 0.42              |
| 36:DM:73:ILE:HA    | 36:DM:73:ILE:HD13  | 1.77                     | 0.42              |
| 38:DO:41:ALA:O     | 38:DO:43:ASN:N     | 2.52                     | 0.42              |
| 39:DP:87:ARG:HG2   | 39:DP:88:ARG:N     | 2.34                     | 0.42              |
| 39:DP:91:VAL:HG11  | 39:DP:96:LEU:HD21  | 2.02                     | 0.42              |
| 45:DV:31:TYR:C     | 45:DV:31:TYR:CD1   | 2.93                     | 0.42              |
| 24:DA:857:G:O2'    | 46:DW:19:ARG:CZ    | 2.68                     | 0.42              |
| 46:DW:32:ALA:O     | 46:DW:34:SER:N     | 2.52                     | 0.42              |
| 21:AA:1032:G:O2'   | 21:AA:1033:G:C5'   | 2.65                     | 0.41              |
| 21:AA:1134:G:C6    | 21:AA:1135:U:N3    | 2.88                     | 0.41              |
| 21:AA:1151:A:HO2'  | 21:AA:1152:A:P     | 2.43                     | 0.41              |
| 21:AA:1258:G:O2'   | 21:AA:1259:C:H6    | 2.02                     | 0.41              |
| 21:AA:126:G:C2'    | 21:AA:127:G:O5'    | 2.68                     | 0.41              |
| 21:AA:130:A:O2'    | 21:AA:131:A:O5'    | 2.37                     | 0.41              |
| 21:AA:1323:G:H2'   | 21:AA:1324:A:C8    | 2.54                     | 0.41              |
| 21:AA:140:U:H2'    | 21:AA:141:G:O4'    | 2.20                     | 0.41              |
| 15:AP:70:ARG:HH12  | 21:AA:451:A:H5'    | 1.85                     | 0.41              |
| 21:AA:472:U:C4     | 21:AA:473:U:O4     | 2.73                     | 0.41              |
| 21:AA:545:C:O2'    | 21:AA:549:C:H5''   | 2.20                     | 0.41              |
| 21:AA:596:A:N1     | 21:AA:645:G:C4     | 2.88                     | 0.41              |
| 21:AA:793:U:O4     | 21:AA:1517:G:H5''  | 2.20                     | 0.41              |
| 21:AA:973:G:H3'    | 21:AA:974:A:H5''   | 2.01                     | 0.41              |
| 21:AA:9:G:C6       | 21:AA:26:A:C6      | 3.08                     | 0.41              |
| 1:AB:103:TRP:HE1   | 1:AB:150:ILE:HG13  | 1.85                     | 0.41              |
| 1:AB:168:GLU:O     | 1:AB:172:ILE:HG13  | 2.20                     | 0.41              |
| 4:AE:56:PRO:O      | 4:AE:58:ALA:N      | 2.53                     | 0.41              |
| 4:AE:94:PHE:CZ     | 4:AE:96:GLN:HG2    | 2.55                     | 0.41              |
| 5:AF:11:HIS:HA     | 5:AF:12:PRO:HD2    | 1.91                     | 0.41              |
| 5:AF:21:MET:HE2    | 5:AF:25:TYR:CE1    | 2.55                     | 0.41              |
| 5:AF:8:PHE:HB3     | 5:AF:78:PHE:CE1    | 2.55                     | 0.41              |
| 6:AG:132:THR:O     | 6:AG:135:LYS:HB3   | 2.20                     | 0.41              |
| 6:AG:34:LYS:NZ     | 21:AA:1290:G:H5'   | 2.34                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:AL:2:THR:HB     | 11:AL:5:GLN:CB    | 2.50                     | 0.41              |
| 13:AN:63:CYS:O     | 13:AN:65:GLN:N    | 2.53                     | 0.41              |
| 15:AP:41:PRO:HB2   | 21:AA:450:G:H4'   | 2.01                     | 0.41              |
| 24:BA:1073:A:N7    | 24:BA:1074:G:H8   | 2.18                     | 0.41              |
| 24:BA:1304:A:C2    | 24:BA:1305:C:C2   | 3.08                     | 0.41              |
| 24:BA:1342:A:C6    | 24:BA:1345:C:N3   | 2.88                     | 0.41              |
| 24:BA:1917:U:O2'   | 24:BA:1918:A:H5'  | 2.19                     | 0.41              |
| 24:BA:2062:A:O2'   | 24:BA:2063:C:H5'  | 2.19                     | 0.41              |
| 24:BA:2077:A:C2    | 24:BA:2078:C:C5   | 3.09                     | 0.41              |
| 24:BA:2081:U:C5    | 24:BA:2237:G:N1   | 2.88                     | 0.41              |
| 24:BA:2415:G:H4'   | 35:BL:66:PHE:HB2  | 2.02                     | 0.41              |
| 24:BA:2617:U:C2'   | 24:BA:2618:G:H5'  | 2.50                     | 0.41              |
| 24:BA:2841:C:H2'   | 24:BA:2842:G:C8   | 2.55                     | 0.41              |
| 24:BA:536:G:C2     | 24:BA:558:U:O2    | 2.73                     | 0.41              |
| 24:BA:635:C:C2'    | 24:BA:636:G:H5'   | 2.50                     | 0.41              |
| 24:BA:672:C:C2'    | 24:BA:673:C:H5'   | 2.50                     | 0.41              |
| 24:BA:695:G:H1'    | 24:BA:768:G:N2    | 2.35                     | 0.41              |
| 24:BA:812:C:O2'    | 24:BA:813:U:H5'   | 2.20                     | 0.41              |
| 24:BA:92:U:H5''    | 24:BA:92:U:C6     | 2.52                     | 0.41              |
| 24:BA:954:G:C6     | 24:BA:955:U:C5    | 3.08                     | 0.41              |
| 24:BA:977:G:C4     | 24:BA:978:G:C8    | 3.08                     | 0.41              |
| 26:BC:104:LEU:HB3  | 26:BC:105:ALA:H   | 1.63                     | 0.41              |
| 27:BD:124:ARG:HG2  | 27:BD:125:TRP:CD1 | 2.54                     | 0.41              |
| 28:BE:150:THR:HG23 | 28:BE:153:LEU:H   | 1.85                     | 0.41              |
| 28:BE:23:PHE:CE1   | 28:BE:28:VAL:HG11 | 2.55                     | 0.41              |
| 28:BE:84:THR:HB    | 28:BE:85:PHE:CD2  | 2.55                     | 0.41              |
| 29:BF:39:VAL:HG13  | 29:BF:84:ILE:HD12 | 2.02                     | 0.41              |
| 30:BG:9:VAL:O      | 30:BG:11:PRO:HD3  | 2.20                     | 0.41              |
| 31:BH:95:GLY:C     | 31:BH:97:ARG:N    | 2.73                     | 0.41              |
| 32:BI:53:PRO:HB2   | 32:BI:74:PRO:CG   | 2.50                     | 0.41              |
| 36:BM:47:GLU:O     | 36:BM:50:ARG:N    | 2.53                     | 0.41              |
| 37:BN:52:ILE:O     | 37:BN:54:LEU:N    | 2.53                     | 0.41              |
| 37:BN:71:ARG:NH2   | 37:BN:71:ARG:HG3  | 2.35                     | 0.41              |
| 38:BO:5:SER:O      | 38:BO:6:ALA:C     | 2.59                     | 0.41              |
| 25:BB:51:G:H5''    | 38:BO:64:TYR:CD2  | 2.54                     | 0.41              |
| 39:BP:21:PRO:HA    | 39:BP:46:VAL:HG12 | 2.02                     | 0.41              |
| 40:BQ:16:ILE:O     | 40:BQ:17:LEU:C    | 2.58                     | 0.41              |
| 45:BV:88:HIS:CG    | 45:BV:89:ILE:N    | 2.88                     | 0.41              |
| 24:BA:2232:C:P     | 47:BX:26:ARG:HH22 | 2.43                     | 0.41              |
| 48:BY:18:LEU:HD22  | 48:BY:18:LEU:HA   | 1.84                     | 0.41              |
| 49:BZ:22:THR:HG23  | 49:BZ:46:MET:HB3  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:110:C:O2'   | 55:CA:111:G:O4'   | 2.32                     | 0.41              |
| 55:CA:1208:C:C2   | 55:CA:1209:C:C6   | 3.08                     | 0.41              |
| 55:CA:1301:U:H4'  | 55:CA:1302:C:OP1  | 2.20                     | 0.41              |
| 55:CA:1484:C:H2'  | 55:CA:1485:U:H6   | 1.84                     | 0.41              |
| 55:CA:177:G:C2'   | 55:CA:178:C:H5'   | 2.48                     | 0.41              |
| 55:CA:198:G:O2'   | 55:CA:199:A:C5'   | 2.68                     | 0.41              |
| 55:CA:339:C:O2    | 55:CA:351:G:N2    | 2.53                     | 0.41              |
| 55:CA:577:G:O2'   | 55:CA:578:C:O5'   | 2.36                     | 0.41              |
| 55:CA:596:A:O2'   | 55:CA:597:G:C5'   | 2.68                     | 0.41              |
| 10:CK:117:HIS:ND1 | 55:CA:675:A:H1'   | 2.34                     | 0.41              |
| 55:CA:765:G:N7    | 55:CA:812:G:C4    | 2.88                     | 0.41              |
| 55:CA:924:C:O2'   | 55:CA:925:G:H5'   | 2.20                     | 0.41              |
| 55:CA:954:G:C5    | 55:CA:955:U:N3    | 2.88                     | 0.41              |
| 55:CA:966:G:H2'   | 55:CA:967:C:C6    | 2.55                     | 0.41              |
| 1:CB:81:ASP:CG    | 1:CB:82:ALA:N     | 2.73                     | 0.41              |
| 2:CC:149:LYS:HB3  | 2:CC:149:LYS:HE2  | 1.93                     | 0.41              |
| 2:CC:203:LYS:HB3  | 2:CC:203:LYS:HE3  | 1.94                     | 0.41              |
| 3:CD:167:PRO:CG   | 3:CD:170:LEU:HD11 | 2.50                     | 0.41              |
| 6:CG:75:LYS:HE2   | 6:CG:76:SER:N     | 2.26                     | 0.41              |
| 7:CH:1:SER:C      | 7:CH:3:GLN:N      | 2.74                     | 0.41              |
| 9:CJ:82:LYS:HZ2   | 9:CJ:82:LYS:HG3   | 1.78                     | 0.41              |
| 12:CM:18:LEU:N    | 12:CM:18:LEU:HD12 | 2.35                     | 0.41              |
| 24:DA:1071:G:O5'  | 24:DA:1072:C:H5   | 2.03                     | 0.41              |
| 24:DA:1203:U:H3   | 24:DA:1204:A:N6   | 2.17                     | 0.41              |
| 24:DA:1537:G:O2'  | 24:DA:1538:G:H4'  | 2.17                     | 0.41              |
| 24:DA:1613:G:C6   | 24:DA:1619:G:C6   | 3.08                     | 0.41              |
| 24:DA:1631:G:H1'  | 24:DA:1635:A:N6   | 2.35                     | 0.41              |
| 24:DA:1517:G:N2   | 24:DA:1732:C:C6   | 2.88                     | 0.41              |
| 24:DA:1889:A:C6   | 24:DA:1890:A:C6   | 3.07                     | 0.41              |
| 24:DA:1919:A:O5'  | 24:DA:1919:A:C8   | 2.60                     | 0.41              |
| 24:DA:197:A:N3    | 24:DA:197:A:H2'   | 2.33                     | 0.41              |
| 24:DA:2062:A:C6   | 24:DA:2503:A:N7   | 2.88                     | 0.41              |
| 24:DA:2397:G:C6   | 24:DA:2420:C:N3   | 2.87                     | 0.41              |
| 24:DA:240:C:OP2   | 24:DA:241:A:H3'   | 2.19                     | 0.41              |
| 24:DA:2511:U:H3'  | 24:DA:2511:U:H6   | 1.83                     | 0.41              |
| 24:DA:2592:G:H2'  | 24:DA:2593:U:C6   | 2.47                     | 0.41              |
| 24:DA:2624:G:C5   | 24:DA:2625:G:C8   | 3.08                     | 0.41              |
| 24:DA:2644:G:C6   | 24:DA:2645:G:C2   | 3.08                     | 0.41              |
| 24:DA:320:A:N7    | 28:DE:132:LYS:HB2 | 2.35                     | 0.41              |
| 24:DA:396:G:O2'   | 24:DA:397:U:H5'   | 2.20                     | 0.41              |
| 24:DA:866:A:O2'   | 24:DA:867:C:C5'   | 2.68                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:DB:14:U:H6      | 56:DB:14:U:H2'     | 1.64                     | 0.41              |
| 26:DC:171:VAL:HG12 | 26:DC:173:LEU:HD13 | 2.01                     | 0.41              |
| 29:DF:109:ARG:NH1  | 29:DF:135:ILE:HG21 | 2.35                     | 0.41              |
| 29:DF:49:LEU:HD13  | 29:DF:149:ARG:HH21 | 1.84                     | 0.41              |
| 29:DF:41:GLU:HG2   | 29:DF:42:ALA:N     | 2.26                     | 0.41              |
| 31:DH:53:GLU:C     | 31:DH:55:GLU:N     | 2.74                     | 0.41              |
| 32:DI:69:VAL:O     | 32:DI:69:VAL:HG13  | 2.19                     | 0.41              |
| 33:DJ:116:ARG:HD2  | 33:DJ:116:ARG:HA   | 1.84                     | 0.41              |
| 33:DJ:74:TYR:CE2   | 33:DJ:103:ILE:HD11 | 2.55                     | 0.41              |
| 34:DK:22:ILE:HG12  | 34:DK:40:LYS:O     | 2.19                     | 0.41              |
| 55:CA:1422:G:H5''  | 34:DK:48:PRO:HB3   | 2.00                     | 0.41              |
| 34:DK:11:ALA:HB2   | 34:DK:64:ARG:NH1   | 2.35                     | 0.41              |
| 24:DA:1653:G:O6    | 37:DN:10:LEU:O     | 2.38                     | 0.41              |
| 40:DQ:27:ARG:HE    | 40:DQ:37:ALA:HB1   | 1.85                     | 0.41              |
| 40:DQ:91:ARG:CZ    | 41:DR:11:GLN:H     | 2.33                     | 0.41              |
| 42:DS:32:ALA:HA    | 42:DS:35:ILE:CD1   | 2.47                     | 0.41              |
| 43:DT:53:VAL:HG21  | 43:DT:92:ASN:HD22  | 1.85                     | 0.41              |
| 45:DV:63:ILE:HD12  | 45:DV:63:ILE:N     | 2.34                     | 0.41              |
| 45:DV:77:VAL:HG11  | 45:DV:79:ARG:HH21  | 1.84                     | 0.41              |
| 47:DX:26:ARG:O     | 47:DX:27:ARG:HB3   | 2.20                     | 0.41              |
| 49:DZ:31:ILE:O     | 49:DZ:31:ILE:HG13  | 2.19                     | 0.41              |
| 21:AA:1007:U:C4    | 21:AA:1008:U:H5    | 2.38                     | 0.41              |
| 21:AA:920:U:O4'    | 21:AA:1080:A:C2    | 2.73                     | 0.41              |
| 21:AA:1154:G:O2'   | 21:AA:1155:A:H5'   | 2.20                     | 0.41              |
| 21:AA:1219:A:N1    | 21:AA:1220:G:C6    | 2.88                     | 0.41              |
| 21:AA:1283:U:O2'   | 21:AA:1284:C:O4'   | 2.29                     | 0.41              |
| 21:AA:1363:A:C4    | 21:AA:1365:G:C6    | 3.08                     | 0.41              |
| 21:AA:1533:C:H3'   | 21:AA:1534:A:C5'   | 2.43                     | 0.41              |
| 21:AA:212:G:O2'    | 21:AA:213:G:P      | 2.78                     | 0.41              |
| 21:AA:439:U:H2'    | 21:AA:440:C:C5'    | 2.50                     | 0.41              |
| 21:AA:624:C:H2'    | 21:AA:625:U:O4'    | 2.20                     | 0.41              |
| 21:AA:675:A:H2'    | 21:AA:676:A:O4'    | 2.20                     | 0.41              |
| 21:AA:859:G:H2'    | 21:AA:860:A:C8     | 2.55                     | 0.41              |
| 1:AB:209:VAL:O     | 1:AB:210:THR:C     | 2.59                     | 0.41              |
| 1:AB:53:LEU:HA     | 1:AB:56:LEU:CB     | 2.46                     | 0.41              |
| 2:AC:190:THR:HG21  | 2:AC:192:TYR:OH    | 2.20                     | 0.41              |
| 3:AD:28:ASP:OD1    | 3:AD:33:ILE:HG12   | 2.19                     | 0.41              |
| 3:AD:62:ARG:CA     | 3:AD:62:ARG:NE     | 2.77                     | 0.41              |
| 4:AE:57:ALA:HA     | 4:AE:60:GLN:OE1    | 2.19                     | 0.41              |
| 7:AH:118:ALA:HB3   | 7:AH:120:LEU:HD11  | 2.02                     | 0.41              |
| 8:AI:12:LYS:HD3    | 21:AA:1371:G:OP1   | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AK:81:LEU:H     | 10:AK:81:LEU:HD23  | 1.85                     | 0.41              |
| 11:AL:118:VAL:HG12 | 11:AL:119:LYS:N    | 2.36                     | 0.41              |
| 12:AM:102:LYS:O    | 12:AM:103:THR:HG23 | 2.19                     | 0.41              |
| 14:AO:67:ASP:O     | 14:AO:70:LYS:HB3   | 2.19                     | 0.41              |
| 15:AP:1:MET:HG2    | 15:AP:2:VAL:N      | 2.34                     | 0.41              |
| 51:B1:9:LYS:HG2    | 51:B1:9:LYS:O      | 2.20                     | 0.41              |
| 53:B3:16:THR:HB    | 53:B3:17:GLY:H     | 1.53                     | 0.41              |
| 24:BA:1080:A:C2    | 24:BA:1081:U:C6    | 3.08                     | 0.41              |
| 24:BA:1082:U:C2    | 24:BA:1086:A:N6    | 2.87                     | 0.41              |
| 24:BA:1187:G:HO2'  | 24:BA:1188:U:H6    | 1.65                     | 0.41              |
| 24:BA:1257:C:C4    | 24:BA:1258:U:C5    | 3.08                     | 0.41              |
| 24:BA:1555:G:HO2'  | 24:BA:1556:C:H5'   | 1.81                     | 0.41              |
| 24:BA:1608:A:C5    | 24:BA:1611:C:C4    | 3.08                     | 0.41              |
| 24:BA:1853:A:N1    | 24:BA:1854:A:C2    | 2.89                     | 0.41              |
| 24:BA:1911:U:C4    | 24:BA:1918:A:C5    | 3.07                     | 0.41              |
| 24:BA:2453:A:O2'   | 24:BA:2572:A:H1'   | 2.20                     | 0.41              |
| 24:BA:1638:C:H4'   | 24:BA:2710:C:O2    | 2.20                     | 0.41              |
| 24:BA:83:A:H5''    | 24:BA:84:A:P       | 2.60                     | 0.41              |
| 24:BA:929:U:O2     | 49:BZ:25:GLY:HA2   | 2.19                     | 0.41              |
| 25:BB:104:A:H2'    | 25:BB:105:G:O4'    | 2.20                     | 0.41              |
| 25:BB:71:C:H2'     | 25:BB:72:G:C5'     | 2.50                     | 0.41              |
| 29:BF:137:PHE:HA   | 29:BF:138:PRO:HD3  | 1.90                     | 0.41              |
| 30:BG:115:GLN:HG2  | 30:BG:115:GLN:O    | 2.19                     | 0.41              |
| 24:BA:558:U:H5''   | 33:BJ:111:LYS:CE   | 2.50                     | 0.41              |
| 33:BJ:102:GLU:HG3  | 33:BJ:124:VAL:HG11 | 2.01                     | 0.41              |
| 33:BJ:16:TYR:CA    | 33:BJ:138:GLN:O    | 2.67                     | 0.41              |
| 36:BM:31:PHE:O     | 36:BM:104:GLU:HA   | 2.20                     | 0.41              |
| 36:BM:43:ALA:HA    | 36:BM:46:ILE:CG1   | 2.51                     | 0.41              |
| 36:BM:35:ALA:HB3   | 36:BM:99:GLY:H     | 1.84                     | 0.41              |
| 37:BN:96:ARG:HH22  | 37:BN:116:VAL:HG23 | 1.85                     | 0.41              |
| 40:BQ:51:GLN:O     | 40:BQ:52:ARG:C     | 2.59                     | 0.41              |
| 24:BA:995:C:OP2    | 40:BQ:53:LYS:HE2   | 2.20                     | 0.41              |
| 48:BY:53:VAL:O     | 48:BY:56:LEU:O     | 2.38                     | 0.41              |
| 55:CA:1052:U:O4    | 55:CA:1200:C:C2    | 2.73                     | 0.41              |
| 55:CA:1161:C:O2'   | 55:CA:1162:C:O5'   | 2.38                     | 0.41              |
| 55:CA:1163:A:H2'   | 55:CA:1164:G:C8    | 2.55                     | 0.41              |
| 55:CA:1220:G:C2    | 55:CA:1221:G:C4    | 3.09                     | 0.41              |
| 55:CA:1293:C:H2'   | 55:CA:1294:G:H8    | 1.81                     | 0.41              |
| 55:CA:1268:G:N2    | 55:CA:1327:C:H1'   | 2.35                     | 0.41              |
| 55:CA:313:A:H2'    | 55:CA:314:C:H6     | 1.83                     | 0.41              |
| 55:CA:407:U:C2     | 55:CA:408:A:C8     | 3.08                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:426:U:H2'   | 55:CA:427:U:H6    | 1.85                     | 0.41              |
| 55:CA:837:U:H2'   | 55:CA:838:G:C8    | 2.54                     | 0.41              |
| 55:CA:848:C:H2'   | 55:CA:849:G:O4'   | 2.20                     | 0.41              |
| 55:CA:934:C:H4'   | 55:CA:935:A:OP1   | 2.20                     | 0.41              |
| 1:CB:137:THR:O    | 1:CB:140:LEU:N    | 2.53                     | 0.41              |
| 3:CD:98:ASP:HB3   | 3:CD:132:ALA:HB1  | 2.03                     | 0.41              |
| 4:CE:39:GLY:HA2   | 4:CE:45:VAL:HA    | 2.01                     | 0.41              |
| 4:CE:80:LEU:CB    | 4:CE:97:PRO:HB3   | 2.49                     | 0.41              |
| 4:CE:145:ASN:O    | 7:CH:72:GLU:OE2   | 2.38                     | 0.41              |
| 7:CH:89:ASP:N     | 7:CH:89:ASP:OD1   | 2.53                     | 0.41              |
| 7:CH:94:VAL:HG23  | 7:CH:101:ALA:HB2  | 2.02                     | 0.41              |
| 12:CM:47:LEU:HD21 | 12:CM:52:ILE:HG22 | 2.02                     | 0.41              |
| 14:CO:41:HIS:O    | 14:CO:45:HIS:CE1  | 2.73                     | 0.41              |
| 17:CR:32:ILE:HG22 | 17:CR:38:ILE:HA   | 2.01                     | 0.41              |
| 22:CV:33:U:H2'    | 22:CV:35:A:N7     | 2.34                     | 0.41              |
| 53:D3:41:ARG:CG   | 53:D3:41:ARG:NH2  | 2.75                     | 0.41              |
| 24:DA:1127:A:O2'  | 24:DA:1128:G:C5'  | 2.62                     | 0.41              |
| 24:DA:1149:G:C6   | 24:DA:1150:C:C4   | 3.08                     | 0.41              |
| 24:DA:1238:G:C2   | 24:DA:1239:G:C5   | 3.08                     | 0.41              |
| 24:DA:1373:A:H2'  | 24:DA:1374:G:O4'  | 2.20                     | 0.41              |
| 24:DA:142:A:C4    | 24:DA:143:C:C5    | 3.07                     | 0.41              |
| 24:DA:1270:C:C4   | 24:DA:1648:U:C4   | 3.08                     | 0.41              |
| 24:DA:1680:U:C4   | 24:DA:1681:G:C2   | 3.08                     | 0.41              |
| 24:DA:1742:U:H2'  | 24:DA:1743:G:C8   | 2.55                     | 0.41              |
| 24:DA:1767:G:N2   | 24:DA:1986:C:C2   | 2.88                     | 0.41              |
| 24:DA:1766:G:C2   | 24:DA:1987:A:N3   | 2.88                     | 0.41              |
| 24:DA:2027:G:C6   | 24:DA:2028:U:C4   | 3.08                     | 0.41              |
| 24:DA:206:U:HO2'  | 24:DA:207:A:H5'   | 1.78                     | 0.41              |
| 24:DA:212:G:H2'   | 24:DA:213:A:O4'   | 2.19                     | 0.41              |
| 24:DA:2238:G:H8   | 59:DA:3525:HOH:O  | 2.03                     | 0.41              |
| 24:DA:2297:A:O2'  | 24:DA:2298:A:H5'  | 2.20                     | 0.41              |
| 24:DA:2349:G:C2   | 24:DA:2350:C:H1'  | 2.55                     | 0.41              |
| 24:DA:2411:A:H2'  | 24:DA:2412:A:C8   | 2.55                     | 0.41              |
| 24:DA:2574:G:C5   | 24:DA:2575:C:C5   | 3.08                     | 0.41              |
| 24:DA:2654:A:H4'  | 24:DA:2655:G:O5'  | 2.19                     | 0.41              |
| 24:DA:2665:A:C2   | 24:DA:2666:C:C2   | 3.08                     | 0.41              |
| 24:DA:2837:A:N6   | 24:DA:2882:A:C6   | 2.88                     | 0.41              |
| 24:DA:2850:A:H2'  | 24:DA:2851:A:C8   | 2.55                     | 0.41              |
| 24:DA:301:G:C4    | 24:DA:302:C:C4    | 3.08                     | 0.41              |
| 24:DA:389:G:C4    | 24:DA:2413:G:H4'  | 2.54                     | 0.41              |
| 24:DA:379:G:N1    | 24:DA:396:G:C6    | 2.88                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:DA:36:G:N1      | 24:DA:445:C:C4    | 2.88                     | 0.41              |
| 24:DA:737:C:H2'    | 24:DA:738:G:O4'   | 2.20                     | 0.41              |
| 24:DA:690:G:H1'    | 24:DA:779:U:O3'   | 2.20                     | 0.41              |
| 56:DB:37:C:C4      | 56:DB:49:C:H1'    | 2.55                     | 0.41              |
| 30:DG:145:ALA:HA   | 30:DG:148:ARG:HG2 | 2.01                     | 0.41              |
| 35:DL:112:LEU:HD23 | 35:DL:112:LEU:O   | 2.20                     | 0.41              |
| 37:DN:55:ALA:CB    | 37:DN:79:LEU:HD22 | 2.51                     | 0.41              |
| 41:DR:2:TYR:CD2    | 41:DR:42:ALA:HB2  | 2.56                     | 0.41              |
| 41:DR:2:TYR:H      | 41:DR:42:ALA:HB2  | 1.86                     | 0.41              |
| 41:DR:38:VAL:N     | 41:DR:53:PHE:HB3  | 2.36                     | 0.41              |
| 41:DR:86:GLN:HE21  | 41:DR:86:GLN:HB2  | 1.67                     | 0.41              |
| 44:DU:82:VAL:HG23  | 44:DU:83:GLY:H    | 1.85                     | 0.41              |
| 45:DV:26:PHE:CD2   | 45:DV:42:LEU:HB2  | 2.56                     | 0.41              |
| 48:DY:37:LEU:HD13  | 48:DY:42:LEU:CD1  | 2.50                     | 0.41              |
| 21:AA:1099:G:C6    | 21:AA:1100:C:N3   | 2.88                     | 0.41              |
| 21:AA:1220:G:C2    | 21:AA:1221:G:C4   | 3.08                     | 0.41              |
| 21:AA:1443:C:H2'   | 21:AA:1444:U:H6   | 1.86                     | 0.41              |
| 21:AA:146:G:C6     | 21:AA:147:G:C5    | 3.09                     | 0.41              |
| 21:AA:188:C:O2     | 21:AA:188:C:H2'   | 2.19                     | 0.41              |
| 21:AA:289:G:N1     | 21:AA:290:C:C4    | 2.88                     | 0.41              |
| 21:AA:327:A:O3'    | 21:AA:328:C:H4'   | 2.20                     | 0.41              |
| 21:AA:344:A:O2'    | 39:BP:36:LYS:HE2  | 2.20                     | 0.41              |
| 21:AA:346:G:N2     | 21:AA:347:G:C4    | 2.88                     | 0.41              |
| 21:AA:43:C:H2'     | 21:AA:44:A:O4'    | 2.20                     | 0.41              |
| 21:AA:489:C:O2'    | 21:AA:490:C:H5'   | 2.20                     | 0.41              |
| 1:AB:89:PHE:HD2    | 1:AB:148:GLY:O    | 2.03                     | 0.41              |
| 4:AE:93:VAL:CG2    | 4:AE:138:ALA:HB3  | 2.50                     | 0.41              |
| 4:AE:61:LYS:NZ     | 21:AA:1073:U:P    | 2.93                     | 0.41              |
| 6:AG:145:GLU:HA    | 6:AG:148:LYS:HE2  | 2.03                     | 0.41              |
| 13:AN:22:LYS:HG3   | 13:AN:23:ARG:N    | 2.36                     | 0.41              |
| 15:AP:52:LEU:CD2   | 15:AP:75:ILE:HG12 | 2.45                     | 0.41              |
| 24:BA:1037:G:C2    | 24:BA:1119:U:O2   | 2.73                     | 0.41              |
| 24:BA:1056:G:H21   | 24:BA:1103:A:H62  | 1.68                     | 0.41              |
| 24:BA:1085:A:H1'   | 24:BA:1105:U:H1'  | 2.01                     | 0.41              |
| 24:BA:1217:U:H2'   | 24:BA:1218:G:O5'  | 2.21                     | 0.41              |
| 24:BA:1286:A:C6    | 24:BA:1329:U:C2   | 3.09                     | 0.41              |
| 24:BA:1343:G:C6    | 24:BA:1344:U:O4   | 2.73                     | 0.41              |
| 24:BA:1423:G:N2    | 24:BA:1424:G:H1'  | 2.35                     | 0.41              |
| 24:BA:1484:U:H2'   | 24:BA:1485:U:H6   | 1.85                     | 0.41              |
| 24:BA:14:A:H3'     | 24:BA:15:G:H5''   | 2.01                     | 0.41              |
| 24:BA:1662:U:O2    | 24:BA:2687:U:H4'  | 2.21                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:BA:1709:U:H2'   | 24:BA:1710:G:H8   | 1.84                     | 0.41              |
| 24:BA:1959:G:C6    | 24:BA:1960:A:C5   | 3.08                     | 0.41              |
| 24:BA:1900:A:C2    | 24:BA:1970:A:C5   | 3.08                     | 0.41              |
| 24:BA:207:A:H2'    | 24:BA:208:C:O4'   | 2.19                     | 0.41              |
| 24:BA:2146:C:H4'   | 24:BA:2147:A:C4'  | 2.50                     | 0.41              |
| 24:BA:2305:U:H1'   | 29:BF:132:ARG:N   | 2.28                     | 0.41              |
| 24:BA:2305:U:H5''  | 29:BF:130:GLY:CA  | 2.45                     | 0.41              |
| 24:BA:2357:G:N2    | 24:BA:2361:G:C5   | 2.88                     | 0.41              |
| 24:BA:2582:G:H2'   | 24:BA:2582:G:N3   | 2.35                     | 0.41              |
| 24:BA:2577:A:H1'   | 24:BA:2612:C:N3   | 2.34                     | 0.41              |
| 24:BA:579:G:C8     | 24:BA:2017:U:C4   | 3.08                     | 0.41              |
| 24:BA:991:C:N3     | 24:BA:1185:G:C6   | 2.88                     | 0.41              |
| 25:BB:20:G:N2      | 25:BB:64:G:C4     | 2.89                     | 0.41              |
| 26:BC:195:GLY:O    | 26:BC:196:ASN:CB  | 2.68                     | 0.41              |
| 26:BC:43:ASN:CG    | 26:BC:44:ASN:H    | 2.22                     | 0.41              |
| 26:BC:70:LYS:HD2   | 26:BC:99:GLU:OE1  | 2.21                     | 0.41              |
| 26:BC:90:ILE:CG2   | 26:BC:102:TYR:HD1 | 2.32                     | 0.41              |
| 27:BD:151:THR:O    | 27:BD:152:PRO:C   | 2.58                     | 0.41              |
| 28:BE:178:VAL:HG13 | 28:BE:179:SER:H   | 1.85                     | 0.41              |
| 24:BA:659:G:H21    | 28:BE:30:GLN:NE2  | 2.18                     | 0.41              |
| 31:BH:2:GLN:O      | 31:BH:3:VAL:CG2   | 2.62                     | 0.41              |
| 31:BH:72:ILE:O     | 31:BH:72:ILE:HG23 | 2.19                     | 0.41              |
| 31:BH:94:ILE:HD12  | 31:BH:98:ASP:O    | 2.19                     | 0.41              |
| 36:BM:96:ILE:CD1   | 36:BM:96:ILE:C    | 2.85                     | 0.41              |
| 39:BP:28:LYS:HB2   | 39:BP:82:SER:HB3  | 2.02                     | 0.41              |
| 39:BP:5:LYS:C      | 39:BP:7:LEU:N     | 2.73                     | 0.41              |
| 39:BP:85:VAL:HG13  | 39:BP:86:LYS:N    | 2.34                     | 0.41              |
| 40:BQ:98:ALA:HB2   | 40:BQ:105:PHE:CE2 | 2.55                     | 0.41              |
| 40:BQ:63:ARG:NH2   | 40:BQ:96:ASP:CA   | 2.83                     | 0.41              |
| 44:BU:48:VAL:O     | 44:BU:48:VAL:HG13 | 2.20                     | 0.41              |
| 45:BV:26:PHE:HZ    | 45:BV:47:VAL:HG11 | 1.85                     | 0.41              |
| 55:CA:1043:G:C6    | 55:CA:1044:A:N6   | 2.89                     | 0.41              |
| 55:CA:1053:G:O5'   | 55:CA:1054:C:H3'  | 2.20                     | 0.41              |
| 55:CA:1134:G:N2    | 55:CA:1141:C:C2   | 2.88                     | 0.41              |
| 55:CA:1120:C:C2    | 55:CA:1154:G:N2   | 2.88                     | 0.41              |
| 55:CA:1250:A:C2    | 55:CA:1370:G:H1'  | 2.56                     | 0.41              |
| 55:CA:1448:C:O2'   | 55:CA:1449:C:H6   | 2.02                     | 0.41              |
| 55:CA:243:A:C2     | 55:CA:245:U:H2'   | 2.54                     | 0.41              |
| 55:CA:596:A:O2'    | 55:CA:597:G:O5'   | 2.38                     | 0.41              |
| 55:CA:939:G:C6     | 55:CA:940:C:N4    | 2.88                     | 0.41              |
| 55:CA:961:U:N3     | 55:CA:983:A:C2    | 2.88                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:977:A:H4'   | 55:CA:981:U:O2    | 2.20                     | 0.41              |
| 1:CB:100:LEU:N    | 1:CB:100:LEU:HD12 | 2.35                     | 0.41              |
| 3:CD:166:LYS:HA   | 3:CD:167:PRO:HD2  | 1.70                     | 0.41              |
| 3:CD:33:ILE:HD12  | 3:CD:34:GLU:H     | 1.83                     | 0.41              |
| 5:CF:47:LEU:HD12  | 5:CF:55:HIS:HA    | 2.02                     | 0.41              |
| 6:CG:100:MET:H    | 6:CG:100:MET:CE   | 2.28                     | 0.41              |
| 6:CG:59:GLU:HG3   | 6:CG:60:ALA:H     | 1.83                     | 0.41              |
| 9:CJ:76:ILE:HG22  | 9:CJ:77:VAL:H     | 1.84                     | 0.41              |
| 12:CM:5:GLY:C     | 12:CM:6:ILE:HG13  | 2.40                     | 0.41              |
| 12:CM:72:ILE:HG13 | 55:CA:1309:G:O2'  | 2.20                     | 0.41              |
| 13:CN:100:TRP:CD1 | 13:CN:100:TRP:C   | 2.94                     | 0.41              |
| 16:CQ:12:VAL:HG22 | 16:CQ:12:VAL:O    | 2.21                     | 0.41              |
| 17:CR:49:LYS:HD2  | 17:CR:49:LYS:O    | 2.21                     | 0.41              |
| 18:CS:57:VAL:HA   | 18:CS:58:PRO:HD2  | 1.88                     | 0.41              |
| 18:CS:60:PHE:CG   | 18:CS:61:VAL:N    | 2.87                     | 0.41              |
| 19:CT:42:ASP:O    | 19:CT:44:ALA:N    | 2.53                     | 0.41              |
| 51:D1:16:THR:CG2  | 51:D1:41:VAL:HB   | 2.50                     | 0.41              |
| 24:DA:1057:A:C6   | 24:DA:1058:U:C4   | 3.08                     | 0.41              |
| 24:DA:1112:G:H2'  | 24:DA:1113:U:C5   | 2.55                     | 0.41              |
| 24:DA:120:U:C2    | 24:DA:149:A:C5    | 3.08                     | 0.41              |
| 24:DA:1288:G:C8   | 24:DA:1327:A:N6   | 2.88                     | 0.41              |
| 24:DA:1301:A:N3   | 24:DA:1301:A:H2'  | 2.35                     | 0.41              |
| 24:DA:139:U:H5''  | 24:DA:140:C:C5    | 2.56                     | 0.41              |
| 24:DA:1437:C:C2   | 24:DA:1438:U:C5   | 3.08                     | 0.41              |
| 24:DA:1449:G:H2'  | 24:DA:1450:G:O4'  | 2.20                     | 0.41              |
| 24:DA:1597:A:O3'  | 24:DA:1598:A:H8   | 2.03                     | 0.41              |
| 24:DA:1848:A:C2   | 24:DA:1849:G:C4   | 3.09                     | 0.41              |
| 24:DA:2006:C:C2   | 24:DA:2007:U:C5   | 3.08                     | 0.41              |
| 24:DA:2254:C:H2'  | 24:DA:2255:G:O4'  | 2.20                     | 0.41              |
| 24:DA:2287:A:HO2' | 24:DA:2288:A:C3'  | 2.22                     | 0.41              |
| 24:DA:2329:U:H2'  | 24:DA:2330:G:O4'  | 2.19                     | 0.41              |
| 24:DA:2348:U:O2'  | 24:DA:2349:G:C5'  | 2.69                     | 0.41              |
| 24:DA:2643:G:H2'  | 24:DA:2644:G:H8   | 1.85                     | 0.41              |
| 24:DA:2800:A:N1   | 24:DA:2801:G:N3   | 2.68                     | 0.41              |
| 24:DA:296:U:H5''  | 44:DU:91:LYS:HZ3  | 1.85                     | 0.41              |
| 24:DA:395:U:O2'   | 24:DA:396:G:O5'   | 2.38                     | 0.41              |
| 24:DA:447:A:H5'   | 24:DA:449:A:C4    | 2.56                     | 0.41              |
| 24:DA:454:A:HO2'  | 24:DA:455:C:P     | 2.43                     | 0.41              |
| 24:DA:657:U:O2'   | 24:DA:658:U:C5'   | 2.68                     | 0.41              |
| 24:DA:806:C:O2'   | 24:DA:807:U:H5'   | 2.20                     | 0.41              |
| 24:DA:866:A:N6    | 24:DA:913:U:O2'   | 2.46                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:DC:105:ALA:HA  | 26:DC:106:PRO:HD3  | 1.68                     | 0.41              |
| 26:DC:31:PRO:C    | 26:DC:32:LEU:HG    | 2.41                     | 0.41              |
| 26:DC:77:VAL:HG23 | 26:DC:111:ALA:HA   | 2.01                     | 0.41              |
| 27:DD:4:LEU:HD23  | 27:DD:101:PHE:CZ   | 2.54                     | 0.41              |
| 29:DF:102:LEU:C   | 29:DF:103:ILE:HD12 | 2.41                     | 0.41              |
| 29:DF:13:LYS:N    | 29:DF:13:LYS:HD2   | 2.35                     | 0.41              |
| 30:DG:169:ARG:O   | 30:DG:170:THR:HB   | 2.20                     | 0.41              |
| 34:DK:104:THR:C   | 34:DK:106:GLU:H    | 2.24                     | 0.41              |
| 24:DA:666:A:H5''  | 35:DL:48:ARG:HG2   | 2.03                     | 0.41              |
| 24:DA:1248:G:C4   | 40:DQ:2:ARG:HG2    | 2.55                     | 0.41              |
| 40:DQ:40:LYS:HD2  | 40:DQ:44:TYR:HE2   | 1.85                     | 0.41              |
| 42:DS:5:ALA:HB3   | 42:DS:54:ALA:HB2   | 2.01                     | 0.41              |
| 47:DX:9:LYS:HD2   | 47:DX:53:LYS:HE3   | 2.01                     | 0.41              |
| 47:DX:63:ILE:HG13 | 47:DX:63:ILE:H     | 1.59                     | 0.41              |
| 21:AA:1049:U:H4'  | 21:AA:1050:G:H5'   | 2.02                     | 0.41              |
| 21:AA:1131:G:O2'  | 21:AA:1132:C:O5'   | 2.33                     | 0.41              |
| 21:AA:1220:G:C6   | 21:AA:1221:G:C5    | 3.08                     | 0.41              |
| 21:AA:1356:G:C2   | 21:AA:1367:C:O2    | 2.74                     | 0.41              |
| 21:AA:144:G:C2    | 21:AA:145:G:C4     | 3.08                     | 0.41              |
| 21:AA:1433:A:C4   | 21:AA:1468:A:C2    | 3.08                     | 0.41              |
| 21:AA:1478:U:H2'  | 21:AA:1479:C:H6    | 1.84                     | 0.41              |
| 21:AA:203:G:N2    | 21:AA:215:C:C2     | 2.89                     | 0.41              |
| 21:AA:39:G:H2'    | 21:AA:40:C:H6      | 1.85                     | 0.41              |
| 2:AC:191:THR:HG21 | 21:AA:421:U:O2     | 2.20                     | 0.41              |
| 21:AA:515:G:C6    | 21:AA:516:U:N3     | 2.89                     | 0.41              |
| 21:AA:695:A:H61   | 21:AA:797:C:H1'    | 1.85                     | 0.41              |
| 1:AB:164:ASP:OD1  | 1:AB:203:ASP:OD1   | 2.38                     | 0.41              |
| 1:AB:68:PHE:HD2   | 1:AB:89:PHE:O      | 2.03                     | 0.41              |
| 1:AB:73:ARG:O     | 1:AB:73:ARG:HG3    | 2.20                     | 0.41              |
| 3:AD:115:GLN:CD   | 3:AD:119:HIS:CE1   | 2.94                     | 0.41              |
| 5:AF:46:GLN:HE21  | 5:AF:56:LYS:HG2    | 1.84                     | 0.41              |
| 7:AH:29:SER:HB2   | 7:AH:32:LYS:HZ2    | 1.81                     | 0.41              |
| 7:AH:52:GLY:HA3   | 7:AH:56:PRO:HA     | 2.01                     | 0.41              |
| 11:AL:2:THR:HB    | 11:AL:5:GLN:HB2    | 2.02                     | 0.41              |
| 14:AO:31:LEU:HD13 | 14:AO:58:MET:O     | 2.20                     | 0.41              |
| 15:AP:17:TYR:CD1  | 15:AP:17:TYR:N     | 2.87                     | 0.41              |
| 18:AS:77:ARG:HD2  | 21:AA:1225:A:H1'   | 2.01                     | 0.41              |
| 50:B0:38:LEU:H    | 50:B0:38:LEU:HG    | 1.65                     | 0.41              |
| 54:B4:9:LYS:HB2   | 54:B4:9:LYS:HE2    | 1.92                     | 0.41              |
| 24:BA:1000:A:C4   | 24:BA:1155:A:C6    | 3.08                     | 0.41              |
| 24:BA:1276:A:C2   | 24:BA:1277:G:N7    | 2.88                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:146:A:C2    | 24:BA:147:C:C2    | 3.09                     | 0.41              |
| 24:BA:1495:A:H2'  | 24:BA:1496:A:C8   | 2.54                     | 0.41              |
| 24:BA:1859:U:H2'  | 24:BA:1860:G:C8   | 2.56                     | 0.41              |
| 24:BA:200:U:C2'   | 24:BA:201:C:H5'   | 2.51                     | 0.41              |
| 24:BA:2097:A:C2   | 24:BA:2193:G:C2   | 3.08                     | 0.41              |
| 24:BA:2390:U:O2   | 24:BA:2391:G:C8   | 2.73                     | 0.41              |
| 24:BA:2557:G:C4   | 24:BA:2558:C:C5   | 3.08                     | 0.41              |
| 24:BA:2673:G:H2'  | 24:BA:2674:G:H8   | 1.84                     | 0.41              |
| 24:BA:288:U:H2'   | 24:BA:289:G:C8    | 2.50                     | 0.41              |
| 24:BA:310:A:OP1   | 44:BU:15:GLY:N    | 2.52                     | 0.41              |
| 24:BA:391:A:C5    | 24:BA:411:G:C2    | 3.08                     | 0.41              |
| 24:BA:503:A:H5''  | 24:BA:504:A:OP1   | 2.20                     | 0.41              |
| 24:BA:584:C:N4    | 24:BA:585:G:C6    | 2.89                     | 0.41              |
| 24:BA:698:C:C4    | 24:BA:762:U:C4    | 3.09                     | 0.41              |
| 24:BA:778:G:C5    | 24:BA:779:U:C5    | 3.09                     | 0.41              |
| 25:BB:90:C:H6     | 25:BB:90:C:C5'    | 2.26                     | 0.41              |
| 26:BC:67:LYS:HE2  | 26:BC:149:LYS:O   | 2.20                     | 0.41              |
| 27:BD:124:ARG:HG2 | 27:BD:125:TRP:NE1 | 2.35                     | 0.41              |
| 28:BE:52:VAL:O    | 28:BE:74:LYS:HE2  | 2.20                     | 0.41              |
| 30:BG:29:ASN:OD1  | 30:BG:30:GLY:N    | 2.53                     | 0.41              |
| 24:BA:2198:A:C2   | 31:BH:29:PHE:HB2  | 2.56                     | 0.41              |
| 31:BH:67:ALA:HA   | 31:BH:138:VAL:CB  | 2.48                     | 0.41              |
| 32:BI:30:GLN:NE2  | 32:BI:32:VAL:HB   | 2.35                     | 0.41              |
| 34:BK:118:LEU:N   | 34:BK:118:LEU:CD1 | 2.84                     | 0.41              |
| 36:BM:33:LEU:HD21 | 36:BM:128:THR:HB  | 2.01                     | 0.41              |
| 36:BM:68:PHE:HA   | 36:BM:69:PRO:HD2  | 1.77                     | 0.41              |
| 38:BO:10:ARG:NH2  | 38:BO:96:GLY:O    | 2.49                     | 0.41              |
| 40:BQ:69:ARG:HB2  | 40:BQ:69:ARG:NH2  | 2.08                     | 0.41              |
| 41:BR:93:PHE:CD1  | 41:BR:93:PHE:C    | 2.93                     | 0.41              |
| 43:BT:19:LYS:O    | 43:BT:23:ALA:CB   | 2.68                     | 0.41              |
| 25:BB:94:A:OP1    | 45:BV:19:ARG:HD3  | 2.20                     | 0.41              |
| 55:CA:1162:C:O2'  | 55:CA:1163:A:O4'  | 2.29                     | 0.41              |
| 55:CA:1213:A:C8   | 55:CA:1215:G:N7   | 2.88                     | 0.41              |
| 55:CA:1463:U:H2'  | 55:CA:1464:U:H6   | 1.85                     | 0.41              |
| 55:CA:152:A:H3'   | 55:CA:153:C:H6    | 1.85                     | 0.41              |
| 55:CA:299:G:H2'   | 55:CA:300:A:C8    | 2.55                     | 0.41              |
| 55:CA:401:C:C2    | 55:CA:402:G:C8    | 3.09                     | 0.41              |
| 55:CA:669:G:C2    | 55:CA:670:G:C4    | 3.09                     | 0.41              |
| 55:CA:709:U:O2'   | 55:CA:710:G:H5'   | 2.20                     | 0.41              |
| 55:CA:735:C:O2'   | 55:CA:736:C:C5'   | 2.69                     | 0.41              |
| 55:CA:874:G:O2'   | 55:CA:875:U:C5'   | 2.64                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:938:A:C6    | 55:CA:939:G:C6    | 3.08                     | 0.41              |
| 2:CC:84:GLU:HA    | 2:CC:87:ARG:HB2   | 2.03                     | 0.41              |
| 3:CD:109:THR:O    | 3:CD:113:ALA:N    | 2.46                     | 0.41              |
| 6:CG:2:ARG:HG2    | 6:CG:3:ARG:N      | 2.34                     | 0.41              |
| 6:CG:69:ARG:HA    | 6:CG:70:PRO:HD3   | 1.79                     | 0.41              |
| 6:CG:89:GLU:O     | 6:CG:90:VAL:HG13  | 2.20                     | 0.41              |
| 10:CK:90:PRO:O    | 10:CK:91:GLY:C    | 2.59                     | 0.41              |
| 11:CL:32:VAL:O    | 11:CL:33:CYS:HB3  | 2.20                     | 0.41              |
| 11:CL:3:VAL:HG23  | 11:CL:4:ASN:N     | 2.36                     | 0.41              |
| 13:CN:22:LYS:O    | 13:CN:26:LEU:HB2  | 2.20                     | 0.41              |
| 13:CN:76:PHE:CE2  | 13:CN:92:ILE:HG21 | 2.56                     | 0.41              |
| 18:CS:11:ASP:N    | 18:CS:11:ASP:OD1  | 2.53                     | 0.41              |
| 18:CS:6:LYS:N     | 18:CS:6:LYS:HD2   | 2.35                     | 0.41              |
| 19:CT:59:ARG:C    | 19:CT:61:ALA:H    | 2.23                     | 0.41              |
| 20:CU:31:VAL:HG12 | 20:CU:32:ARG:N    | 2.36                     | 0.41              |
| 20:CU:3:ILE:O     | 20:CU:4:LYS:HG2   | 2.21                     | 0.41              |
| 22:CV:37:A:C6     | 22:CV:38:A:C4     | 3.08                     | 0.41              |
| 24:DA:2284:A:OP1  | 51:D1:4:ILE:HB    | 2.19                     | 0.41              |
| 24:DA:103:A:O2'   | 24:DA:104:A:H5'   | 2.20                     | 0.41              |
| 24:DA:1313:U:C2'  | 24:DA:1313:U:O2   | 2.66                     | 0.41              |
| 24:DA:1400:U:C2'  | 24:DA:1401:G:O4'  | 2.65                     | 0.41              |
| 24:DA:1878:G:H2'  | 24:DA:1879:C:C6   | 2.55                     | 0.41              |
| 24:DA:1941:C:O2'  | 24:DA:1942:C:C5'  | 2.68                     | 0.41              |
| 24:DA:1955:U:H5'  | 24:DA:2551:C:O2'  | 2.21                     | 0.41              |
| 24:DA:1667:G:N2   | 24:DA:1992:G:OP2  | 2.42                     | 0.41              |
| 24:DA:215:G:C4'   | 24:DA:216:A:H4'   | 2.50                     | 0.41              |
| 24:DA:2197:U:O2'  | 24:DA:2198:A:O5'  | 2.38                     | 0.41              |
| 24:DA:2458:G:O2'  | 24:DA:2460:U:O4   | 2.36                     | 0.41              |
| 24:DA:2489:U:O4   | 24:DA:2490:G:N1   | 2.52                     | 0.41              |
| 24:DA:2620:C:H2'  | 24:DA:2621:G:O4'  | 2.20                     | 0.41              |
| 24:DA:2641:G:H5'' | 33:DJ:78:THR:HB   | 2.02                     | 0.41              |
| 24:DA:36:G:C2     | 24:DA:445:C:C4    | 3.09                     | 0.41              |
| 24:DA:70:G:H8     | 24:DA:70:G:OP2    | 2.03                     | 0.41              |
| 24:DA:762:U:O2    | 24:DA:1431:A:H5'' | 2.20                     | 0.41              |
| 24:DA:764:A:H5''  | 26:DC:208:GLY:HA3 | 2.03                     | 0.41              |
| 24:DA:815:C:H2'   | 24:DA:816:C:C6    | 2.55                     | 0.41              |
| 26:DC:44:ASN:O    | 26:DC:46:GLY:N    | 2.53                     | 0.41              |
| 27:DD:56:LYS:HB3  | 27:DD:56:LYS:NZ   | 2.35                     | 0.41              |
| 29:DF:11:VAL:HG13 | 29:DF:171:ALA:HB2 | 2.03                     | 0.41              |
| 30:DG:117:PRO:HG2 | 30:DG:143:VAL:CG1 | 2.49                     | 0.41              |
| 30:DG:157:LYS:HB2 | 30:DG:157:LYS:HE2 | 1.84                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:DG:31:GLU:O    | 30:DG:32:LEU:HB2  | 2.19                     | 0.41              |
| 30:DG:92:GLY:O    | 30:DG:93:TYR:C    | 2.59                     | 0.41              |
| 31:DH:53:GLU:C    | 31:DH:55:GLU:H    | 2.23                     | 0.41              |
| 32:DI:49:GLU:HG3  | 32:DI:54:ILE:HD11 | 2.02                     | 0.41              |
| 34:DK:59:LYS:HG2  | 34:DK:89:ASN:HA   | 2.01                     | 0.41              |
| 34:DK:7:MET:HA    | 34:DK:7:MET:HE3   | 2.01                     | 0.41              |
| 38:DO:51:ALA:HB2  | 38:DO:81:ARG:HD2  | 2.02                     | 0.41              |
| 24:DA:995:C:H1'   | 40:DQ:60:TRP:CZ2  | 2.55                     | 0.41              |
| 41:DR:19:THR:HG22 | 41:DR:20:VAL:H    | 1.84                     | 0.41              |
| 41:DR:19:THR:HG22 | 41:DR:20:VAL:N    | 2.35                     | 0.41              |
| 42:DS:66:ILE:CD1  | 42:DS:66:ILE:H    | 2.33                     | 0.41              |
| 44:DU:90:LYS:HB2  | 44:DU:92:VAL:HG13 | 2.03                     | 0.41              |
| 45:DV:14:LYS:O    | 45:DV:15:GLY:C    | 2.58                     | 0.41              |
| 21:AA:1130:A:H61  | 21:AA:1144:G:H1'  | 1.84                     | 0.41              |
| 21:AA:1166:G:H8   | 21:AA:1166:G:O5'  | 2.04                     | 0.41              |
| 21:AA:1228:C:O2'  | 21:AA:1229:A:O5'  | 2.38                     | 0.41              |
| 21:AA:1310:G:H2'  | 21:AA:1311:A:O4'  | 2.20                     | 0.41              |
| 21:AA:1403:C:O2'  | 21:AA:1404:C:H5'  | 2.20                     | 0.41              |
| 19:AT:73:ARG:HD3  | 21:AA:261:U:O4    | 2.20                     | 0.41              |
| 21:AA:9:G:O6      | 21:AA:26:A:N6     | 2.52                     | 0.41              |
| 21:AA:330:C:O2'   | 21:AA:331:G:C8    | 2.69                     | 0.41              |
| 21:AA:414:A:O2'   | 21:AA:415:A:C5'   | 2.46                     | 0.41              |
| 21:AA:481:G:H4'   | 21:AA:481:G:OP1   | 2.21                     | 0.41              |
| 21:AA:502:A:C4    | 21:AA:503:C:C6    | 3.09                     | 0.41              |
| 21:AA:582:C:C4    | 21:AA:583:A:N7    | 2.89                     | 0.41              |
| 1:AB:162:VAL:HG22 | 1:AB:184:ALA:CB   | 2.50                     | 0.41              |
| 1:AB:165:ALA:HA   | 1:AB:172:ILE:HD11 | 2.03                     | 0.41              |
| 3:AD:56:GLU:HA    | 3:AD:56:GLU:OE1   | 2.20                     | 0.41              |
| 3:AD:77:GLU:OE1   | 3:AD:77:GLU:HA    | 2.20                     | 0.41              |
| 4:AE:91:SER:OG    | 4:AE:134:ASN:HB2  | 2.21                     | 0.41              |
| 4:AE:94:PHE:C     | 4:AE:94:PHE:CD1   | 2.91                     | 0.41              |
| 6:AG:30:MET:HG3   | 6:AG:34:LYS:O     | 2.20                     | 0.41              |
| 6:AG:38:ALA:O     | 6:AG:42:VAL:HG23  | 2.21                     | 0.41              |
| 7:AH:94:VAL:O     | 7:AH:95:MET:C     | 2.59                     | 0.41              |
| 11:AL:6:LEU:HD21  | 11:AL:11:ARG:NE   | 2.35                     | 0.41              |
| 15:AP:62:GLY:C    | 15:AP:64:GLY:H    | 2.22                     | 0.41              |
| 19:AT:30:PHE:O    | 19:AT:33:LYS:HB2  | 2.20                     | 0.41              |
| 24:BA:1021:A:C2'  | 24:BA:1021:A:N3   | 2.84                     | 0.41              |
| 24:BA:107:G:C2    | 24:BA:108:G:C8    | 3.09                     | 0.41              |
| 24:BA:1145:C:H2'  | 24:BA:1146:C:C6   | 2.56                     | 0.41              |
| 24:BA:1349:C:H2'  | 24:BA:1350:C:C6   | 2.55                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:1496:A:H4'  | 24:BA:1497:U:H5    | 1.84                     | 0.41              |
| 24:BA:1754:A:N1   | 24:BA:2716:C:O2'   | 2.53                     | 0.41              |
| 24:BA:1866:A:C4   | 24:BA:1876:A:C6    | 3.09                     | 0.41              |
| 24:BA:1829:A:N6   | 24:BA:1977:A:N6    | 2.69                     | 0.41              |
| 24:BA:2210:U:H4'  | 24:BA:2211:A:O5'   | 2.21                     | 0.41              |
| 24:BA:2518:A:H2'  | 24:BA:2518:A:N3    | 2.36                     | 0.41              |
| 24:BA:2602:A:H4'  | 24:BA:2603:G:H5'   | 2.03                     | 0.41              |
| 24:BA:261:G:N3    | 24:BA:261:G:H2'    | 2.35                     | 0.41              |
| 24:BA:2851:A:N6   | 24:BA:2852:G:C6    | 2.88                     | 0.41              |
| 24:BA:302:C:H5'   | 44:BU:78:LYS:HZ3   | 1.86                     | 0.41              |
| 24:BA:399:U:C2'   | 24:BA:400:G:H5'    | 2.50                     | 0.41              |
| 24:BA:406:G:H2'   | 24:BA:407:G:C8     | 2.55                     | 0.41              |
| 24:BA:480:A:OP2   | 44:BU:43:LYS:HD2   | 2.20                     | 0.41              |
| 24:BA:513:A:H2'   | 24:BA:514:A:C8     | 2.55                     | 0.41              |
| 24:BA:542:C:O2    | 24:BA:542:C:C2'    | 2.67                     | 0.41              |
| 24:BA:563:A:C2    | 24:BA:2018:G:H1'   | 2.55                     | 0.41              |
| 24:BA:622:G:C6    | 24:BA:623:C:N4     | 2.88                     | 0.41              |
| 24:BA:636:G:H4'   | 24:BA:638:G:O3'    | 2.20                     | 0.41              |
| 24:BA:916:G:H8    | 24:BA:916:G:O5'    | 2.04                     | 0.41              |
| 24:BA:958:U:H3    | 36:BM:16:ARG:HD3   | 1.85                     | 0.41              |
| 24:BA:972:A:H8    | 24:BA:972:A:O5'    | 2.04                     | 0.41              |
| 24:BA:97:C:C2     | 24:BA:98:G:C8      | 3.09                     | 0.41              |
| 24:BA:992:C:C2    | 24:BA:993:G:C8     | 3.08                     | 0.41              |
| 26:BC:12:ARG:HD2  | 26:BC:15:VAL:HG21  | 2.01                     | 0.41              |
| 26:BC:239:PHE:O   | 26:BC:241:LYS:HG2  | 2.20                     | 0.41              |
| 26:BC:250:GLN:NE2 | 26:BC:250:GLN:H    | 2.17                     | 0.41              |
| 27:BD:186:LEU:HA  | 27:BD:186:LEU:HD12 | 1.71                     | 0.41              |
| 28:BE:160:ALA:C   | 28:BE:162:ARG:H    | 2.24                     | 0.41              |
| 28:BE:57:LYS:CG   | 28:BE:58:LYS:N     | 2.78                     | 0.41              |
| 29:BF:135:ILE:C   | 29:BF:137:PHE:N    | 2.74                     | 0.41              |
| 29:BF:40:GLY:C    | 29:BF:84:ILE:HD11  | 2.41                     | 0.41              |
| 30:BG:164:ALA:C   | 30:BG:166:GLU:N    | 2.74                     | 0.41              |
| 30:BG:24:THR:OG1  | 30:BG:34:ARG:HB3   | 2.20                     | 0.41              |
| 33:BJ:37:ARG:HG3  | 33:BJ:118:MET:HE1  | 2.03                     | 0.41              |
| 33:BJ:140:LEU:CD1 | 33:BJ:140:LEU:C    | 2.89                     | 0.41              |
| 34:BK:99:ILE:CG2  | 34:BK:100:PHE:N    | 2.82                     | 0.41              |
| 36:BM:43:ALA:HA   | 36:BM:46:ILE:HG12  | 2.02                     | 0.41              |
| 39:BP:69:VAL:HG22 | 39:BP:69:VAL:O     | 2.17                     | 0.41              |
| 43:BT:29:THR:HA   | 43:BT:86:THR:CA    | 2.51                     | 0.41              |
| 44:BU:66:VAL:O    | 44:BU:69:VAL:HG22  | 2.21                     | 0.41              |
| 49:BZ:43:ILE:O    | 49:BZ:47:ILE:HG13  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 49:BZ:53:MET:O    | 49:BZ:54:VAL:HG13 | 2.21                     | 0.41              |
| 55:CA:1099:G:C6   | 55:CA:1100:C:N3   | 2.88                     | 0.41              |
| 55:CA:1256:A:C2   | 55:CA:1278:G:H2'  | 2.56                     | 0.41              |
| 55:CA:1304:G:H1'  | 55:CA:1333:A:H61  | 1.85                     | 0.41              |
| 55:CA:1386:G:H2'  | 55:CA:1387:G:C8   | 2.54                     | 0.41              |
| 55:CA:302:G:C5    | 55:CA:303:A:N7    | 2.89                     | 0.41              |
| 55:CA:370:C:H2'   | 55:CA:371:A:C8    | 2.53                     | 0.41              |
| 55:CA:814:A:C5'   | 55:CA:1511:G:H4'  | 2.51                     | 0.41              |
| 55:CA:829:G:C6    | 55:CA:858:G:N2    | 2.88                     | 0.41              |
| 55:CA:914:A:O2'   | 55:CA:915:A:O4'   | 2.39                     | 0.41              |
| 55:CA:976:G:N7    | 55:CA:1358:U:C2   | 2.88                     | 0.41              |
| 1:CB:212:TYR:C    | 1:CB:215:ALA:H    | 2.24                     | 0.41              |
| 2:CC:83:VAL:O     | 2:CC:87:ARG:HG3   | 2.20                     | 0.41              |
| 4:CE:38:VAL:CG1   | 4:CE:39:GLY:H     | 2.11                     | 0.41              |
| 4:CE:68:ARG:O     | 4:CE:69:ASN:C     | 2.58                     | 0.41              |
| 6:CG:25:PHE:HD1   | 6:CG:100:MET:SD   | 2.44                     | 0.41              |
| 9:CJ:92:LEU:H     | 9:CJ:92:LEU:HD22  | 1.86                     | 0.41              |
| 10:CK:90:PRO:HB2  | 10:CK:91:GLY:H    | 1.65                     | 0.41              |
| 14:CO:63:ARG:HB2  | 14:CO:63:ARG:HE   | 1.58                     | 0.41              |
| 17:CR:22:TYR:CE1  | 17:CR:64:LEU:HD12 | 2.52                     | 0.41              |
| 18:CS:59:VAL:HG11 | 18:CS:73:PHE:HB3  | 2.03                     | 0.41              |
| 20:CU:13:VAL:CG2  | 20:CU:15:LEU:HD23 | 2.47                     | 0.41              |
| 50:D0:28:SER:HB3  | 50:D0:39:ARG:CZ   | 2.50                     | 0.41              |
| 51:D1:5:ARG:CD    | 51:D1:25:ASN:HB2  | 2.50                     | 0.41              |
| 52:D2:35:ARG:C    | 52:D2:38:GLY:H    | 2.24                     | 0.41              |
| 53:D3:63:TYR:O    | 53:D3:64:ALA:O    | 2.38                     | 0.41              |
| 24:DA:1049:C:H2'  | 24:DA:1049:C:H6   | 1.41                     | 0.41              |
| 24:DA:1345:C:H2'  | 24:DA:1346:G:H8   | 1.85                     | 0.41              |
| 24:DA:726:G:H3'   | 24:DA:1432:G:O2'  | 2.21                     | 0.41              |
| 24:DA:147:C:O2'   | 24:DA:148:U:H5'   | 2.20                     | 0.41              |
| 24:DA:1659:G:C2   | 24:DA:2002:G:N3   | 2.88                     | 0.41              |
| 24:DA:1742:U:C4   | 24:DA:1743:G:C6   | 3.08                     | 0.41              |
| 24:DA:1796:U:H2'  | 24:DA:1797:G:C8   | 2.56                     | 0.41              |
| 24:DA:1809:A:O2'  | 24:DA:1810:A:P    | 2.78                     | 0.41              |
| 24:DA:1853:A:H1'  | 24:DA:2234:G:H5'  | 2.03                     | 0.41              |
| 24:DA:197:A:N7    | 24:DA:2430:A:C8   | 2.89                     | 0.41              |
| 24:DA:2287:A:HO2' | 24:DA:2288:A:C5'  | 2.27                     | 0.41              |
| 24:DA:2446:G:C5   | 24:DA:2501:C:H2'  | 2.55                     | 0.41              |
| 24:DA:2454:G:N2   | 24:DA:2499:C:C2   | 2.88                     | 0.41              |
| 24:DA:2524:G:O2'  | 24:DA:2741:A:N1   | 2.40                     | 0.41              |
| 24:DA:363:G:H2'   | 24:DA:364:C:H5    | 1.85                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:389:G:H8    | 24:DA:389:G:O5'    | 2.03                     | 0.41              |
| 24:DA:408:G:H2'   | 24:DA:409:G:H8     | 1.85                     | 0.41              |
| 24:DA:415:A:C6    | 24:DA:416:U:C4     | 3.07                     | 0.41              |
| 24:DA:511:U:H5'   | 24:DA:1236:G:OP1   | 2.20                     | 0.41              |
| 24:DA:604:G:N3    | 24:DA:605:G:C8     | 2.89                     | 0.41              |
| 24:DA:614:A:H4'   | 24:DA:616:A:N7     | 2.35                     | 0.41              |
| 24:DA:70:G:HO2'   | 24:DA:71:A:H2      | 1.60                     | 0.41              |
| 24:DA:771:G:N3    | 24:DA:772:C:C6     | 2.88                     | 0.41              |
| 24:DA:800:A:N1    | 24:DA:802:A:C8     | 2.88                     | 0.41              |
| 24:DA:945:A:C8    | 24:DA:2448:A:C2    | 3.08                     | 0.41              |
| 56:DB:115:A:H2'   | 56:DB:116:G:H8     | 1.80                     | 0.41              |
| 26:DC:189:ALA:O   | 26:DC:190:THR:HB   | 2.21                     | 0.41              |
| 28:DE:3:LEU:HA    | 28:DE:3:LEU:HD12   | 1.95                     | 0.41              |
| 29:DF:37:MET:N    | 29:DF:151:LEU:HB3  | 2.35                     | 0.41              |
| 29:DF:8:LYS:HB2   | 29:DF:8:LYS:HZ1    | 1.83                     | 0.41              |
| 31:DH:83:LYS:HG3  | 31:DH:149:GLU:HB2  | 2.02                     | 0.41              |
| 33:DJ:37:ARG:NH2  | 33:DJ:39:LYS:HZ1   | 2.18                     | 0.41              |
| 33:DJ:49:ASP:HB2  | 33:DJ:121:LYS:NZ   | 2.35                     | 0.41              |
| 34:DK:71:ARG:HD2  | 34:DK:71:ARG:HA    | 1.89                     | 0.41              |
| 34:DK:13:ASN:ND2  | 34:DK:97:THR:H     | 2.04                     | 0.41              |
| 34:DK:99:ILE:HG13 | 34:DK:118:LEU:HD12 | 2.03                     | 0.41              |
| 35:DL:111:ILE:HA  | 35:DL:128:THR:OG1  | 2.21                     | 0.41              |
| 39:DP:54:LEU:HG   | 39:DP:54:LEU:O     | 2.20                     | 0.41              |
| 42:DS:9:HIS:H     | 42:DS:102:HIS:CE1  | 2.38                     | 0.41              |
| 44:DU:16:LYS:HA   | 44:DU:16:LYS:HD3   | 1.87                     | 0.41              |
| 44:DU:58:VAL:CG1  | 44:DU:60:LYS:HG2   | 2.51                     | 0.41              |
| 21:AA:1294:G:C6   | 21:AA:1295:U:N3    | 2.89                     | 0.41              |
| 21:AA:1449:C:O2'  | 21:AA:1450:U:O4'   | 2.30                     | 0.41              |
| 21:AA:1501:C:C5   | 21:AA:1504:G:C4    | 3.09                     | 0.41              |
| 20:AU:38:GLU:CG   | 21:AA:1527:U:OP2   | 2.69                     | 0.41              |
| 21:AA:253:A:H2'   | 21:AA:254:G:H8     | 1.84                     | 0.41              |
| 21:AA:50:A:O2'    | 21:AA:360:G:N2     | 2.53                     | 0.41              |
| 21:AA:511:C:C4    | 21:AA:512:U:C4     | 3.09                     | 0.41              |
| 21:AA:57:G:C6     | 21:AA:58:C:N4      | 2.89                     | 0.41              |
| 21:AA:774:G:C5    | 21:AA:775:G:N7     | 2.89                     | 0.41              |
| 21:AA:778:G:H2'   | 21:AA:779:C:C6     | 2.55                     | 0.41              |
| 21:AA:925:G:H2'   | 21:AA:927:G:H8     | 1.86                     | 0.41              |
| 21:AA:961:U:O2'   | 21:AA:962:C:H5'    | 2.20                     | 0.41              |
| 21:AA:982:U:C2    | 21:AA:983:A:N1     | 2.89                     | 0.41              |
| 1:AB:185:ILE:HG22 | 1:AB:199:ILE:HB    | 2.03                     | 0.41              |
| 1:AB:32:GLY:HA3   | 1:AB:39:ILE:CG1    | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AB:67:LEU:HD22  | 1:AB:69:VAL:CG2   | 2.50                     | 0.41              |
| 2:AC:111:ASP:O    | 2:AC:115:VAL:HG23 | 2.21                     | 0.41              |
| 2:AC:41:TYR:CZ    | 2:AC:89:VAL:HG21  | 2.55                     | 0.41              |
| 8:AI:33:SER:OG    | 8:AI:34:LEU:N     | 2.53                     | 0.41              |
| 9:AJ:11:LYS:HB3   | 9:AJ:71:LEU:CD1   | 2.47                     | 0.41              |
| 9:AJ:38:GLY:O     | 9:AJ:74:VAL:O     | 2.38                     | 0.41              |
| 13:AN:68:ARG:HA   | 13:AN:69:PRO:HD2  | 1.79                     | 0.41              |
| 16:AQ:68:LYS:O    | 21:AA:254:G:OP1   | 2.39                     | 0.41              |
| 54:B4:15:LYS:O    | 54:B4:16:ILE:O    | 2.38                     | 0.41              |
| 24:BA:1062:G:N7   | 24:BA:1088:A:C8   | 2.88                     | 0.41              |
| 24:BA:1122:G:N3   | 24:BA:1122:G:C2'  | 2.84                     | 0.41              |
| 24:BA:1567:G:H2'  | 26:BC:84:PRO:HG3  | 2.03                     | 0.41              |
| 24:BA:1654:A:N3   | 24:BA:1655:A:C8   | 2.88                     | 0.41              |
| 24:BA:1731:G:H1'  | 24:BA:1733:G:C8   | 2.55                     | 0.41              |
| 24:BA:1798:U:P    | 26:BC:255:LYS:O   | 2.79                     | 0.41              |
| 24:BA:1803:A:H5'' | 24:BA:1804:C:OP2  | 2.20                     | 0.41              |
| 24:BA:1899:A:H3'  | 24:BA:1899:A:C8   | 2.56                     | 0.41              |
| 24:BA:1652:A:H2   | 24:BA:2006:C:N3   | 2.13                     | 0.41              |
| 24:BA:1255:U:H3   | 24:BA:2060:A:C5'  | 2.34                     | 0.41              |
| 24:BA:2235:G:H2'  | 24:BA:2236:U:C6   | 2.56                     | 0.41              |
| 24:BA:2287:A:C5   | 24:BA:2289:G:N7   | 2.89                     | 0.41              |
| 24:BA:2353:G:O2'  | 46:BW:31:LEU:CD2  | 2.65                     | 0.41              |
| 24:BA:1864:U:OP1  | 24:BA:2411:A:H5'  | 2.20                     | 0.41              |
| 24:BA:2534:A:H2'  | 24:BA:2535:G:O4'  | 2.21                     | 0.41              |
| 24:BA:2853:C:C2'  | 24:BA:2854:G:H5'  | 2.50                     | 0.41              |
| 24:BA:2897:U:H2'  | 24:BA:2898:U:C6   | 2.56                     | 0.41              |
| 24:BA:312:G:N3    | 24:BA:313:G:C8    | 2.89                     | 0.41              |
| 24:BA:342:A:N1    | 24:BA:343:C:C2    | 2.88                     | 0.41              |
| 24:BA:607:U:O4    | 24:BA:620:G:O4'   | 2.38                     | 0.41              |
| 24:BA:611:C:C2'   | 24:BA:612:G:H5'   | 2.51                     | 0.41              |
| 24:BA:640:C:O2'   | 24:BA:641:U:H5'   | 2.20                     | 0.41              |
| 24:BA:662:G:O3'   | 35:BL:16:GLY:HA2  | 2.20                     | 0.41              |
| 24:BA:78:U:C2     | 24:BA:79:C:C5     | 3.09                     | 0.41              |
| 24:BA:971:G:C6    | 24:BA:972:A:C4    | 3.09                     | 0.41              |
| 24:BA:987:C:N4    | 24:BA:988:A:C5    | 2.89                     | 0.41              |
| 29:BF:125:GLY:O   | 29:BF:126:ASN:OD1 | 2.39                     | 0.41              |
| 31:BH:85:GLY:HA3  | 31:BH:91:PHE:HB3  | 2.01                     | 0.41              |
| 32:BI:50:LYS:HE2  | 32:BI:50:LYS:HB2  | 1.87                     | 0.41              |
| 34:BK:2:ILE:CD1   | 34:BK:2:ILE:N     | 2.82                     | 0.41              |
| 36:BM:133:LYS:O   | 36:BM:134:THR:CB  | 2.63                     | 0.41              |
| 36:BM:46:ILE:O    | 36:BM:47:GLU:C    | 2.59                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:1652:A:H62  | 37:BN:11:ASN:HD21 | 1.69                     | 0.41              |
| 37:BN:64:ARG:O    | 37:BN:67:PHE:HB3  | 2.21                     | 0.41              |
| 38:BO:31:THR:HG22 | 38:BO:34:HIS:O    | 2.20                     | 0.41              |
| 39:BP:24:THR:HG22 | 39:BP:87:ARG:N    | 2.33                     | 0.41              |
| 43:BT:19:LYS:O    | 43:BT:20:ALA:C    | 2.58                     | 0.41              |
| 43:BT:28:ASN:C    | 43:BT:91:GLN:HE22 | 2.24                     | 0.41              |
| 46:BW:74:LYS:O    | 46:BW:75:ASN:C    | 2.58                     | 0.41              |
| 48:BY:42:LEU:O    | 48:BY:43:LEU:C    | 2.58                     | 0.41              |
| 55:CA:1250:A:C5   | 55:CA:1287:A:C5   | 3.09                     | 0.41              |
| 55:CA:198:G:O2'   | 55:CA:199:A:O4'   | 2.37                     | 0.41              |
| 55:CA:316:C:C2    | 55:CA:317:U:C5    | 3.09                     | 0.41              |
| 55:CA:317:U:N3    | 55:CA:337:G:C2    | 2.89                     | 0.41              |
| 55:CA:411:A:C6    | 55:CA:429:U:C5    | 3.08                     | 0.41              |
| 55:CA:397:A:C6    | 55:CA:548:G:C5    | 3.08                     | 0.41              |
| 55:CA:562:U:C4    | 55:CA:884:U:C5    | 3.09                     | 0.41              |
| 55:CA:727:G:C2    | 55:CA:731:G:C2    | 3.07                     | 0.41              |
| 55:CA:763:G:C4    | 55:CA:764:C:C5    | 3.09                     | 0.41              |
| 55:CA:833:G:C2    | 55:CA:834:U:C2    | 3.08                     | 0.41              |
| 55:CA:914:A:H2'   | 55:CA:915:A:C8    | 2.56                     | 0.41              |
| 55:CA:946:A:H2'   | 55:CA:947:G:H8    | 1.85                     | 0.41              |
| 1:CB:151:LYS:HG3  | 1:CB:152:ASP:H    | 1.85                     | 0.41              |
| 1:CB:169:HIS:CG   | 1:CB:170:ILE:N    | 2.89                     | 0.41              |
| 1:CB:25:LYS:O     | 1:CB:192:PRO:HG3  | 2.20                     | 0.41              |
| 1:CB:96:LEU:HD22  | 55:CA:1103:C:C5'  | 2.51                     | 0.41              |
| 2:CC:131:ARG:CA   | 2:CC:134:LYS:HD2  | 2.50                     | 0.41              |
| 2:CC:152:VAL:HG23 | 2:CC:156:LEU:HD11 | 2.03                     | 0.41              |
| 2:CC:99:GLN:O     | 2:CC:100:ILE:C    | 2.59                     | 0.41              |
| 6:CG:112:ASP:CB   | 6:CG:118:ARG:HA   | 2.51                     | 0.41              |
| 9:CJ:71:LEU:HD12  | 9:CJ:72:ARG:H     | 1.86                     | 0.41              |
| 15:CP:66:THR:CG2  | 15:CP:67:ILE:N    | 2.83                     | 0.41              |
| 16:CQ:24:ILE:N    | 16:CQ:24:ILE:HD12 | 2.35                     | 0.41              |
| 5:CF:59:TYR:HE2   | 17:CR:66:LEU:CD2  | 2.33                     | 0.41              |
| 17:CR:70:THR:OG1  | 17:CR:71:ASP:N    | 2.53                     | 0.41              |
| 18:CS:50:VAL:CG1  | 18:CS:70:LEU:HB3  | 2.48                     | 0.41              |
| 24:DA:1047:G:C2   | 24:DA:1110:G:C4   | 3.08                     | 0.41              |
| 24:DA:1062:G:O2'  | 24:DA:1063:G:C8   | 2.29                     | 0.41              |
| 24:DA:1287:A:OP1  | 37:DN:103:ARG:CG  | 2.69                     | 0.41              |
| 24:DA:132:G:H2'   | 24:DA:133:U:C6    | 2.55                     | 0.41              |
| 24:DA:1355:G:C6   | 24:DA:1377:G:C2   | 3.09                     | 0.41              |
| 24:DA:13:A:C5'    | 24:DA:14:A:OP1    | 2.67                     | 0.41              |
| 24:DA:1753:G:C2   | 24:DA:1756:G:C2   | 3.09                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:DA:1707:G:C8   | 24:DA:1756:G:N7   | 2.89                     | 0.41              |
| 24:DA:1830:C:H5'  | 26:DC:14:HIS:HE1  | 1.80                     | 0.41              |
| 24:DA:1844:C:N3   | 24:DA:1845:G:N7   | 2.69                     | 0.41              |
| 24:DA:2136:G:H2'  | 24:DA:2137:U:H6   | 1.83                     | 0.41              |
| 24:DA:2285:C:OP2  | 51:D1:5:ARG:NH1   | 2.54                     | 0.41              |
| 24:DA:229:C:HO2'  | 24:DA:230:G:P     | 2.43                     | 0.41              |
| 24:DA:241:A:C1'   | 24:DA:243:U:C4    | 3.03                     | 0.41              |
| 24:DA:2439:A:H1'  | 24:DA:2587:A:H5'  | 2.02                     | 0.41              |
| 24:DA:2654:A:H4'  | 24:DA:2655:G:OP1  | 2.19                     | 0.41              |
| 24:DA:2823:A:C4   | 24:DA:2824:C:C6   | 3.08                     | 0.41              |
| 24:DA:2850:A:N7   | 24:DA:2868:A:O2'  | 2.53                     | 0.41              |
| 24:DA:302:C:O2'   | 24:DA:303:G:O5'   | 2.38                     | 0.41              |
| 24:DA:61:C:N4     | 24:DA:94:A:C6     | 2.89                     | 0.41              |
| 24:DA:719:C:O2'   | 24:DA:720:U:H5'   | 2.20                     | 0.41              |
| 24:DA:735:A:H2'   | 24:DA:735:A:N3    | 2.36                     | 0.41              |
| 24:DA:738:G:N1    | 24:DA:739:A:C2    | 2.89                     | 0.41              |
| 24:DA:79:C:O2'    | 24:DA:346:A:H1'   | 2.20                     | 0.41              |
| 56:DB:66:A:C6     | 56:DB:107:G:C4    | 3.09                     | 0.41              |
| 56:DB:42:C:O2     | 29:DF:89:THR:N    | 2.52                     | 0.41              |
| 56:DB:98:G:H1     | 45:DV:14:LYS:H    | 1.68                     | 0.41              |
| 27:DD:15:PHE:HA   | 27:DD:20:VAL:O    | 2.21                     | 0.41              |
| 27:DD:40:LEU:HD12 | 27:DD:40:LEU:N    | 2.35                     | 0.41              |
| 28:DE:134:LEU:HA  | 28:DE:137:LYS:CB  | 2.51                     | 0.41              |
| 28:DE:46:GLN:CB   | 28:DE:86:ALA:HB1  | 2.45                     | 0.41              |
| 29:DF:82:TYR:HA   | 29:DF:83:PRO:HD2  | 1.86                     | 0.41              |
| 33:DJ:123:LYS:N   | 33:DJ:123:LYS:HD2 | 2.35                     | 0.41              |
| 33:DJ:97:PRO:C    | 33:DJ:99:ARG:N    | 2.74                     | 0.41              |
| 37:DN:51:LEU:HA   | 37:DN:51:LEU:HD23 | 1.87                     | 0.41              |
| 38:DO:18:LEU:HD21 | 38:DO:91:SER:CB   | 2.50                     | 0.41              |
| 39:DP:54:LEU:HA   | 39:DP:76:HIS:CD2  | 2.55                     | 0.41              |
| 41:DR:68:ARG:NH1  | 41:DR:90:ARG:HG2  | 2.34                     | 0.41              |
| 42:DS:27:LYS:O    | 42:DS:28:LYS:C    | 2.59                     | 0.41              |
| 44:DU:100:GLU:O   | 44:DU:101:THR:C   | 2.59                     | 0.41              |
| 46:DW:17:ALA:O    | 46:DW:18:LYS:CB   | 2.56                     | 0.41              |
| 21:AA:1039:G:C6   | 21:AA:1040:U:C4   | 3.08                     | 0.41              |
| 21:AA:1081:A:C2   | 21:AA:1082:A:C8   | 3.09                     | 0.41              |
| 21:AA:112:G:C6    | 21:AA:330:C:N4    | 2.89                     | 0.41              |
| 21:AA:113:G:H1'   | 21:AA:354:G:H5'   | 2.03                     | 0.41              |
| 18:AS:77:ARG:NH2  | 21:AA:1322:C:P    | 2.92                     | 0.41              |
| 21:AA:1382:C:O2'  | 21:AA:1383:C:C6   | 2.69                     | 0.41              |
| 21:AA:1501:C:C6   | 21:AA:1504:G:C8   | 3.09                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 21:AA:211:G:H2'  | 21:AA:212:G:O4'   | 2.20                     | 0.41              |
| 21:AA:252:U:O2'  | 21:AA:275:G:N2    | 2.54                     | 0.41              |
| 21:AA:109:A:C5   | 21:AA:326:G:C2    | 3.09                     | 0.41              |
| 21:AA:454:G:C2'  | 21:AA:455:G:H5'   | 2.50                     | 0.41              |
| 21:AA:506:G:C6   | 21:AA:507:C:C4    | 3.09                     | 0.41              |
| 21:AA:62:U:H2'   | 21:AA:63:C:C6     | 2.56                     | 0.41              |
| 5:AF:53:LYS:HZ3  | 21:AA:710:G:H5''  | 1.79                     | 0.41              |
| 21:AA:868:C:H2'  | 21:AA:869:G:O4'   | 2.21                     | 0.41              |
| 1:AB:67:LEU:HG   | 1:AB:149:GLY:HA3  | 2.02                     | 0.41              |
| 1:AB:81:ASP:CG   | 1:AB:82:ALA:H     | 2.24                     | 0.41              |
| 3:AD:117:VAL:HA  | 3:AD:122:ILE:CD1  | 2.48                     | 0.41              |
| 4:AE:57:ALA:HA   | 4:AE:60:GLN:HB3   | 2.03                     | 0.41              |
| 5:AF:71:ILE:HD11 | 5:AF:89:VAL:HG21  | 2.02                     | 0.41              |
| 9:AJ:74:VAL:O    | 9:AJ:75:ASP:CB    | 2.67                     | 0.41              |
| 10:AK:22:ILE:CG1 | 10:AK:85:VAL:HA   | 2.50                     | 0.41              |
| 10:AK:25:SER:OG  | 10:AK:26:PHE:N    | 2.53                     | 0.41              |
| 10:AK:44:ALA:HB3 | 10:AK:69:CYS:HB2  | 2.01                     | 0.41              |
| 11:AL:82:ARG:HG2 | 11:AL:82:ARG:HH11 | 1.84                     | 0.41              |
| 12:AM:70:ARG:HG2 | 12:AM:71:GLU:CB   | 2.50                     | 0.41              |
| 14:AO:20:ASP:OD1 | 21:AA:750:C:O2'   | 2.37                     | 0.41              |
| 14:AO:68:TYR:OH  | 21:AA:752:G:O3'   | 2.38                     | 0.41              |
| 18:AS:79:TYR:O   | 18:AS:80:ARG:HB3  | 2.21                     | 0.41              |
| 10:AK:125:LYS:O  | 20:AU:33:ARG:CZ   | 2.68                     | 0.41              |
| 22:AV:27:G:C5'   | 22:AV:27:G:H8     | 2.28                     | 0.41              |
| 24:BA:1125:G:N1  | 24:BA:1126:A:N6   | 2.69                     | 0.41              |
| 24:BA:1300:G:C4' | 24:BA:1301:A:H5'' | 2.49                     | 0.41              |
| 24:BA:1753:G:N1  | 24:BA:1756:G:OP2  | 2.53                     | 0.41              |
| 24:BA:1970:A:H1' | 24:BA:1972:G:C8   | 2.55                     | 0.41              |
| 24:BA:2149:U:H2' | 24:BA:2150:C:O4'  | 2.20                     | 0.41              |
| 24:BA:2185:U:H6  | 24:BA:2185:U:OP2  | 2.04                     | 0.41              |
| 24:BA:2186:G:C2  | 24:BA:2187:U:H1'  | 2.56                     | 0.41              |
| 24:BA:217:A:C4   | 24:BA:218:A:C8    | 3.08                     | 0.41              |
| 24:BA:2207:C:C2  | 24:BA:2218:G:C2   | 3.09                     | 0.41              |
| 24:BA:2291:U:N3  | 24:BA:2292:U:C4   | 2.89                     | 0.41              |
| 24:BA:2516:A:C6  | 24:BA:2517:C:C4   | 3.09                     | 0.41              |
| 24:BA:2667:C:C2' | 24:BA:2668:G:H5'  | 2.51                     | 0.41              |
| 24:BA:2824:C:H2' | 24:BA:2825:G:O5'  | 2.20                     | 0.41              |
| 24:BA:445:C:O2   | 24:BA:449:A:H2    | 2.04                     | 0.41              |
| 24:BA:477:A:H2'  | 24:BA:478:A:C8    | 2.55                     | 0.41              |
| 24:BA:528:A:H2   | 24:BA:2043:C:C5'  | 2.30                     | 0.41              |
| 24:BA:602:A:H1'  | 24:BA:656:G:N2    | 2.36                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BA:681:G:C4     | 24:BA:682:G:C8     | 3.09                     | 0.41              |
| 24:BA:705:A:C2     | 24:BA:706:A:C4     | 3.08                     | 0.41              |
| 24:BA:783:A:H2'    | 24:BA:784:G:H4'    | 2.02                     | 0.41              |
| 24:BA:988:A:C2     | 24:BA:989:G:N2     | 2.88                     | 0.41              |
| 24:BA:1655:A:H5'   | 27:BD:118:PHE:CD2  | 2.56                     | 0.41              |
| 28:BE:172:ALA:O    | 28:BE:175:ILE:HG22 | 2.21                     | 0.41              |
| 28:BE:176:ASP:OD2  | 28:BE:179:SER:HB3  | 2.21                     | 0.41              |
| 24:BA:448:U:H5'    | 28:BE:79:ARG:NH2   | 2.36                     | 0.41              |
| 30:BG:102:ILE:HG21 | 30:BG:130:ILE:HD13 | 2.03                     | 0.41              |
| 30:BG:1:SER:O      | 30:BG:2:ARG:HB2    | 2.20                     | 0.41              |
| 30:BG:83:THR:O     | 30:BG:84:LYS:HD3   | 2.20                     | 0.41              |
| 32:BI:72:THR:HB    | 32:BI:112:LYS:HZ1  | 1.84                     | 0.41              |
| 36:BM:33:LEU:HD23  | 36:BM:33:LEU:HA    | 1.83                     | 0.41              |
| 39:BP:20:ARG:HA    | 39:BP:21:PRO:HD2   | 1.85                     | 0.41              |
| 41:BR:49:ILE:HG22  | 41:BR:54:VAL:N     | 2.35                     | 0.41              |
| 42:BS:46:LEU:HD23  | 42:BS:46:LEU:HA    | 1.88                     | 0.41              |
| 24:BA:747:U:O3'    | 42:BS:89:ALA:HB3   | 2.21                     | 0.41              |
| 24:BA:1398:C:H5''  | 43:BT:59:ASN:HD21  | 1.84                     | 0.41              |
| 43:BT:32:LEU:N     | 43:BT:83:ALA:HB3   | 2.31                     | 0.41              |
| 46:BW:14:ASP:HB3   | 46:BW:15:SER:H     | 1.31                     | 0.41              |
| 49:BZ:8:GLN:HB3    | 49:BZ:31:ILE:HA    | 2.02                     | 0.41              |
| 55:CA:1026:G:H22   | 55:CA:1036:A:N6    | 2.17                     | 0.41              |
| 55:CA:1042:A:H2'   | 55:CA:1043:G:O4'   | 2.21                     | 0.41              |
| 1:CB:94:ARG:HE     | 55:CA:1099:G:H5''  | 1.86                     | 0.41              |
| 55:CA:1065:U:O4    | 55:CA:1189:U:N3    | 2.53                     | 0.41              |
| 55:CA:1441:A:N6    | 55:CA:1462:C:H1'   | 2.36                     | 0.41              |
| 55:CA:468:A:H5''   | 55:CA:469:C:H5     | 1.86                     | 0.41              |
| 55:CA:640:A:C2     | 55:CA:642:A:N6     | 2.88                     | 0.41              |
| 55:CA:669:G:H2'    | 55:CA:670:G:H8     | 1.84                     | 0.41              |
| 14:CO:53:ARG:NH1   | 55:CA:728:A:C8     | 2.88                     | 0.41              |
| 55:CA:809:G:C6     | 55:CA:810:C:C5     | 3.09                     | 0.41              |
| 55:CA:663:A:H5'    | 55:CA:836:G:OP1    | 2.20                     | 0.41              |
| 55:CA:85:U:O2      | 55:CA:85:U:O4'     | 2.38                     | 0.41              |
| 55:CA:981:U:C5     | 55:CA:982:U:O2     | 2.74                     | 0.41              |
| 2:CC:36:PHE:HE1    | 13:CN:91:GLU:OE1   | 2.03                     | 0.41              |
| 3:CD:32:LYS:HE3    | 55:CA:413:G:C2     | 2.55                     | 0.41              |
| 4:CE:104:ILE:CG2   | 4:CE:104:ILE:O     | 2.68                     | 0.41              |
| 4:CE:148:SER:O     | 4:CE:152:VAL:N     | 2.53                     | 0.41              |
| 9:CJ:92:LEU:O      | 9:CJ:94:ALA:N      | 2.54                     | 0.41              |
| 11:CL:113:ARG:NH2  | 11:CL:120:ARG:HA   | 2.35                     | 0.41              |
| 12:CM:27:THR:HG21  | 55:CA:1328:C:H5''  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:CO:69:LEU:CD1  | 14:CO:77:TYR:HB2  | 2.50                     | 0.41              |
| 15:CP:32:PHE:HD1  | 15:CP:32:PHE:O    | 2.04                     | 0.41              |
| 18:CS:46:LEU:H    | 18:CS:46:LEU:HD23 | 1.85                     | 0.41              |
| 19:CT:23:ARG:CB   | 19:CT:65:LEU:HD11 | 2.51                     | 0.41              |
| 17:CR:37:LYS:CD   | 20:CU:22:CYS:HB3  | 2.51                     | 0.41              |
| 20:CU:24:LYS:HZ2  | 20:CU:25:ALA:HB2  | 1.86                     | 0.41              |
| 22:CV:30:G:C2     | 22:CV:31:A:N9     | 2.89                     | 0.41              |
| 50:D0:43:THR:HG23 | 50:D0:47:TYR:O    | 2.21                     | 0.41              |
| 51:D1:36:LYS:HA   | 51:D1:47:ILE:HA   | 2.03                     | 0.41              |
| 24:DA:682:G:H5'   | 52:D2:26:ASN:OD1  | 2.20                     | 0.41              |
| 24:DA:1136:G:O2'  | 24:DA:1137:G:C8   | 2.70                     | 0.41              |
| 24:DA:1398:C:O2'  | 24:DA:1399:C:O5'  | 2.39                     | 0.41              |
| 24:DA:1407:G:H2'  | 24:DA:1408:G:H8   | 1.86                     | 0.41              |
| 24:DA:1475:G:N3   | 24:DA:1514:G:O6   | 2.54                     | 0.41              |
| 24:DA:1923:U:O2'  | 24:DA:1924:C:H5'  | 2.20                     | 0.41              |
| 24:DA:2235:G:O2'  | 24:DA:2236:U:H5'  | 2.21                     | 0.41              |
| 24:DA:228:C:H4'   | 24:DA:229:C:C6    | 2.56                     | 0.41              |
| 24:DA:2413:G:C4   | 24:DA:2414:G:C8   | 3.09                     | 0.41              |
| 24:DA:2426:A:H3'  | 24:DA:2427:C:C5'  | 2.50                     | 0.41              |
| 24:DA:2577:A:H2   | 50:D0:1:ALA:H2    | 1.65                     | 0.41              |
| 24:DA:2647:U:O2'  | 24:DA:2648:G:H5'  | 2.20                     | 0.41              |
| 24:DA:2543:G:N3   | 24:DA:2765:A:H2'  | 2.35                     | 0.41              |
| 24:DA:30:G:OP1    | 40:DQ:4:LYS:HG3   | 2.21                     | 0.41              |
| 24:DA:363:G:H2'   | 24:DA:364:C:C5    | 2.56                     | 0.41              |
| 24:DA:379:G:O6    | 24:DA:380:G:C6    | 2.73                     | 0.41              |
| 24:DA:396:G:O2'   | 24:DA:397:U:C6    | 2.55                     | 0.41              |
| 24:DA:411:G:C4'   | 24:DA:412:A:OP1   | 2.67                     | 0.41              |
| 24:DA:511:U:H4'   | 24:DA:1235:G:H4'  | 2.02                     | 0.41              |
| 24:DA:50:U:H4'    | 24:DA:51:G:OP2    | 2.20                     | 0.41              |
| 24:DA:728:G:C4    | 24:DA:730:A:C8    | 3.09                     | 0.41              |
| 24:DA:71:A:C8     | 24:DA:73:A:N6     | 2.89                     | 0.41              |
| 24:DA:807:U:C1'   | 24:DA:2445:G:H5'  | 2.51                     | 0.41              |
| 24:DA:810:U:HO2'  | 24:DA:811:U:H5    | 1.68                     | 0.41              |
| 24:DA:866:A:C8    | 24:DA:914:G:C6    | 3.09                     | 0.41              |
| 24:DA:903:C:H2'   | 24:DA:904:G:H8    | 1.83                     | 0.41              |
| 24:DA:948:C:H2'   | 24:DA:949:G:H8    | 1.84                     | 0.41              |
| 24:DA:959:A:O2'   | 24:DA:960:A:O4'   | 2.32                     | 0.41              |
| 24:DA:963:U:O2'   | 24:DA:964:C:C6    | 2.72                     | 0.41              |
| 24:DA:952:G:C4    | 24:DA:966:G:N2    | 2.89                     | 0.41              |
| 24:DA:8:C:O2'     | 24:DA:9:G:H5'     | 2.21                     | 0.41              |
| 56:DB:51:G:H3'    | 38:DO:64:TYR:CE1  | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 56:DB:52:A:H1'    | 56:DB:53:A:N7     | 2.36                     | 0.41              |
| 29:DF:122:ASP:HB3 | 29:DF:126:ASN:ND2 | 2.36                     | 0.41              |
| 29:DF:33:ILE:HB   | 29:DF:90:LEU:HD23 | 2.03                     | 0.41              |
| 29:DF:48:LEU:O    | 29:DF:52:ALA:CB   | 2.69                     | 0.41              |
| 29:DF:74:ALA:HB1  | 29:DF:76:PHE:CE2  | 2.54                     | 0.41              |
| 30:DG:94:ARG:HG2  | 30:DG:104:LEU:HA  | 2.03                     | 0.41              |
| 24:DA:2751:G:N3   | 30:DG:2:ARG:NH2   | 2.69                     | 0.41              |
| 31:DH:2:GLN:HB3   | 31:DH:18:GLN:CG   | 2.51                     | 0.41              |
| 31:DH:4:ILE:O     | 31:DH:36:ALA:HB1  | 2.20                     | 0.41              |
| 33:DJ:15:TRP:HA   | 33:DJ:53:TYR:O    | 2.20                     | 0.41              |
| 33:DJ:35:ARG:HA   | 33:DJ:40:HIS:CD2  | 2.56                     | 0.41              |
| 33:DJ:64:VAL:CG1  | 33:DJ:65:THR:N    | 2.83                     | 0.41              |
| 34:DK:61:VAL:HG13 | 34:DK:87:LEU:HD21 | 2.03                     | 0.41              |
| 35:DL:96:LYS:HE2  | 35:DL:102:GLY:O   | 2.21                     | 0.41              |
| 39:DP:24:THR:O    | 39:DP:25:VAL:C    | 2.58                     | 0.41              |
| 24:DA:1392:A:H61  | 43:DT:18:GLU:HG3  | 1.86                     | 0.41              |
| 43:DT:18:GLU:HB2  | 43:DT:19:LYS:H    | 1.45                     | 0.41              |
| 43:DT:61:LEU:C    | 43:DT:61:LEU:HD12 | 2.41                     | 0.41              |
| 45:DV:15:GLY:O    | 45:DV:19:ARG:HG3  | 2.20                     | 0.41              |
| 56:DB:76:G:O2'    | 45:DV:21:ARG:NH2  | 2.53                     | 0.41              |
| 46:DW:17:ALA:CB   | 46:DW:36:ILE:HA   | 2.50                     | 0.41              |
| 24:DA:380:G:H4'   | 47:DX:15:ASN:O    | 2.21                     | 0.41              |
| 21:AA:1261:A:C2   | 21:AA:1275:A:C5   | 3.09                     | 0.41              |
| 21:AA:1356:G:N2   | 21:AA:1357:A:N3   | 2.69                     | 0.41              |
| 21:AA:1453:G:N3   | 21:AA:1453:G:C2'  | 2.76                     | 0.41              |
| 21:AA:1487:G:H2'  | 21:AA:1488:G:H8   | 1.86                     | 0.41              |
| 19:AT:4:LYS:HB3   | 21:AA:332:G:OP2   | 2.20                     | 0.41              |
| 3:AD:119:HIS:HA   | 21:AA:439:U:O4'   | 2.21                     | 0.41              |
| 21:AA:451:A:N7    | 21:AA:481:G:C2    | 2.89                     | 0.41              |
| 21:AA:530:G:O2'   | 21:AA:531:U:P     | 2.79                     | 0.41              |
| 21:AA:613:C:H6    | 21:AA:613:C:O5'   | 2.04                     | 0.41              |
| 1:AB:219:THR:HG23 | 1:AB:220:VAL:H    | 1.86                     | 0.41              |
| 3:AD:109:THR:HG23 | 3:AD:112:GLU:CB   | 2.51                     | 0.41              |
| 3:AD:191:SER:O    | 3:AD:192:ALA:CB   | 2.69                     | 0.41              |
| 4:AE:155:LYS:HG2  | 7:AH:65:PHE:CB    | 2.51                     | 0.41              |
| 5:AF:40:GLU:HB2   | 5:AF:42:TRP:NE1   | 2.28                     | 0.41              |
| 8:AI:79:ARG:O     | 8:AI:79:ARG:HD2   | 2.20                     | 0.41              |
| 10:AK:32:THR:HG23 | 10:AK:42:GLY:O    | 2.20                     | 0.41              |
| 2:AC:17:TRP:CZ2   | 13:AN:95:LEU:O    | 2.72                     | 0.41              |
| 14:AO:16:ARG:HD3  | 14:AO:20:ASP:OD2  | 2.21                     | 0.41              |
| 14:AO:44:GLU:O    | 14:AO:45:HIS:HB2  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:AQ:46:HIS:HE2  | 16:AQ:48:GLU:HB2   | 1.85                     | 0.41              |
| 18:AS:43:MET:HA   | 18:AS:46:LEU:HD12  | 2.02                     | 0.41              |
| 19:AT:79:THR:O    | 19:AT:80:ALA:C     | 2.59                     | 0.41              |
| 20:AU:13:VAL:HG13 | 20:AU:15:LEU:HD11  | 2.02                     | 0.41              |
| 20:AU:46:ARG:HA   | 20:AU:49:ALA:HB3   | 2.02                     | 0.41              |
| 51:B1:34:GLU:HG2  | 51:B1:49:LYS:HG3   | 2.02                     | 0.41              |
| 54:B4:37:GLN:O    | 54:B4:37:GLN:HG2   | 2.21                     | 0.41              |
| 24:BA:990:A:N6    | 24:BA:1186:G:H1'   | 2.35                     | 0.41              |
| 24:BA:1214:A:H2'  | 24:BA:1215:G:O4'   | 2.20                     | 0.41              |
| 24:BA:1321:A:H2'  | 24:BA:1322:A:O4'   | 2.20                     | 0.41              |
| 24:BA:1353:A:H2'  | 24:BA:1354:A:C8    | 2.55                     | 0.41              |
| 24:BA:1421:G:N3   | 24:BA:1422:G:C8    | 2.88                     | 0.41              |
| 24:BA:14:A:C5'    | 24:BA:15:G:OP2     | 2.65                     | 0.41              |
| 24:BA:1805:A:H2'  | 24:BA:1806:C:H6    | 1.86                     | 0.41              |
| 24:BA:1809:A:O2'  | 24:BA:1810:A:O4'   | 2.39                     | 0.41              |
| 24:BA:1838:C:N4   | 24:BA:1899:A:C4    | 2.88                     | 0.41              |
| 24:BA:2037:A:C6   | 24:BA:2038:G:C6    | 3.09                     | 0.41              |
| 24:BA:2195:U:O2'  | 24:BA:2196:C:H5'   | 2.20                     | 0.41              |
| 24:BA:2262:U:O2'  | 24:BA:2328:A:H1'   | 2.21                     | 0.41              |
| 24:BA:2534:A:C5   | 24:BA:2535:G:C8    | 3.09                     | 0.41              |
| 24:BA:2564:A:N1   | 24:BA:2646:C:O2'   | 2.50                     | 0.41              |
| 24:BA:2808:G:C2   | 24:BA:2891:U:C6    | 3.08                     | 0.41              |
| 24:BA:301:G:C6    | 24:BA:302:C:N4     | 2.89                     | 0.41              |
| 24:BA:307:G:N2    | 24:BA:309:A:H3'    | 2.35                     | 0.41              |
| 24:BA:36:G:C5     | 24:BA:37:C:C5      | 3.08                     | 0.41              |
| 24:BA:590:A:H2'   | 24:BA:591:U:C6     | 2.56                     | 0.41              |
| 24:BA:626:A:H2'   | 35:BL:78:ARG:NH1   | 2.36                     | 0.41              |
| 24:BA:752:A:O2'   | 24:BA:753:A:P      | 2.79                     | 0.41              |
| 24:BA:988:A:H2    | 24:BA:989:G:N2     | 2.19                     | 0.41              |
| 25:BB:105:G:O2'   | 25:BB:106:G:H5'    | 2.21                     | 0.41              |
| 25:BB:97:C:H2'    | 25:BB:98:G:O4'     | 2.21                     | 0.41              |
| 26:BC:185:ALA:C   | 26:BC:187:CYS:H    | 2.24                     | 0.41              |
| 28:BE:62:GLN:HB2  | 28:BE:62:GLN:HE21  | 1.58                     | 0.41              |
| 24:BA:2305:U:H6   | 29:BF:152:ASP:HB3  | 1.85                     | 0.41              |
| 30:BG:25:ILE:HG22 | 30:BG:78:VAL:HG21  | 2.01                     | 0.41              |
| 33:BJ:69:ARG:O    | 33:BJ:90:GLU:HG2   | 2.20                     | 0.41              |
| 34:BK:113:MET:SD  | 34:BK:116:ILE:HD11 | 2.61                     | 0.41              |
| 34:BK:118:LEU:HB3 | 34:BK:119:ALA:H    | 1.58                     | 0.41              |
| 34:BK:7:MET:SD    | 34:BK:20:MET:HB2   | 2.61                     | 0.41              |
| 34:BK:61:VAL:HG22 | 34:BK:87:LEU:HD11  | 2.02                     | 0.41              |
| 36:BM:97:GLN:CD   | 36:BM:97:GLN:H     | 2.24                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:BO:57:ALA:C    | 38:BO:59:ALA:N    | 2.74                     | 0.41              |
| 39:BP:112:ARG:O   | 39:BP:113:LEU:C   | 2.58                     | 0.41              |
| 39:BP:26:GLU:HB2  | 39:BP:43:GLU:HB2  | 2.02                     | 0.41              |
| 44:BU:48:VAL:O    | 44:BU:53:GLN:HB3  | 2.21                     | 0.41              |
| 47:BX:34:SER:CA   | 47:BX:49:ARG:HA   | 2.46                     | 0.41              |
| 24:BA:1157:G:O2'  | 49:BZ:31:ILE:HD11 | 2.21                     | 0.41              |
| 55:CA:1073:U:H2'  | 55:CA:1074:G:O4'  | 2.21                     | 0.41              |
| 55:CA:1386:G:C2   | 55:CA:1387:G:C5   | 3.09                     | 0.41              |
| 55:CA:236:A:H2'   | 55:CA:237:G:H8    | 1.86                     | 0.41              |
| 55:CA:10:A:C6     | 55:CA:25:C:N3     | 2.89                     | 0.41              |
| 3:CD:145:ARG:NH2  | 55:CA:490:C:OP1   | 2.54                     | 0.41              |
| 55:CA:506:G:H2'   | 55:CA:507:C:C6    | 2.55                     | 0.41              |
| 55:CA:519:C:O2'   | 55:CA:520:A:H5'   | 2.21                     | 0.41              |
| 55:CA:71:A:C5     | 55:CA:100:G:C4    | 3.09                     | 0.41              |
| 55:CA:818:G:H3'   | 55:CA:819:A:C5'   | 2.51                     | 0.41              |
| 55:CA:976:G:OP1   | 55:CA:976:G:H4'   | 2.20                     | 0.41              |
| 55:CA:994:A:N6    | 55:CA:1215:G:O2'  | 2.54                     | 0.41              |
| 1:CB:125:PHE:N    | 1:CB:125:PHE:HD2  | 2.18                     | 0.41              |
| 1:CB:74:ALA:C     | 1:CB:206:ILE:HD11 | 2.41                     | 0.41              |
| 2:CC:2:GLN:HE21   | 2:CC:2:GLN:HB3    | 1.51                     | 0.41              |
| 3:CD:103:ARG:O    | 3:CD:104:MET:HB2  | 2.21                     | 0.41              |
| 4:CE:74:ALA:O     | 4:CE:75:LEU:HB2   | 2.20                     | 0.41              |
| 5:CF:35:LYS:HE2   | 5:CF:37:HIS:CE1   | 2.52                     | 0.41              |
| 9:CJ:52:LEU:HA    | 9:CJ:62:ARG:HA    | 2.01                     | 0.41              |
| 9:CJ:52:LEU:HB2   | 13:CN:80:ARG:HD2  | 2.03                     | 0.41              |
| 11:CL:98:ARG:O    | 11:CL:117:GLY:HA3 | 2.20                     | 0.41              |
| 11:CL:118:VAL:O   | 55:CA:36:C:H4'    | 2.21                     | 0.41              |
| 15:CP:4:ILE:O     | 15:CP:71:VAL:HG11 | 2.21                     | 0.41              |
| 20:CU:31:VAL:HG12 | 20:CU:32:ARG:H    | 1.86                     | 0.41              |
| 52:D2:28:ARG:C    | 52:D2:30:VAL:N    | 2.74                     | 0.41              |
| 24:DA:1064:C:C4   | 24:DA:1065:U:C4   | 3.09                     | 0.41              |
| 24:DA:1139:G:C6   | 24:DA:1140:C:C4   | 3.08                     | 0.41              |
| 24:DA:1223:G:O5'  | 24:DA:1223:G:H8   | 2.04                     | 0.41              |
| 24:DA:1308:A:H3'  | 24:DA:1309:G:C8   | 2.55                     | 0.41              |
| 24:DA:1380:G:C2   | 24:DA:1381:G:C8   | 3.09                     | 0.41              |
| 24:DA:1442:U:C4   | 24:DA:1443:U:O4   | 2.74                     | 0.41              |
| 24:DA:183:C:H2'   | 24:DA:184:C:H5'   | 2.03                     | 0.41              |
| 24:DA:1879:C:H2'  | 24:DA:1880:U:O4'  | 2.20                     | 0.41              |
| 24:DA:1994:C:H2'  | 24:DA:1995:U:C6   | 2.46                     | 0.41              |
| 24:DA:216:A:O2'   | 24:DA:217:A:C8    | 2.25                     | 0.41              |
| 24:DA:647:G:N2    | 24:DA:2350:C:O2'  | 2.47                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:2693:G:N3   | 24:DA:2694:G:C8    | 2.89                     | 0.41              |
| 24:DA:2744:G:C6   | 24:DA:2761:A:C6    | 3.09                     | 0.41              |
| 24:DA:2787:C:O2'  | 24:DA:2788:C:H5'   | 2.21                     | 0.41              |
| 24:DA:181:A:C2    | 24:DA:434:U:H1'    | 2.55                     | 0.41              |
| 24:DA:42:A:C2     | 24:DA:438:G:C2     | 3.09                     | 0.41              |
| 24:DA:527:C:O2    | 24:DA:527:C:C2'    | 2.69                     | 0.41              |
| 24:DA:790:U:O2'   | 24:DA:791:C:H6     | 2.03                     | 0.41              |
| 24:DA:900:A:H3'   | 24:DA:901:C:C6     | 2.56                     | 0.41              |
| 24:DA:957:C:OP2   | 36:DM:75:GLU:HA    | 2.21                     | 0.41              |
| 26:DC:141:HIS:HB3 | 26:DC:190:THR:HB   | 2.01                     | 0.41              |
| 26:DC:19:VAL:O    | 26:DC:19:VAL:HG12  | 2.21                     | 0.41              |
| 26:DC:67:LYS:HD3  | 26:DC:148:GLY:O    | 2.21                     | 0.41              |
| 31:DH:66:ASN:O    | 31:DH:67:ALA:HB3   | 2.21                     | 0.41              |
| 32:DI:112:LYS:HZ3 | 32:DI:128:ILE:HD12 | 1.85                     | 0.41              |
| 33:DJ:48:VAL:HG12 | 33:DJ:49:ASP:N     | 2.36                     | 0.41              |
| 34:DK:22:ILE:HD11 | 34:DK:40:LYS:HG3   | 2.03                     | 0.41              |
| 35:DL:121:THR:OG1 | 35:DL:141:LYS:HE3  | 2.20                     | 0.41              |
| 38:DO:2:ASP:O     | 38:DO:4:LYS:N      | 2.53                     | 0.41              |
| 38:DO:77:ALA:O    | 38:DO:81:ARG:HG3   | 2.20                     | 0.41              |
| 40:DQ:23:TYR:HB2  | 40:DQ:28:SER:HB3   | 2.02                     | 0.41              |
| 44:DU:80:ASP:OD1  | 44:DU:80:ASP:N     | 2.53                     | 0.41              |
| 44:DU:94:PHE:HD2  | 44:DU:94:PHE:O     | 2.04                     | 0.41              |
| 46:DW:28:GLU:H    | 46:DW:31:LEU:CD2   | 2.19                     | 0.41              |
| 46:DW:37:VAL:CG2  | 46:DW:38:ARG:HH11  | 2.33                     | 0.41              |
| 48:DY:27:ASN:HA   | 48:DY:27:ASN:HD22  | 1.73                     | 0.41              |
| 21:AA:1167:A:C8   | 21:AA:1169:A:N6    | 2.89                     | 0.41              |
| 21:AA:1211:U:O2'  | 21:AA:1212:U:OP2   | 2.35                     | 0.41              |
| 21:AA:1534:A:N3   | 21:AA:1534:A:H2'   | 2.36                     | 0.41              |
| 15:AP:5:ARG:HB2   | 21:AA:376:G:H5''   | 2.03                     | 0.41              |
| 21:AA:652:U:O2'   | 21:AA:653:U:H6     | 2.02                     | 0.41              |
| 21:AA:694:A:H2'   | 21:AA:695:A:O4'    | 2.20                     | 0.41              |
| 21:AA:760:G:H2'   | 21:AA:761:G:C5'    | 2.51                     | 0.41              |
| 21:AA:770:C:O2    | 21:AA:810:C:O2     | 2.38                     | 0.41              |
| 1:AB:44:LYS:HA    | 1:AB:44:LYS:HD2    | 1.76                     | 0.41              |
| 2:AC:155:ARG:HG2  | 2:AC:159:ALA:O     | 2.21                     | 0.41              |
| 2:AC:120:THR:HG23 | 2:AC:188:ALA:CB    | 2.50                     | 0.41              |
| 3:AD:69:ARG:HE    | 3:AD:69:ARG:HA     | 1.86                     | 0.41              |
| 5:AF:79:ARG:CA    | 5:AF:79:ARG:NE     | 2.84                     | 0.41              |
| 5:AF:98:GLU:HG3   | 5:AF:99:ALA:N      | 2.36                     | 0.41              |
| 6:AG:128:GLU:O    | 6:AG:130:LYS:HG2   | 2.21                     | 0.41              |
| 7:AH:85:TYR:HE2   | 7:AH:123:GLU:OE2   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:AH:84:ILE:HA    | 7:AH:84:ILE:HD13   | 1.75                     | 0.41              |
| 11:AL:115:LYS:O   | 11:AL:116:TYR:CB   | 2.68                     | 0.41              |
| 11:AL:43:LYS:N    | 11:AL:43:LYS:CD    | 2.80                     | 0.41              |
| 12:AM:75:SER:O    | 12:AM:78:ARG:HB3   | 2.21                     | 0.41              |
| 14:AO:57:ARG:HB3  | 14:AO:57:ARG:HH11  | 1.83                     | 0.41              |
| 15:AP:25:ARG:HE   | 15:AP:25:ARG:HB2   | 1.62                     | 0.41              |
| 16:AQ:32:ILE:HG22 | 16:AQ:33:TYR:N     | 2.35                     | 0.41              |
| 20:AU:52:VAL:CG1  | 20:AU:53:LYS:H     | 2.23                     | 0.41              |
| 24:BA:1853:A:N1   | 24:BA:2087:G:H1'   | 2.35                     | 0.41              |
| 24:BA:2550:G:C6   | 24:BA:2551:C:N4    | 2.89                     | 0.41              |
| 24:BA:2597:G:H2'  | 24:BA:2598:A:C8    | 2.56                     | 0.41              |
| 24:BA:1755:A:N6   | 24:BA:2694:G:O2'   | 2.53                     | 0.41              |
| 24:BA:2840:C:H2'  | 24:BA:2841:C:H6    | 1.85                     | 0.41              |
| 24:BA:433:C:H2'   | 24:BA:433:C:O2     | 2.18                     | 0.41              |
| 24:BA:556:A:C8    | 24:BA:557:C:C5     | 3.09                     | 0.41              |
| 24:BA:851:C:H2'   | 24:BA:852:U:C6     | 2.56                     | 0.41              |
| 24:BA:864:G:C6    | 24:BA:865:C:C4     | 3.09                     | 0.41              |
| 24:BA:972:A:H3'   | 24:BA:973:A:H2'    | 2.02                     | 0.41              |
| 26:BC:108:GLY:O   | 26:BC:109:LEU:C    | 2.59                     | 0.41              |
| 26:BC:144:GLU:HG2 | 26:BC:151:GLY:N    | 2.35                     | 0.41              |
| 26:BC:255:LYS:C   | 26:BC:257:ARG:N    | 2.73                     | 0.41              |
| 27:BD:4:LEU:CD1   | 27:BD:100:LEU:HD23 | 2.50                     | 0.41              |
| 27:BD:91:THR:OG1  | 27:BD:91:THR:O     | 2.38                     | 0.41              |
| 28:BE:7:ASP:CG    | 28:BE:8:ALA:N      | 2.74                     | 0.41              |
| 29:BF:53:ALA:C    | 29:BF:55:ASP:N     | 2.74                     | 0.41              |
| 30:BG:72:ASN:C    | 30:BG:72:ASN:ND2   | 2.74                     | 0.41              |
| 32:BI:49:GLU:HG2  | 32:BI:50:LYS:H     | 1.85                     | 0.41              |
| 32:BI:80:LYS:HA   | 32:BI:85:ILE:O     | 2.21                     | 0.41              |
| 33:BJ:35:ARG:O    | 33:BJ:36:LEU:C     | 2.57                     | 0.41              |
| 34:BK:58:LEU:N    | 34:BK:58:LEU:HD23  | 2.36                     | 0.41              |
| 37:BN:116:VAL:O   | 37:BN:117:ASP:CB   | 2.69                     | 0.41              |
| 38:BO:93:ASP:C    | 38:BO:95:SER:N     | 2.74                     | 0.41              |
| 40:BQ:56:PHE:HB3  | 40:BQ:60:TRP:CZ2   | 2.55                     | 0.41              |
| 42:BS:29:VAL:O    | 42:BS:33:LEU:HD22  | 2.21                     | 0.41              |
| 43:BT:49:LYS:O    | 43:BT:50:LEU:C     | 2.58                     | 0.41              |
| 47:BX:50:VAL:HG12 | 47:BX:51:SER:N     | 2.35                     | 0.41              |
| 55:CA:51:A:C5     | 55:CA:116:A:C8     | 3.09                     | 0.41              |
| 55:CA:1216:A:O2'  | 55:CA:1217:C:C5'   | 2.69                     | 0.41              |
| 55:CA:1295:U:O5'  | 55:CA:1295:U:H6    | 2.04                     | 0.41              |
| 55:CA:1395:C:O2'  | 55:CA:1396:A:H5'   | 2.20                     | 0.41              |
| 55:CA:166:U:C2'   | 55:CA:167:A:H5'    | 2.49                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:315:A:C5'   | 55:CA:317:U:OP2   | 2.68                     | 0.41              |
| 55:CA:513:C:H2'   | 55:CA:514:C:C6    | 2.55                     | 0.41              |
| 55:CA:675:A:H2'   | 55:CA:676:A:O4'   | 2.21                     | 0.41              |
| 55:CA:859:G:H2'   | 55:CA:860:A:C8    | 2.56                     | 0.41              |
| 55:CA:86:G:O2'    | 55:CA:87:C:P      | 2.79                     | 0.41              |
| 1:CB:212:TYR:O    | 1:CB:216:VAL:N    | 2.49                     | 0.41              |
| 1:CB:67:LEU:HD23  | 1:CB:67:LEU:HA    | 1.87                     | 0.41              |
| 3:CD:98:ASP:O     | 3:CD:113:ALA:HB1  | 2.21                     | 0.41              |
| 4:CE:47:PHE:CD1   | 4:CE:140:ILE:HD12 | 2.56                     | 0.41              |
| 6:CG:52:ARG:C     | 6:CG:54:GLY:H     | 2.23                     | 0.41              |
| 10:CK:19:VAL:CB   | 10:CK:34:THR:O    | 2.68                     | 0.41              |
| 10:CK:73:VAL:C    | 10:CK:75:GLU:H    | 2.24                     | 0.41              |
| 11:CL:24:GLU:O    | 11:CL:25:ALA:CB   | 2.66                     | 0.41              |
| 14:CO:44:GLU:HG2  | 14:CO:45:HIS:N    | 2.36                     | 0.41              |
| 53:D3:50:SER:O    | 53:D3:52:GLY:N    | 2.54                     | 0.41              |
| 24:DA:1171:G:H2'  | 24:DA:1172:C:C1'  | 2.51                     | 0.41              |
| 24:DA:1276:A:N1   | 24:DA:1277:G:C6   | 2.88                     | 0.41              |
| 24:DA:1477:A:C8   | 24:DA:1515:A:N6   | 2.89                     | 0.41              |
| 24:DA:1507:C:C2   | 24:DA:1508:A:H1'  | 2.56                     | 0.41              |
| 24:DA:1670:C:N4   | 24:DA:1674:G:O5'  | 2.54                     | 0.41              |
| 24:DA:1812:U:H1'  | 26:DC:43:ASN:ND2  | 2.36                     | 0.41              |
| 24:DA:1917:U:H2'  | 24:DA:1918:A:H5'  | 2.03                     | 0.41              |
| 24:DA:2023:C:O2'  | 24:DA:2024:G:P    | 2.78                     | 0.41              |
| 24:DA:214:G:O2'   | 24:DA:216:A:O3'   | 2.31                     | 0.41              |
| 24:DA:2347:C:HO2' | 24:DA:2348:U:H6   | 1.65                     | 0.41              |
| 24:DA:2349:G:C6   | 24:DA:2350:C:C2   | 3.08                     | 0.41              |
| 24:DA:2363:G:C6   | 24:DA:2364:C:C4   | 3.09                     | 0.41              |
| 24:DA:2389:G:H5'' | 24:DA:2390:U:H5'  | 2.02                     | 0.41              |
| 24:DA:2435:A:C4   | 24:DA:2436:G:C8   | 3.08                     | 0.41              |
| 24:DA:243:U:H2'   | 24:DA:244:A:H8    | 1.86                     | 0.41              |
| 24:DA:2902:C:O2'  | 24:DA:2903:U:C6   | 2.73                     | 0.41              |
| 24:DA:362:A:N7    | 24:DA:363:G:N7    | 2.68                     | 0.41              |
| 24:DA:528:A:H2    | 24:DA:2043:C:C5'  | 2.34                     | 0.41              |
| 24:DA:591:U:N3    | 24:DA:592:A:C5    | 2.89                     | 0.41              |
| 24:DA:76:C:O3'    | 48:DY:52:ARG:HG2  | 2.20                     | 0.41              |
| 24:DA:790:U:HO2'  | 24:DA:791:C:P     | 2.44                     | 0.41              |
| 24:DA:975:A:C2'   | 24:DA:976:G:H8    | 2.29                     | 0.41              |
| 24:DA:980:A:N6    | 24:DA:2027:G:O2'  | 2.54                     | 0.41              |
| 24:DA:98:G:N3     | 24:DA:98:G:H2'    | 2.36                     | 0.41              |
| 27:DD:16:THR:HG22 | 27:DD:20:VAL:HB   | 2.02                     | 0.41              |
| 27:DD:14:ILE:HG23 | 27:DD:22:ILE:HB   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DD:22:ILE:HA   | 27:DD:23:PRO:HD2   | 1.97                     | 0.41              |
| 29:DF:137:PHE:O   | 29:DF:138:PRO:C    | 2.59                     | 0.41              |
| 32:DI:54:ILE:HG23 | 32:DI:70:THR:HG21  | 2.03                     | 0.41              |
| 33:DJ:89:PHE:CE2  | 33:DJ:100:VAL:HG11 | 2.56                     | 0.41              |
| 37:DN:97:ILE:HD12 | 37:DN:99:LYS:HD3   | 2.03                     | 0.41              |
| 38:DO:26:LEU:HB3  | 38:DO:92:PHE:CD1   | 2.55                     | 0.41              |
| 38:DO:34:HIS:O    | 38:DO:35:ILE:HG12  | 2.21                     | 0.41              |
| 40:DQ:69:ARG:NH2  | 40:DQ:74:SER:HB2   | 2.35                     | 0.41              |
| 40:DQ:91:ARG:CZ   | 40:DQ:93:ILE:HG21  | 2.51                     | 0.41              |
| 43:DT:39:THR:CG2  | 43:DT:42:GLU:HB2   | 2.31                     | 0.41              |
| 24:DA:856:G:H1'   | 46:DW:23:LYS:HB3   | 2.03                     | 0.41              |
| 47:DX:58:ILE:HG12 | 47:DX:66:VAL:HG11  | 2.03                     | 0.41              |
| 21:AA:1050:G:N1   | 21:AA:1209:C:C2    | 2.89                     | 0.41              |
| 21:AA:1360:A:C2'  | 21:AA:1361:G:H8    | 2.33                     | 0.41              |
| 21:AA:1528:U:O2'  | 21:AA:1529:G:H3'   | 2.20                     | 0.41              |
| 21:AA:312:C:H2'   | 21:AA:313:A:O4'    | 2.20                     | 0.41              |
| 21:AA:625:U:H2'   | 21:AA:625:U:O2     | 2.20                     | 0.41              |
| 21:AA:760:G:H2'   | 21:AA:761:G:H5'    | 2.03                     | 0.41              |
| 21:AA:76:G:N2     | 21:AA:95:C:N3      | 2.68                     | 0.41              |
| 21:AA:76:G:N2     | 21:AA:95:C:C4      | 2.88                     | 0.41              |
| 21:AA:977:A:O2'   | 21:AA:978:A:H5''   | 2.21                     | 0.41              |
| 1:AB:131:LYS:HG3  | 1:AB:135:MET:HE3   | 2.02                     | 0.41              |
| 4:AE:34:ALA:O     | 4:AE:49:TYR:CD2    | 2.74                     | 0.41              |
| 5:AF:4:TYR:O      | 5:AF:63:ASN:HA     | 2.21                     | 0.41              |
| 7:AH:74:ILE:HD13  | 7:AH:128:VAL:HG22  | 2.01                     | 0.41              |
| 7:AH:79:ARG:HG3   | 7:AH:82:LEU:H      | 1.86                     | 0.41              |
| 8:AI:11:ARG:HA    | 8:AI:105:ARG:HH12  | 1.86                     | 0.41              |
| 8:AI:21:LYS:HE3   | 8:AI:61:ASP:HB3    | 2.03                     | 0.41              |
| 8:AI:28:VAL:O     | 8:AI:28:VAL:HG12   | 2.20                     | 0.41              |
| 9:AJ:74:VAL:HB    | 9:AJ:75:ASP:H      | 1.67                     | 0.41              |
| 10:AK:96:ILE:HG13 | 10:AK:97:ARG:N     | 2.35                     | 0.41              |
| 11:AL:43:LYS:HB2  | 11:AL:44:PRO:HD3   | 2.03                     | 0.41              |
| 15:AP:51:ARG:O    | 15:AP:52:LEU:HB2   | 2.20                     | 0.41              |
| 20:AU:43:GLU:C    | 20:AU:45:LYS:N     | 2.75                     | 0.41              |
| 20:AU:44:ARG:HD2  | 20:AU:44:ARG:H     | 1.85                     | 0.41              |
| 23:AW:5:U:C4      | 23:AW:6:U:O4       | 2.74                     | 0.41              |
| 24:BA:1071:G:H4'  | 24:BA:1088:A:O2'   | 2.21                     | 0.41              |
| 24:BA:1071:G:C4   | 24:BA:1089:A:C6    | 3.09                     | 0.41              |
| 24:BA:1022:G:C6   | 24:BA:1140:C:C4    | 3.09                     | 0.41              |
| 24:BA:1205:A:C6   | 28:BE:165:HIS:CG   | 3.08                     | 0.41              |
| 24:BA:1253:A:C3'  | 24:BA:1254:A:C5'   | 2.99                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BA:1416:G:O2'  | 24:BA:1417:C:P     | 2.78                     | 0.41              |
| 24:BA:1450:G:H2'  | 24:BA:1451:C:H6    | 1.86                     | 0.41              |
| 24:BA:1528:A:C2'  | 24:BA:1529:G:H5'   | 2.50                     | 0.41              |
| 24:BA:1623:G:C2   | 24:BA:1624:U:C6    | 3.09                     | 0.41              |
| 24:BA:1730:C:O2'  | 24:BA:1731:G:H5''  | 2.21                     | 0.41              |
| 24:BA:1760:C:H2'  | 24:BA:1761:C:C6    | 2.56                     | 0.41              |
| 24:BA:1882:U:O2'  | 24:BA:1883:U:H5'   | 2.20                     | 0.41              |
| 24:BA:235:U:O2    | 24:BA:430:A:C5     | 2.74                     | 0.41              |
| 24:BA:2455:G:N2   | 24:BA:2456:C:C2    | 2.89                     | 0.41              |
| 24:BA:2702:G:H2'  | 24:BA:2703:C:C6    | 2.56                     | 0.41              |
| 24:BA:341:C:H2'   | 24:BA:342:A:O4'    | 2.21                     | 0.41              |
| 24:BA:414:C:H2'   | 24:BA:415:A:C8     | 2.56                     | 0.41              |
| 24:BA:447:A:C8    | 24:BA:473:G:C6     | 3.09                     | 0.41              |
| 24:BA:615:U:C3'   | 24:BA:616:A:H5'    | 2.50                     | 0.41              |
| 24:BA:656:G:O2'   | 24:BA:657:U:H5'    | 2.21                     | 0.41              |
| 24:BA:769:U:H2'   | 24:BA:770:G:O4'    | 2.20                     | 0.41              |
| 24:BA:817:C:H2'   | 24:BA:818:G:O4'    | 2.21                     | 0.41              |
| 24:BA:992:C:O2    | 24:BA:992:C:H2'    | 2.20                     | 0.41              |
| 25:BB:46:A:C5     | 25:BB:47:C:C4      | 3.09                     | 0.41              |
| 25:BB:54:G:N3     | 25:BB:55:U:C6      | 2.89                     | 0.41              |
| 26:BC:247:TRP:C   | 26:BC:249:VAL:H    | 2.24                     | 0.41              |
| 26:BC:47:ARG:HG3  | 26:BC:47:ARG:NH1   | 2.36                     | 0.41              |
| 27:BD:174:SER:O   | 27:BD:175:LEU:HB2  | 2.21                     | 0.41              |
| 28:BE:5:LEU:HA    | 28:BE:120:VAL:HG13 | 2.02                     | 0.41              |
| 28:BE:24:ASN:C    | 28:BE:24:ASN:ND2   | 2.74                     | 0.41              |
| 28:BE:72:SER:O    | 28:BE:74:LYS:N     | 2.54                     | 0.41              |
| 12:AM:70:ARG:HG3  | 29:BF:112:ASP:HA   | 2.03                     | 0.41              |
| 29:BF:144:LYS:HA  | 29:BF:144:LYS:HD3  | 1.90                     | 0.41              |
| 31:BH:90:LEU:HD22 | 31:BH:123:ARG:HA   | 2.02                     | 0.41              |
| 32:BI:57:VAL:HG12 | 32:BI:58:ILE:N     | 2.36                     | 0.41              |
| 35:BL:18:ARG:HH11 | 35:BL:18:ARG:HD3   | 1.71                     | 0.41              |
| 35:BL:47:ARG:HG3  | 35:BL:50:PHE:HB2   | 2.03                     | 0.41              |
| 37:BN:33:ILE:HG13 | 37:BN:118:ARG:HD2  | 2.03                     | 0.41              |
| 37:BN:37:THR:OG1  | 37:BN:40:LYS:HD2   | 2.21                     | 0.41              |
| 37:BN:49:GLU:HB2  | 37:BN:50:PRO:HD3   | 2.03                     | 0.41              |
| 38:BO:85:LYS:HB3  | 38:BO:85:LYS:HE3   | 1.87                     | 0.41              |
| 39:BP:19:PHE:CD2  | 39:BP:19:PHE:N     | 2.85                     | 0.41              |
| 40:BQ:114:ALA:C   | 40:BQ:116:LEU:N    | 2.74                     | 0.41              |
| 43:BT:7:LEU:C     | 43:BT:9:LYS:H      | 2.24                     | 0.41              |
| 44:BU:35:VAL:CB   | 44:BU:38:ILE:HG13  | 2.48                     | 0.41              |
| 44:BU:94:PHE:CD1  | 44:BU:94:PHE:O     | 2.73                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:BW:10:ARG:O    | 46:BW:11:ASN:HB2  | 2.21                     | 0.41              |
| 24:BA:857:G:H1'   | 46:BW:19:ARG:CD   | 2.51                     | 0.41              |
| 46:BW:47:GLY:C    | 46:BW:49:ASN:N    | 2.75                     | 0.41              |
| 47:BX:54:GLY:O    | 47:BX:57:VAL:HB   | 2.20                     | 0.41              |
| 47:BX:5:GLN:HE21  | 47:BX:49:ARG:CB   | 2.34                     | 0.41              |
| 55:CA:1162:C:O2'  | 55:CA:1163:A:H5'  | 2.21                     | 0.41              |
| 55:CA:1165:U:C4   | 55:CA:1166:G:C5   | 3.09                     | 0.41              |
| 6:CG:118:ARG:HH12 | 55:CA:1239:A:H5'' | 1.85                     | 0.41              |
| 55:CA:1242:G:O2'  | 55:CA:1243:C:P    | 2.79                     | 0.41              |
| 55:CA:198:G:C6    | 55:CA:220:G:C2    | 3.09                     | 0.41              |
| 55:CA:204:G:C4    | 55:CA:205:A:C8    | 3.09                     | 0.41              |
| 55:CA:206:C:O5'   | 55:CA:207:C:OP2   | 2.38                     | 0.41              |
| 55:CA:242:G:C6    | 55:CA:245:U:O4    | 2.74                     | 0.41              |
| 55:CA:277:C:O2'   | 55:CA:278:G:H5'   | 2.21                     | 0.41              |
| 55:CA:330:C:HO2'  | 55:CA:331:G:H8    | 1.68                     | 0.41              |
| 55:CA:353:A:C2'   | 55:CA:354:G:OP2   | 2.69                     | 0.41              |
| 55:CA:410:G:C2    | 55:CA:429:U:C2    | 3.09                     | 0.41              |
| 17:CR:69:TYR:CE2  | 55:CA:674:G:H1'   | 2.56                     | 0.41              |
| 55:CA:980:C:C4    | 55:CA:981:U:C2    | 3.09                     | 0.41              |
| 1:CB:100:LEU:C    | 1:CB:102:ASN:N    | 2.74                     | 0.41              |
| 1:CB:134:LEU:HD22 | 1:CB:138:ARG:HH21 | 1.85                     | 0.41              |
| 3:CD:75:TYR:OH    | 3:CD:204:SER:HB3  | 2.21                     | 0.41              |
| 4:CE:37:VAL:HG11  | 4:CE:116:VAL:HG21 | 2.03                     | 0.41              |
| 4:CE:75:LEU:HA    | 4:CE:75:LEU:HD22  | 1.73                     | 0.41              |
| 6:CG:48:THR:O     | 6:CG:52:ARG:HD3   | 2.20                     | 0.41              |
| 7:CH:1:SER:H1     | 55:CA:877:G:N2    | 2.17                     | 0.41              |
| 7:CH:33:VAL:C     | 7:CH:35:ILE:N     | 2.75                     | 0.41              |
| 8:CI:49:GLN:O     | 8:CI:50:PRO:C     | 2.58                     | 0.41              |
| 11:CL:71:HIS:HB3  | 11:CL:98:ARG:NH2  | 2.36                     | 0.41              |
| 2:CC:36:PHE:CE1   | 13:CN:91:GLU:HB3  | 2.55                     | 0.41              |
| 9:CJ:64:GLN:CB    | 13:CN:98:ALA:HB3  | 2.51                     | 0.41              |
| 18:CS:51:HIS:HA   | 18:CS:55:GLN:O    | 2.21                     | 0.41              |
| 19:CT:61:ALA:CA   | 19:CT:67:HIS:HA   | 2.51                     | 0.41              |
| 52:D2:6:GLN:HA    | 52:D2:7:PRO:HD2   | 1.80                     | 0.41              |
| 53:D3:57:VAL:HG12 | 53:D3:61:LEU:HD11 | 2.03                     | 0.41              |
| 24:DA:1071:G:H2'  | 24:DA:1072:C:C6   | 2.56                     | 0.41              |
| 24:DA:1171:G:C6   | 24:DA:1179:G:C2   | 3.08                     | 0.41              |
| 24:DA:1376:C:C4   | 24:DA:1377:G:C6   | 3.09                     | 0.41              |
| 24:DA:1435:G:C2   | 24:DA:1436:G:C8   | 3.09                     | 0.41              |
| 24:DA:145:C:H2'   | 24:DA:146:A:C8    | 2.56                     | 0.41              |
| 24:DA:1652:A:H3'  | 24:DA:1653:G:H8   | 1.80                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:DA:1816:C:O3'   | 24:DA:1817:G:C8   | 2.64                     | 0.41              |
| 24:DA:181:A:H1'    | 24:DA:435:C:O4'   | 2.21                     | 0.41              |
| 24:DA:1844:C:N3    | 24:DA:1845:G:C8   | 2.89                     | 0.41              |
| 24:DA:202:U:N3     | 24:DA:203:A:C2    | 2.89                     | 0.41              |
| 24:DA:2070:A:C2    | 24:DA:2442:C:C2   | 3.08                     | 0.41              |
| 24:DA:2199:A:O2'   | 24:DA:2200:C:H5'  | 2.21                     | 0.41              |
| 24:DA:2283:C:H2'   | 24:DA:2284:A:C8   | 2.55                     | 0.41              |
| 24:DA:2360:G:O4'   | 35:DL:60:ARG:NH2  | 2.53                     | 0.41              |
| 24:DA:2595:G:C6    | 24:DA:2599:G:C6   | 3.09                     | 0.41              |
| 24:DA:2654:A:C4    | 24:DA:2656:U:N3   | 2.88                     | 0.41              |
| 24:DA:2697:G:C5    | 24:DA:2698:U:C5   | 3.08                     | 0.41              |
| 24:DA:2902:C:O2'   | 24:DA:2903:U:P    | 2.79                     | 0.41              |
| 24:DA:456:C:O2'    | 43:DT:73:ARG:CG   | 2.64                     | 0.41              |
| 24:DA:520:G:H2'    | 24:DA:521:U:H6    | 1.80                     | 0.41              |
| 24:DA:601:C:H2'    | 24:DA:602:A:O4'   | 2.21                     | 0.41              |
| 24:DA:605:G:C5     | 24:DA:606:U:C5    | 3.09                     | 0.41              |
| 24:DA:607:U:C5     | 24:DA:619:G:C5    | 3.03                     | 0.41              |
| 24:DA:739:A:HO2'   | 24:DA:740:C:H5    | 1.66                     | 0.41              |
| 24:DA:845:A:C2     | 24:DA:847:U:N1    | 2.89                     | 0.41              |
| 24:DA:876:C:O2     | 24:DA:876:C:O4'   | 2.38                     | 0.41              |
| 56:DB:104:A:H2'    | 56:DB:105:G:C5'   | 2.51                     | 0.41              |
| 56:DB:13:G:O2'     | 56:DB:14:U:H5''   | 2.21                     | 0.41              |
| 56:DB:16:G:O6      | 56:DB:69:G:C5     | 2.73                     | 0.41              |
| 26:DC:209:ALA:O    | 26:DC:212:TRP:CD1 | 2.74                     | 0.41              |
| 27:DD:16:THR:CG2   | 27:DD:20:VAL:HB   | 2.51                     | 0.41              |
| 28:DE:149:ILE:HG12 | 28:DE:188:MET:HG3 | 2.02                     | 0.41              |
| 29:DF:92:GLY:O     | 29:DF:95:MET:HB3  | 2.19                     | 0.41              |
| 24:DA:2429:G:N7    | 35:DL:55:MET:HE3  | 2.35                     | 0.41              |
| 35:DL:93:ASN:O     | 35:DL:95:LEU:HG   | 2.20                     | 0.41              |
| 38:DO:7:ARG:NH2    | 38:DO:29:HIS:HD2  | 2.19                     | 0.41              |
| 40:DQ:61:ILE:HD12  | 40:DQ:61:ILE:H    | 1.83                     | 0.41              |
| 41:DR:33:VAL:CG2   | 41:DR:61:ALA:HB3  | 2.48                     | 0.41              |
| 43:DT:28:ASN:O     | 43:DT:29:THR:CG2  | 2.69                     | 0.41              |
| 21:AA:1023:U:H2'   | 21:AA:1024:G:O4'  | 2.21                     | 0.41              |
| 21:AA:1072:G:C5    | 21:AA:1073:U:C4   | 3.09                     | 0.41              |
| 21:AA:1170:A:O2'   | 21:AA:1171:A:H5'  | 2.21                     | 0.41              |
| 21:AA:1175:G:C2    | 21:AA:1176:A:C8   | 3.09                     | 0.41              |
| 21:AA:1234:C:C2'   | 21:AA:1235:U:H5'  | 2.51                     | 0.41              |
| 21:AA:201:G:H2'    | 21:AA:202:G:O4'   | 2.21                     | 0.41              |
| 21:AA:251:G:C2     | 21:AA:266:G:C6    | 3.09                     | 0.41              |
| 21:AA:567:G:H1'    | 59:AA:1818:HOH:O  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:AA:615:G:N3    | 21:AA:616:G:C8     | 2.89                     | 0.41              |
| 21:AA:78:A:O5'    | 21:AA:78:A:H8      | 2.04                     | 0.41              |
| 21:AA:827:U:C4    | 21:AA:870:U:C2     | 3.09                     | 0.41              |
| 21:AA:893:C:H2'   | 21:AA:894:G:C8     | 2.55                     | 0.41              |
| 3:AD:154:VAL:O    | 3:AD:157:ALA:HB3   | 2.20                     | 0.41              |
| 4:AE:35:LEU:HD12  | 4:AE:36:THR:O      | 2.20                     | 0.41              |
| 5:AF:68:GLN:HB3   | 5:AF:68:GLN:HE21   | 1.57                     | 0.41              |
| 6:AG:78:ARG:HD2   | 6:AG:83:THR:CA     | 2.44                     | 0.41              |
| 6:AG:91:ARG:HA    | 6:AG:92:PRO:HD3    | 1.96                     | 0.41              |
| 8:AI:43:ALA:HB1   | 8:AI:46:VAL:HG21   | 2.02                     | 0.41              |
| 8:AI:51:LEU:HA    | 8:AI:54:VAL:HG23   | 2.03                     | 0.41              |
| 10:AK:122:PRO:O   | 10:AK:123:PRO:O    | 2.39                     | 0.41              |
| 11:AL:20:VAL:N    | 11:AL:21:PRO:CD    | 2.84                     | 0.41              |
| 15:AP:28:ARG:HH11 | 15:AP:29:ASN:ND2   | 2.15                     | 0.41              |
| 16:AQ:29:LYS:HE2  | 16:AQ:29:LYS:HB3   | 1.89                     | 0.41              |
| 20:AU:24:LYS:CG   | 20:AU:25:ALA:H     | 2.33                     | 0.41              |
| 22:AV:34:G:OP1    | 22:AV:34:G:C8      | 2.66                     | 0.41              |
| 51:B1:29:LYS:HB3  | 51:B1:29:LYS:NZ    | 2.36                     | 0.41              |
| 51:B1:9:LYS:NZ    | 51:B1:50:GLU:OE2   | 2.47                     | 0.41              |
| 54:B4:1:MET:SD    | 54:B4:36:ARG:HB2   | 2.61                     | 0.41              |
| 24:BA:1429:G:C2   | 24:BA:1430:G:C5    | 3.09                     | 0.41              |
| 24:BA:1567:G:H1'  | 24:BA:1568:G:C6    | 2.55                     | 0.41              |
| 24:BA:1677:A:N6   | 24:BA:1678:A:N6    | 2.69                     | 0.41              |
| 24:BA:1703:G:H2'  | 24:BA:1703:G:N3    | 2.36                     | 0.41              |
| 24:BA:1981:A:H8   | 24:BA:1981:A:H2'   | 1.53                     | 0.41              |
| 24:BA:1649:G:C6   | 24:BA:2009:A:N6    | 2.89                     | 0.41              |
| 24:BA:827:U:H2'   | 24:BA:2068:U:O2    | 2.21                     | 0.41              |
| 24:BA:858:G:C4    | 24:BA:2268:A:C2    | 3.08                     | 0.41              |
| 24:BA:2521:C:C4   | 24:BA:2522:U:C4    | 3.09                     | 0.41              |
| 24:BA:2860:A:C3'  | 24:BA:2860:A:H8    | 2.30                     | 0.41              |
| 24:BA:532:A:H4'   | 24:BA:533:G:C8     | 2.56                     | 0.41              |
| 24:BA:789:A:OP1   | 24:BA:790:U:C5     | 2.70                     | 0.41              |
| 24:BA:854:C:H2'   | 24:BA:855:G:H5'    | 2.02                     | 0.41              |
| 25:BB:58:A:H2'    | 25:BB:59:A:H8      | 1.86                     | 0.41              |
| 29:BF:42:ALA:HB2  | 29:BF:49:LEU:HB2   | 2.01                     | 0.41              |
| 30:BG:149:ALA:O   | 30:BG:151:ARG:N    | 2.53                     | 0.41              |
| 31:BH:14:SER:OG   | 31:BH:17:ASP:HB2   | 2.21                     | 0.41              |
| 31:BH:75:LEU:HD22 | 31:BH:143:ILE:HG12 | 2.02                     | 0.41              |
| 32:BI:85:ILE:HG13 | 32:BI:85:ILE:H     | 1.66                     | 0.41              |
| 33:BJ:25:LEU:HD13 | 33:BJ:25:LEU:O     | 2.20                     | 0.41              |
| 33:BJ:40:HIS:H    | 33:BJ:40:HIS:CD2   | 2.38                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:BK:5:GLN:NE2    | 34:BK:5:GLN:HA    | 2.35                     | 0.41              |
| 35:BL:127:VAL:HG23 | 35:BL:131:ALA:HB3 | 2.01                     | 0.41              |
| 28:BE:25:GLU:OE1   | 35:BL:6:LEU:HA    | 2.21                     | 0.41              |
| 24:BA:626:A:H2'    | 35:BL:78:ARG:CZ   | 2.51                     | 0.41              |
| 38:BO:16:ARG:HD3   | 38:BO:16:ARG:HA   | 1.81                     | 0.41              |
| 41:BR:10:LYS:HZ2   | 41:BR:10:LYS:HG2  | 1.49                     | 0.41              |
| 42:BS:19:LEU:HA    | 42:BS:19:LEU:HD12 | 1.87                     | 0.41              |
| 25:BB:12:C:C4      | 46:BW:72:GLY:HA3  | 2.56                     | 0.41              |
| 47:BX:40:GLU:HG3   | 47:BX:43:LYS:NZ   | 2.36                     | 0.41              |
| 55:CA:10:A:N6      | 55:CA:25:C:N4     | 2.69                     | 0.41              |
| 55:CA:1160:G:C6    | 55:CA:1181:G:C6   | 3.08                     | 0.41              |
| 55:CA:149:A:C2     | 55:CA:150:U:C2    | 3.08                     | 0.41              |
| 55:CA:18:C:C4      | 55:CA:19:A:N7     | 2.89                     | 0.41              |
| 55:CA:513:C:HO2'   | 55:CA:514:C:H6    | 1.68                     | 0.41              |
| 55:CA:560:A:C8     | 55:CA:566:G:C4    | 3.09                     | 0.41              |
| 55:CA:885:G:OP2    | 55:CA:885:G:H8    | 2.03                     | 0.41              |
| 55:CA:922:G:C6     | 55:CA:923:A:C6    | 3.09                     | 0.41              |
| 2:CC:35:ASP:CG     | 2:CC:56:ILE:HD12  | 2.42                     | 0.41              |
| 4:CE:114:LEU:CD1   | 4:CE:122:VAL:HG11 | 2.51                     | 0.41              |
| 5:CF:90:MET:HE3    | 17:CR:60:ARG:NH1  | 2.36                     | 0.41              |
| 6:CG:14:ASP:OD2    | 6:CG:15:PRO:CD    | 2.69                     | 0.41              |
| 6:CG:14:ASP:HA     | 6:CG:15:PRO:HD2   | 1.84                     | 0.41              |
| 6:CG:92:PRO:CA     | 6:CG:95:ARG:HB2   | 2.51                     | 0.41              |
| 7:CH:55:LYS:NZ     | 55:CA:653:U:H5'   | 2.36                     | 0.41              |
| 8:CI:63:TYR:C      | 8:CI:63:TYR:HD1   | 2.23                     | 0.41              |
| 9:CJ:40:ILE:HA     | 9:CJ:41:PRO:HD2   | 1.90                     | 0.41              |
| 9:CJ:5:ARG:HH21    | 9:CJ:77:VAL:HG22  | 1.86                     | 0.41              |
| 15:CP:75:ILE:C     | 15:CP:77:GLU:H    | 2.23                     | 0.41              |
| 20:CU:3:ILE:HG22   | 20:CU:19:LYS:NZ   | 2.35                     | 0.41              |
| 54:D4:7:VAL:HG22   | 54:D4:25:VAL:CG2  | 2.52                     | 0.41              |
| 24:DA:1000:A:N6    | 24:DA:1001:A:C6   | 2.89                     | 0.41              |
| 24:DA:1169:A:C2    | 24:DA:1181:U:O2   | 2.74                     | 0.41              |
| 24:DA:117:G:C6     | 24:DA:119:A:N6    | 2.89                     | 0.41              |
| 24:DA:515:A:C2     | 24:DA:1260:A:N3   | 2.84                     | 0.41              |
| 24:DA:55:G:N2      | 24:DA:127:A:C2    | 2.85                     | 0.41              |
| 24:DA:1314:C:O2'   | 24:DA:1315:C:H5'  | 2.21                     | 0.41              |
| 24:DA:1354:A:H2'   | 24:DA:1355:G:O4'  | 2.20                     | 0.41              |
| 24:DA:1637:A:H4'   | 24:DA:2711:A:O2'  | 2.21                     | 0.41              |
| 24:DA:743:A:O2'    | 24:DA:1659:G:OP1  | 2.39                     | 0.41              |
| 24:DA:1968:G:O2'   | 24:DA:1973:G:H4'  | 2.21                     | 0.41              |
| 24:DA:2084:C:C5    | 24:DA:2085:U:C5   | 3.09                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DA:2154:A:OP2   | 24:DA:2154:A:H8    | 2.04                     | 0.41              |
| 24:DA:2248:C:H3'   | 24:DA:2249:U:C6    | 2.56                     | 0.41              |
| 24:DA:2259:U:O2'   | 24:DA:2260:C:H5'   | 2.21                     | 0.41              |
| 24:DA:2265:U:O2'   | 36:DM:13:HIS:CE1   | 2.74                     | 0.41              |
| 24:DA:2293:G:H5''  | 38:DO:94:ARG:NH1   | 2.36                     | 0.41              |
| 24:DA:2306:C:H3'   | 24:DA:2307:G:C5'   | 2.51                     | 0.41              |
| 24:DA:2372:U:H2'   | 24:DA:2373:G:C8    | 2.56                     | 0.41              |
| 24:DA:2409:G:C6    | 24:DA:2410:G:C5    | 3.08                     | 0.41              |
| 24:DA:2459:A:N6    | 24:DA:2494:G:C2    | 2.89                     | 0.41              |
| 24:DA:249:C:P      | 24:DA:2394:C:O2'   | 2.79                     | 0.41              |
| 24:DA:2598:A:H8    | 24:DA:2598:A:O5'   | 2.04                     | 0.41              |
| 24:DA:26:G:N2      | 24:DA:513:A:N7     | 2.69                     | 0.41              |
| 24:DA:2746:U:C2    | 24:DA:2759:G:C2    | 3.09                     | 0.41              |
| 24:DA:366:C:H2'    | 24:DA:367:G:O5'    | 2.21                     | 0.41              |
| 24:DA:37:C:H2'     | 24:DA:38:A:C8      | 2.56                     | 0.41              |
| 24:DA:383:C:C2     | 24:DA:385:C:C5     | 3.09                     | 0.41              |
| 24:DA:227:A:N6     | 24:DA:410:G:H1'    | 2.35                     | 0.41              |
| 24:DA:412:A:N6     | 24:DA:2411:A:C2'   | 2.84                     | 0.41              |
| 24:DA:507:A:H5''   | 24:DA:509:C:C2     | 2.55                     | 0.41              |
| 24:DA:529:A:C4     | 24:DA:2023:C:C4    | 3.09                     | 0.41              |
| 24:DA:980:A:H2     | 24:DA:2038:G:H1'   | 1.85                     | 0.41              |
| 24:DA:991:C:OP2    | 24:DA:1186:G:OP2   | 2.39                     | 0.41              |
| 26:DC:212:TRP:O    | 26:DC:212:TRP:HD1  | 2.03                     | 0.41              |
| 26:DC:180:MET:CE   | 26:DC:268:ARG:HE   | 2.33                     | 0.41              |
| 24:DA:1805:A:O2'   | 26:DC:49:THR:HA    | 2.21                     | 0.41              |
| 26:DC:83:ASP:HA    | 26:DC:84:PRO:HD2   | 1.89                     | 0.41              |
| 28:DE:28:VAL:HG23  | 35:DL:6:LEU:HD21   | 2.02                     | 0.41              |
| 29:DF:169:LEU:HD23 | 29:DF:176:PHE:CZ   | 2.55                     | 0.41              |
| 30:DG:25:ILE:HG22  | 30:DG:25:ILE:O     | 2.20                     | 0.41              |
| 30:DG:43:LYS:HB2   | 30:DG:50:THR:O     | 2.21                     | 0.41              |
| 36:DM:38:ARG:HG2   | 36:DM:98:PRO:CG    | 2.51                     | 0.41              |
| 37:DN:28:LEU:O     | 37:DN:32:GLU:N     | 2.42                     | 0.41              |
| 56:DB:113:C:O2'    | 38:DO:46:GLU:HA    | 2.20                     | 0.41              |
| 39:DP:3:ILE:C      | 39:DP:5:LYS:H      | 2.25                     | 0.41              |
| 40:DQ:63:ARG:O     | 40:DQ:64:ILE:C     | 2.59                     | 0.41              |
| 41:DR:1:MET:CG     | 41:DR:101:ILE:HD12 | 2.42                     | 0.41              |
| 42:DS:31:GLN:O     | 42:DS:33:LEU:N     | 2.54                     | 0.41              |
| 45:DV:87:GLN:O     | 45:DV:88:HIS:HB2   | 2.21                     | 0.41              |
| 47:DX:1:SER:O      | 47:DX:2:ARG:C      | 2.59                     | 0.41              |
| 48:DY:45:GLN:C     | 48:DY:47:ARG:N     | 2.74                     | 0.41              |
| 21:AA:1015:G:O2'   | 21:AA:1016:A:H5'   | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:AA:1097:C:N4   | 21:AA:1098:C:N4   | 2.69                     | 0.40              |
| 21:AA:1256:A:C1'  | 21:AA:1258:G:C5   | 3.02                     | 0.40              |
| 21:AA:1234:C:O2'  | 21:AA:1364:U:H6   | 2.00                     | 0.40              |
| 15:AP:29:ASN:O    | 21:AA:309:A:H5''  | 2.20                     | 0.40              |
| 21:AA:615:G:C6    | 21:AA:626:G:C6    | 3.09                     | 0.40              |
| 17:AR:37:LYS:CB   | 21:AA:719:C:H1'   | 2.51                     | 0.40              |
| 21:AA:734:G:C5    | 21:AA:735:C:C4    | 3.09                     | 0.40              |
| 1:AB:23:ASN:HA    | 1:AB:24:PRO:HD3   | 1.85                     | 0.40              |
| 1:AB:46:VAL:N     | 1:AB:47:PRO:CD    | 2.84                     | 0.40              |
| 1:AB:53:LEU:HD13  | 1:AB:56:LEU:HG    | 2.02                     | 0.40              |
| 3:AD:29:THR:C     | 3:AD:30:LYS:HE2   | 2.41                     | 0.40              |
| 4:AE:135:VAL:HG13 | 4:AE:136:VAL:N    | 2.36                     | 0.40              |
| 4:AE:30:PHE:CD1   | 4:AE:30:PHE:N     | 2.89                     | 0.40              |
| 5:AF:79:ARG:N     | 5:AF:79:ARG:HE    | 2.20                     | 0.40              |
| 7:AH:10:LEU:HB3   | 7:AH:74:ILE:HG12  | 2.01                     | 0.40              |
| 7:AH:13:ILE:HD11  | 7:AH:60:LEU:HD12  | 2.02                     | 0.40              |
| 9:AJ:73:LEU:HD13  | 9:AJ:73:LEU:O     | 2.21                     | 0.40              |
| 10:AK:93:GLU:O    | 10:AK:96:ILE:HG12 | 2.20                     | 0.40              |
| 15:AP:6:LEU:HB2   | 21:AA:375:U:O3'   | 2.20                     | 0.40              |
| 18:AS:17:LYS:HE3  | 18:AS:32:THR:HG23 | 2.03                     | 0.40              |
| 51:B1:18:HIS:CG   | 51:B1:19:PHE:N    | 2.89                     | 0.40              |
| 53:B3:31:ILE:O    | 53:B3:35:LYS:HE3  | 2.21                     | 0.40              |
| 24:BA:1065:U:O4   | 24:BA:1074:G:N3   | 2.54                     | 0.40              |
| 24:BA:110:G:C2    | 24:BA:111:A:C8    | 3.09                     | 0.40              |
| 24:BA:1154:G:H5'' | 24:BA:1155:A:OP2  | 2.21                     | 0.40              |
| 24:BA:1385:A:H1'  | 24:BA:1386:C:C5   | 2.55                     | 0.40              |
| 24:BA:1388:G:C4   | 24:BA:1389:G:C8   | 3.09                     | 0.40              |
| 24:BA:1404:C:C2   | 24:BA:1405:U:C5   | 3.09                     | 0.40              |
| 24:BA:1659:G:H2'  | 24:BA:1660:G:O5'  | 2.21                     | 0.40              |
| 24:BA:1661:G:C6   | 24:BA:1662:U:C4   | 3.10                     | 0.40              |
| 24:BA:1716:U:O2'  | 24:BA:1717:A:C5'  | 2.67                     | 0.40              |
| 24:BA:1735:A:C4   | 24:BA:1736:U:C5   | 3.09                     | 0.40              |
| 24:BA:1806:C:H2'  | 24:BA:1806:C:O2   | 2.21                     | 0.40              |
| 24:BA:1844:C:C2'  | 24:BA:1845:G:H5'  | 2.51                     | 0.40              |
| 24:BA:2194:U:C4   | 24:BA:2195:U:C4   | 3.08                     | 0.40              |
| 24:BA:2255:G:N7   | 24:BA:2256:G:N7   | 2.69                     | 0.40              |
| 24:BA:2327:A:H2'  | 24:BA:2328:A:H8   | 1.75                     | 0.40              |
| 24:BA:2442:C:H2'  | 24:BA:2443:C:H6   | 1.85                     | 0.40              |
| 24:BA:2525:G:N2   | 24:BA:2539:C:C2   | 2.89                     | 0.40              |
| 24:BA:2607:G:H2'  | 24:BA:2608:G:O4'  | 2.20                     | 0.40              |
| 24:BA:2799:A:C5   | 24:BA:2801:G:C8   | 3.09                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:2816:G:O2'  | 24:BA:2817:U:H5'  | 2.21                     | 0.40              |
| 24:BA:2816:G:H2'  | 24:BA:2817:U:H6   | 1.86                     | 0.40              |
| 24:BA:292:U:N3    | 24:BA:293:U:C5    | 2.89                     | 0.40              |
| 24:BA:498:G:N3    | 24:BA:499:U:C6    | 2.89                     | 0.40              |
| 24:BA:640:C:H2'   | 24:BA:641:U:C6    | 2.56                     | 0.40              |
| 24:BA:791:C:N4    | 24:BA:794:A:H1'   | 2.36                     | 0.40              |
| 24:BA:81:G:C2     | 24:BA:106:C:C2    | 3.09                     | 0.40              |
| 27:BD:12:THR:HG22 | 27:BD:13:ARG:H    | 1.80                     | 0.40              |
| 27:BD:39:ASP:OD2  | 27:BD:40:LEU:N    | 2.54                     | 0.40              |
| 29:BF:12:VAL:HG13 | 29:BF:13:LYS:H    | 1.86                     | 0.40              |
| 30:BG:84:LYS:CD   | 30:BG:133:LYS:HG2 | 2.51                     | 0.40              |
| 33:BJ:132:HIS:O   | 33:BJ:133:ALA:C   | 2.59                     | 0.40              |
| 36:BM:47:GLU:OE2  | 36:BM:51:ARG:NH1  | 2.53                     | 0.40              |
| 38:BO:61:GLN:O    | 38:BO:61:GLN:HG3  | 2.21                     | 0.40              |
| 39:BP:13:LYS:HG3  | 39:BP:76:HIS:HA   | 2.03                     | 0.40              |
| 44:BU:5:ARG:O     | 44:BU:6:ARG:C     | 2.59                     | 0.40              |
| 45:BV:44:HIS:CE1  | 45:BV:85:LYS:HB2  | 2.56                     | 0.40              |
| 48:BY:19:LEU:HA   | 48:BY:22:LEU:HB3  | 2.03                     | 0.40              |
| 49:BZ:5:LYS:HA    | 49:BZ:35:VAL:O    | 2.22                     | 0.40              |
| 55:CA:1242:G:C2   | 55:CA:1243:C:C1'  | 2.99                     | 0.40              |
| 55:CA:1242:G:H2'  | 55:CA:1243:C:O5'  | 2.20                     | 0.40              |
| 55:CA:1244:G:C5   | 55:CA:1245:C:C4   | 3.09                     | 0.40              |
| 55:CA:1255:G:C6   | 55:CA:1279:G:C5   | 3.09                     | 0.40              |
| 55:CA:1410:A:C6   | 55:CA:1411:C:N4   | 2.89                     | 0.40              |
| 55:CA:149:A:N6    | 55:CA:174:A:N6    | 2.68                     | 0.40              |
| 16:CQ:67:SER:HA   | 55:CA:265:G:O3'   | 2.21                     | 0.40              |
| 55:CA:329:A:C4    | 55:CA:332:G:C5    | 3.10                     | 0.40              |
| 55:CA:352:C:H5''  | 55:CA:352:C:C6    | 2.53                     | 0.40              |
| 55:CA:393:A:C4    | 55:CA:394:G:C8    | 3.09                     | 0.40              |
| 55:CA:550:G:H2'   | 55:CA:551:U:H6    | 1.85                     | 0.40              |
| 55:CA:563:A:N6    | 59:CA:1821:HOH:O  | 2.54                     | 0.40              |
| 7:CH:87:ARG:NH2   | 55:CA:633:G:OP2   | 2.54                     | 0.40              |
| 55:CA:650:G:N3    | 55:CA:650:G:H2'   | 2.37                     | 0.40              |
| 55:CA:733:G:HO2'  | 55:CA:734:G:P     | 2.44                     | 0.40              |
| 55:CA:780:A:C2    | 55:CA:803:G:C6    | 3.09                     | 0.40              |
| 55:CA:577:G:H4'   | 55:CA:816:A:H2'   | 2.03                     | 0.40              |
| 1:CB:206:ILE:HD13 | 1:CB:209:VAL:CG2  | 2.51                     | 0.40              |
| 1:CB:68:PHE:HB2   | 1:CB:90:PHE:CB    | 2.51                     | 0.40              |
| 2:CC:80:GLY:HA2   | 2:CC:83:VAL:HG13  | 2.02                     | 0.40              |
| 3:CD:63:ILE:O     | 3:CD:110:ARG:HD2  | 2.20                     | 0.40              |
| 4:CE:43:GLY:HA2   | 4:CE:117:ALA:O    | 2.21                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:CF:67:PRO:O      | 5:CF:69:GLU:N     | 2.54                     | 0.40              |
| 9:CJ:28:THR:O      | 9:CJ:32:THR:HG22  | 2.21                     | 0.40              |
| 10:CK:126:ARG:HH21 | 55:CA:796:C:C3'   | 2.33                     | 0.40              |
| 10:CK:13:LYS:H     | 10:CK:13:LYS:HG3  | 1.75                     | 0.40              |
| 10:CK:78:ILE:HD13  | 10:CK:78:ILE:H    | 1.87                     | 0.40              |
| 15:CP:35:ARG:NH1   | 15:CP:38:PHE:HB3  | 2.35                     | 0.40              |
| 16:CQ:66:LEU:O     | 16:CQ:67:SER:HB3  | 2.20                     | 0.40              |
| 17:CR:27:THR:O     | 17:CR:30:ASN:HB3  | 2.21                     | 0.40              |
| 18:CS:52:ASN:HD21  | 18:CS:55:GLN:N    | 2.15                     | 0.40              |
| 19:CT:9:ARG:HG2    | 55:CA:108:G:C6    | 2.56                     | 0.40              |
| 10:CK:121:ARG:NH2  | 20:CU:35:GLU:HB2  | 2.36                     | 0.40              |
| 53:D3:35:LYS:HB2   | 53:D3:40:LYS:HD3  | 2.03                     | 0.40              |
| 24:DA:1034:G:O6    | 24:DA:1122:G:C6   | 2.75                     | 0.40              |
| 24:DA:1062:G:H8    | 24:DA:1070:A:OP2  | 2.04                     | 0.40              |
| 24:DA:1557:C:C4    | 24:DA:1558:C:C2   | 3.09                     | 0.40              |
| 24:DA:1599:U:OP1   | 43:DT:40:LYS:HB2  | 2.21                     | 0.40              |
| 24:DA:1676:A:H2'   | 24:DA:1677:A:C8   | 2.56                     | 0.40              |
| 24:DA:1945:G:H2'   | 24:DA:1946:U:C5   | 2.55                     | 0.40              |
| 24:DA:1955:U:O2'   | 24:DA:1956:U:P    | 2.78                     | 0.40              |
| 24:DA:2010:G:C5    | 24:DA:2011:U:C5   | 3.10                     | 0.40              |
| 24:DA:2251:G:H2'   | 24:DA:2252:G:C8   | 2.56                     | 0.40              |
| 24:DA:2262:U:H4'   | 24:DA:2328:A:N3   | 2.37                     | 0.40              |
| 24:DA:2635:A:C2    | 24:DA:2784:U:N3   | 2.89                     | 0.40              |
| 24:DA:2644:G:N1    | 24:DA:2645:G:N2   | 2.68                     | 0.40              |
| 24:DA:2674:G:C4    | 24:DA:2675:A:C8   | 3.09                     | 0.40              |
| 24:DA:2756:U:C1'   | 24:DA:2757:A:H5'' | 2.50                     | 0.40              |
| 24:DA:324:A:H2'    | 24:DA:325:G:H8    | 1.86                     | 0.40              |
| 24:DA:538:A:O2'    | 24:DA:539:G:H5'   | 2.20                     | 0.40              |
| 24:DA:668:A:C5     | 24:DA:670:A:C8    | 3.09                     | 0.40              |
| 24:DA:685:A:C5     | 24:DA:774:G:N2    | 2.88                     | 0.40              |
| 24:DA:685:A:C8     | 24:DA:774:G:N1    | 2.89                     | 0.40              |
| 24:DA:807:U:H2'    | 24:DA:808:G:C8    | 2.56                     | 0.40              |
| 24:DA:845:A:N3     | 24:DA:847:U:H1'   | 2.36                     | 0.40              |
| 56:DB:44:G:OP1     | 29:DF:91:ARG:NH1  | 2.54                     | 0.40              |
| 26:DC:99:GLU:HG2   | 26:DC:100:ARG:H   | 1.84                     | 0.40              |
| 26:DC:44:ASN:C     | 26:DC:46:GLY:N    | 2.74                     | 0.40              |
| 27:DD:150:GLN:O    | 27:DD:151:THR:C   | 2.59                     | 0.40              |
| 27:DD:94:GLN:O     | 27:DD:95:SER:C    | 2.58                     | 0.40              |
| 29:DF:11:VAL:O     | 29:DF:12:VAL:HB   | 2.21                     | 0.40              |
| 30:DG:102:ILE:HB   | 30:DG:114:HIS:O   | 2.21                     | 0.40              |
| 30:DG:34:ARG:O     | 30:DG:35:THR:HG23 | 2.21                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:DJ:54:ILE:O     | 33:DJ:122:LEU:HD12 | 2.21                     | 0.40              |
| 33:DJ:22:GLY:O     | 33:DJ:23:LYS:C     | 2.59                     | 0.40              |
| 34:DK:108:ARG:CA   | 34:DK:116:ILE:HD13 | 2.49                     | 0.40              |
| 34:DK:4:GLU:HA     | 34:DK:21:CYS:SG    | 2.61                     | 0.40              |
| 35:DL:128:THR:HG22 | 35:DL:129:LYS:N    | 2.36                     | 0.40              |
| 35:DL:4:ASN:HD22   | 35:DL:4:ASN:HA     | 1.58                     | 0.40              |
| 36:DM:41:LEU:HB3   | 36:DM:46:ILE:HG23  | 2.02                     | 0.40              |
| 39:DP:90:ALA:HB3   | 39:DP:110:LYS:HB2  | 2.03                     | 0.40              |
| 39:DP:25:VAL:HG23  | 39:DP:25:VAL:O     | 2.21                     | 0.40              |
| 39:DP:91:VAL:HG11  | 39:DP:96:LEU:CD1   | 2.49                     | 0.40              |
| 41:DR:48:LYS:N     | 41:DR:48:LYS:HD2   | 2.33                     | 0.40              |
| 43:DT:55:VAL:HG22  | 43:DT:56:GLU:N     | 2.36                     | 0.40              |
| 44:DU:40:LEU:HA    | 44:DU:61:GLU:HA    | 2.03                     | 0.40              |
| 21:AA:1061:G:C6    | 21:AA:1062:U:N3    | 2.90                     | 0.40              |
| 21:AA:1092:A:C6    | 21:AA:1093:A:C6    | 3.10                     | 0.40              |
| 21:AA:1120:C:O2'   | 21:AA:1121:U:H5'   | 2.21                     | 0.40              |
| 21:AA:116:A:H8     | 21:AA:116:A:O5'    | 2.04                     | 0.40              |
| 2:AC:4:VAL:HB      | 21:AA:1190:G:P     | 2.61                     | 0.40              |
| 21:AA:1225:A:N3    | 21:AA:1225:A:C2'   | 2.81                     | 0.40              |
| 21:AA:1282:C:O2'   | 21:AA:1283:U:C6    | 2.68                     | 0.40              |
| 21:AA:1312:G:N2    | 21:AA:1326:U:C2    | 2.89                     | 0.40              |
| 6:AG:35:LYS:HD2    | 21:AA:1373:G:H5''  | 2.02                     | 0.40              |
| 21:AA:1508:A:H2'   | 21:AA:1509:C:O4'   | 2.22                     | 0.40              |
| 21:AA:155:A:C2     | 21:AA:167:A:C2     | 3.09                     | 0.40              |
| 21:AA:624:C:C4     | 21:AA:625:U:C5     | 3.09                     | 0.40              |
| 21:AA:901:A:C5     | 21:AA:902:G:H1'    | 2.56                     | 0.40              |
| 21:AA:940:C:H2'    | 21:AA:941:G:O4'    | 2.21                     | 0.40              |
| 1:AB:185:ILE:HG13  | 1:AB:203:ASP:HB3   | 2.03                     | 0.40              |
| 1:AB:56:LEU:HD11   | 1:AB:220:VAL:HG23  | 2.02                     | 0.40              |
| 2:AC:129:PHE:C     | 2:AC:129:PHE:CD2   | 2.95                     | 0.40              |
| 3:AD:187:ARG:HD2   | 3:AD:187:ARG:HA    | 1.89                     | 0.40              |
| 4:AE:107:GLY:O     | 4:AE:111:ARG:CZ    | 2.68                     | 0.40              |
| 4:AE:32:PHE:CE2    | 4:AE:54:GLU:HA     | 2.57                     | 0.40              |
| 8:AI:105:ARG:HE    | 21:AA:1117:A:C4'   | 2.33                     | 0.40              |
| 8:AI:98:ARG:NE     | 8:AI:103:VAL:HG21  | 2.36                     | 0.40              |
| 14:AO:54:GLY:O     | 14:AO:58:MET:HG3   | 2.22                     | 0.40              |
| 15:AP:42:ILE:O     | 15:AP:43:ALA:HB3   | 2.21                     | 0.40              |
| 20:AU:24:LYS:CG    | 20:AU:25:ALA:N     | 2.84                     | 0.40              |
| 20:AU:9:GLU:C      | 2:CC:48:LYS:HZ3    | 2.24                     | 0.40              |
| 51:B1:39:ASP:HA    | 51:B1:40:PRO:HD2   | 1.79                     | 0.40              |
| 24:BA:1255:U:H3    | 24:BA:2060:A:H5'   | 1.87                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BA:1299:G:H2'  | 24:BA:1639:C:N4   | 2.37                     | 0.40              |
| 24:BA:1352:U:C2'  | 24:BA:1353:A:H5'  | 2.50                     | 0.40              |
| 24:BA:1403:A:C4   | 24:BA:1404:C:C5   | 3.09                     | 0.40              |
| 24:BA:1427:A:C4   | 24:BA:1428:C:N4   | 2.89                     | 0.40              |
| 24:BA:1528:A:H2'  | 24:BA:1529:G:H5'  | 2.03                     | 0.40              |
| 24:BA:1574:C:H6   | 24:BA:1574:C:O5'  | 2.04                     | 0.40              |
| 24:BA:1829:A:O2'  | 26:BC:14:HIS:CE1  | 2.74                     | 0.40              |
| 24:BA:1878:G:H2'  | 24:BA:1879:C:O4'  | 2.22                     | 0.40              |
| 24:BA:2186:G:C6   | 24:BA:2187:U:C2   | 3.10                     | 0.40              |
| 24:BA:2204:G:C6   | 24:BA:2205:A:C5   | 3.10                     | 0.40              |
| 24:BA:2263:C:O2'  | 24:BA:2264:C:H5'  | 2.21                     | 0.40              |
| 24:BA:2282:G:C6   | 24:BA:2425:A:N1   | 2.90                     | 0.40              |
| 24:BA:2470:G:C2'  | 24:BA:2471:A:H5'  | 2.51                     | 0.40              |
| 24:BA:2862:G:H2'  | 24:BA:2863:C:C6   | 2.56                     | 0.40              |
| 24:BA:352:A:OP2   | 24:BA:352:A:H8    | 2.05                     | 0.40              |
| 24:BA:656:G:H2'   | 24:BA:657:U:O4'   | 2.21                     | 0.40              |
| 24:BA:827:U:OP2   | 24:BA:828:U:C2    | 2.74                     | 0.40              |
| 24:BA:855:G:N3    | 46:BW:23:LYS:HG2  | 2.36                     | 0.40              |
| 25:BB:16:G:C5     | 25:BB:69:G:C2     | 3.09                     | 0.40              |
| 24:BA:1800:C:OP1  | 26:BC:259:ASN:ND2 | 2.54                     | 0.40              |
| 26:BC:43:ASN:ND2  | 26:BC:44:ASN:H    | 2.19                     | 0.40              |
| 29:BF:8:LYS:O     | 29:BF:12:VAL:CG1  | 2.70                     | 0.40              |
| 32:BI:58:ILE:HG22 | 32:BI:60:VAL:CG2  | 2.52                     | 0.40              |
| 33:BJ:114:LEU:CD2 | 33:BJ:114:LEU:O   | 2.68                     | 0.40              |
| 35:BL:21:ARG:HA   | 35:BL:21:ARG:HD3  | 1.49                     | 0.40              |
| 36:BM:45:GLN:NE2  | 36:BM:125:PRO:HD3 | 2.35                     | 0.40              |
| 36:BM:47:GLU:O    | 36:BM:48:ALA:C    | 2.60                     | 0.40              |
| 40:BQ:77:LYS:O    | 40:BQ:78:PHE:C    | 2.59                     | 0.40              |
| 43:BT:22:THR:HA   | 43:BT:25:GLU:HB3  | 2.04                     | 0.40              |
| 44:BU:100:GLU:O   | 44:BU:101:THR:CB  | 2.69                     | 0.40              |
| 49:BZ:23:LEU:HD21 | 49:BZ:53:MET:HE1  | 2.02                     | 0.40              |
| 55:CA:1144:G:N2   | 55:CA:1146:A:H62  | 2.20                     | 0.40              |
| 55:CA:1156:G:HO2' | 55:CA:1180:A:N6   | 2.18                     | 0.40              |
| 55:CA:1201:A:HO2' | 55:CA:1202:U:P    | 2.39                     | 0.40              |
| 55:CA:1242:G:N2   | 55:CA:1302:C:O2   | 2.54                     | 0.40              |
| 55:CA:1258:G:O2'  | 55:CA:1259:C:H5'  | 2.20                     | 0.40              |
| 55:CA:241:G:N2    | 55:CA:286:C:C2    | 2.89                     | 0.40              |
| 55:CA:109:A:N6    | 55:CA:326:G:N7    | 2.69                     | 0.40              |
| 55:CA:330:C:O2'   | 55:CA:331:G:H5'   | 2.20                     | 0.40              |
| 55:CA:562:U:H4'   | 55:CA:563:A:O5'   | 2.21                     | 0.40              |
| 55:CA:61:G:C6     | 55:CA:107:G:N1    | 2.89                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CA:687:A:C2    | 55:CA:704:A:N6    | 2.89                     | 0.40              |
| 55:CA:803:G:C6    | 55:CA:804:U:N3    | 2.89                     | 0.40              |
| 55:CA:853:C:O2'   | 55:CA:854:U:H5'   | 2.20                     | 0.40              |
| 55:CA:987:G:H2'   | 55:CA:988:G:H8    | 1.86                     | 0.40              |
| 1:CB:46:VAL:HA    | 1:CB:49:PHE:CE2   | 2.56                     | 0.40              |
| 1:CB:55:GLU:N     | 1:CB:55:GLU:OE1   | 2.54                     | 0.40              |
| 2:CC:127:VAL:HG23 | 2:CC:127:VAL:O    | 2.21                     | 0.40              |
| 2:CC:109:GLU:CB   | 2:CC:143:LEU:HD22 | 2.47                     | 0.40              |
| 5:AF:16:GLU:HB2   | 3:CD:188:SER:HA   | 2.03                     | 0.40              |
| 4:CE:104:ILE:H    | 4:CE:122:VAL:H    | 1.70                     | 0.40              |
| 4:CE:95:MET:CA    | 4:CE:124:ALA:HB2  | 2.47                     | 0.40              |
| 4:CE:94:PHE:CG    | 4:CE:95:MET:N     | 2.89                     | 0.40              |
| 5:CF:57:ALA:HB3   | 5:CF:59:TYR:CE1   | 2.55                     | 0.40              |
| 10:CK:34:THR:CB   | 10:CK:40:ALA:HA   | 2.52                     | 0.40              |
| 11:CL:19:ASN:HD22 | 11:CL:19:ASN:H    | 1.65                     | 0.40              |
| 11:CL:43:LYS:CB   | 11:CL:44:PRO:CD   | 2.74                     | 0.40              |
| 12:CM:11:HIS:O    | 12:CM:12:LYS:HG2  | 2.21                     | 0.40              |
| 19:CT:4:LYS:C     | 19:CT:6:ALA:N     | 2.75                     | 0.40              |
| 52:D2:43:THR:HG23 | 52:D2:45:SER:OG   | 2.21                     | 0.40              |
| 24:DA:1113:U:O2'  | 24:DA:1114:C:P    | 2.80                     | 0.40              |
| 24:DA:577:G:O2'   | 24:DA:1254:A:OP1  | 2.39                     | 0.40              |
| 24:DA:1280:G:C2'  | 24:DA:1281:G:H5'  | 2.52                     | 0.40              |
| 24:DA:1296:G:C2   | 24:DA:1645:G:C5   | 3.09                     | 0.40              |
| 24:DA:1415:U:C2   | 24:DA:1588:G:N1   | 2.89                     | 0.40              |
| 24:DA:1616:A:C2   | 24:DA:1647:U:C5   | 3.09                     | 0.40              |
| 24:DA:1819:A:OP1  | 26:DC:155:ARG:N   | 2.50                     | 0.40              |
| 24:DA:1878:G:C6   | 24:DA:1879:C:C4   | 3.09                     | 0.40              |
| 24:DA:1910:G:C2   | 24:DA:1921:G:C4   | 3.09                     | 0.40              |
| 24:DA:194:G:C6    | 24:DA:195:A:C5    | 3.09                     | 0.40              |
| 24:DA:1956:U:O2'  | 24:DA:1957:C:O5'  | 2.40                     | 0.40              |
| 24:DA:2261:C:O2'  | 24:DA:2262:U:C5'  | 2.69                     | 0.40              |
| 24:DA:2286:G:H4'  | 24:DA:2287:A:C1'  | 2.51                     | 0.40              |
| 24:DA:2345:G:C6   | 24:DA:2347:C:N4   | 2.89                     | 0.40              |
| 24:DA:241:A:C8    | 24:DA:243:U:N3    | 2.89                     | 0.40              |
| 24:DA:2539:C:N4   | 24:DA:2540:C:H41  | 2.19                     | 0.40              |
| 24:DA:2567:G:H2'  | 24:DA:2568:U:C6   | 2.56                     | 0.40              |
| 24:DA:264:C:H5'   | 24:DA:265:A:OP1   | 2.22                     | 0.40              |
| 24:DA:2665:A:H2'  | 24:DA:2666:C:O2   | 2.21                     | 0.40              |
| 24:DA:1456:G:N2   | 24:DA:2704:C:C2   | 2.90                     | 0.40              |
| 24:DA:2543:G:C1'  | 24:DA:2766:A:H5'' | 2.51                     | 0.40              |
| 24:DA:2844:G:O2'  | 24:DA:2845:U:H5'  | 2.21                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:DA:2868:A:O2'   | 24:DA:2869:G:C5'  | 2.69                     | 0.40              |
| 24:DA:364:C:H2'    | 24:DA:365:U:H6    | 1.73                     | 0.40              |
| 24:DA:408:G:N3     | 24:DA:409:G:C8    | 2.90                     | 0.40              |
| 24:DA:410:G:C6     | 24:DA:2407:A:N6   | 2.89                     | 0.40              |
| 24:DA:605:G:O2'    | 24:DA:606:U:C5'   | 2.69                     | 0.40              |
| 24:DA:671:C:O2'    | 24:DA:672:C:P     | 2.79                     | 0.40              |
| 24:DA:734:A:H2'    | 24:DA:735:A:H8    | 1.86                     | 0.40              |
| 24:DA:849:A:C4     | 24:DA:850:U:C5    | 3.10                     | 0.40              |
| 24:DA:964:C:O3'    | 24:DA:2273:A:O2'  | 2.33                     | 0.40              |
| 26:DC:212:TRP:HD1  | 26:DC:212:TRP:C   | 2.25                     | 0.40              |
| 26:DC:2:VAL:O      | 26:DC:3:VAL:CB    | 2.66                     | 0.40              |
| 28:DE:147:LEU:HD21 | 28:DE:179:SER:HB2 | 2.02                     | 0.40              |
| 30:DG:91:VAL:N     | 30:DG:93:TYR:CD2  | 2.90                     | 0.40              |
| 32:DI:72:THR:HA    | 32:DI:73:PRO:HD2  | 1.83                     | 0.40              |
| 35:DL:29:LYS:O     | 35:DL:29:LYS:HG2  | 2.21                     | 0.40              |
| 35:DL:56:PRO:CB    | 35:DL:58:TYR:CE2  | 3.03                     | 0.40              |
| 35:DL:95:LEU:HA    | 35:DL:98:ALA:HB3  | 2.03                     | 0.40              |
| 39:DP:83:ILE:O     | 39:DP:83:ILE:HD13 | 2.21                     | 0.40              |
| 40:DQ:63:ARG:NH1   | 40:DQ:99:VAL:CG2  | 2.84                     | 0.40              |
| 42:DS:6:LYS:HB2    | 42:DS:103:ILE:O   | 2.21                     | 0.40              |
| 44:DU:64:ILE:HG12  | 44:DU:64:ILE:O    | 2.21                     | 0.40              |
| 56:DB:73:A:H2      | 45:DV:37:PRO:HB3  | 1.87                     | 0.40              |
| 47:DX:62:GLY:O     | 47:DX:66:VAL:HG23 | 2.21                     | 0.40              |
| 21:AA:1068:G:OP2   | 21:AA:1094:G:H8   | 2.04                     | 0.40              |
| 21:AA:1463:U:H2'   | 21:AA:1464:U:H6   | 1.86                     | 0.40              |
| 21:AA:126:G:N1     | 21:AA:236:A:C6    | 2.90                     | 0.40              |
| 3:AD:36:ALA:HB1    | 21:AA:426:U:H5''  | 2.02                     | 0.40              |
| 21:AA:587:G:O2'    | 21:AA:588:G:H5'   | 2.21                     | 0.40              |
| 21:AA:595:A:C5     | 21:AA:641:U:C4    | 3.09                     | 0.40              |
| 21:AA:670:G:C6     | 21:AA:671:G:N7    | 2.90                     | 0.40              |
| 21:AA:792:A:C5     | 21:AA:794:A:N6    | 2.89                     | 0.40              |
| 21:AA:792:A:C1'    | 21:AA:794:A:N7    | 2.84                     | 0.40              |
| 21:AA:920:U:O2'    | 21:AA:921:U:H5'   | 2.21                     | 0.40              |
| 21:AA:928:G:H2'    | 21:AA:929:G:H8    | 1.87                     | 0.40              |
| 6:AG:101:ARG:CZ    | 21:AA:939:G:H5'   | 2.51                     | 0.40              |
| 21:AA:956:U:N3     | 21:AA:957:U:C5    | 2.89                     | 0.40              |
| 1:AB:137:THR:CA    | 1:AB:140:LEU:HD13 | 2.30                     | 0.40              |
| 1:AB:52:ALA:O      | 1:AB:54:ALA:N     | 2.55                     | 0.40              |
| 2:AC:135:ARG:HA    | 2:AC:135:ARG:HD3  | 1.89                     | 0.40              |
| 2:AC:5:HIS:NE2     | 2:AC:7:ASN:HB3    | 2.36                     | 0.40              |
| 6:AG:100:MET:HB2   | 6:AG:100:MET:HE3  | 1.99                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:AI:17:ARG:HH22  | 21:AA:1129:C:H5'   | 1.85                     | 0.40              |
| 10:AK:124:LYS:O   | 10:AK:125:LYS:O    | 2.39                     | 0.40              |
| 10:AK:34:THR:OG1  | 10:AK:39:ASN:N     | 2.52                     | 0.40              |
| 15:AP:36:VAL:HG22 | 15:AP:36:VAL:O     | 2.22                     | 0.40              |
| 18:AS:29:PRO:HA   | 18:AS:47:THR:OG1   | 2.21                     | 0.40              |
| 51:B1:27:ARG:C    | 51:B1:29:LYS:H     | 2.25                     | 0.40              |
| 24:BA:1072:C:N4   | 24:BA:1093:G:H1    | 2.19                     | 0.40              |
| 24:BA:1266:G:N7   | 42:BS:16:LYS:HE3   | 2.35                     | 0.40              |
| 24:BA:1327:A:OP2  | 59:BA:3618:HOH:O   | 2.21                     | 0.40              |
| 24:BA:1340:U:C5   | 24:BA:1603:A:C8    | 3.08                     | 0.40              |
| 24:BA:1380:G:C2   | 24:BA:1381:G:N7    | 2.90                     | 0.40              |
| 24:BA:144:A:C6    | 24:BA:145:C:C4     | 3.10                     | 0.40              |
| 24:BA:1471:G:H2'  | 24:BA:1472:C:C6    | 2.56                     | 0.40              |
| 24:BA:1821:A:O5'  | 24:BA:1821:A:H8    | 2.04                     | 0.40              |
| 24:BA:1839:G:C8   | 24:BA:1927:A:O4'   | 2.75                     | 0.40              |
| 24:BA:1899:A:C2'  | 24:BA:1900:A:OP2   | 2.70                     | 0.40              |
| 24:BA:2261:C:H1'  | 24:BA:2388:A:N3    | 2.36                     | 0.40              |
| 24:BA:2716:C:H2'  | 24:BA:2717:C:H6    | 1.86                     | 0.40              |
| 24:BA:2814:A:O5'  | 24:BA:2814:A:H8    | 2.04                     | 0.40              |
| 24:BA:2047:C:O2'  | 24:BA:2823:A:N1    | 2.43                     | 0.40              |
| 24:BA:2843:G:H21  | 24:BA:2844:G:H1'   | 1.86                     | 0.40              |
| 24:BA:506:G:H4'   | 24:BA:509:C:O2     | 2.21                     | 0.40              |
| 24:BA:944:C:H2'   | 59:BA:3356:HOH:O   | 2.22                     | 0.40              |
| 24:BA:995:C:OP2   | 40:BQ:53:LYS:HE3   | 2.20                     | 0.40              |
| 25:BB:14:U:C3'    | 25:BB:15:A:H5''    | 2.51                     | 0.40              |
| 25:BB:67:G:N2     | 25:BB:68:C:H1'     | 2.36                     | 0.40              |
| 25:BB:71:C:H2'    | 25:BB:72:G:H5'     | 2.03                     | 0.40              |
| 25:BB:80:U:H2'    | 25:BB:81:G:C8      | 2.57                     | 0.40              |
| 24:BA:764:A:OP1   | 26:BC:206:LYS:HE3  | 2.22                     | 0.40              |
| 27:BD:16:THR:CG2  | 27:BD:18:ASP:OD1   | 2.61                     | 0.40              |
| 27:BD:34:VAL:HG22 | 27:BD:94:GLN:N     | 2.35                     | 0.40              |
| 24:BA:2784:U:H4'  | 27:BD:42:ASN:HD21  | 1.86                     | 0.40              |
| 29:BF:147:ARG:HG3 | 29:BF:149:ARG:H    | 1.87                     | 0.40              |
| 30:BG:93:TYR:HA   | 30:BG:93:TYR:HD2   | 1.65                     | 0.40              |
| 35:BL:92:LEU:HD23 | 35:BL:125:LEU:HD23 | 2.04                     | 0.40              |
| 36:BM:43:ALA:C    | 36:BM:45:GLN:N     | 2.74                     | 0.40              |
| 37:BN:55:ALA:HA   | 37:BN:80:PHE:CD1   | 2.57                     | 0.40              |
| 37:BN:69:ARG:H    | 37:BN:69:ARG:HG2   | 1.42                     | 0.40              |
| 39:BP:48:ALA:CB   | 39:BP:95:LYS:HG3   | 2.51                     | 0.40              |
| 39:BP:50:ARG:HB3  | 39:BP:57:ALA:O     | 2.21                     | 0.40              |
| 40:BQ:57:ARG:HA   | 40:BQ:60:TRP:CE3   | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:BS:66:ILE:HD13 | 42:BS:67:ASP:N    | 2.36                     | 0.40              |
| 43:BT:32:LEU:CD2  | 43:BT:32:LEU:N    | 2.83                     | 0.40              |
| 43:BT:29:THR:CA   | 43:BT:86:THR:H    | 2.34                     | 0.40              |
| 44:BU:44:HIS:O    | 44:BU:45:GLN:C    | 2.59                     | 0.40              |
| 44:BU:92:VAL:HG13 | 44:BU:93:ARG:O    | 2.21                     | 0.40              |
| 44:BU:94:PHE:O    | 44:BU:94:PHE:CG   | 2.75                     | 0.40              |
| 48:BY:19:LEU:HD12 | 48:BY:22:LEU:HD23 | 2.03                     | 0.40              |
| 55:CA:1023:U:C2   | 55:CA:1024:G:N7   | 2.90                     | 0.40              |
| 55:CA:1163:A:C6   | 55:CA:1174:G:C6   | 3.09                     | 0.40              |
| 55:CA:1246:A:O2'  | 55:CA:1247:U:C5'  | 2.69                     | 0.40              |
| 55:CA:1266:G:N1   | 55:CA:1270:G:O6   | 2.54                     | 0.40              |
| 55:CA:1266:G:N2   | 55:CA:1269:A:OP2  | 2.54                     | 0.40              |
| 55:CA:1361:G:H2'  | 55:CA:1362:A:H5'' | 2.04                     | 0.40              |
| 55:CA:1507:A:C6   | 55:CA:1530:G:C5   | 3.08                     | 0.40              |
| 55:CA:253:A:O2'   | 55:CA:254:G:O5'   | 2.35                     | 0.40              |
| 55:CA:291:U:O2'   | 55:CA:292:G:H5'   | 2.21                     | 0.40              |
| 55:CA:39:G:H2'    | 55:CA:40:C:C6     | 2.56                     | 0.40              |
| 55:CA:571:U:H3'   | 55:CA:572:A:H5''  | 2.03                     | 0.40              |
| 55:CA:764:C:N4    | 55:CA:812:G:N1    | 2.70                     | 0.40              |
| 55:CA:767:A:C4    | 55:CA:768:A:C8    | 3.10                     | 0.40              |
| 55:CA:880:C:C2'   | 55:CA:880:C:O2    | 2.58                     | 0.40              |
| 55:CA:928:G:O2'   | 55:CA:1533:C:P    | 2.78                     | 0.40              |
| 1:CB:34:ARG:HD3   | 1:CB:35:ASN:N     | 2.36                     | 0.40              |
| 1:CB:80:LYS:C     | 1:CB:81:ASP:OD1   | 2.60                     | 0.40              |
| 2:CC:162:ALA:HB2  | 55:CA:1056:U:O5'  | 2.20                     | 0.40              |
| 2:CC:39:ARG:HG2   | 2:CC:54:ILE:HG21  | 2.03                     | 0.40              |
| 2:CC:59:PRO:HB2   | 2:CC:60:ALA:H     | 1.58                     | 0.40              |
| 3:CD:107:GLY:N    | 3:CD:157:ALA:CB   | 2.84                     | 0.40              |
| 4:CE:75:LEU:HD13  | 4:CE:79:THR:O     | 2.21                     | 0.40              |
| 5:CF:49:TYR:CE1   | 17:CR:65:SER:HA   | 2.56                     | 0.40              |
| 6:CG:94:ARG:HB3   | 6:CG:98:LEU:HD11  | 2.03                     | 0.40              |
| 8:CI:128:LYS:HA   | 8:CI:128:LYS:HD2  | 1.83                     | 0.40              |
| 8:CI:5:TYR:O      | 8:CI:19:PHE:HA    | 2.21                     | 0.40              |
| 8:CI:59:LYS:HE2   | 8:CI:59:LYS:HB3   | 1.63                     | 0.40              |
| 12:CM:105:ALA:O   | 12:CM:109:LYS:N   | 2.54                     | 0.40              |
| 12:CM:2:ARG:HH11  | 12:CM:8:ILE:HG21  | 1.86                     | 0.40              |
| 15:CP:26:ASN:OD1  | 15:CP:31:ARG:HB3  | 2.21                     | 0.40              |
| 20:CU:9:GLU:HB2   | 20:CU:11:PHE:CE2  | 2.57                     | 0.40              |
| 51:D1:52:LYS:HB2  | 51:D1:52:LYS:NZ   | 2.36                     | 0.40              |
| 24:DA:1112:G:O2'  | 24:DA:1113:U:C6   | 2.66                     | 0.40              |
| 24:DA:1203:U:C4   | 24:DA:1204:A:C5   | 3.09                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:1345:C:C2   | 24:DA:1346:G:C8    | 3.09                     | 0.40              |
| 24:DA:1442:U:C4   | 24:DA:1443:U:C4    | 3.09                     | 0.40              |
| 24:DA:1493:C:OP2  | 24:DA:1493:C:H6    | 2.03                     | 0.40              |
| 24:DA:14:A:C6     | 24:DA:526:A:C2     | 3.09                     | 0.40              |
| 24:DA:1655:A:H4'  | 27:DD:118:PHE:CE1  | 2.55                     | 0.40              |
| 24:DA:1721:G:O2'  | 24:DA:1739:A:N6    | 2.53                     | 0.40              |
| 24:DA:1833:C:O2   | 24:DA:1969:A:H2    | 2.03                     | 0.40              |
| 24:DA:1851:U:H2'  | 24:DA:1852:U:O4'   | 2.22                     | 0.40              |
| 24:DA:2262:U:H5'' | 46:DW:38:ARG:HH22  | 1.86                     | 0.40              |
| 24:DA:2365:G:OP1  | 46:DW:54:ARG:HG3   | 2.22                     | 0.40              |
| 24:DA:2423:U:C1'  | 24:DA:2425:A:N7    | 2.83                     | 0.40              |
| 24:DA:2558:C:C2'  | 24:DA:2559:C:H5'   | 2.52                     | 0.40              |
| 24:DA:2560:A:C6   | 24:DA:2561:U:C4    | 3.10                     | 0.40              |
| 24:DA:2611:C:C2'  | 24:DA:2612:C:H6    | 2.35                     | 0.40              |
| 24:DA:2697:G:O2'  | 24:DA:2698:U:H5'   | 2.21                     | 0.40              |
| 24:DA:271:G:C4    | 24:DA:272:A:N7     | 2.89                     | 0.40              |
| 24:DA:432:A:H2'   | 24:DA:433:C:C6     | 2.57                     | 0.40              |
| 24:DA:571:U:N3    | 24:DA:2030:A:C6    | 2.89                     | 0.40              |
| 24:DA:64:A:C6     | 24:DA:91:A:N6      | 2.89                     | 0.40              |
| 24:DA:70:G:H5'    | 24:DA:71:A:OP1     | 2.21                     | 0.40              |
| 24:DA:929:U:N3    | 24:DA:930:G:C5     | 2.89                     | 0.40              |
| 24:DA:975:A:N6    | 24:DA:989:G:HI1'   | 2.36                     | 0.40              |
| 24:DA:996:A:C4    | 24:DA:997:G:C8     | 3.10                     | 0.40              |
| 56:DB:78:A:C2     | 56:DB:99:A:C4      | 3.09                     | 0.40              |
| 26:DC:6:LYS:HA    | 26:DC:7:PRO:HD3    | 1.94                     | 0.40              |
| 28:DE:141:MET:O   | 28:DE:142:ALA:HB3  | 2.22                     | 0.40              |
| 32:DI:5:GLN:HB2   | 32:DI:7:TYR:CE2    | 2.56                     | 0.40              |
| 32:DI:64:ARG:HB2  | 32:DI:64:ARG:CZ    | 2.51                     | 0.40              |
| 33:DJ:23:LYS:HE2  | 33:DJ:142:ILE:HG13 | 2.04                     | 0.40              |
| 36:DM:72:PRO:HA   | 36:DM:92:TRP:CE3   | 2.56                     | 0.40              |
| 24:DA:2378:A:O2'  | 38:DO:21:LEU:HD13  | 2.21                     | 0.40              |
| 41:DR:39:LEU:HB2  | 41:DR:49:ILE:CD1   | 2.51                     | 0.40              |
| 44:DU:20:LYS:C    | 44:DU:20:LYS:HD3   | 2.42                     | 0.40              |
| 44:DU:64:ILE:O    | 44:DU:65:GLN:O     | 2.40                     | 0.40              |
| 45:DV:80:HIS:CD2  | 45:DV:83:LYS:N     | 2.89                     | 0.40              |
| 45:DV:21:ARG:HE   | 45:DV:87:GLN:HG2   | 1.86                     | 0.40              |
| 46:DW:25:PHE:CG   | 46:DW:26:GLY:N     | 2.88                     | 0.40              |
| 21:AA:1022:A:C6   | 21:AA:1023:U:N3    | 2.90                     | 0.40              |
| 21:AA:1171:A:C6   | 21:AA:1172:C:C4    | 3.09                     | 0.40              |
| 21:AA:1239:A:C6   | 21:AA:1298:U:C5    | 3.10                     | 0.40              |
| 21:AA:313:A:H2'   | 21:AA:314:C:C6     | 2.56                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:328:C:O2     | 21:AA:328:C:H2'    | 2.22                     | 0.40              |
| 21:AA:469:C:C4     | 21:AA:470:C:C4     | 3.10                     | 0.40              |
| 21:AA:953:G:C6     | 21:AA:954:G:C5     | 3.09                     | 0.40              |
| 1:AB:116:LEU:O     | 1:AB:119:GLN:NE2   | 2.54                     | 0.40              |
| 1:AB:153:MET:CE    | 1:AB:157:PRO:HG3   | 2.51                     | 0.40              |
| 1:AB:177:ASN:C     | 1:AB:177:ASN:OD1   | 2.59                     | 0.40              |
| 1:AB:30:ILE:HD11   | 1:AB:38:HIS:CD2    | 2.57                     | 0.40              |
| 2:AC:108:PRO:CB    | 2:AC:114:LEU:HD13  | 2.52                     | 0.40              |
| 2:AC:78:LYS:O      | 2:AC:79:LYS:HB2    | 2.22                     | 0.40              |
| 3:AD:21:LYS:O      | 3:AD:22:SER:C      | 2.59                     | 0.40              |
| 4:AE:17:VAL:HA     | 4:AE:33:THR:O      | 2.22                     | 0.40              |
| 10:AK:71:ASP:OD1   | 10:AK:72:ALA:N     | 2.55                     | 0.40              |
| 13:AN:78:LEU:HB2   | 13:AN:83:VAL:CG2   | 2.51                     | 0.40              |
| 22:AV:35:A:C2'     | 22:AV:36:A:O5'     | 2.70                     | 0.40              |
| 24:BA:1014:A:H2'   | 24:BA:1015:U:C6    | 2.56                     | 0.40              |
| 24:BA:996:A:C6     | 24:BA:1160:G:C6    | 3.08                     | 0.40              |
| 24:BA:1538:G:O2'   | 24:BA:1539:U:C5'   | 2.69                     | 0.40              |
| 24:BA:1569:A:C6    | 24:BA:1570:A:N1    | 2.90                     | 0.40              |
| 24:BA:1601:G:H2'   | 24:BA:1602:U:O4'   | 2.22                     | 0.40              |
| 24:BA:1730:C:OP1   | 24:BA:1730:C:H4'   | 2.20                     | 0.40              |
| 24:BA:1787:A:O2'   | 24:BA:1788:C:H5'   | 2.21                     | 0.40              |
| 24:BA:1997:C:O2'   | 24:BA:1998:A:C5'   | 2.64                     | 0.40              |
| 24:BA:2093:G:C5    | 24:BA:2225:A:C5    | 3.09                     | 0.40              |
| 24:BA:2096:C:H2'   | 24:BA:2097:A:C8    | 2.57                     | 0.40              |
| 24:BA:2182:U:C2'   | 24:BA:2183:A:OP1   | 2.69                     | 0.40              |
| 24:BA:2214:C:H6    | 24:BA:2214:C:H5'   | 1.85                     | 0.40              |
| 24:BA:2255:G:C5    | 24:BA:2256:G:C8    | 3.09                     | 0.40              |
| 24:BA:2283:C:N4    | 24:BA:2389:G:C5    | 2.90                     | 0.40              |
| 24:BA:2545:G:H2'   | 24:BA:2546:U:H5'   | 2.03                     | 0.40              |
| 24:BA:2765:A:N3    | 24:BA:2766:A:H5'   | 2.36                     | 0.40              |
| 24:BA:2791:G:C4    | 24:BA:2792:A:C8    | 3.09                     | 0.40              |
| 24:BA:287:G:N2     | 24:BA:354:A:C4     | 2.89                     | 0.40              |
| 24:BA:35:G:HO2'    | 24:BA:36:G:C5'     | 2.30                     | 0.40              |
| 24:BA:30:G:C6      | 24:BA:511:U:O2     | 2.75                     | 0.40              |
| 24:BA:725:G:O6     | 24:BA:726:G:N1     | 2.54                     | 0.40              |
| 25:BB:116:G:H4'    | 38:BO:54:VAL:HG22  | 2.03                     | 0.40              |
| 26:BC:245:THR:C    | 26:BC:247:TRP:N    | 2.74                     | 0.40              |
| 26:BC:245:THR:C    | 26:BC:247:TRP:H    | 2.25                     | 0.40              |
| 28:BE:133:LEU:HD23 | 28:BE:133:LEU:HA   | 1.89                     | 0.40              |
| 28:BE:108:ILE:HD11 | 28:BE:180:LEU:HD13 | 2.03                     | 0.40              |
| 29:BF:100:GLU:O    | 29:BF:102:LEU:N    | 2.55                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:BF:41:GLU:HB2   | 29:BF:48:LEU:HD23  | 2.04                     | 0.40              |
| 29:BF:8:LYS:HB2    | 29:BF:9:ASP:H      | 1.62                     | 0.40              |
| 30:BG:26:LYS:HB3   | 30:BG:32:LEU:CB    | 2.51                     | 0.40              |
| 30:BG:26:LYS:HB3   | 30:BG:32:LEU:HA    | 2.03                     | 0.40              |
| 30:BG:95:ALA:HB2   | 30:BG:104:LEU:HD23 | 2.02                     | 0.40              |
| 32:BI:52:LEU:HA    | 32:BI:53:PRO:HD3   | 1.97                     | 0.40              |
| 32:BI:64:ARG:HA    | 32:BI:64:ARG:HD2   | 1.98                     | 0.40              |
| 33:BJ:37:ARG:HA    | 33:BJ:118:MET:HE2  | 2.02                     | 0.40              |
| 34:BK:116:ILE:HG13 | 34:BK:116:ILE:H    | 1.74                     | 0.40              |
| 36:BM:136:MET:HE2  | 36:BM:136:MET:HB3  | 1.87                     | 0.40              |
| 36:BM:43:ALA:O     | 36:BM:47:GLU:HB2   | 2.21                     | 0.40              |
| 36:BM:96:ILE:CD1   | 36:BM:96:ILE:O     | 2.70                     | 0.40              |
| 38:BO:34:HIS:CD2   | 38:BO:53:THR:OG1   | 2.74                     | 0.40              |
| 39:BP:50:ARG:H     | 39:BP:50:ARG:HG3   | 1.72                     | 0.40              |
| 43:BT:34:VAL:O     | 43:BT:34:VAL:HG23  | 2.21                     | 0.40              |
| 46:BW:51:GLY:O     | 46:BW:52:CYS:C     | 2.58                     | 0.40              |
| 55:CA:1201:A:H4'   | 55:CA:1203:C:OP2   | 2.20                     | 0.40              |
| 55:CA:1292:G:C6    | 55:CA:1293:C:C4    | 3.10                     | 0.40              |
| 12:CM:97:ARG:HB3   | 55:CA:1308:U:OP2   | 2.22                     | 0.40              |
| 55:CA:162:A:H2'    | 55:CA:163:C:O4'    | 2.22                     | 0.40              |
| 19:CT:81:GLN:HE22  | 55:CA:258:G:H5'    | 1.76                     | 0.40              |
| 55:CA:615:G:N2     | 55:CA:626:G:C4     | 2.90                     | 0.40              |
| 55:CA:876:C:H2'    | 55:CA:877:G:H8     | 1.87                     | 0.40              |
| 55:CA:889:A:O2'    | 55:CA:890:G:H4'    | 2.21                     | 0.40              |
| 55:CA:94:G:H4'     | 55:CA:95:C:H5''    | 2.03                     | 0.40              |
| 2:CC:168:ARG:CG    | 2:CC:169:GLU:N     | 2.84                     | 0.40              |
| 5:CF:43:GLY:O      | 5:CF:44:ARG:C      | 2.59                     | 0.40              |
| 6:CG:135:LYS:O     | 6:CG:139:ASP:N     | 2.54                     | 0.40              |
| 7:CH:76:ARG:HD3    | 7:CH:76:ARG:C      | 2.41                     | 0.40              |
| 9:CJ:48:ARG:HB3    | 13:CN:100:TRP:HZ2  | 1.86                     | 0.40              |
| 9:CJ:47:GLU:CB     | 9:CJ:67:ILE:HG13   | 2.44                     | 0.40              |
| 13:CN:2:LYS:HA     | 55:CA:1048:G:OP1   | 2.22                     | 0.40              |
| 13:CN:19:TYR:CE2   | 13:CN:51:PRO:HG3   | 2.56                     | 0.40              |
| 18:CS:72:GLU:HG2   | 55:CA:1320:C:H4'   | 2.03                     | 0.40              |
| 19:CT:22:SER:HA    | 19:CT:25:SER:OG    | 2.21                     | 0.40              |
| 19:CT:73:ARG:NH1   | 55:CA:261:U:C5     | 2.89                     | 0.40              |
| 20:CU:15:LEU:HD13  | 20:CU:17:ARG:HE    | 1.86                     | 0.40              |
| 50:D0:21:LEU:HD23  | 50:D0:21:LEU:HA    | 1.94                     | 0.40              |
| 51:D1:43:ARG:HB2   | 51:D1:43:ARG:NH2   | 2.36                     | 0.40              |
| 51:D1:8:ILE:HG21   | 51:D1:51:ALA:HB1   | 2.03                     | 0.40              |
| 24:DA:126:A:H8     | 52:D2:46:LYS:HE2   | 1.86                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DA:1047:G:N2   | 24:DA:1110:G:C4    | 2.89                     | 0.40              |
| 24:DA:1055:G:H3'  | 24:DA:1056:G:H5'   | 2.02                     | 0.40              |
| 24:DA:1343:G:H2'  | 24:DA:1344:U:C5    | 2.56                     | 0.40              |
| 24:DA:1803:A:H3'  | 24:DA:1804:C:C6    | 2.56                     | 0.40              |
| 24:DA:1959:G:C6   | 24:DA:1960:A:C5    | 3.10                     | 0.40              |
| 24:DA:1965:C:H3'  | 24:DA:1966:A:H5''  | 2.00                     | 0.40              |
| 24:DA:2051:A:C4'  | 24:DA:2052:A:OP1   | 2.54                     | 0.40              |
| 24:DA:2102:G:C2   | 24:DA:2188:U:C2    | 3.09                     | 0.40              |
| 24:DA:187:G:C2    | 24:DA:210:C:C2     | 3.10                     | 0.40              |
| 24:DA:252:G:N2    | 24:DA:253:C:C2     | 2.89                     | 0.40              |
| 24:DA:38:A:C6     | 24:DA:39:G:C5      | 3.10                     | 0.40              |
| 24:DA:447:A:H5'   | 24:DA:449:A:C8     | 2.57                     | 0.40              |
| 24:DA:36:G:H4'    | 24:DA:451:U:N3     | 2.37                     | 0.40              |
| 24:DA:511:U:H5''  | 24:DA:512:G:OP2    | 2.21                     | 0.40              |
| 24:DA:19:A:N1     | 24:DA:522:A:C6     | 2.90                     | 0.40              |
| 24:DA:532:A:H5'   | 24:DA:533:G:O4'    | 2.22                     | 0.40              |
| 24:DA:567:U:N3    | 24:DA:568:U:C4     | 2.89                     | 0.40              |
| 24:DA:825:A:C6    | 24:DA:826:U:N3     | 2.89                     | 0.40              |
| 24:DA:871:U:H2'   | 24:DA:872:U:C6     | 2.57                     | 0.40              |
| 56:DB:54:G:H2'    | 56:DB:55:U:C6      | 2.57                     | 0.40              |
| 56:DB:57:A:H2'    | 56:DB:58:A:H8      | 1.85                     | 0.40              |
| 26:DC:94:LEU:HB2  | 26:DC:100:ARG:HD2  | 2.03                     | 0.40              |
| 27:DD:138:LEU:N   | 27:DD:138:LEU:HD13 | 2.37                     | 0.40              |
| 27:DD:202:ILE:N   | 27:DD:202:ILE:HD12 | 2.37                     | 0.40              |
| 29:DF:146:ASP:HB3 | 29:DF:147:ARG:H    | 1.60                     | 0.40              |
| 33:DJ:30:THR:CG2  | 33:DJ:31:GLU:H     | 2.34                     | 0.40              |
| 37:DN:57:THR:O    | 37:DN:80:PHE:HD1   | 2.04                     | 0.40              |
| 40:DQ:48:ASP:HA   | 40:DQ:51:GLN:HB2   | 2.04                     | 0.40              |
| 42:DS:24:ILE:HB   | 42:DS:32:ALA:HB1   | 2.03                     | 0.40              |
| 42:DS:4:ILE:CG2   | 42:DS:106:VAL:HG22 | 2.51                     | 0.40              |
| 47:DX:2:ARG:HH21  | 47:DX:32:LEU:HD23  | 1.87                     | 0.40              |
| 21:AA:1075:U:H4'  | 21:AA:1101:A:N6    | 2.36                     | 0.40              |
| 21:AA:1081:A:C2   | 21:AA:1082:A:N9    | 2.90                     | 0.40              |
| 21:AA:1106:G:C6   | 21:AA:1107:C:C5    | 3.10                     | 0.40              |
| 21:AA:1124:G:N2   | 21:AA:1150:A:C2    | 2.90                     | 0.40              |
| 21:AA:148:G:N3    | 21:AA:1446:A:H2    | 2.19                     | 0.40              |
| 21:AA:158:G:H2'   | 21:AA:159:G:H5''   | 2.02                     | 0.40              |
| 21:AA:19:A:C6     | 21:AA:20:U:C4      | 3.10                     | 0.40              |
| 21:AA:613:C:H2'   | 21:AA:614:C:C6     | 2.57                     | 0.40              |
| 21:AA:666:G:N1    | 21:AA:741:G:C5     | 2.90                     | 0.40              |
| 21:AA:724:G:H4'   | 21:AA:724:G:OP2    | 2.22                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AA:838:G:H1'    | 21:AA:849:G:N2     | 2.36                     | 0.40              |
| 21:AA:845:A:H8     | 21:AA:846:G:C4'    | 2.35                     | 0.40              |
| 21:AA:878:A:H2'    | 21:AA:879:C:O4'    | 2.21                     | 0.40              |
| 21:AA:961:U:C2     | 21:AA:983:A:C4     | 3.10                     | 0.40              |
| 2:AC:116:ALA:HB1   | 2:AC:186:SER:HB3   | 2.04                     | 0.40              |
| 2:AC:41:TYR:OH     | 2:AC:89:VAL:HG21   | 2.22                     | 0.40              |
| 2:AC:63:ILE:O      | 2:AC:98:ALA:HA     | 2.21                     | 0.40              |
| 3:AD:195:ASN:ND2   | 3:AD:195:ASN:N     | 2.66                     | 0.40              |
| 6:AG:149:ALA:HB1   | 10:AK:58:THR:CB    | 2.52                     | 0.40              |
| 11:AL:14:LYS:HB2   | 11:AL:14:LYS:HE3   | 1.77                     | 0.40              |
| 16:AQ:12:VAL:CG1   | 16:AQ:16:MET:HE1   | 2.49                     | 0.40              |
| 20:AU:9:GLU:N      | 20:AU:10:PRO:CD    | 2.84                     | 0.40              |
| 50:B0:54:ILE:HA    | 50:B0:54:ILE:HD13  | 1.93                     | 0.40              |
| 54:B4:30:GLU:HB3   | 54:B4:33:HIS:CE1   | 2.57                     | 0.40              |
| 24:BA:55:G:N3      | 24:BA:127:A:H2     | 2.20                     | 0.40              |
| 24:BA:1655:A:H3'   | 24:BA:1656:C:C6    | 2.57                     | 0.40              |
| 24:BA:1767:G:C2    | 24:BA:1768:C:C6    | 3.10                     | 0.40              |
| 24:BA:760:G:H4'    | 24:BA:1776:G:OP1   | 2.21                     | 0.40              |
| 24:BA:177:G:H3'    | 24:BA:178:G:C8     | 2.56                     | 0.40              |
| 24:BA:1819:A:H5''  | 26:BC:159:THR:HG21 | 2.03                     | 0.40              |
| 24:BA:1853:A:C6    | 24:BA:1854:A:N1    | 2.89                     | 0.40              |
| 24:BA:2248:C:H2'   | 24:BA:2248:C:O2    | 2.22                     | 0.40              |
| 24:BA:827:U:C4     | 24:BA:2430:A:C5    | 3.09                     | 0.40              |
| 24:BA:262:A:H2'    | 24:BA:263:G:O4'    | 2.22                     | 0.40              |
| 24:BA:1297:C:OP1   | 24:BA:2710:C:H4'   | 2.21                     | 0.40              |
| 24:BA:2714:G:H2'   | 24:BA:2715:C:C6    | 2.56                     | 0.40              |
| 24:BA:2782:G:C2'   | 24:BA:2783:U:H5'   | 2.52                     | 0.40              |
| 24:BA:27:G:C2      | 24:BA:512:G:O2'    | 2.74                     | 0.40              |
| 24:BA:2818:U:H1'   | 24:BA:2829:A:H2    | 1.85                     | 0.40              |
| 24:BA:2840:C:H5''  | 37:BN:53:THR:HG21  | 2.03                     | 0.40              |
| 24:BA:327:G:C5     | 24:BA:328:U:C4     | 3.09                     | 0.40              |
| 24:BA:363:G:H2'    | 24:BA:364:C:C5     | 2.57                     | 0.40              |
| 24:BA:541:A:C6     | 24:BA:553:G:C6     | 3.09                     | 0.40              |
| 24:BA:556:A:N7     | 24:BA:557:C:C5     | 2.90                     | 0.40              |
| 24:BA:580:U:O3'    | 40:BQ:30:VAL:CG1   | 2.69                     | 0.40              |
| 24:BA:594:U:H2'    | 24:BA:595:C:C6     | 2.57                     | 0.40              |
| 24:BA:63:A:H2'     | 24:BA:64:A:H8      | 1.87                     | 0.40              |
| 24:BA:751:A:C2     | 24:BA:789:A:C4     | 3.09                     | 0.40              |
| 24:BA:861:A:H2'    | 24:BA:862:G:O4'    | 2.21                     | 0.40              |
| 26:BC:163:ILE:HD13 | 26:BC:173:LEU:HD11 | 2.03                     | 0.40              |
| 26:BC:268:ARG:HH11 | 26:BC:268:ARG:CB   | 2.34                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BD:90:PHE:O    | 27:BD:92:VAL:N    | 2.55                     | 0.40              |
| 28:BE:47:LYS:HD3  | 28:BE:51:GLU:O    | 2.21                     | 0.40              |
| 29:BF:127:TYR:O   | 29:BF:128:SER:CB  | 2.69                     | 0.40              |
| 30:BG:11:PRO:O    | 30:BG:12:ALA:C    | 2.60                     | 0.40              |
| 31:BH:133:GLN:HA  | 31:BH:133:GLN:OE1 | 2.22                     | 0.40              |
| 33:BJ:13:ARG:HD3  | 33:BJ:51:GLY:O    | 2.22                     | 0.40              |
| 34:BK:1:MET:CE    | 34:BK:32:TYR:CE1  | 3.04                     | 0.40              |
| 34:BK:68:GLY:O    | 34:BK:69:VAL:HG23 | 2.21                     | 0.40              |
| 36:BM:5:LYS:O     | 36:BM:6:ARG:HB2   | 2.21                     | 0.40              |
| 36:BM:81:ARG:HA   | 36:BM:81:ARG:HD3  | 1.80                     | 0.40              |
| 38:BO:53:THR:OG1  | 38:BO:53:THR:O    | 2.39                     | 0.40              |
| 38:BO:76:LYS:O    | 38:BO:79:ALA:HB3  | 2.22                     | 0.40              |
| 43:BT:68:LYS:CG   | 43:BT:69:ARG:H    | 2.35                     | 0.40              |
| 46:BW:9:THR:HG23  | 46:BW:10:ARG:N    | 2.36                     | 0.40              |
| 46:BW:23:LYS:CD   | 46:BW:24:ARG:N    | 2.83                     | 0.40              |
| 47:BX:70:LEU:O    | 47:BX:74:GLY:N    | 2.51                     | 0.40              |
| 48:BY:47:ARG:CG   | 48:BY:47:ARG:HH21 | 2.34                     | 0.40              |
| 49:BZ:19:HIS:O    | 49:BZ:22:THR:HB   | 2.22                     | 0.40              |
| 55:CA:1115:U:H2'  | 55:CA:1116:U:H6   | 1.87                     | 0.40              |
| 55:CA:1117:A:C5   | 55:CA:1184:G:O6   | 2.74                     | 0.40              |
| 6:CG:29:LEU:HG    | 55:CA:1240:U:N3   | 2.37                     | 0.40              |
| 55:CA:1301:U:H5'' | 55:CA:1302:C:OP1  | 2.21                     | 0.40              |
| 55:CA:1289:A:H2   | 55:CA:1371:G:H21  | 1.69                     | 0.40              |
| 6:CG:78:ARG:NH2   | 55:CA:1382:C:H4'  | 2.37                     | 0.40              |
| 55:CA:1410:A:N1   | 55:CA:1491:G:C6   | 2.90                     | 0.40              |
| 55:CA:1497:G:C2'  | 55:CA:1498:U:O5'  | 2.70                     | 0.40              |
| 55:CA:173:U:H5'   | 55:CA:197:A:O4'   | 2.21                     | 0.40              |
| 55:CA:345:C:H4'   | 55:CA:346:G:H5''  | 2.03                     | 0.40              |
| 55:CA:451:A:H61   | 55:CA:481:G:H5'   | 1.86                     | 0.40              |
| 55:CA:545:C:H2'   | 55:CA:546:A:O4'   | 2.21                     | 0.40              |
| 55:CA:859:G:C8    | 55:CA:869:G:N2    | 2.90                     | 0.40              |
| 1:CB:153:MET:C    | 1:CB:155:GLY:H    | 2.24                     | 0.40              |
| 2:CC:131:ARG:O    | 2:CC:132:ALA:C    | 2.59                     | 0.40              |
| 2:CC:183:TYR:CE1  | 2:CC:200:TRP:CE2  | 3.10                     | 0.40              |
| 3:CD:80:ARG:HG3   | 3:CD:80:ARG:H     | 1.58                     | 0.40              |
| 4:CE:111:ARG:O    | 4:CE:113:VAL:N    | 2.55                     | 0.40              |
| 4:CE:152:VAL:C    | 4:CE:154:ALA:H    | 2.24                     | 0.40              |
| 4:CE:55:VAL:N     | 4:CE:56:PRO:CD    | 2.83                     | 0.40              |
| 4:CE:76:ASN:O     | 4:CE:79:THR:HG22  | 2.22                     | 0.40              |
| 5:CF:12:PRO:HA    | 5:CF:15:SER:HB2   | 2.03                     | 0.40              |
| 14:CO:87:ARG:HD2  | 14:CO:87:ARG:HA   | 1.93                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:CQ:26:ARG:CG   | 16:CQ:39:ARG:HB2  | 2.52                     | 0.40              |
| 16:CQ:10:ARG:HA   | 16:CQ:57:VAL:HA   | 2.03                     | 0.40              |
| 51:D1:29:LYS:HE2  | 51:D1:31:GLU:OE2  | 2.21                     | 0.40              |
| 52:D2:31:LEU:CA   | 52:D2:34:ARG:HB2  | 2.44                     | 0.40              |
| 24:DA:1048:A:N6   | 24:DA:1111:A:C5   | 2.89                     | 0.40              |
| 24:DA:1060:U:H1'  | 24:DA:1062:G:OP2  | 2.21                     | 0.40              |
| 24:DA:1062:G:OP1  | 24:DA:1070:A:C4'  | 2.66                     | 0.40              |
| 24:DA:1085:A:H3'  | 24:DA:1086:A:C2   | 2.57                     | 0.40              |
| 24:DA:1210:G:P    | 24:DA:1212:G:H5'  | 2.62                     | 0.40              |
| 24:DA:1300:G:H5'' | 24:DA:1301:A:O5'  | 2.21                     | 0.40              |
| 24:DA:1351:C:H4'  | 24:DA:1572:A:O4'  | 2.22                     | 0.40              |
| 24:DA:1819:A:H1'  | 24:DA:1821:A:C5   | 2.56                     | 0.40              |
| 24:DA:183:C:C2'   | 24:DA:184:C:H5'   | 2.51                     | 0.40              |
| 24:DA:1951:U:C2   | 24:DA:1953:A:OP2  | 2.74                     | 0.40              |
| 24:DA:197:A:C6    | 24:DA:2430:A:N3   | 2.89                     | 0.40              |
| 24:DA:2024:G:C5   | 24:DA:2040:G:C2   | 3.10                     | 0.40              |
| 24:DA:2074:U:C4   | 24:DA:2075:U:O4   | 2.73                     | 0.40              |
| 24:DA:2289:G:H2'  | 24:DA:2290:G:H8   | 1.86                     | 0.40              |
| 24:DA:2298:A:N1   | 24:DA:2321:U:C5   | 2.90                     | 0.40              |
| 24:DA:2438:U:H5'' | 24:DA:2600:A:OP1  | 2.21                     | 0.40              |
| 24:DA:2453:A:O2'  | 24:DA:2572:A:H1'  | 2.21                     | 0.40              |
| 24:DA:246:C:C2'   | 24:DA:247:G:H5'   | 2.51                     | 0.40              |
| 24:DA:2558:C:C4   | 24:DA:2559:C:C4   | 3.09                     | 0.40              |
| 24:DA:2768:U:C4   | 24:DA:2769:U:C4   | 3.10                     | 0.40              |
| 24:DA:392:U:H2'   | 24:DA:393:C:C6    | 2.56                     | 0.40              |
| 24:DA:370:G:O6    | 24:DA:424:G:C6    | 2.75                     | 0.40              |
| 24:DA:539:G:C2    | 24:DA:540:C:C2    | 3.10                     | 0.40              |
| 24:DA:581:C:H2'   | 24:DA:582:A:O4'   | 2.21                     | 0.40              |
| 24:DA:86:G:C2     | 24:DA:87:U:C5     | 3.10                     | 0.40              |
| 24:DA:961:C:C4    | 24:DA:2031:A:C4   | 3.10                     | 0.40              |
| 24:DA:980:A:H2    | 24:DA:2038:G:C1'  | 2.35                     | 0.40              |
| 56:DB:102:G:C5    | 56:DB:103:U:C5    | 3.10                     | 0.40              |
| 56:DB:34:A:C5     | 56:DB:44:G:N7     | 2.89                     | 0.40              |
| 26:DC:198:GLU:O   | 26:DC:198:GLU:HG3 | 2.22                     | 0.40              |
| 26:DC:65:ASP:OD2  | 26:DC:68:ARG:HG2  | 2.22                     | 0.40              |
| 27:DD:78:GLY:C    | 27:DD:79:LEU:HD13 | 2.42                     | 0.40              |
| 30:DG:122:ALA:HB2 | 30:DG:132:LEU:HA  | 2.03                     | 0.40              |
| 33:DJ:125:TYR:HE2 | 33:DJ:132:HIS:CD2 | 2.40                     | 0.40              |
| 33:DJ:18:VAL:HG12 | 33:DJ:54:ILE:HD11 | 2.03                     | 0.40              |
| 33:DJ:37:ARG:NH2  | 33:DJ:39:LYS:NZ   | 2.69                     | 0.40              |
| 33:DJ:56:VAL:CG2  | 33:DJ:124:VAL:HA  | 2.51                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:DL:79:LEU:HD22 | 35:DL:115:GLU:O   | 2.21                     | 0.40              |
| 36:DM:108:VAL:HA  | 36:DM:109:PRO:HD3 | 1.85                     | 0.40              |
| 36:DM:76:LYS:HA   | 36:DM:77:PRO:HD3  | 1.87                     | 0.40              |
| 37:DN:14:SER:C    | 37:DN:16:HIS:N    | 2.75                     | 0.40              |
| 40:DQ:26:ALA:O    | 40:DQ:30:VAL:HB   | 2.22                     | 0.40              |
| 43:DT:12:ARG:HG3  | 48:DY:29:ARG:NH1  | 2.37                     | 0.40              |
| 43:DT:28:ASN:O    | 43:DT:29:THR:HG22 | 2.22                     | 0.40              |
| 45:DV:26:PHE:HA   | 45:DV:27:PRO:HD2  | 1.75                     | 0.40              |
| 46:DW:44:PHE:HE2  | 46:DW:76:ARG:HE   | 1.66                     | 0.40              |
| 47:DX:39:VAL:O    | 47:DX:41:SER:N    | 2.49                     | 0.40              |
| 47:DX:36:ARG:HA   | 47:DX:47:THR:HA   | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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 |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | AB    | 216/241 (90%) | 119 (55%) | 69 (32%) | 28 (13%) | 0           | 6  |
| 1   | CB    | 216/241 (90%) | 144 (67%) | 50 (23%) | 22 (10%) | 1           | 11 |
| 2   | AC    | 204/233 (88%) | 140 (69%) | 48 (24%) | 16 (8%)  | 1           | 17 |
| 2   | CC    | 204/233 (88%) | 136 (67%) | 52 (26%) | 16 (8%)  | 1           | 17 |
| 3   | AD    | 203/206 (98%) | 143 (70%) | 43 (21%) | 17 (8%)  | 1           | 14 |
| 3   | CD    | 203/206 (98%) | 136 (67%) | 46 (23%) | 21 (10%) | 0           | 10 |
| 4   | AE    | 148/167 (89%) | 105 (71%) | 27 (18%) | 16 (11%) | 0           | 9  |
| 4   | CE    | 148/167 (89%) | 100 (68%) | 34 (23%) | 14 (10%) | 1           | 12 |
| 5   | AF    | 98/135 (73%)  | 68 (69%)  | 22 (22%) | 8 (8%)   | 1           | 15 |
| 5   | CF    | 98/135 (73%)  | 65 (66%)  | 27 (28%) | 6 (6%)   | 2           | 23 |
| 6   | AG    | 149/179 (83%) | 103 (69%) | 36 (24%) | 10 (7%)  | 1           | 21 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 6   | CG    | 148/179 (83%) | 84 (57%)  | 44 (30%) | 20 (14%) | 0           | 5   |
| 7   | AH    | 127/130 (98%) | 90 (71%)  | 27 (21%) | 10 (8%)  | 1           | 16  |
| 7   | CH    | 127/130 (98%) | 88 (69%)  | 30 (24%) | 9 (7%)   | 1           | 20  |
| 8   | AI    | 125/130 (96%) | 81 (65%)  | 32 (26%) | 12 (10%) | 1           | 12  |
| 8   | CI    | 125/130 (96%) | 88 (70%)  | 33 (26%) | 4 (3%)   | 5           | 40  |
| 9   | AJ    | 96/103 (93%)  | 69 (72%)  | 16 (17%) | 11 (12%) | 0           | 8   |
| 9   | CJ    | 96/103 (93%)  | 62 (65%)  | 22 (23%) | 12 (12%) | 0           | 7   |
| 10  | AK    | 115/129 (89%) | 84 (73%)  | 22 (19%) | 9 (8%)   | 1           | 17  |
| 10  | CK    | 115/129 (89%) | 86 (75%)  | 19 (16%) | 10 (9%)  | 1           | 14  |
| 11  | AL    | 121/124 (98%) | 82 (68%)  | 27 (22%) | 12 (10%) | 1           | 11  |
| 11  | CL    | 121/124 (98%) | 86 (71%)  | 26 (22%) | 9 (7%)   | 1           | 18  |
| 12  | AM    | 112/118 (95%) | 89 (80%)  | 16 (14%) | 7 (6%)   | 1           | 23  |
| 12  | CM    | 111/118 (94%) | 71 (64%)  | 28 (25%) | 12 (11%) | 0           | 9   |
| 13  | AN    | 92/101 (91%)  | 63 (68%)  | 18 (20%) | 11 (12%) | 0           | 7   |
| 13  | CN    | 91/101 (90%)  | 62 (68%)  | 24 (26%) | 5 (6%)   | 2           | 26  |
| 14  | AO    | 86/89 (97%)   | 64 (74%)  | 20 (23%) | 2 (2%)   | 7           | 47  |
| 14  | CO    | 86/89 (97%)   | 67 (78%)  | 19 (22%) | 0        | 100         | 100 |
| 15  | AP    | 80/82 (98%)   | 52 (65%)  | 22 (28%) | 6 (8%)   | 1           | 18  |
| 15  | CP    | 78/82 (95%)   | 52 (67%)  | 20 (26%) | 6 (8%)   | 1           | 17  |
| 16  | AQ    | 78/84 (93%)   | 47 (60%)  | 20 (26%) | 11 (14%) | 0           | 5   |
| 16  | CQ    | 78/84 (93%)   | 57 (73%)  | 16 (20%) | 5 (6%)   | 1           | 23  |
| 17  | AR    | 53/75 (71%)   | 39 (74%)  | 11 (21%) | 3 (6%)   | 2           | 25  |
| 17  | CR    | 53/75 (71%)   | 39 (74%)  | 11 (21%) | 3 (6%)   | 2           | 25  |
| 18  | AS    | 77/92 (84%)   | 61 (79%)  | 13 (17%) | 3 (4%)   | 3           | 34  |
| 18  | CS    | 77/92 (84%)   | 55 (71%)  | 20 (26%) | 2 (3%)   | 6           | 44  |
| 19  | AT    | 83/87 (95%)   | 63 (76%)  | 14 (17%) | 6 (7%)   | 1           | 19  |
| 19  | CT    | 83/87 (95%)   | 59 (71%)  | 21 (25%) | 3 (4%)   | 4           | 37  |
| 20  | AU    | 49/71 (69%)   | 26 (53%)  | 16 (33%) | 7 (14%)  | 0           | 5   |
| 20  | CU    | 49/71 (69%)   | 23 (47%)  | 17 (35%) | 9 (18%)  | 0           | 2   |
| 26  | BC    | 269/273 (98%) | 192 (71%) | 48 (18%) | 29 (11%) | 0           | 9   |
| 26  | DC    | 269/273 (98%) | 169 (63%) | 73 (27%) | 27 (10%) | 1           | 11  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 27  | BD    | 207/209 (99%) | 141 (68%) | 35 (17%) | 31 (15%) | 0           | 4  |
| 27  | DD    | 207/209 (99%) | 129 (62%) | 48 (23%) | 30 (14%) | 0           | 5  |
| 28  | BE    | 199/201 (99%) | 138 (69%) | 41 (21%) | 20 (10%) | 1           | 11 |
| 28  | DE    | 199/201 (99%) | 129 (65%) | 49 (25%) | 21 (11%) | 0           | 9  |
| 29  | BF    | 175/179 (98%) | 133 (76%) | 26 (15%) | 16 (9%)  | 1           | 13 |
| 29  | DF    | 176/179 (98%) | 94 (53%)  | 43 (24%) | 39 (22%) | 0           | 1  |
| 30  | BG    | 174/177 (98%) | 114 (66%) | 34 (20%) | 26 (15%) | 0           | 4  |
| 30  | DG    | 174/177 (98%) | 109 (63%) | 36 (21%) | 29 (17%) | 0           | 4  |
| 31  | BH    | 147/149 (99%) | 63 (43%)  | 53 (36%) | 31 (21%) | 0           | 2  |
| 31  | DH    | 147/149 (99%) | 78 (53%)  | 48 (33%) | 21 (14%) | 0           | 5  |
| 32  | BI    | 139/142 (98%) | 84 (60%)  | 42 (30%) | 13 (9%)  | 1           | 12 |
| 32  | DI    | 139/142 (98%) | 81 (58%)  | 39 (28%) | 19 (14%) | 0           | 5  |
| 33  | BJ    | 140/142 (99%) | 100 (71%) | 22 (16%) | 18 (13%) | 0           | 6  |
| 33  | DJ    | 140/142 (99%) | 95 (68%)  | 31 (22%) | 14 (10%) | 1           | 11 |
| 34  | BK    | 120/123 (98%) | 86 (72%)  | 17 (14%) | 17 (14%) | 0           | 5  |
| 34  | DK    | 120/123 (98%) | 79 (66%)  | 22 (18%) | 19 (16%) | 0           | 4  |
| 35  | BL    | 141/144 (98%) | 106 (75%) | 23 (16%) | 12 (8%)  | 1           | 14 |
| 35  | DL    | 141/144 (98%) | 80 (57%)  | 42 (30%) | 19 (14%) | 0           | 5  |
| 36  | BM    | 134/136 (98%) | 95 (71%)  | 16 (12%) | 23 (17%) | 0           | 3  |
| 36  | DM    | 134/136 (98%) | 89 (66%)  | 32 (24%) | 13 (10%) | 1           | 12 |
| 37  | BN    | 118/127 (93%) | 85 (72%)  | 23 (20%) | 10 (8%)  | 1           | 14 |
| 37  | DN    | 118/127 (93%) | 73 (62%)  | 32 (27%) | 13 (11%) | 0           | 9  |
| 38  | BO    | 114/117 (97%) | 84 (74%)  | 20 (18%) | 10 (9%)  | 1           | 14 |
| 38  | DO    | 114/117 (97%) | 80 (70%)  | 28 (25%) | 6 (5%)   | 2           | 26 |
| 39  | BP    | 112/115 (97%) | 74 (66%)  | 23 (20%) | 15 (13%) | 0           | 5  |
| 39  | DP    | 112/115 (97%) | 67 (60%)  | 30 (27%) | 15 (13%) | 0           | 5  |
| 40  | BQ    | 115/118 (98%) | 85 (74%)  | 23 (20%) | 7 (6%)   | 2           | 23 |
| 40  | DQ    | 115/118 (98%) | 85 (74%)  | 22 (19%) | 8 (7%)   | 1           | 20 |
| 41  | BR    | 101/103 (98%) | 75 (74%)  | 14 (14%) | 12 (12%) | 0           | 7  |
| 41  | DR    | 101/103 (98%) | 71 (70%)  | 20 (20%) | 10 (10%) | 1           | 11 |
| 42  | BS    | 108/110 (98%) | 81 (75%)  | 20 (18%) | 7 (6%)   | 1           | 22 |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 42  | DS    | 108/110 (98%)     | 80 (74%)   | 18 (17%)   | 10 (9%)    | 1           | 13 |
| 43  | BT    | 91/100 (91%)      | 55 (60%)   | 20 (22%)   | 16 (18%)   | 0           | 3  |
| 43  | DT    | 91/100 (91%)      | 47 (52%)   | 30 (33%)   | 14 (15%)   | 0           | 4  |
| 44  | BU    | 100/104 (96%)     | 68 (68%)   | 16 (16%)   | 16 (16%)   | 0           | 4  |
| 44  | DU    | 100/104 (96%)     | 49 (49%)   | 29 (29%)   | 22 (22%)   | 0           | 1  |
| 45  | BV    | 92/94 (98%)       | 76 (83%)   | 15 (16%)   | 1 (1%)     | 17          | 61 |
| 45  | DV    | 92/94 (98%)       | 59 (64%)   | 25 (27%)   | 8 (9%)     | 1           | 14 |
| 46  | BW    | 77/85 (91%)       | 32 (42%)   | 18 (23%)   | 27 (35%)   | 0           | 0  |
| 46  | DW    | 77/85 (91%)       | 34 (44%)   | 25 (32%)   | 18 (23%)   | 0           | 1  |
| 47  | BX    | 75/78 (96%)       | 58 (77%)   | 12 (16%)   | 5 (7%)     | 1           | 21 |
| 47  | DX    | 75/78 (96%)       | 49 (65%)   | 19 (25%)   | 7 (9%)     | 1           | 13 |
| 48  | BY    | 61/63 (97%)       | 39 (64%)   | 15 (25%)   | 7 (12%)    | 0           | 8  |
| 48  | DY    | 61/63 (97%)       | 45 (74%)   | 11 (18%)   | 5 (8%)     | 1           | 15 |
| 49  | BZ    | 56/59 (95%)       | 43 (77%)   | 10 (18%)   | 3 (5%)     | 2           | 26 |
| 49  | DZ    | 56/59 (95%)       | 35 (62%)   | 14 (25%)   | 7 (12%)    | 0           | 7  |
| 50  | B0    | 54/57 (95%)       | 39 (72%)   | 8 (15%)    | 7 (13%)    | 0           | 6  |
| 50  | D0    | 54/57 (95%)       | 39 (72%)   | 8 (15%)    | 7 (13%)    | 0           | 6  |
| 51  | B1    | 48/55 (87%)       | 32 (67%)   | 9 (19%)    | 7 (15%)    | 0           | 5  |
| 51  | D1    | 48/55 (87%)       | 37 (77%)   | 7 (15%)    | 4 (8%)     | 1           | 15 |
| 52  | B2    | 44/46 (96%)       | 36 (82%)   | 6 (14%)    | 2 (4%)     | 3           | 30 |
| 52  | D2    | 44/46 (96%)       | 30 (68%)   | 9 (20%)    | 5 (11%)    | 0           | 8  |
| 53  | B3    | 62/65 (95%)       | 50 (81%)   | 10 (16%)   | 2 (3%)     | 5           | 40 |
| 53  | D3    | 62/65 (95%)       | 42 (68%)   | 15 (24%)   | 5 (8%)     | 1           | 16 |
| 54  | B4    | 36/38 (95%)       | 27 (75%)   | 6 (17%)    | 3 (8%)     | 1           | 15 |
| 54  | D4    | 36/38 (95%)       | 22 (61%)   | 8 (22%)    | 6 (17%)    | 0           | 4  |
| All | All   | 11238/11970 (94%) | 7515 (67%) | 2516 (22%) | 1207 (11%) | 0           | 9  |

All (1207) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AB    | 20  | ARG  |
| 1   | AB    | 22  | TRP  |
| 1   | AB    | 37  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AB    | 71  | THR  |
| 1   | AB    | 125 | PHE  |
| 1   | AB    | 127 | LYS  |
| 1   | AB    | 200 | PRO  |
| 2   | AC    | 11  | LEU  |
| 2   | AC    | 16  | PRO  |
| 2   | AC    | 100 | ILE  |
| 2   | AC    | 145 | ALA  |
| 3   | AD    | 22  | SER  |
| 3   | AD    | 28  | ASP  |
| 3   | AD    | 124 | VAL  |
| 3   | AD    | 192 | ALA  |
| 4   | AE    | 110 | MET  |
| 4   | AE    | 121 | ASN  |
| 5   | AF    | 86  | ARG  |
| 6   | AG    | 145 | GLU  |
| 7   | AH    | 66  | GLN  |
| 8   | AI    | 40  | ARG  |
| 8   | AI    | 43  | ALA  |
| 8   | AI    | 71  | ILE  |
| 9   | AJ    | 57  | VAL  |
| 9   | AJ    | 61  | ALA  |
| 10  | AK    | 13  | LYS  |
| 10  | AK    | 123 | PRO  |
| 10  | AK    | 125 | LYS  |
| 10  | AK    | 126 | ARG  |
| 11  | AL    | 23  | LEU  |
| 11  | AL    | 33  | CYS  |
| 11  | AL    | 73  | LEU  |
| 11  | AL    | 75  | GLU  |
| 12  | AM    | 46  | GLU  |
| 13  | AN    | 33  | VAL  |
| 13  | AN    | 51  | PRO  |
| 13  | AN    | 61  | ASN  |
| 16  | AQ    | 12  | VAL  |
| 16  | AQ    | 17  | GLU  |
| 16  | AQ    | 50  | ASN  |
| 16  | AQ    | 52  | CYS  |
| 16  | AQ    | 70  | LYS  |
| 17  | AR    | 47  | ARG  |
| 18  | AS    | 48  | ILE  |
| 19  | AT    | 67  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | AU    | 8   | ASN  |
| 20  | AU    | 34  | ARG  |
| 20  | AU    | 36  | PHE  |
| 26  | BC    | 35  | LYS  |
| 26  | BC    | 77  | VAL  |
| 26  | BC    | 104 | LEU  |
| 26  | BC    | 106 | PRO  |
| 26  | BC    | 110 | LYS  |
| 26  | BC    | 120 | ASP  |
| 26  | BC    | 121 | ALA  |
| 26  | BC    | 196 | ASN  |
| 27  | BD    | 43  | ASP  |
| 27  | BD    | 54  | ALA  |
| 27  | BD    | 73  | VAL  |
| 27  | BD    | 99  | GLU  |
| 27  | BD    | 103 | ASP  |
| 27  | BD    | 104 | VAL  |
| 27  | BD    | 119 | ALA  |
| 27  | BD    | 122 | VAL  |
| 27  | BD    | 169 | ARG  |
| 27  | BD    | 192 | ALA  |
| 28  | BE    | 6   | LYS  |
| 28  | BE    | 8   | ALA  |
| 28  | BE    | 46  | GLN  |
| 28  | BE    | 153 | LEU  |
| 28  | BE    | 175 | ILE  |
| 29  | BF    | 8   | LYS  |
| 29  | BF    | 111 | ARG  |
| 29  | BF    | 134 | GLN  |
| 30  | BG    | 7   | PRO  |
| 30  | BG    | 8   | VAL  |
| 30  | BG    | 9   | VAL  |
| 30  | BG    | 33  | THR  |
| 30  | BG    | 53  | PRO  |
| 30  | BG    | 84  | LYS  |
| 30  | BG    | 94  | ARG  |
| 30  | BG    | 118 | ALA  |
| 30  | BG    | 170 | THR  |
| 31  | BH    | 3   | VAL  |
| 31  | BH    | 8   | LYS  |
| 31  | BH    | 9   | VAL  |
| 31  | BH    | 10  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | BH    | 14  | SER  |
| 31  | BH    | 28  | ASN  |
| 31  | BH    | 30  | LEU  |
| 31  | BH    | 31  | VAL  |
| 31  | BH    | 32  | PRO  |
| 31  | BH    | 33  | GLN  |
| 31  | BH    | 35  | LYS  |
| 31  | BH    | 121 | VAL  |
| 32  | BI    | 65  | SER  |
| 32  | BI    | 92  | PRO  |
| 33  | BJ    | 2   | LYS  |
| 33  | BJ    | 4   | PHE  |
| 33  | BJ    | 14  | ASP  |
| 33  | BJ    | 21  | THR  |
| 33  | BJ    | 44  | TYR  |
| 33  | BJ    | 45  | THR  |
| 33  | BJ    | 73  | VAL  |
| 33  | BJ    | 81  | ILE  |
| 33  | BJ    | 111 | LYS  |
| 34  | BK    | 13  | ASN  |
| 34  | BK    | 16  | ALA  |
| 34  | BK    | 35  | VAL  |
| 34  | BK    | 49  | ARG  |
| 34  | BK    | 71  | ARG  |
| 34  | BK    | 72  | PRO  |
| 34  | BK    | 118 | LEU  |
| 34  | BK    | 119 | ALA  |
| 35  | BL    | 15  | ALA  |
| 35  | BL    | 66  | PHE  |
| 35  | BL    | 81  | ASP  |
| 35  | BL    | 88  | GLY  |
| 36  | BM    | 2   | LEU  |
| 36  | BM    | 13  | HIS  |
| 36  | BM    | 15  | GLY  |
| 36  | BM    | 35  | ALA  |
| 36  | BM    | 36  | VAL  |
| 36  | BM    | 54  | THR  |
| 36  | BM    | 55  | ARG  |
| 36  | BM    | 60  | GLN  |
| 36  | BM    | 69  | PRO  |
| 36  | BM    | 77  | PRO  |
| 37  | BN    | 2   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | BN    | 15  | SER  |
| 38  | BO    | 3   | LYS  |
| 38  | BO    | 68  | LYS  |
| 39  | BP    | 25  | VAL  |
| 39  | BP    | 50  | ARG  |
| 39  | BP    | 103 | THR  |
| 39  | BP    | 105 | LYS  |
| 40  | BQ    | 87  | VAL  |
| 41  | BR    | 55  | ASP  |
| 41  | BR    | 91  | GLN  |
| 42  | BS    | 3   | THR  |
| 42  | BS    | 14  | ALA  |
| 42  | BS    | 19  | LEU  |
| 43  | BT    | 16  | VAL  |
| 43  | BT    | 27  | SER  |
| 43  | BT    | 29  | THR  |
| 43  | BT    | 49  | LYS  |
| 43  | BT    | 69  | ARG  |
| 43  | BT    | 88  | LYS  |
| 44  | BU    | 6   | ARG  |
| 44  | BU    | 18  | LYS  |
| 44  | BU    | 51  | LEU  |
| 44  | BU    | 88  | ASP  |
| 44  | BU    | 98  | ASN  |
| 45  | BV    | 69  | GLU  |
| 46  | BW    | 9   | THR  |
| 46  | BW    | 23  | LYS  |
| 46  | BW    | 30  | VAL  |
| 46  | BW    | 36  | ILE  |
| 46  | BW    | 51  | GLY  |
| 47  | BX    | 34  | SER  |
| 48  | BY    | 22  | LEU  |
| 48  | BY    | 23  | ARG  |
| 49  | BZ    | 3   | THR  |
| 50  | B0    | 35  | GLU  |
| 50  | B0    | 54  | ILE  |
| 51  | B1    | 4   | ILE  |
| 52  | B2    | 44  | VAL  |
| 53  | B3    | 22  | LYS  |
| 53  | B3    | 31  | ILE  |
| 54  | B4    | 4   | ARG  |
| 1   | CB    | 80  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CB    | 129 | THR  |
| 1   | CB    | 150 | ILE  |
| 1   | CB    | 188 | THR  |
| 2   | CC    | 87  | ARG  |
| 2   | CC    | 112 | ALA  |
| 2   | CC    | 130 | ARG  |
| 3   | CD    | 24  | VAL  |
| 3   | CD    | 25  | ARG  |
| 3   | CD    | 33  | ILE  |
| 3   | CD    | 35  | GLN  |
| 3   | CD    | 80  | ARG  |
| 3   | CD    | 104 | MET  |
| 3   | CD    | 181 | PHE  |
| 3   | CD    | 186 | GLU  |
| 4   | CE    | 89  | THR  |
| 4   | CE    | 108 | GLY  |
| 5   | CF    | 68  | GLN  |
| 5   | CF    | 98  | GLU  |
| 6   | CG    | 29  | LEU  |
| 6   | CG    | 30  | MET  |
| 6   | CG    | 31  | VAL  |
| 6   | CG    | 62  | GLU  |
| 8   | CI    | 71  | ILE  |
| 8   | CI    | 122 | ARG  |
| 9   | CJ    | 46  | LYS  |
| 9   | CJ    | 93  | ALA  |
| 10  | CK    | 90  | PRO  |
| 10  | CK    | 125 | LYS  |
| 10  | CK    | 126 | ARG  |
| 11  | CL    | 34  | THR  |
| 11  | CL    | 43  | LYS  |
| 11  | CL    | 92  | VAL  |
| 12  | CM    | 14  | ALA  |
| 12  | CM    | 46  | GLU  |
| 13  | CN    | 95  | LEU  |
| 20  | CU    | 4   | LYS  |
| 20  | CU    | 15  | LEU  |
| 20  | CU    | 23  | GLU  |
| 20  | CU    | 31  | VAL  |
| 20  | CU    | 34  | ARG  |
| 26  | DC    | 9   | SER  |
| 26  | DC    | 28  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | DC    | 186 | ASP  |
| 26  | DC    | 269 | ARG  |
| 27  | DD    | 11  | MET  |
| 27  | DD    | 14  | ILE  |
| 27  | DD    | 31  | ALA  |
| 27  | DD    | 74  | GLU  |
| 27  | DD    | 77  | ARG  |
| 27  | DD    | 136 | ASN  |
| 27  | DD    | 150 | GLN  |
| 27  | DD    | 164 | GLN  |
| 27  | DD    | 170 | VAL  |
| 27  | DD    | 175 | LEU  |
| 27  | DD    | 194 | PRO  |
| 28  | DE    | 41  | GLN  |
| 28  | DE    | 55  | SER  |
| 28  | DE    | 99  | LYS  |
| 28  | DE    | 116 | ASP  |
| 29  | DF    | 10  | GLU  |
| 29  | DF    | 12  | VAL  |
| 29  | DF    | 32  | LYS  |
| 29  | DF    | 36  | ASN  |
| 29  | DF    | 42  | ALA  |
| 29  | DF    | 112 | ASP  |
| 29  | DF    | 114 | ARG  |
| 29  | DF    | 120 | SER  |
| 29  | DF    | 122 | ASP  |
| 29  | DF    | 137 | PHE  |
| 29  | DF    | 138 | PRO  |
| 30  | DG    | 49  | LEU  |
| 30  | DG    | 95  | ALA  |
| 30  | DG    | 149 | ALA  |
| 30  | DG    | 164 | ALA  |
| 30  | DG    | 165 | ASP  |
| 31  | DH    | 3   | VAL  |
| 31  | DH    | 9   | VAL  |
| 31  | DH    | 10  | ALA  |
| 31  | DH    | 49  | ALA  |
| 31  | DH    | 72  | ILE  |
| 31  | DH    | 76  | GLU  |
| 31  | DH    | 98  | ASP  |
| 31  | DH    | 102 | ALA  |
| 32  | DI    | 22  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | DI    | 23  | VAL  |
| 32  | DI    | 29  | GLN  |
| 32  | DI    | 52  | LEU  |
| 32  | DI    | 58  | ILE  |
| 32  | DI    | 69  | VAL  |
| 33  | DJ    | 45  | THR  |
| 33  | DJ    | 81  | ILE  |
| 33  | DJ    | 87  | ALA  |
| 33  | DJ    | 95  | ARG  |
| 34  | DK    | 18  | ARG  |
| 34  | DK    | 35  | VAL  |
| 34  | DK    | 49  | ARG  |
| 34  | DK    | 71  | ARG  |
| 34  | DK    | 72  | PRO  |
| 34  | DK    | 93  | GLN  |
| 34  | DK    | 110 | GLU  |
| 34  | DK    | 120 | PRO  |
| 35  | DL    | 4   | ASN  |
| 35  | DL    | 41  | ARG  |
| 35  | DL    | 82  | LEU  |
| 35  | DL    | 85  | VAL  |
| 35  | DL    | 89  | VAL  |
| 35  | DL    | 101 | ILE  |
| 35  | DL    | 111 | ILE  |
| 36  | DM    | 2   | LEU  |
| 36  | DM    | 72  | PRO  |
| 36  | DM    | 77  | PRO  |
| 36  | DM    | 135 | VAL  |
| 37  | DN    | 30  | ARG  |
| 37  | DN    | 63  | ARG  |
| 37  | DN    | 104 | ALA  |
| 38  | DO    | 90  | VAL  |
| 39  | DP    | 25  | VAL  |
| 39  | DP    | 50  | ARG  |
| 39  | DP    | 83  | ILE  |
| 39  | DP    | 109 | ILE  |
| 39  | DP    | 112 | ARG  |
| 42  | DS    | 28  | LYS  |
| 42  | DS    | 33  | LEU  |
| 42  | DS    | 72  | THR  |
| 43  | DT    | 14  | PRO  |
| 43  | DT    | 15  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | DT    | 20  | ALA  |
| 43  | DT    | 29  | THR  |
| 43  | DT    | 56  | GLU  |
| 43  | DT    | 88  | LYS  |
| 44  | DU    | 65  | GLN  |
| 44  | DU    | 82  | VAL  |
| 44  | DU    | 92  | VAL  |
| 44  | DU    | 95  | PHE  |
| 44  | DU    | 96  | LYS  |
| 44  | DU    | 97  | SER  |
| 45  | DV    | 56  | PHE  |
| 45  | DV    | 58  | SER  |
| 46  | DW    | 9   | THR  |
| 46  | DW    | 34  | SER  |
| 46  | DW    | 35  | ILE  |
| 47  | DX    | 2   | ARG  |
| 49  | DZ    | 13  | ILE  |
| 49  | DZ    | 30  | ARG  |
| 50  | D0    | 54  | ILE  |
| 53  | D3    | 29  | ARG  |
| 54  | D4    | 8   | LYS  |
| 54  | D4    | 20  | ASP  |
| 1   | AB    | 18  | GLN  |
| 1   | AB    | 40  | ILE  |
| 1   | AB    | 52  | ALA  |
| 1   | AB    | 72  | LYS  |
| 1   | AB    | 119 | GLN  |
| 1   | AB    | 120 | SER  |
| 1   | AB    | 187 | ASP  |
| 1   | AB    | 189 | ASN  |
| 2   | AC    | 35  | ASP  |
| 2   | AC    | 60  | ALA  |
| 2   | AC    | 99  | GLN  |
| 2   | AC    | 167 | TYR  |
| 3   | AD    | 32  | LYS  |
| 3   | AD    | 150 | LYS  |
| 3   | AD    | 174 | ALA  |
| 3   | AD    | 197 | HIS  |
| 4   | AE    | 77  | ASN  |
| 4   | AE    | 97  | PRO  |
| 4   | AE    | 137 | ARG  |
| 5   | AF    | 54  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | AG    | 16  | LYS  |
| 6   | AG    | 78  | ARG  |
| 7   | AH    | 77  | VAL  |
| 7   | AH    | 78  | SER  |
| 7   | AH    | 87  | ARG  |
| 8   | AI    | 8   | THR  |
| 8   | AI    | 128 | LYS  |
| 9   | AJ    | 75  | ASP  |
| 9   | AJ    | 92  | LEU  |
| 11  | AL    | 24  | GLU  |
| 12  | AM    | 3   | ILE  |
| 12  | AM    | 6   | ILE  |
| 13  | AN    | 28  | ALA  |
| 13  | AN    | 52  | ARG  |
| 15  | AP    | 10  | GLY  |
| 15  | AP    | 52  | LEU  |
| 15  | AP    | 80  | LYS  |
| 16  | AQ    | 11  | VAL  |
| 18  | AS    | 61  | VAL  |
| 20  | AU    | 12  | ASP  |
| 20  | AU    | 23  | GLU  |
| 26  | BC    | 9   | SER  |
| 26  | BC    | 22  | GLU  |
| 26  | BC    | 43  | ASN  |
| 26  | BC    | 57  | HIS  |
| 26  | BC    | 140 | VAL  |
| 26  | BC    | 141 | HIS  |
| 26  | BC    | 239 | PHE  |
| 27  | BD    | 72  | GLY  |
| 27  | BD    | 77  | ARG  |
| 27  | BD    | 92  | VAL  |
| 27  | BD    | 94  | GLN  |
| 27  | BD    | 107 | VAL  |
| 27  | BD    | 144 | GLY  |
| 27  | BD    | 183 | GLU  |
| 27  | BD    | 191 | GLY  |
| 28  | BE    | 11  | ALA  |
| 28  | BE    | 43  | THR  |
| 28  | BE    | 78  | TRP  |
| 29  | BF    | 113 | PHE  |
| 29  | BF    | 149 | ARG  |
| 29  | BF    | 175 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | BG    | 28  | LYS  |
| 30  | BG    | 30  | GLY  |
| 30  | BG    | 31  | GLU  |
| 30  | BG    | 44  | HIS  |
| 30  | BG    | 45  | ALA  |
| 30  | BG    | 60  | GLY  |
| 30  | BG    | 164 | ALA  |
| 30  | BG    | 168 | VAL  |
| 31  | BH    | 25  | TYR  |
| 31  | BH    | 34  | GLY  |
| 31  | BH    | 54  | LEU  |
| 31  | BH    | 81  | ALA  |
| 31  | BH    | 83  | LYS  |
| 31  | BH    | 101 | ASP  |
| 31  | BH    | 131 | SER  |
| 32  | BI    | 30  | GLN  |
| 32  | BI    | 59  | THR  |
| 33  | BJ    | 13  | ARG  |
| 33  | BJ    | 39  | LYS  |
| 33  | BJ    | 41  | LYS  |
| 34  | BK    | 3   | GLN  |
| 34  | BK    | 93  | GLN  |
| 34  | BK    | 108 | ARG  |
| 35  | BL    | 65  | GLY  |
| 35  | BL    | 111 | ILE  |
| 36  | BM    | 14  | LYS  |
| 36  | BM    | 56  | ALA  |
| 37  | BN    | 3   | HIS  |
| 37  | BN    | 101 | GLY  |
| 37  | BN    | 117 | ASP  |
| 37  | BN    | 118 | ARG  |
| 38  | BO    | 22  | GLY  |
| 38  | BO    | 95  | SER  |
| 38  | BO    | 100 | HIS  |
| 38  | BO    | 112 | GLU  |
| 39  | BP    | 2   | ASN  |
| 39  | BP    | 4   | ILE  |
| 39  | BP    | 15  | ASP  |
| 39  | BP    | 65  | ASN  |
| 39  | BP    | 93  | LYS  |
| 40  | BQ    | 86  | SER  |
| 42  | BS    | 64  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | BT    | 35  | ALA  |
| 43  | BT    | 68  | LYS  |
| 43  | BT    | 70  | HIS  |
| 43  | BT    | 84  | TYR  |
| 43  | BT    | 86  | THR  |
| 44  | BU    | 16  | LYS  |
| 44  | BU    | 87  | GLU  |
| 46  | BW    | 15  | SER  |
| 46  | BW    | 17  | ALA  |
| 46  | BW    | 18  | LYS  |
| 46  | BW    | 25  | PHE  |
| 46  | BW    | 26  | GLY  |
| 46  | BW    | 27  | GLY  |
| 46  | BW    | 33  | GLY  |
| 46  | BW    | 47  | GLY  |
| 46  | BW    | 50  | VAL  |
| 47  | BX    | 18  | SER  |
| 47  | BX    | 53  | LYS  |
| 48  | BY    | 24  | GLU  |
| 48  | BY    | 37  | LEU  |
| 48  | BY    | 44  | LYS  |
| 50  | B0    | 34  | GLY  |
| 50  | B0    | 51  | ARG  |
| 51  | B1    | 51  | ALA  |
| 54  | B4    | 16  | ILE  |
| 1   | CB    | 10  | LYS  |
| 1   | CB    | 22  | TRP  |
| 1   | CB    | 85  | SER  |
| 1   | CB    | 163 | ILE  |
| 1   | CB    | 203 | ASP  |
| 1   | CB    | 218 | ALA  |
| 2   | CC    | 27  | GLU  |
| 2   | CC    | 47  | ALA  |
| 2   | CC    | 59  | PRO  |
| 2   | CC    | 188 | ALA  |
| 3   | CD    | 27  | ILE  |
| 3   | CD    | 69  | ARG  |
| 3   | CD    | 107 | GLY  |
| 4   | CE    | 31  | SER  |
| 4   | CE    | 56  | PRO  |
| 4   | CE    | 75  | LEU  |
| 4   | CE    | 81  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | CG    | 9   | ARG  |
| 6   | CG    | 10  | LYS  |
| 6   | CG    | 36  | SER  |
| 6   | CG    | 52  | ARG  |
| 6   | CG    | 95  | ARG  |
| 6   | CG    | 107 | ALA  |
| 6   | CG    | 113 | LYS  |
| 6   | CG    | 133 | ALA  |
| 7   | CH    | 29  | SER  |
| 8   | CI    | 58  | GLU  |
| 9   | CJ    | 57  | VAL  |
| 9   | CJ    | 87  | LEU  |
| 10  | CK    | 40  | ALA  |
| 10  | CK    | 70  | ALA  |
| 11  | CL    | 88  | ASP  |
| 12  | CM    | 4   | ALA  |
| 12  | CM    | 65  | GLU  |
| 12  | CM    | 76  | ILE  |
| 13  | CN    | 52  | ARG  |
| 15  | CP    | 47  | GLU  |
| 15  | CP    | 53  | ASP  |
| 15  | CP    | 54  | LEU  |
| 15  | CP    | 78  | VAL  |
| 16  | CQ    | 78  | VAL  |
| 17  | CR    | 69  | TYR  |
| 18  | CS    | 46  | LEU  |
| 19  | CT    | 43  | LYS  |
| 19  | CT    | 82  | ILE  |
| 20  | CU    | 7   | GLU  |
| 20  | CU    | 8   | ASN  |
| 26  | DC    | 3   | VAL  |
| 26  | DC    | 37  | SER  |
| 26  | DC    | 45  | ASN  |
| 26  | DC    | 94  | LEU  |
| 26  | DC    | 121 | ALA  |
| 26  | DC    | 140 | VAL  |
| 26  | DC    | 195 | GLY  |
| 26  | DC    | 232 | GLY  |
| 26  | DC    | 239 | PHE  |
| 27  | DD    | 93  | GLY  |
| 27  | DD    | 102 | ALA  |
| 27  | DD    | 107 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | DD    | 112 | THR  |
| 27  | DD    | 118 | PHE  |
| 27  | DD    | 119 | ALA  |
| 27  | DD    | 120 | GLY  |
| 28  | DE    | 62  | GLN  |
| 28  | DE    | 79  | ARG  |
| 28  | DE    | 80  | SER  |
| 28  | DE    | 127 | GLU  |
| 28  | DE    | 153 | LEU  |
| 29  | DF    | 8   | LYS  |
| 29  | DF    | 37  | MET  |
| 29  | DF    | 43  | ILE  |
| 29  | DF    | 67  | THR  |
| 29  | DF    | 76  | PHE  |
| 29  | DF    | 113 | PHE  |
| 29  | DF    | 133 | GLU  |
| 29  | DF    | 145 | VAL  |
| 29  | DF    | 148 | VAL  |
| 30  | DG    | 59  | ASP  |
| 30  | DG    | 80  | GLU  |
| 30  | DG    | 83  | THR  |
| 30  | DG    | 85  | LYS  |
| 30  | DG    | 86  | LEU  |
| 30  | DG    | 93  | TYR  |
| 30  | DG    | 150 | TYR  |
| 31  | DH    | 61  | VAL  |
| 31  | DH    | 66  | ASN  |
| 31  | DH    | 86  | ASP  |
| 31  | DH    | 97  | ARG  |
| 32  | DI    | 9   | LYS  |
| 32  | DI    | 30  | GLN  |
| 32  | DI    | 51  | GLY  |
| 32  | DI    | 62  | ALA  |
| 32  | DI    | 140 | GLU  |
| 33  | DJ    | 112 | GLY  |
| 34  | DK    | 16  | ALA  |
| 34  | DK    | 46  | ALA  |
| 34  | DK    | 104 | THR  |
| 35  | DL    | 29  | LYS  |
| 36  | DM    | 14  | LYS  |
| 36  | DM    | 73  | ILE  |
| 37  | DN    | 8   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | DN    | 105 | GLY  |
| 38  | DO    | 3   | LYS  |
| 38  | DO    | 8   | ILE  |
| 38  | DO    | 72  | ALA  |
| 39  | DP    | 32  | VAL  |
| 39  | DP    | 33  | GLU  |
| 39  | DP    | 85  | VAL  |
| 39  | DP    | 108 | ARG  |
| 40  | DQ    | 23  | TYR  |
| 40  | DQ    | 86  | SER  |
| 40  | DQ    | 88  | GLU  |
| 40  | DQ    | 91  | ARG  |
| 41  | DR    | 3   | ALA  |
| 41  | DR    | 40  | MET  |
| 42  | DS    | 3   | THR  |
| 42  | DS    | 40  | ASN  |
| 43  | DT    | 39  | THR  |
| 43  | DT    | 68  | LYS  |
| 44  | DU    | 4   | ILE  |
| 44  | DU    | 54  | PRO  |
| 44  | DU    | 87  | GLU  |
| 44  | DU    | 88  | ASP  |
| 44  | DU    | 89  | GLY  |
| 45  | DV    | 33  | GLY  |
| 45  | DV    | 55  | GLU  |
| 46  | DW    | 18  | LYS  |
| 46  | DW    | 24  | ARG  |
| 46  | DW    | 33  | GLY  |
| 46  | DW    | 39  | GLN  |
| 46  | DW    | 53  | GLY  |
| 46  | DW    | 57  | THR  |
| 46  | DW    | 71  | LYS  |
| 46  | DW    | 83  | ALA  |
| 47  | DX    | 41  | SER  |
| 47  | DX    | 49  | ARG  |
| 47  | DX    | 63  | ILE  |
| 48  | DY    | 9   | LYS  |
| 48  | DY    | 22  | LEU  |
| 48  | DY    | 37  | LEU  |
| 49  | DZ    | 4   | ILE  |
| 50  | D0    | 21  | LEU  |
| 50  | D0    | 55  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | D1    | 4   | ILE  |
| 51  | D1    | 36  | LYS  |
| 52  | D2    | 24  | THR  |
| 52  | D2    | 40  | ALA  |
| 53  | D3    | 3   | ILE  |
| 53  | D3    | 6   | VAL  |
| 53  | D3    | 51  | LYS  |
| 54  | D4    | 4   | ARG  |
| 1   | AB    | 63  | LYS  |
| 1   | AB    | 94  | ARG  |
| 1   | AB    | 95  | TRP  |
| 1   | AB    | 105 | THR  |
| 1   | AB    | 128 | LEU  |
| 1   | AB    | 147 | LEU  |
| 2   | AC    | 26  | LYS  |
| 2   | AC    | 192 | TYR  |
| 3   | AD    | 125 | ASN  |
| 3   | AD    | 155 | LYS  |
| 3   | AD    | 166 | LYS  |
| 3   | AD    | 172 | VAL  |
| 4   | AE    | 50  | GLY  |
| 4   | AE    | 56  | PRO  |
| 4   | AE    | 57  | ALA  |
| 4   | AE    | 79  | THR  |
| 4   | AE    | 124 | ALA  |
| 5   | AF    | 39  | LEU  |
| 6   | AG    | 95  | ARG  |
| 6   | AG    | 112 | ASP  |
| 6   | AG    | 129 | ASN  |
| 8   | AI    | 9   | GLY  |
| 8   | AI    | 13  | SER  |
| 8   | AI    | 120 | ALA  |
| 9   | AJ    | 36  | VAL  |
| 9   | AJ    | 74  | VAL  |
| 9   | AJ    | 101 | SER  |
| 10  | AK    | 105 | ARG  |
| 11  | AL    | 22  | ALA  |
| 11  | AL    | 43  | LYS  |
| 11  | AL    | 87  | LYS  |
| 12  | AM    | 4   | ALA  |
| 12  | AM    | 23  | GLY  |
| 12  | AM    | 70  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | AM    | 84  | CYS  |
| 13  | AN    | 27  | LYS  |
| 15  | AP    | 49  | GLY  |
| 16  | AQ    | 5   | ARG  |
| 17  | AR    | 54  | LEU  |
| 18  | AS    | 27  | LYS  |
| 19  | AT    | 4   | LYS  |
| 19  | AT    | 5   | SER  |
| 19  | AT    | 40  | ALA  |
| 26  | BC    | 8   | THR  |
| 26  | BC    | 94  | LEU  |
| 26  | BC    | 105 | ALA  |
| 26  | BC    | 157 | ALA  |
| 26  | BC    | 189 | ALA  |
| 26  | BC    | 237 | ARG  |
| 26  | BC    | 243 | PRO  |
| 27  | BD    | 17  | GLU  |
| 27  | BD    | 106 | LYS  |
| 27  | BD    | 118 | PHE  |
| 27  | BD    | 184 | ARG  |
| 27  | BD    | 190 | LYS  |
| 28  | BE    | 79  | ARG  |
| 28  | BE    | 80  | SER  |
| 29  | BF    | 11  | VAL  |
| 29  | BF    | 20  | ASN  |
| 29  | BF    | 133 | GLU  |
| 29  | BF    | 147 | ARG  |
| 29  | BF    | 174 | PHE  |
| 30  | BG    | 61  | TRP  |
| 31  | BH    | 40  | THR  |
| 31  | BH    | 106 | ALA  |
| 31  | BH    | 111 | ALA  |
| 32  | BI    | 105 | LEU  |
| 33  | BJ    | 65  | THR  |
| 33  | BJ    | 68  | LYS  |
| 34  | BK    | 17  | ARG  |
| 34  | BK    | 46  | ALA  |
| 34  | BK    | 50  | GLY  |
| 35  | BL    | 29  | LYS  |
| 35  | BL    | 30  | THR  |
| 36  | BM    | 59  | ARG  |
| 36  | BM    | 79  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | BM    | 81  | ARG  |
| 37  | BN    | 80  | PHE  |
| 38  | BO    | 58  | ILE  |
| 38  | BO    | 94  | ARG  |
| 38  | BO    | 113 | ALA  |
| 39  | BP    | 5   | LYS  |
| 39  | BP    | 20  | ARG  |
| 39  | BP    | 34  | GLY  |
| 39  | BP    | 51  | ASN  |
| 39  | BP    | 86  | LYS  |
| 40  | BQ    | 5   | ARG  |
| 40  | BQ    | 90  | ASP  |
| 41  | BR    | 31  | GLU  |
| 41  | BR    | 53  | PHE  |
| 42  | BS    | 18  | ARG  |
| 43  | BT    | 38  | ALA  |
| 43  | BT    | 39  | THR  |
| 44  | BU    | 38  | ILE  |
| 44  | BU    | 39  | ASN  |
| 44  | BU    | 74  | ALA  |
| 44  | BU    | 83  | GLY  |
| 44  | BU    | 92  | VAL  |
| 46  | BW    | 16  | GLU  |
| 46  | BW    | 29  | SER  |
| 46  | BW    | 34  | SER  |
| 46  | BW    | 74  | LYS  |
| 47  | BX    | 17  | ARG  |
| 47  | BX    | 20  | ALA  |
| 48  | BY    | 57  | LEU  |
| 49  | BZ    | 34  | THR  |
| 50  | B0    | 12  | ARG  |
| 51  | B1    | 18  | HIS  |
| 51  | B1    | 26  | LYS  |
| 51  | B1    | 43  | ARG  |
| 51  | B1    | 50  | GLU  |
| 1   | CB    | 17  | HIS  |
| 1   | CB    | 44  | LYS  |
| 1   | CB    | 81  | ASP  |
| 1   | CB    | 148 | GLY  |
| 1   | CB    | 149 | GLY  |
| 1   | CB    | 205 | ALA  |
| 3   | CD    | 29  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CD    | 47  | LEU  |
| 3   | CD    | 82  | LYS  |
| 3   | CD    | 166 | LYS  |
| 3   | CD    | 187 | ARG  |
| 3   | CD    | 192 | ALA  |
| 4   | CE    | 29  | ILE  |
| 4   | CE    | 51  | LYS  |
| 5   | CF    | 85  | ILE  |
| 5   | CF    | 99  | ALA  |
| 6   | CG    | 15  | PRO  |
| 6   | CG    | 17  | PHE  |
| 6   | CG    | 49  | LEU  |
| 6   | CG    | 75  | LYS  |
| 7   | CH    | 30  | LYS  |
| 7   | CH    | 78  | SER  |
| 7   | CH    | 98  | LEU  |
| 8   | CI    | 119 | LYS  |
| 9   | CJ    | 82  | LYS  |
| 10  | CK    | 120 | CYS  |
| 11  | CL    | 22  | ALA  |
| 11  | CL    | 121 | PRO  |
| 12  | CM    | 45  | SER  |
| 12  | CM    | 92  | ARG  |
| 13  | CN    | 99  | SER  |
| 15  | CP    | 28  | ARG  |
| 16  | CQ    | 29  | LYS  |
| 16  | CQ    | 81  | ALA  |
| 20  | CU    | 37  | TYR  |
| 26  | DC    | 36  | ASN  |
| 26  | DC    | 59  | GLN  |
| 26  | DC    | 69  | ASN  |
| 26  | DC    | 98  | GLY  |
| 26  | DC    | 141 | HIS  |
| 26  | DC    | 147 | PRO  |
| 26  | DC    | 237 | ARG  |
| 27  | DD    | 95  | SER  |
| 27  | DD    | 99  | GLU  |
| 27  | DD    | 162 | ALA  |
| 28  | DE    | 13  | THR  |
| 28  | DE    | 63  | LYS  |
| 28  | DE    | 165 | HIS  |
| 28  | DE    | 187 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | DE    | 188 | MET  |
| 29  | DF    | 41  | GLU  |
| 29  | DF    | 70  | ARG  |
| 29  | DF    | 116 | LEU  |
| 30  | DG    | 9   | VAL  |
| 30  | DG    | 11  | PRO  |
| 30  | DG    | 46  | ASP  |
| 30  | DG    | 91  | VAL  |
| 30  | DG    | 117 | PRO  |
| 30  | DG    | 125 | PRO  |
| 30  | DG    | 169 | ARG  |
| 31  | DH    | 99  | ILE  |
| 31  | DH    | 144 | VAL  |
| 32  | DI    | 35  | MET  |
| 33  | DJ    | 13  | ARG  |
| 33  | DJ    | 44  | TYR  |
| 34  | DK    | 14  | SER  |
| 34  | DK    | 17  | ARG  |
| 34  | DK    | 103 | VAL  |
| 35  | DL    | 19  | LEU  |
| 35  | DL    | 99  | ASN  |
| 35  | DL    | 100 | ILE  |
| 35  | DL    | 115 | GLU  |
| 36  | DM    | 16  | ARG  |
| 36  | DM    | 111 | GLU  |
| 37  | DN    | 2   | ARG  |
| 37  | DN    | 5   | LYS  |
| 37  | DN    | 10  | LEU  |
| 37  | DN    | 13  | ASN  |
| 39  | DP    | 94  | ALA  |
| 39  | DP    | 113 | LEU  |
| 40  | DQ    | 6   | GLY  |
| 40  | DQ    | 29  | ARG  |
| 40  | DQ    | 87  | VAL  |
| 41  | DR    | 98  | ILE  |
| 42  | DS    | 61  | ASN  |
| 43  | DT    | 19  | LYS  |
| 43  | DT    | 38  | ALA  |
| 44  | DU    | 8   | ASP  |
| 44  | DU    | 40  | LEU  |
| 45  | DV    | 79  | ARG  |
| 46  | DW    | 36  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | DW    | 46  | ALA  |
| 47  | DX    | 35  | HIS  |
| 47  | DX    | 69  | GLU  |
| 50  | D0    | 32  | THR  |
| 51  | D1    | 35  | LEU  |
| 52  | D2    | 29  | GLN  |
| 52  | D2    | 39  | ARG  |
| 53  | D3    | 22  | LYS  |
| 54  | D4    | 3   | VAL  |
| 54  | D4    | 37  | GLN  |
| 1   | AB    | 21  | TYR  |
| 2   | AC    | 92  | ASP  |
| 2   | AC    | 107 | LYS  |
| 2   | AC    | 171 | ARG  |
| 3   | AD    | 24  | VAL  |
| 3   | AD    | 29  | THR  |
| 4   | AE    | 24  | VAL  |
| 4   | AE    | 132 | PRO  |
| 5   | AF    | 7   | VAL  |
| 5   | AF    | 69  | GLU  |
| 6   | AG    | 71  | THR  |
| 8   | AI    | 33  | SER  |
| 8   | AI    | 54  | VAL  |
| 8   | AI    | 55  | ASP  |
| 9   | AJ    | 35  | GLN  |
| 10  | AK    | 119 | GLY  |
| 11  | AL    | 28  | GLN  |
| 13  | AN    | 2   | LYS  |
| 13  | AN    | 21  | ALA  |
| 13  | AN    | 64  | ARG  |
| 14  | AO    | 43  | ALA  |
| 15  | AP    | 36  | VAL  |
| 16  | AQ    | 10  | ARG  |
| 16  | AQ    | 49  | ASN  |
| 19  | AT    | 10  | ALA  |
| 20  | AU    | 11  | PHE  |
| 26  | BC    | 109 | LEU  |
| 26  | BC    | 204 | LEU  |
| 26  | BC    | 246 | PRO  |
| 27  | BD    | 164 | GLN  |
| 27  | BD    | 170 | VAL  |
| 27  | BD    | 182 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | BD    | 187 | LEU  |
| 28  | BE    | 45  | ALA  |
| 28  | BE    | 49  | ARG  |
| 28  | BE    | 73  | ILE  |
| 29  | BF    | 2   | LYS  |
| 29  | BF    | 54  | ALA  |
| 30  | BG    | 55  | ASP  |
| 30  | BG    | 97  | VAL  |
| 30  | BG    | 113 | ASP  |
| 30  | BG    | 117 | PRO  |
| 31  | BH    | 7   | ASP  |
| 31  | BH    | 29  | PHE  |
| 31  | BH    | 67  | ALA  |
| 31  | BH    | 89  | LYS  |
| 31  | BH    | 96  | THR  |
| 32  | BI    | 6   | ALA  |
| 33  | BJ    | 36  | LEU  |
| 33  | BJ    | 102 | GLU  |
| 33  | BJ    | 125 | TYR  |
| 34  | BK    | 48  | PRO  |
| 34  | BK    | 69  | VAL  |
| 35  | BL    | 25  | SER  |
| 35  | BL    | 64  | PHE  |
| 36  | BM    | 84  | LYS  |
| 36  | BM    | 134 | THR  |
| 37  | BN    | 17  | ARG  |
| 38  | BO    | 77  | ALA  |
| 39  | BP    | 33  | GLU  |
| 40  | BQ    | 4   | LYS  |
| 41  | BR    | 49  | ILE  |
| 41  | BR    | 71  | LYS  |
| 42  | BS    | 96  | ILE  |
| 43  | BT    | 18  | GLU  |
| 46  | BW    | 14  | ASP  |
| 46  | BW    | 56  | HIS  |
| 50  | B0    | 3   | GLN  |
| 51  | B1    | 16  | THR  |
| 52  | B2    | 2   | LYS  |
| 54  | B4    | 37  | GLN  |
| 1   | CB    | 26  | MET  |
| 1   | CB    | 86  | CYS  |
| 1   | CB    | 101 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CC    | 100 | ILE  |
| 2   | CC    | 180 | ASP  |
| 3   | CD    | 21  | LYS  |
| 3   | CD    | 39  | GLN  |
| 4   | CE    | 69  | ASN  |
| 4   | CE    | 111 | ARG  |
| 5   | CF    | 63  | ASN  |
| 6   | CG    | 88  | VAL  |
| 7   | CH    | 22  | ALA  |
| 7   | CH    | 47  | ASP  |
| 7   | CH    | 107 | LYS  |
| 10  | CK    | 88  | PRO  |
| 10  | CK    | 91  | GLY  |
| 10  | CK    | 118 | ASN  |
| 12  | CM    | 42  | VAL  |
| 12  | CM    | 77  | LYS  |
| 13  | CN    | 51  | PRO  |
| 15  | CP    | 42  | ILE  |
| 16  | CQ    | 67  | SER  |
| 16  | CQ    | 79  | GLU  |
| 18  | CS    | 29  | PRO  |
| 19  | CT    | 65  | LEU  |
| 26  | DC    | 106 | PRO  |
| 26  | DC    | 196 | ASN  |
| 26  | DC    | 204 | LEU  |
| 27  | DD    | 48  | ILE  |
| 27  | DD    | 197 | THR  |
| 28  | DE    | 69  | ARG  |
| 28  | DE    | 96  | VAL  |
| 28  | DE    | 126 | VAL  |
| 28  | DE    | 148 | ILE  |
| 29  | DF    | 94  | ARG  |
| 29  | DF    | 104 | THR  |
| 29  | DF    | 130 | GLY  |
| 30  | DG    | 40  | VAL  |
| 30  | DG    | 45  | ALA  |
| 30  | DG    | 123 | GLU  |
| 31  | DH    | 39  | ALA  |
| 31  | DH    | 105 | ALA  |
| 32  | DI    | 19  | PRO  |
| 32  | DI    | 87  | SER  |
| 32  | DI    | 119 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | DJ    | 5   | THR  |
| 33  | DJ    | 6   | ALA  |
| 33  | DJ    | 25  | LEU  |
| 33  | DJ    | 113 | PRO  |
| 34  | DK    | 5   | GLN  |
| 34  | DK    | 6   | THR  |
| 35  | DL    | 30  | THR  |
| 36  | DM    | 13  | HIS  |
| 36  | DM    | 106 | ASP  |
| 37  | DN    | 82  | GLU  |
| 39  | DP    | 20  | ARG  |
| 39  | DP    | 51  | ASN  |
| 40  | DQ    | 58  | GLN  |
| 41  | DR    | 15  | SER  |
| 41  | DR    | 29  | THR  |
| 41  | DR    | 65  | ALA  |
| 42  | DS    | 71  | VAL  |
| 43  | DT    | 11  | LEU  |
| 46  | DW    | 23  | LYS  |
| 46  | DW    | 41  | GLY  |
| 48  | DY    | 2   | LYS  |
| 48  | DY    | 46  | VAL  |
| 49  | DZ    | 52  | PHE  |
| 50  | D0    | 26  | SER  |
| 50  | D0    | 53  | VAL  |
| 54  | D4    | 16  | ILE  |
| 1   | AB    | 85  | SER  |
| 1   | AB    | 150 | ILE  |
| 2   | AC    | 53  | ARG  |
| 2   | AC    | 65  | VAL  |
| 3   | AD    | 191 | SER  |
| 5   | AF    | 63  | ASN  |
| 5   | AF    | 94  | HIS  |
| 5   | AF    | 99  | ALA  |
| 6   | AG    | 120 | ALA  |
| 7   | AH    | 49  | LYS  |
| 7   | AH    | 69  | ALA  |
| 7   | AH    | 99  | GLY  |
| 7   | AH    | 103 | VAL  |
| 9   | AJ    | 33  | GLY  |
| 9   | AJ    | 39  | PRO  |
| 9   | AJ    | 41  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | AK    | 14  | GLN  |
| 11  | AL    | 72  | ASN  |
| 11  | AL    | 77  | SER  |
| 13  | AN    | 80  | ARG  |
| 14  | AO    | 45  | HIS  |
| 17  | AR    | 24  | ASP  |
| 26  | BC    | 37  | SER  |
| 26  | BC    | 64  | VAL  |
| 26  | BC    | 150 | GLY  |
| 27  | BD    | 109 | VAL  |
| 27  | BD    | 145 | SER  |
| 27  | BD    | 151 | THR  |
| 28  | BE    | 59  | PRO  |
| 28  | BE    | 71  | GLY  |
| 28  | BE    | 83  | VAL  |
| 28  | BE    | 96  | VAL  |
| 30  | BG    | 16  | VAL  |
| 30  | BG    | 32  | LEU  |
| 30  | BG    | 109 | SER  |
| 31  | BH    | 103 | VAL  |
| 32  | BI    | 3   | LYS  |
| 32  | BI    | 7   | TYR  |
| 32  | BI    | 20  | SER  |
| 32  | BI    | 64  | ARG  |
| 32  | BI    | 83  | ALA  |
| 34  | BK    | 92  | GLU  |
| 36  | BM    | 47  | GLU  |
| 36  | BM    | 73  | ILE  |
| 43  | BT    | 28  | ASN  |
| 43  | BT    | 55  | VAL  |
| 44  | BU    | 63  | ALA  |
| 44  | BU    | 67  | SER  |
| 44  | BU    | 85  | ARG  |
| 46  | BW    | 40  | ARG  |
| 46  | BW    | 78  | PHE  |
| 48  | BY    | 17  | GLU  |
| 49  | BZ    | 4   | ILE  |
| 2   | CC    | 46  | LEU  |
| 2   | CC    | 140 | ALA  |
| 2   | CC    | 145 | ALA  |
| 2   | CC    | 167 | TYR  |
| 3   | CD    | 38  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | CE    | 144 | GLU  |
| 7   | CH    | 72  | GLU  |
| 9   | CJ    | 36  | VAL  |
| 9   | CJ    | 75  | ASP  |
| 11  | CL    | 60  | PHE  |
| 12  | CM    | 62  | PHE  |
| 13  | CN    | 50  | LEU  |
| 17  | CR    | 72  | ARG  |
| 26  | DC    | 64  | VAL  |
| 26  | DC    | 246 | PRO  |
| 27  | DD    | 106 | LYS  |
| 27  | DD    | 109 | VAL  |
| 27  | DD    | 169 | ARG  |
| 28  | DE    | 60  | TRP  |
| 29  | DF    | 82  | TYR  |
| 29  | DF    | 125 | GLY  |
| 29  | DF    | 156 | THR  |
| 30  | DG    | 39  | ALA  |
| 30  | DG    | 119 | GLY  |
| 30  | DG    | 126 | THR  |
| 30  | DG    | 136 | ASP  |
| 30  | DG    | 152 | ARG  |
| 31  | DH    | 89  | LYS  |
| 31  | DH    | 121 | VAL  |
| 31  | DH    | 124 | THR  |
| 31  | DH    | 143 | ILE  |
| 33  | DJ    | 43  | GLU  |
| 34  | DK    | 119 | ALA  |
| 35  | DL    | 48  | ARG  |
| 35  | DL    | 88  | GLY  |
| 35  | DL    | 93  | ASN  |
| 36  | DM    | 69  | PRO  |
| 36  | DM    | 134 | THR  |
| 37  | DN    | 59  | SER  |
| 37  | DN    | 71  | ARG  |
| 37  | DN    | 72  | ASP  |
| 39  | DP    | 63  | ILE  |
| 41  | DR    | 53  | PHE  |
| 42  | DS    | 32  | ALA  |
| 43  | DT    | 18  | GLU  |
| 43  | DT    | 50  | LEU  |
| 44  | DU    | 6   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | DU    | 41  | VAL  |
| 44  | DU    | 52  | ASN  |
| 44  | DU    | 101 | THR  |
| 47  | DX    | 17  | ARG  |
| 49  | DZ    | 27  | GLY  |
| 50  | D0    | 33  | SER  |
| 51  | D1    | 50  | GLU  |
| 1   | AB    | 53  | LEU  |
| 1   | AB    | 75  | ALA  |
| 3   | AD    | 31  | CYS  |
| 4   | AE    | 152 | VAL  |
| 6   | AG    | 57  | GLU  |
| 7   | AH    | 96  | ALA  |
| 10  | AK    | 97  | ARG  |
| 13  | AN    | 44  | VAL  |
| 15  | AP    | 42  | ILE  |
| 26  | BC    | 226 | PRO  |
| 28  | BE    | 123 | LYS  |
| 28  | BE    | 148 | ILE  |
| 29  | BF    | 61  | GLY  |
| 29  | BF    | 83  | PRO  |
| 31  | BH    | 13  | GLY  |
| 31  | BH    | 107 | GLY  |
| 33  | BJ    | 96  | ARG  |
| 35  | BL    | 23  | ILE  |
| 35  | BL    | 40  | SER  |
| 36  | BM    | 46  | ILE  |
| 36  | BM    | 133 | LYS  |
| 37  | BN    | 32  | GLU  |
| 40  | BQ    | 43  | GLN  |
| 40  | BQ    | 115 | ALA  |
| 41  | BR    | 28  | ALA  |
| 41  | BR    | 51  | VAL  |
| 41  | BR    | 65  | ALA  |
| 41  | BR    | 98  | ILE  |
| 42  | BS    | 29  | VAL  |
| 44  | BU    | 53  | GLN  |
| 46  | BW    | 68  | PHE  |
| 1   | CB    | 128 | LEU  |
| 2   | CC    | 65  | VAL  |
| 3   | CD    | 191 | SER  |
| 4   | CE    | 58  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | CE    | 104 | ILE  |
| 5   | CF    | 7   | VAL  |
| 6   | CG    | 74  | VAL  |
| 9   | CJ    | 42  | LEU  |
| 9   | CJ    | 74  | VAL  |
| 10  | CK    | 127 | ARG  |
| 17  | CR    | 51  | GLN  |
| 28  | DE    | 45  | ALA  |
| 29  | DF    | 68  | LYS  |
| 29  | DF    | 69  | ALA  |
| 29  | DF    | 83  | PRO  |
| 29  | DF    | 86  | CYS  |
| 30  | DG    | 92  | GLY  |
| 30  | DG    | 170 | THR  |
| 32  | DI    | 31  | GLY  |
| 32  | DI    | 83  | ALA  |
| 35  | DL    | 36  | LYS  |
| 35  | DL    | 66  | PHE  |
| 38  | DO    | 42  | PRO  |
| 44  | DU    | 12  | VAL  |
| 44  | DU    | 35  | VAL  |
| 44  | DU    | 47  | PRO  |
| 45  | DV    | 57  | TYR  |
| 45  | DV    | 84  | PRO  |
| 46  | DW    | 16  | GLU  |
| 49  | DZ    | 29  | ARG  |
| 49  | DZ    | 32  | GLY  |
| 52  | D2    | 43  | THR  |
| 2   | AC    | 14  | VAL  |
| 3   | AD    | 100 | VAL  |
| 11  | AL    | 41  | PRO  |
| 28  | BE    | 187 | VAL  |
| 30  | BG    | 110 | HIS  |
| 32  | BI    | 31  | GLY  |
| 36  | BM    | 72  | PRO  |
| 41  | BR    | 64  | VAL  |
| 46  | BW    | 41  | GLY  |
| 1   | CB    | 200 | PRO  |
| 6   | CG    | 68  | VAL  |
| 9   | CJ    | 33  | GLY  |
| 27  | DD    | 44  | GLY  |
| 27  | DD    | 143 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | DE    | 129 | PRO  |
| 29  | DF    | 175 | PRO  |
| 32  | DI    | 138 | VAL  |
| 33  | DJ    | 96  | ARG  |
| 38  | DO    | 27  | VAL  |
| 39  | DP    | 4   | ILE  |
| 41  | DR    | 8   | GLY  |
| 46  | DW    | 26  | GLY  |
| 1   | AB    | 163 | ILE  |
| 4   | AE    | 78  | GLY  |
| 4   | AE    | 131 | ASN  |
| 20  | AU    | 52  | VAL  |
| 27  | BD    | 93  | GLY  |
| 46  | BW    | 37  | VAL  |
| 46  | BW    | 73  | PRO  |
| 1   | CB    | 154 | GLY  |
| 2   | CC    | 77  | GLY  |
| 9   | CJ    | 38  | GLY  |
| 12  | CM    | 3   | ILE  |
| 26  | DC    | 2   | VAL  |
| 27  | DD    | 122 | VAL  |
| 27  | DD    | 144 | GLY  |
| 29  | DF    | 88  | VAL  |
| 32  | DI    | 28  | GLY  |
| 34  | DK    | 2   | ILE  |
| 41  | DR    | 27  | ILE  |
| 42  | DS    | 96  | ILE  |
| 43  | DT    | 16  | VAL  |
| 46  | DW    | 22  | VAL  |
| 8   | AI    | 25  | GLY  |
| 10  | AK    | 38  | GLY  |
| 31  | BH    | 80  | ILE  |
| 20  | CU    | 9   | GLU  |
| 29  | DF    | 81  | GLY  |
| 29  | DF    | 136 | ILE  |
| 31  | DH    | 103 | VAL  |
| 36  | DM    | 36  | VAL  |
| 41  | DR    | 75  | VAL  |
| 44  | DU    | 64  | ILE  |
| 45  | DV    | 15  | GLY  |
| 1   | AB    | 181 | PRO  |
| 4   | AE    | 104 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | AG    | 79  | VAL  |
| 7   | AH    | 102 | VAL  |
| 16  | AQ    | 57  | VAL  |
| 19  | AT    | 3   | ILE  |
| 29  | BF    | 135 | ILE  |
| 32  | BI    | 23  | VAL  |
| 36  | BM    | 23  | GLY  |
| 37  | BN    | 84  | GLY  |
| 46  | BW    | 70  | VAL  |
| 50  | B0    | 53  | VAL  |
| 2   | CC    | 76  | ILE  |
| 4   | CE    | 116 | VAL  |
| 6   | CG    | 92  | PRO  |
| 7   | CH    | 6   | ILE  |
| 9   | CJ    | 84  | VAL  |
| 11  | CL    | 83  | GLY  |
| 29  | DF    | 108 | PRO  |
| 33  | DJ    | 56  | VAL  |
| 34  | DK    | 48  | PRO  |
| 35  | DL    | 114 | GLY  |
| 44  | DU    | 33  | VAL  |
| 16  | AQ    | 9   | GLY  |
| 41  | BR    | 30  | GLY  |
| 11  | CL    | 117 | GLY  |
| 12  | CM    | 93  | GLY  |
| 26  | DC    | 217 | PRO  |
| 29  | DF    | 84  | ILE  |
| 42  | DS    | 29  | 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 X-ray entries followed by that with respect to entries of similar resolution.

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 |
|-----|-------|---------------|-----------|----------|-------------|
| 1   | AB    | 180/199 (90%) | 147 (82%) | 33 (18%) | 2 13        |
| 1   | CB    | 180/199 (90%) | 158 (88%) | 22 (12%) | 6 31        |
| 2   | AC    | 170/190 (90%) | 148 (87%) | 22 (13%) | 5 29        |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2   | CC    | 170/190 (90%) | 146 (86%) | 24 (14%) | 4           | 26 |
| 3   | AD    | 172/173 (99%) | 147 (86%) | 25 (14%) | 4           | 25 |
| 3   | CD    | 172/173 (99%) | 152 (88%) | 20 (12%) | 6           | 34 |
| 4   | AE    | 113/126 (90%) | 93 (82%)  | 20 (18%) | 2           | 15 |
| 4   | CE    | 113/126 (90%) | 100 (88%) | 13 (12%) | 6           | 34 |
| 5   | AF    | 87/116 (75%)  | 75 (86%)  | 12 (14%) | 4           | 27 |
| 5   | CF    | 87/116 (75%)  | 74 (85%)  | 13 (15%) | 3           | 24 |
| 6   | AG    | 124/147 (84%) | 117 (94%) | 7 (6%)   | 25          | 63 |
| 6   | CG    | 123/147 (84%) | 95 (77%)  | 28 (23%) | 1           | 7  |
| 7   | AH    | 104/105 (99%) | 92 (88%)  | 12 (12%) | 6           | 34 |
| 7   | CH    | 104/105 (99%) | 91 (88%)  | 13 (12%) | 5           | 30 |
| 8   | AI    | 105/107 (98%) | 90 (86%)  | 15 (14%) | 4           | 26 |
| 8   | CI    | 105/107 (98%) | 91 (87%)  | 14 (13%) | 4           | 28 |
| 9   | AJ    | 86/90 (96%)   | 74 (86%)  | 12 (14%) | 4           | 27 |
| 9   | CJ    | 86/90 (96%)   | 77 (90%)  | 9 (10%)  | 8           | 38 |
| 10  | AK    | 90/99 (91%)   | 80 (89%)  | 10 (11%) | 7           | 36 |
| 10  | CK    | 90/99 (91%)   | 80 (89%)  | 10 (11%) | 7           | 36 |
| 11  | AL    | 103/104 (99%) | 85 (82%)  | 18 (18%) | 2           | 15 |
| 11  | CL    | 103/104 (99%) | 88 (85%)  | 15 (15%) | 3           | 24 |
| 12  | AM    | 92/96 (96%)   | 87 (95%)  | 5 (5%)   | 26          | 64 |
| 12  | CM    | 91/96 (95%)   | 74 (81%)  | 17 (19%) | 2           | 12 |
| 13  | AN    | 79/84 (94%)   | 73 (92%)  | 6 (8%)   | 15          | 53 |
| 13  | CN    | 79/84 (94%)   | 68 (86%)  | 11 (14%) | 4           | 27 |
| 14  | AO    | 76/77 (99%)   | 72 (95%)  | 4 (5%)   | 26          | 65 |
| 14  | CO    | 76/77 (99%)   | 72 (95%)  | 4 (5%)   | 26          | 65 |
| 15  | AP    | 65/65 (100%)  | 60 (92%)  | 5 (8%)   | 15          | 52 |
| 15  | CP    | 65/65 (100%)  | 59 (91%)  | 6 (9%)   | 11          | 45 |
| 16  | AQ    | 74/78 (95%)   | 60 (81%)  | 14 (19%) | 2           | 11 |
| 16  | CQ    | 74/78 (95%)   | 64 (86%)  | 10 (14%) | 4           | 28 |
| 17  | AR    | 48/65 (74%)   | 46 (96%)  | 2 (4%)   | 34          | 70 |
| 17  | CR    | 48/65 (74%)   | 46 (96%)  | 2 (4%)   | 34          | 70 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 18  | AS    | 70/79 (89%)    | 63 (90%)  | 7 (10%)  | 9           | 40 |
| 18  | CS    | 70/79 (89%)    | 59 (84%)  | 11 (16%) | 3           | 21 |
| 19  | AT    | 65/66 (98%)    | 55 (85%)  | 10 (15%) | 3           | 22 |
| 19  | CT    | 65/66 (98%)    | 56 (86%)  | 9 (14%)  | 4           | 27 |
| 20  | AU    | 44/61 (72%)    | 37 (84%)  | 7 (16%)  | 3           | 20 |
| 20  | CU    | 44/61 (72%)    | 35 (80%)  | 9 (20%)  | 1           | 9  |
| 26  | BC    | 216/218 (99%)  | 173 (80%) | 43 (20%) | 1           | 10 |
| 26  | DC    | 216/218 (99%)  | 191 (88%) | 25 (12%) | 6           | 34 |
| 27  | BD    | 164/164 (100%) | 136 (83%) | 28 (17%) | 2           | 17 |
| 27  | DD    | 164/164 (100%) | 144 (88%) | 20 (12%) | 6           | 31 |
| 28  | BE    | 165/165 (100%) | 130 (79%) | 35 (21%) | 1           | 8  |
| 28  | DE    | 165/165 (100%) | 152 (92%) | 13 (8%)  | 14          | 51 |
| 29  | BF    | 148/150 (99%)  | 130 (88%) | 18 (12%) | 6           | 31 |
| 29  | DF    | 149/150 (99%)  | 124 (83%) | 25 (17%) | 2           | 17 |
| 30  | BG    | 137/138 (99%)  | 107 (78%) | 30 (22%) | 1           | 7  |
| 30  | DG    | 137/138 (99%)  | 120 (88%) | 17 (12%) | 5           | 31 |
| 31  | BH    | 114/114 (100%) | 97 (85%)  | 17 (15%) | 3           | 24 |
| 31  | DH    | 114/114 (100%) | 95 (83%)  | 19 (17%) | 2           | 18 |
| 32  | BI    | 109/110 (99%)  | 94 (86%)  | 15 (14%) | 4           | 27 |
| 32  | DI    | 109/110 (99%)  | 102 (94%) | 7 (6%)   | 20          | 59 |
| 33  | BJ    | 116/116 (100%) | 90 (78%)  | 26 (22%) | 1           | 7  |
| 33  | DJ    | 116/116 (100%) | 106 (91%) | 10 (9%)  | 12          | 48 |
| 34  | BK    | 103/104 (99%)  | 84 (82%)  | 19 (18%) | 2           | 12 |
| 34  | DK    | 103/104 (99%)  | 85 (82%)  | 18 (18%) | 2           | 15 |
| 35  | BL    | 102/103 (99%)  | 81 (79%)  | 21 (21%) | 1           | 9  |
| 35  | DL    | 102/103 (99%)  | 90 (88%)  | 12 (12%) | 6           | 33 |
| 36  | BM    | 109/109 (100%) | 90 (83%)  | 19 (17%) | 2           | 15 |
| 36  | DM    | 109/109 (100%) | 100 (92%) | 9 (8%)   | 13          | 49 |
| 37  | BN    | 100/103 (97%)  | 81 (81%)  | 19 (19%) | 2           | 11 |
| 37  | DN    | 100/103 (97%)  | 85 (85%)  | 15 (15%) | 3           | 23 |
| 38  | BO    | 86/87 (99%)    | 69 (80%)  | 17 (20%) | 1           | 10 |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |    |
|-----|-------|--------------|-----------|----------|-------------|----|
| 38  | DO    | 86/87 (99%)  | 78 (91%)  | 8 (9%)   | 10          | 44 |
| 39  | BP    | 99/100 (99%) | 79 (80%)  | 20 (20%) | 1           | 10 |
| 39  | DP    | 99/100 (99%) | 91 (92%)  | 8 (8%)   | 14          | 50 |
| 40  | BQ    | 89/90 (99%)  | 73 (82%)  | 16 (18%) | 2           | 14 |
| 40  | DQ    | 89/90 (99%)  | 79 (89%)  | 10 (11%) | 7           | 35 |
| 41  | BR    | 84/84 (100%) | 69 (82%)  | 15 (18%) | 2           | 14 |
| 41  | DR    | 84/84 (100%) | 70 (83%)  | 14 (17%) | 2           | 18 |
| 42  | BS    | 93/93 (100%) | 73 (78%)  | 20 (22%) | 1           | 8  |
| 42  | DS    | 93/93 (100%) | 79 (85%)  | 14 (15%) | 3           | 23 |
| 43  | BT    | 80/84 (95%)  | 61 (76%)  | 19 (24%) | 1           | 6  |
| 43  | DT    | 80/84 (95%)  | 74 (92%)  | 6 (8%)   | 16          | 53 |
| 44  | BU    | 83/85 (98%)  | 69 (83%)  | 14 (17%) | 2           | 17 |
| 44  | DU    | 83/85 (98%)  | 72 (87%)  | 11 (13%) | 4           | 28 |
| 45  | BV    | 78/78 (100%) | 64 (82%)  | 14 (18%) | 2           | 14 |
| 45  | DV    | 78/78 (100%) | 68 (87%)  | 10 (13%) | 5           | 29 |
| 46  | BW    | 59/63 (94%)  | 43 (73%)  | 16 (27%) | 0           | 4  |
| 46  | DW    | 59/63 (94%)  | 44 (75%)  | 15 (25%) | 0           | 5  |
| 47  | BX    | 67/68 (98%)  | 53 (79%)  | 14 (21%) | 1           | 9  |
| 47  | DX    | 67/68 (98%)  | 58 (87%)  | 9 (13%)  | 4           | 28 |
| 48  | BY    | 55/55 (100%) | 44 (80%)  | 11 (20%) | 1           | 10 |
| 48  | DY    | 55/55 (100%) | 52 (94%)  | 3 (6%)   | 25          | 64 |
| 49  | BZ    | 48/49 (98%)  | 34 (71%)  | 14 (29%) | 0           | 3  |
| 49  | DZ    | 48/49 (98%)  | 41 (85%)  | 7 (15%)  | 3           | 24 |
| 50  | B0    | 47/48 (98%)  | 42 (89%)  | 5 (11%)  | 8           | 38 |
| 50  | D0    | 47/48 (98%)  | 42 (89%)  | 5 (11%)  | 8           | 38 |
| 51  | B1    | 45/49 (92%)  | 37 (82%)  | 8 (18%)  | 2           | 14 |
| 51  | D1    | 45/49 (92%)  | 41 (91%)  | 4 (9%)   | 11          | 46 |
| 52  | B2    | 38/38 (100%) | 32 (84%)  | 6 (16%)  | 3           | 21 |
| 52  | D2    | 38/38 (100%) | 34 (90%)  | 4 (10%)  | 8           | 38 |
| 53  | B3    | 51/52 (98%)  | 44 (86%)  | 7 (14%)  | 4           | 27 |
| 53  | D3    | 51/52 (98%)  | 42 (82%)  | 9 (18%)  | 2           | 15 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|-----------------|------------|------------|-------------|----|
| 54  | B4    | 34/34 (100%)    | 30 (88%)   | 4 (12%)    | 6           | 33 |
| 54  | D4    | 34/34 (100%)    | 29 (85%)   | 5 (15%)    | 3           | 24 |
| All | All   | 9331/9756 (96%) | 7983 (86%) | 1348 (14%) | 4           | 25 |

All (1348) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AB    | 8   | MET  |
| 1   | AB    | 10  | LYS  |
| 1   | AB    | 15  | PHE  |
| 1   | AB    | 19  | THR  |
| 1   | AB    | 22  | TRP  |
| 1   | AB    | 30  | ILE  |
| 1   | AB    | 36  | LYS  |
| 1   | AB    | 41  | ASN  |
| 1   | AB    | 48  | MET  |
| 1   | AB    | 57  | ASN  |
| 1   | AB    | 88  | GLN  |
| 1   | AB    | 94  | ARG  |
| 1   | AB    | 100 | LEU  |
| 1   | AB    | 101 | THR  |
| 1   | AB    | 108 | GLN  |
| 1   | AB    | 111 | LYS  |
| 1   | AB    | 115 | ASP  |
| 1   | AB    | 117 | GLU  |
| 1   | AB    | 119 | GLN  |
| 1   | AB    | 125 | PHE  |
| 1   | AB    | 128 | LEU  |
| 1   | AB    | 129 | THR  |
| 1   | AB    | 130 | LYS  |
| 1   | AB    | 138 | ARG  |
| 1   | AB    | 139 | GLU  |
| 1   | AB    | 156 | LEU  |
| 1   | AB    | 158 | ASP  |
| 1   | AB    | 170 | ILE  |
| 1   | AB    | 177 | ASN  |
| 1   | AB    | 183 | PHE  |
| 1   | AB    | 189 | ASN  |
| 1   | AB    | 206 | ILE  |
| 1   | AB    | 219 | THR  |
| 2   | AC    | 2   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 13  | ILE  |
| 2   | AC    | 17  | TRP  |
| 2   | AC    | 24  | ASN  |
| 2   | AC    | 30  | ASP  |
| 2   | AC    | 36  | PHE  |
| 2   | AC    | 57  | GLU  |
| 2   | AC    | 78  | LYS  |
| 2   | AC    | 79  | LYS  |
| 2   | AC    | 101 | ASN  |
| 2   | AC    | 106 | ARG  |
| 2   | AC    | 120 | THR  |
| 2   | AC    | 130 | ARG  |
| 2   | AC    | 139 | ASN  |
| 2   | AC    | 143 | LEU  |
| 2   | AC    | 148 | ILE  |
| 2   | AC    | 149 | LYS  |
| 2   | AC    | 165 | GLU  |
| 2   | AC    | 166 | TRP  |
| 2   | AC    | 167 | TYR  |
| 2   | AC    | 184 | ASN  |
| 2   | AC    | 190 | THR  |
| 3   | AD    | 2   | ARG  |
| 3   | AD    | 10  | LEU  |
| 3   | AD    | 25  | ARG  |
| 3   | AD    | 32  | LYS  |
| 3   | AD    | 43  | ARG  |
| 3   | AD    | 55  | ARG  |
| 3   | AD    | 57  | LYS  |
| 3   | AD    | 58  | GLN  |
| 3   | AD    | 69  | ARG  |
| 3   | AD    | 99  | ASN  |
| 3   | AD    | 103 | ARG  |
| 3   | AD    | 109 | THR  |
| 3   | AD    | 115 | GLN  |
| 3   | AD    | 117 | VAL  |
| 3   | AD    | 122 | ILE  |
| 3   | AD    | 123 | MET  |
| 3   | AD    | 127 | ARG  |
| 3   | AD    | 131 | ILE  |
| 3   | AD    | 141 | VAL  |
| 3   | AD    | 160 | LEU  |
| 3   | AD    | 163 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AD    | 166 | LYS  |
| 3   | AD    | 193 | ASP  |
| 3   | AD    | 195 | ASN  |
| 3   | AD    | 205 | LYS  |
| 4   | AE    | 11  | GLN  |
| 4   | AE    | 14  | LEU  |
| 4   | AE    | 19  | ARG  |
| 4   | AE    | 24  | VAL  |
| 4   | AE    | 25  | LYS  |
| 4   | AE    | 31  | SER  |
| 4   | AE    | 42  | ASN  |
| 4   | AE    | 59  | ILE  |
| 4   | AE    | 77  | ASN  |
| 4   | AE    | 81  | GLN  |
| 4   | AE    | 95  | MET  |
| 4   | AE    | 100 | GLU  |
| 4   | AE    | 113 | VAL  |
| 4   | AE    | 121 | ASN  |
| 4   | AE    | 130 | THR  |
| 4   | AE    | 133 | ILE  |
| 4   | AE    | 139 | THR  |
| 4   | AE    | 144 | GLU  |
| 4   | AE    | 145 | ASN  |
| 4   | AE    | 155 | LYS  |
| 5   | AF    | 14  | GLN  |
| 5   | AF    | 17  | GLN  |
| 5   | AF    | 24  | ARG  |
| 5   | AF    | 39  | LEU  |
| 5   | AF    | 46  | GLN  |
| 5   | AF    | 55  | HIS  |
| 5   | AF    | 62  | MET  |
| 5   | AF    | 68  | GLN  |
| 5   | AF    | 69  | GLU  |
| 5   | AF    | 77  | THR  |
| 5   | AF    | 79  | ARG  |
| 5   | AF    | 86  | ARG  |
| 6   | AG    | 3   | ARG  |
| 6   | AG    | 20  | GLU  |
| 6   | AG    | 85  | GLN  |
| 6   | AG    | 105 | GLU  |
| 6   | AG    | 123 | LEU  |
| 6   | AG    | 142 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | AG    | 147 | ASN  |
| 7   | AH    | 21  | LYS  |
| 7   | AH    | 59  | GLU  |
| 7   | AH    | 76  | ARG  |
| 7   | AH    | 78  | SER  |
| 7   | AH    | 86  | LYS  |
| 7   | AH    | 89  | ASP  |
| 7   | AH    | 98  | LEU  |
| 7   | AH    | 106 | SER  |
| 7   | AH    | 110 | MET  |
| 7   | AH    | 111 | THR  |
| 7   | AH    | 120 | LEU  |
| 7   | AH    | 124 | ILE  |
| 8   | AI    | 21  | LYS  |
| 8   | AI    | 35  | GLU  |
| 8   | AI    | 44  | ARG  |
| 8   | AI    | 48  | ARG  |
| 8   | AI    | 54  | VAL  |
| 8   | AI    | 56  | MET  |
| 8   | AI    | 62  | LEU  |
| 8   | AI    | 67  | LYS  |
| 8   | AI    | 72  | SER  |
| 8   | AI    | 87  | MET  |
| 8   | AI    | 89  | TYR  |
| 8   | AI    | 105 | ARG  |
| 8   | AI    | 115 | VAL  |
| 8   | AI    | 126 | PHE  |
| 8   | AI    | 128 | LYS  |
| 9   | AJ    | 22  | THR  |
| 9   | AJ    | 32  | THR  |
| 9   | AJ    | 35  | GLN  |
| 9   | AJ    | 46  | LYS  |
| 9   | AJ    | 48  | ARG  |
| 9   | AJ    | 59  | LYS  |
| 9   | AJ    | 60  | ASP  |
| 9   | AJ    | 73  | LEU  |
| 9   | AJ    | 76  | ILE  |
| 9   | AJ    | 85  | ASP  |
| 9   | AJ    | 89  | ARG  |
| 9   | AJ    | 91  | ASP  |
| 10  | AK    | 17  | ASP  |
| 10  | AK    | 25  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | AK    | 51  | PHE  |
| 10  | AK    | 64  | VAL  |
| 10  | AK    | 78  | ILE  |
| 10  | AK    | 106 | ILE  |
| 10  | AK    | 124 | LYS  |
| 10  | AK    | 125 | LYS  |
| 10  | AK    | 127 | ARG  |
| 10  | AK    | 128 | VAL  |
| 11  | AL    | 3   | VAL  |
| 11  | AL    | 17  | LYS  |
| 11  | AL    | 20  | VAL  |
| 11  | AL    | 28  | GLN  |
| 11  | AL    | 34  | THR  |
| 11  | AL    | 35  | ARG  |
| 11  | AL    | 40  | THR  |
| 11  | AL    | 43  | LYS  |
| 11  | AL    | 49  | ARG  |
| 11  | AL    | 51  | VAL  |
| 11  | AL    | 63  | THR  |
| 11  | AL    | 66  | ILE  |
| 11  | AL    | 75  | GLU  |
| 11  | AL    | 87  | LYS  |
| 11  | AL    | 88  | ASP  |
| 11  | AL    | 89  | LEU  |
| 11  | AL    | 94  | TYR  |
| 11  | AL    | 109 | ARG  |
| 12  | AM    | 7   | ASN  |
| 12  | AM    | 42  | VAL  |
| 12  | AM    | 70  | ARG  |
| 12  | AM    | 74  | MET  |
| 12  | AM    | 103 | THR  |
| 13  | AN    | 3   | GLN  |
| 13  | AN    | 47  | LEU  |
| 13  | AN    | 59  | GLN  |
| 13  | AN    | 61  | ASN  |
| 13  | AN    | 96  | LYS  |
| 13  | AN    | 99  | SER  |
| 14  | AO    | 16  | ARG  |
| 14  | AO    | 24  | THR  |
| 14  | AO    | 36  | ASN  |
| 14  | AO    | 63  | ARG  |
| 15  | AP    | 6   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | AP    | 16  | PHE  |
| 15  | AP    | 19  | VAL  |
| 15  | AP    | 46  | LYS  |
| 15  | AP    | 52  | LEU  |
| 16  | AQ    | 3   | LYS  |
| 16  | AQ    | 10  | ARG  |
| 16  | AQ    | 16  | MET  |
| 16  | AQ    | 20  | ILE  |
| 16  | AQ    | 28  | VAL  |
| 16  | AQ    | 37  | ILE  |
| 16  | AQ    | 47  | ASP  |
| 16  | AQ    | 49  | ASN  |
| 16  | AQ    | 51  | GLU  |
| 16  | AQ    | 60  | ILE  |
| 16  | AQ    | 64  | ARG  |
| 16  | AQ    | 74  | LEU  |
| 16  | AQ    | 79  | GLU  |
| 16  | AQ    | 80  | LYS  |
| 17  | AR    | 24  | ASP  |
| 17  | AR    | 35  | SER  |
| 18  | AS    | 20  | LYS  |
| 18  | AS    | 32  | THR  |
| 18  | AS    | 42  | ASN  |
| 18  | AS    | 54  | ARG  |
| 18  | AS    | 60  | PHE  |
| 18  | AS    | 61  | VAL  |
| 18  | AS    | 64  | GLU  |
| 19  | AT    | 4   | LYS  |
| 19  | AT    | 13  | SER  |
| 19  | AT    | 23  | ARG  |
| 19  | AT    | 27  | MET  |
| 19  | AT    | 35  | TYR  |
| 19  | AT    | 42  | ASP  |
| 19  | AT    | 67  | HIS  |
| 19  | AT    | 75  | LYS  |
| 19  | AT    | 77  | ASN  |
| 19  | AT    | 84  | LYS  |
| 20  | AU    | 4   | LYS  |
| 20  | AU    | 8   | ASN  |
| 20  | AU    | 18  | PHE  |
| 20  | AU    | 19  | LYS  |
| 20  | AU    | 33  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | AU    | 37  | TYR  |
| 20  | AU    | 42  | THR  |
| 26  | BC    | 12  | ARG  |
| 26  | BC    | 18  | VAL  |
| 26  | BC    | 20  | ASN  |
| 26  | BC    | 27  | LYS  |
| 26  | BC    | 35  | LYS  |
| 26  | BC    | 38  | LYS  |
| 26  | BC    | 43  | ASN  |
| 26  | BC    | 71  | ASP  |
| 26  | BC    | 73  | ILE  |
| 26  | BC    | 77  | VAL  |
| 26  | BC    | 85  | ASN  |
| 26  | BC    | 90  | ILE  |
| 26  | BC    | 93  | VAL  |
| 26  | BC    | 104 | LEU  |
| 26  | BC    | 109 | LEU  |
| 26  | BC    | 110 | LYS  |
| 26  | BC    | 114 | GLN  |
| 26  | BC    | 115 | ILE  |
| 26  | BC    | 120 | ASP  |
| 26  | BC    | 123 | ILE  |
| 26  | BC    | 129 | LEU  |
| 26  | BC    | 132 | ARG  |
| 26  | BC    | 142 | ASN  |
| 26  | BC    | 155 | ARG  |
| 26  | BC    | 164 | VAL  |
| 26  | BC    | 171 | VAL  |
| 26  | BC    | 172 | THR  |
| 26  | BC    | 173 | LEU  |
| 26  | BC    | 175 | LEU  |
| 26  | BC    | 176 | ARG  |
| 26  | BC    | 201 | LEU  |
| 26  | BC    | 202 | ARG  |
| 26  | BC    | 203 | VAL  |
| 26  | BC    | 212 | TRP  |
| 26  | BC    | 213 | ARG  |
| 26  | BC    | 215 | VAL  |
| 26  | BC    | 227 | VAL  |
| 26  | BC    | 250 | GLN  |
| 26  | BC    | 252 | LYS  |
| 26  | BC    | 254 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | BC    | 261 | ARG  |
| 26  | BC    | 268 | ARG  |
| 26  | BC    | 269 | ARG  |
| 27  | BD    | 4   | LEU  |
| 27  | BD    | 14  | ILE  |
| 27  | BD    | 16  | THR  |
| 27  | BD    | 17  | GLU  |
| 27  | BD    | 40  | LEU  |
| 27  | BD    | 42  | ASN  |
| 27  | BD    | 43  | ASP  |
| 27  | BD    | 45  | TYR  |
| 27  | BD    | 60  | VAL  |
| 27  | BD    | 73  | VAL  |
| 27  | BD    | 89  | GLU  |
| 27  | BD    | 90  | PHE  |
| 27  | BD    | 91  | THR  |
| 27  | BD    | 98  | VAL  |
| 27  | BD    | 106 | LYS  |
| 27  | BD    | 114 | LYS  |
| 27  | BD    | 118 | PHE  |
| 27  | BD    | 124 | ARG  |
| 27  | BD    | 131 | ASP  |
| 27  | BD    | 139 | SER  |
| 27  | BD    | 140 | HIS  |
| 27  | BD    | 150 | GLN  |
| 27  | BD    | 159 | LYS  |
| 27  | BD    | 169 | ARG  |
| 27  | BD    | 171 | THR  |
| 27  | BD    | 176 | ASP  |
| 27  | BD    | 183 | GLU  |
| 27  | BD    | 186 | LEU  |
| 28  | BE    | 12  | LEU  |
| 28  | BE    | 14  | VAL  |
| 28  | BE    | 24  | ASN  |
| 28  | BE    | 44  | ARG  |
| 28  | BE    | 48  | THR  |
| 28  | BE    | 61  | ARG  |
| 28  | BE    | 65  | THR  |
| 28  | BE    | 69  | ARG  |
| 28  | BE    | 70  | SER  |
| 28  | BE    | 77  | ILE  |
| 28  | BE    | 78  | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | BE    | 80  | SER  |
| 28  | BE    | 84  | THR  |
| 28  | BE    | 90  | GLN  |
| 28  | BE    | 91  | ASP  |
| 28  | BE    | 108 | ILE  |
| 28  | BE    | 109 | LEU  |
| 28  | BE    | 111 | GLU  |
| 28  | BE    | 113 | VAL  |
| 28  | BE    | 116 | ASP  |
| 28  | BE    | 118 | LEU  |
| 28  | BE    | 119 | ILE  |
| 28  | BE    | 121 | VAL  |
| 28  | BE    | 123 | LYS  |
| 28  | BE    | 127 | GLU  |
| 28  | BE    | 144 | GLU  |
| 28  | BE    | 146 | VAL  |
| 28  | BE    | 153 | LEU  |
| 28  | BE    | 159 | LEU  |
| 28  | BE    | 163 | ASN  |
| 28  | BE    | 170 | ARG  |
| 28  | BE    | 171 | ASP  |
| 28  | BE    | 178 | VAL  |
| 28  | BE    | 186 | VAL  |
| 28  | BE    | 189 | THR  |
| 29  | BF    | 3   | LEU  |
| 29  | BF    | 9   | ASP  |
| 29  | BF    | 12  | VAL  |
| 29  | BF    | 24  | VAL  |
| 29  | BF    | 34  | THR  |
| 29  | BF    | 35  | LEU  |
| 29  | BF    | 36  | ASN  |
| 29  | BF    | 46  | LYS  |
| 29  | BF    | 65  | LEU  |
| 29  | BF    | 82  | TYR  |
| 29  | BF    | 90  | LEU  |
| 29  | BF    | 103 | ILE  |
| 29  | BF    | 109 | ARG  |
| 29  | BF    | 111 | ARG  |
| 29  | BF    | 114 | ARG  |
| 29  | BF    | 132 | ARG  |
| 29  | BF    | 134 | GLN  |
| 29  | BF    | 154 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | BG    | 8   | VAL  |
| 30  | BG    | 15  | ASP  |
| 30  | BG    | 21  | GLN  |
| 30  | BG    | 29  | ASN  |
| 30  | BG    | 32  | LEU  |
| 30  | BG    | 34  | ARG  |
| 30  | BG    | 35  | THR  |
| 30  | BG    | 37  | ASN  |
| 30  | BG    | 40  | VAL  |
| 30  | BG    | 55  | ASP  |
| 30  | BG    | 59  | ASP  |
| 30  | BG    | 68  | ARG  |
| 30  | BG    | 72  | ASN  |
| 30  | BG    | 78  | VAL  |
| 30  | BG    | 80  | GLU  |
| 30  | BG    | 84  | LYS  |
| 30  | BG    | 86  | LEU  |
| 30  | BG    | 91  | VAL  |
| 30  | BG    | 93  | TYR  |
| 30  | BG    | 101 | VAL  |
| 30  | BG    | 116 | LEU  |
| 30  | BG    | 120 | ILE  |
| 30  | BG    | 121 | THR  |
| 30  | BG    | 123 | GLU  |
| 30  | BG    | 126 | THR  |
| 30  | BG    | 132 | LEU  |
| 30  | BG    | 138 | GLN  |
| 30  | BG    | 148 | ARG  |
| 30  | BG    | 170 | THR  |
| 30  | BG    | 174 | LYS  |
| 31  | BH    | 6   | LEU  |
| 31  | BH    | 12  | LEU  |
| 31  | BH    | 14  | SER  |
| 31  | BH    | 15  | LEU  |
| 31  | BH    | 18  | GLN  |
| 31  | BH    | 28  | ASN  |
| 31  | BH    | 31  | VAL  |
| 31  | BH    | 48  | GLU  |
| 31  | BH    | 50  | ARG  |
| 31  | BH    | 54  | LEU  |
| 31  | BH    | 68  | ARG  |
| 31  | BH    | 75  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | BH    | 83  | LYS  |
| 31  | BH    | 96  | THR  |
| 31  | BH    | 97  | ARG  |
| 31  | BH    | 125 | THR  |
| 31  | BH    | 135 | HIS  |
| 32  | BI    | 2   | LYS  |
| 32  | BI    | 10  | LEU  |
| 32  | BI    | 11  | GLN  |
| 32  | BI    | 23  | VAL  |
| 32  | BI    | 37  | PHE  |
| 32  | BI    | 39  | LYS  |
| 32  | BI    | 49  | GLU  |
| 32  | BI    | 61  | TYR  |
| 32  | BI    | 71  | LYS  |
| 32  | BI    | 81  | LYS  |
| 32  | BI    | 86  | LYS  |
| 32  | BI    | 95  | ASP  |
| 32  | BI    | 107 | GLU  |
| 32  | BI    | 126 | ARG  |
| 32  | BI    | 135 | MET  |
| 33  | BJ    | 1   | MET  |
| 33  | BJ    | 2   | LYS  |
| 33  | BJ    | 3   | THR  |
| 33  | BJ    | 7   | LYS  |
| 33  | BJ    | 24  | THR  |
| 33  | BJ    | 25  | LEU  |
| 33  | BJ    | 30  | THR  |
| 33  | BJ    | 31  | GLU  |
| 33  | BJ    | 36  | LEU  |
| 33  | BJ    | 40  | HIS  |
| 33  | BJ    | 41  | LYS  |
| 33  | BJ    | 43  | GLU  |
| 33  | BJ    | 44  | TYR  |
| 33  | BJ    | 54  | ILE  |
| 33  | BJ    | 55  | ILE  |
| 33  | BJ    | 65  | THR  |
| 33  | BJ    | 72  | LYS  |
| 33  | BJ    | 86  | GLN  |
| 33  | BJ    | 88  | THR  |
| 33  | BJ    | 90  | GLU  |
| 33  | BJ    | 103 | ILE  |
| 33  | BJ    | 111 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | BJ    | 114 | LEU  |
| 33  | BJ    | 129 | GLU  |
| 33  | BJ    | 139 | VAL  |
| 33  | BJ    | 140 | LEU  |
| 34  | BK    | 2   | ILE  |
| 34  | BK    | 3   | GLN  |
| 34  | BK    | 8   | LEU  |
| 34  | BK    | 18  | ARG  |
| 34  | BK    | 21  | CYS  |
| 34  | BK    | 23  | LYS  |
| 34  | BK    | 47  | ILE  |
| 34  | BK    | 51  | LYS  |
| 34  | BK    | 52  | VAL  |
| 34  | BK    | 54  | LYS  |
| 34  | BK    | 58  | LEU  |
| 34  | BK    | 69  | VAL  |
| 34  | BK    | 73  | ASP  |
| 34  | BK    | 88  | ASN  |
| 34  | BK    | 89  | ASN  |
| 34  | BK    | 93  | GLN  |
| 34  | BK    | 105 | ARG  |
| 34  | BK    | 111 | LYS  |
| 34  | BK    | 114 | LYS  |
| 35  | BL    | 3   | LEU  |
| 35  | BL    | 4   | ASN  |
| 35  | BL    | 6   | LEU  |
| 35  | BL    | 13  | LYS  |
| 35  | BL    | 14  | LYS  |
| 35  | BL    | 19  | LEU  |
| 35  | BL    | 21  | ARG  |
| 35  | BL    | 27  | LEU  |
| 35  | BL    | 46  | VAL  |
| 35  | BL    | 47  | ARG  |
| 35  | BL    | 55  | MET  |
| 35  | BL    | 61  | LEU  |
| 35  | BL    | 66  | PHE  |
| 35  | BL    | 91  | ASP  |
| 35  | BL    | 93  | ASN  |
| 35  | BL    | 94  | THR  |
| 35  | BL    | 101 | ILE  |
| 35  | BL    | 112 | LEU  |
| 35  | BL    | 121 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | BL    | 122 | VAL  |
| 35  | BL    | 135 | ILE  |
| 36  | BM    | 8   | LYS  |
| 36  | BM    | 10  | ARG  |
| 36  | BM    | 12  | MET  |
| 36  | BM    | 25  | ASP  |
| 36  | BM    | 33  | LEU  |
| 36  | BM    | 36  | VAL  |
| 36  | BM    | 58  | LYS  |
| 36  | BM    | 70  | ASP  |
| 36  | BM    | 75  | GLU  |
| 36  | BM    | 90  | GLU  |
| 36  | BM    | 95  | LEU  |
| 36  | BM    | 96  | ILE  |
| 36  | BM    | 97  | GLN  |
| 36  | BM    | 100 | LYS  |
| 36  | BM    | 102 | LEU  |
| 36  | BM    | 110 | GLU  |
| 36  | BM    | 131 | VAL  |
| 36  | BM    | 133 | LYS  |
| 36  | BM    | 134 | THR  |
| 37  | BN    | 2   | ARG  |
| 37  | BN    | 3   | HIS  |
| 37  | BN    | 8   | ARG  |
| 37  | BN    | 10  | LEU  |
| 37  | BN    | 14  | SER  |
| 37  | BN    | 15  | SER  |
| 37  | BN    | 20  | MET  |
| 37  | BN    | 23  | ASN  |
| 37  | BN    | 33  | ILE  |
| 37  | BN    | 35  | LYS  |
| 37  | BN    | 38  | LEU  |
| 37  | BN    | 51  | LEU  |
| 37  | BN    | 69  | ARG  |
| 37  | BN    | 71  | ARG  |
| 37  | BN    | 75  | ILE  |
| 37  | BN    | 79  | LEU  |
| 37  | BN    | 83  | LEU  |
| 37  | BN    | 95  | THR  |
| 37  | BN    | 120 | GLU  |
| 38  | BO    | 4   | LYS  |
| 38  | BO    | 9   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | BO    | 16  | ARG  |
| 38  | BO    | 17  | LYS  |
| 38  | BO    | 28  | VAL  |
| 38  | BO    | 31  | THR  |
| 38  | BO    | 36  | TYR  |
| 38  | BO    | 52  | SER  |
| 38  | BO    | 53  | THR  |
| 38  | BO    | 65  | THR  |
| 38  | BO    | 80  | GLU  |
| 38  | BO    | 83  | LEU  |
| 38  | BO    | 84  | GLU  |
| 38  | BO    | 94  | ARG  |
| 38  | BO    | 100 | HIS  |
| 38  | BO    | 103 | VAL  |
| 38  | BO    | 111 | ARG  |
| 39  | BP    | 3   | ILE  |
| 39  | BP    | 6   | GLN  |
| 39  | BP    | 14  | GLN  |
| 39  | BP    | 16  | VAL  |
| 39  | BP    | 24  | THR  |
| 39  | BP    | 36  | LYS  |
| 39  | BP    | 37  | LYS  |
| 39  | BP    | 38  | ARG  |
| 39  | BP    | 61  | ARG  |
| 39  | BP    | 69  | VAL  |
| 39  | BP    | 75  | THR  |
| 39  | BP    | 77  | SER  |
| 39  | BP    | 79  | VAL  |
| 39  | BP    | 83  | ILE  |
| 39  | BP    | 91  | VAL  |
| 39  | BP    | 92  | ARG  |
| 39  | BP    | 93  | LYS  |
| 39  | BP    | 95  | LYS  |
| 39  | BP    | 96  | LEU  |
| 39  | BP    | 99  | LEU  |
| 40  | BQ    | 2   | ARG  |
| 40  | BQ    | 8   | ILE  |
| 40  | BQ    | 10  | ARG  |
| 40  | BQ    | 40  | LYS  |
| 40  | BQ    | 50  | ARG  |
| 40  | BQ    | 59  | LEU  |
| 40  | BQ    | 63  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | BQ    | 65  | ASN  |
| 40  | BQ    | 69  | ARG  |
| 40  | BQ    | 88  | GLU  |
| 40  | BQ    | 91  | ARG  |
| 40  | BQ    | 93  | ILE  |
| 40  | BQ    | 94  | LEU  |
| 40  | BQ    | 96  | ASP  |
| 40  | BQ    | 97  | ILE  |
| 40  | BQ    | 103 | VAL  |
| 41  | BR    | 10  | LYS  |
| 41  | BR    | 14  | VAL  |
| 41  | BR    | 37  | GLU  |
| 41  | BR    | 38  | VAL  |
| 41  | BR    | 39  | LEU  |
| 41  | BR    | 43  | ASN  |
| 41  | BR    | 46  | GLU  |
| 41  | BR    | 48  | LYS  |
| 41  | BR    | 54  | VAL  |
| 41  | BR    | 63  | VAL  |
| 41  | BR    | 72  | VAL  |
| 41  | BR    | 83  | TYR  |
| 41  | BR    | 85  | LYS  |
| 41  | BR    | 86  | GLN  |
| 41  | BR    | 97  | LYS  |
| 42  | BS    | 3   | THR  |
| 42  | BS    | 4   | ILE  |
| 42  | BS    | 7   | HIS  |
| 42  | BS    | 30  | SER  |
| 42  | BS    | 36  | LEU  |
| 42  | BS    | 41  | LYS  |
| 42  | BS    | 45  | VAL  |
| 42  | BS    | 48  | LYS  |
| 42  | BS    | 66  | ILE  |
| 42  | BS    | 68  | ASP  |
| 42  | BS    | 70  | LYS  |
| 42  | BS    | 71  | VAL  |
| 42  | BS    | 73  | LYS  |
| 42  | BS    | 76  | VAL  |
| 42  | BS    | 84  | ARG  |
| 42  | BS    | 88  | ARG  |
| 42  | BS    | 96  | ILE  |
| 42  | BS    | 101 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | BS    | 107 | VAL  |
| 42  | BS    | 109 | ASP  |
| 43  | BT    | 2   | ILE  |
| 43  | BT    | 3   | ARG  |
| 43  | BT    | 4   | GLU  |
| 43  | BT    | 8   | LEU  |
| 43  | BT    | 17  | SER  |
| 43  | BT    | 19  | LYS  |
| 43  | BT    | 29  | THR  |
| 43  | BT    | 30  | ILE  |
| 43  | BT    | 31  | VAL  |
| 43  | BT    | 43  | ILE  |
| 43  | BT    | 48  | GLN  |
| 43  | BT    | 49  | LYS  |
| 43  | BT    | 50  | LEU  |
| 43  | BT    | 64  | LYS  |
| 43  | BT    | 67  | VAL  |
| 43  | BT    | 68  | LYS  |
| 43  | BT    | 69  | ARG  |
| 43  | BT    | 73  | ARG  |
| 43  | BT    | 74  | ILE  |
| 44  | BU    | 6   | ARG  |
| 44  | BU    | 8   | ASP  |
| 44  | BU    | 10  | VAL  |
| 44  | BU    | 33  | VAL  |
| 44  | BU    | 42  | LYS  |
| 44  | BU    | 43  | LYS  |
| 44  | BU    | 52  | ASN  |
| 44  | BU    | 61  | GLU  |
| 44  | BU    | 64  | ILE  |
| 44  | BU    | 67  | SER  |
| 44  | BU    | 80  | ASP  |
| 44  | BU    | 86  | PHE  |
| 44  | BU    | 99  | SER  |
| 44  | BU    | 102 | ILE  |
| 45  | BV    | 1   | MET  |
| 45  | BV    | 3   | THR  |
| 45  | BV    | 5   | ASN  |
| 45  | BV    | 8   | VAL  |
| 45  | BV    | 10  | LYS  |
| 45  | BV    | 20  | LEU  |
| 45  | BV    | 29  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | BV    | 41  | GLU  |
| 45  | BV    | 42  | LEU  |
| 45  | BV    | 43  | ASP  |
| 45  | BV    | 46  | LYS  |
| 45  | BV    | 51  | GLN  |
| 45  | BV    | 61  | LEU  |
| 45  | BV    | 66  | ASP  |
| 46  | BW    | 14  | ASP  |
| 46  | BW    | 15  | SER  |
| 46  | BW    | 19  | ARG  |
| 46  | BW    | 23  | LYS  |
| 46  | BW    | 24  | ARG  |
| 46  | BW    | 25  | PHE  |
| 46  | BW    | 38  | ARG  |
| 46  | BW    | 40  | ARG  |
| 46  | BW    | 45  | HIS  |
| 46  | BW    | 49  | ASN  |
| 46  | BW    | 54  | ARG  |
| 46  | BW    | 58  | LEU  |
| 46  | BW    | 67  | LYS  |
| 46  | BW    | 71  | LYS  |
| 46  | BW    | 77  | LYS  |
| 46  | BW    | 80  | SER  |
| 47  | BX    | 6   | VAL  |
| 47  | BX    | 10  | ARG  |
| 47  | BX    | 17  | ARG  |
| 47  | BX    | 19  | HIS  |
| 47  | BX    | 24  | THR  |
| 47  | BX    | 26  | ARG  |
| 47  | BX    | 27  | ARG  |
| 47  | BX    | 29  | LEU  |
| 47  | BX    | 47  | THR  |
| 47  | BX    | 53  | LYS  |
| 47  | BX    | 65  | THR  |
| 47  | BX    | 71  | ARG  |
| 47  | BX    | 73  | ARG  |
| 47  | BX    | 77  | TYR  |
| 48  | BY    | 9   | LYS  |
| 48  | BY    | 10  | SER  |
| 48  | BY    | 14  | LEU  |
| 48  | BY    | 18  | LEU  |
| 48  | BY    | 19  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | BY    | 22  | LEU  |
| 48  | BY    | 37  | LEU  |
| 48  | BY    | 42  | LEU  |
| 48  | BY    | 56  | LEU  |
| 48  | BY    | 57  | LEU  |
| 48  | BY    | 59  | GLU  |
| 49  | BZ    | 2   | LYS  |
| 49  | BZ    | 3   | THR  |
| 49  | BZ    | 4   | ILE  |
| 49  | BZ    | 5   | LYS  |
| 49  | BZ    | 8   | GLN  |
| 49  | BZ    | 9   | THR  |
| 49  | BZ    | 15  | ARG  |
| 49  | BZ    | 23  | LEU  |
| 49  | BZ    | 29  | ARG  |
| 49  | BZ    | 30  | ARG  |
| 49  | BZ    | 37  | ARG  |
| 49  | BZ    | 38  | GLU  |
| 49  | BZ    | 43  | ILE  |
| 49  | BZ    | 58  | GLU  |
| 50  | B0    | 9   | ARG  |
| 50  | B0    | 27  | LEU  |
| 50  | B0    | 28  | SER  |
| 50  | B0    | 39  | ARG  |
| 50  | B0    | 42  | ILE  |
| 51  | B1    | 4   | ILE  |
| 51  | B1    | 9   | LYS  |
| 51  | B1    | 16  | THR  |
| 51  | B1    | 21  | THR  |
| 51  | B1    | 33  | LEU  |
| 51  | B1    | 35  | LEU  |
| 51  | B1    | 42  | VAL  |
| 51  | B1    | 43  | ARG  |
| 52  | B2    | 1   | MET  |
| 52  | B2    | 3   | ARG  |
| 52  | B2    | 12  | ARG  |
| 52  | B2    | 16  | HIS  |
| 52  | B2    | 21  | ARG  |
| 52  | B2    | 39  | ARG  |
| 53  | B3    | 5   | THR  |
| 53  | B3    | 7   | ARG  |
| 53  | B3    | 22  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | B3    | 31  | ILE  |
| 53  | B3    | 34  | LYS  |
| 53  | B3    | 49  | VAL  |
| 53  | B3    | 51  | LYS  |
| 54  | B4    | 1   | MET  |
| 54  | B4    | 4   | ARG  |
| 54  | B4    | 9   | LYS  |
| 54  | B4    | 13  | ASN  |
| 1   | CB    | 8   | MET  |
| 1   | CB    | 10  | LYS  |
| 1   | CB    | 17  | HIS  |
| 1   | CB    | 19  | THR  |
| 1   | CB    | 26  | MET  |
| 1   | CB    | 29  | PHE  |
| 1   | CB    | 34  | ARG  |
| 1   | CB    | 36  | LYS  |
| 1   | CB    | 39  | ILE  |
| 1   | CB    | 46  | VAL  |
| 1   | CB    | 57  | ASN  |
| 1   | CB    | 61  | SER  |
| 1   | CB    | 69  | VAL  |
| 1   | CB    | 88  | GLN  |
| 1   | CB    | 92  | ASN  |
| 1   | CB    | 103 | TRP  |
| 1   | CB    | 124 | THR  |
| 1   | CB    | 125 | PHE  |
| 1   | CB    | 162 | VAL  |
| 1   | CB    | 172 | ILE  |
| 1   | CB    | 191 | ASP  |
| 1   | CB    | 196 | ASP  |
| 2   | CC    | 2   | GLN  |
| 2   | CC    | 26  | LYS  |
| 2   | CC    | 27  | GLU  |
| 2   | CC    | 35  | ASP  |
| 2   | CC    | 38  | VAL  |
| 2   | CC    | 41  | TYR  |
| 2   | CC    | 53  | ARG  |
| 2   | CC    | 54  | ILE  |
| 2   | CC    | 58  | ARG  |
| 2   | CC    | 102 | ILE  |
| 2   | CC    | 106 | ARG  |
| 2   | CC    | 110 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CC    | 123 | LEU  |
| 2   | CC    | 134 | LYS  |
| 2   | CC    | 139 | ASN  |
| 2   | CC    | 161 | ILE  |
| 2   | CC    | 164 | THR  |
| 2   | CC    | 166 | TRP  |
| 2   | CC    | 174 | LEU  |
| 2   | CC    | 178 | ARG  |
| 2   | CC    | 182 | ASP  |
| 2   | CC    | 190 | THR  |
| 2   | CC    | 194 | VAL  |
| 2   | CC    | 205 | GLU  |
| 3   | CD    | 2   | ARG  |
| 3   | CD    | 12  | ARG  |
| 3   | CD    | 30  | LYS  |
| 3   | CD    | 34  | GLU  |
| 3   | CD    | 55  | ARG  |
| 3   | CD    | 57  | LYS  |
| 3   | CD    | 58  | GLN  |
| 3   | CD    | 62  | ARG  |
| 3   | CD    | 99  | ASN  |
| 3   | CD    | 106 | PHE  |
| 3   | CD    | 116 | LEU  |
| 3   | CD    | 125 | ASN  |
| 3   | CD    | 127 | ARG  |
| 3   | CD    | 147 | LYS  |
| 3   | CD    | 153 | ARG  |
| 3   | CD    | 163 | GLN  |
| 3   | CD    | 170 | LEU  |
| 3   | CD    | 187 | ARG  |
| 3   | CD    | 188 | SER  |
| 3   | CD    | 199 | ILE  |
| 4   | CE    | 11  | GLN  |
| 4   | CE    | 13  | LYS  |
| 4   | CE    | 25  | LYS  |
| 4   | CE    | 35  | LEU  |
| 4   | CE    | 59  | ILE  |
| 4   | CE    | 64  | GLU  |
| 4   | CE    | 67  | ARG  |
| 4   | CE    | 75  | LEU  |
| 4   | CE    | 76  | ASN  |
| 4   | CE    | 131 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | CE    | 133 | ILE  |
| 4   | CE    | 136 | VAL  |
| 4   | CE    | 144 | GLU  |
| 5   | CF    | 7   | VAL  |
| 5   | CF    | 17  | GLN  |
| 5   | CF    | 33  | GLU  |
| 5   | CF    | 38  | ARG  |
| 5   | CF    | 56  | LYS  |
| 5   | CF    | 61  | LEU  |
| 5   | CF    | 72  | ASP  |
| 5   | CF    | 73  | GLU  |
| 5   | CF    | 81  | ASN  |
| 5   | CF    | 84  | VAL  |
| 5   | CF    | 85  | ILE  |
| 5   | CF    | 86  | ARG  |
| 5   | CF    | 98  | GLU  |
| 6   | CG    | 3   | ARG  |
| 6   | CG    | 8   | GLN  |
| 6   | CG    | 10  | LYS  |
| 6   | CG    | 11  | ILE  |
| 6   | CG    | 12  | LEU  |
| 6   | CG    | 16  | LYS  |
| 6   | CG    | 22  | LEU  |
| 6   | CG    | 48  | THR  |
| 6   | CG    | 55  | LYS  |
| 6   | CG    | 58  | LEU  |
| 6   | CG    | 59  | GLU  |
| 6   | CG    | 62  | GLU  |
| 6   | CG    | 65  | LEU  |
| 6   | CG    | 66  | GLU  |
| 6   | CG    | 67  | ASN  |
| 6   | CG    | 75  | LYS  |
| 6   | CG    | 77  | ARG  |
| 6   | CG    | 78  | ARG  |
| 6   | CG    | 85  | GLN  |
| 6   | CG    | 100 | MET  |
| 6   | CG    | 102 | TRP  |
| 6   | CG    | 115 | MET  |
| 6   | CG    | 119 | LEU  |
| 6   | CG    | 123 | LEU  |
| 6   | CG    | 137 | ARG  |
| 6   | CG    | 139 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | CG    | 148 | LYS  |
| 6   | CG    | 150 | PHE  |
| 7   | CH    | 2   | MET  |
| 7   | CH    | 29  | SER  |
| 7   | CH    | 33  | VAL  |
| 7   | CH    | 37  | ASN  |
| 7   | CH    | 42  | GLU  |
| 7   | CH    | 45  | ILE  |
| 7   | CH    | 46  | GLU  |
| 7   | CH    | 76  | ARG  |
| 7   | CH    | 82  | LEU  |
| 7   | CH    | 89  | ASP  |
| 7   | CH    | 93  | LYS  |
| 7   | CH    | 98  | LEU  |
| 7   | CH    | 110 | MET  |
| 8   | CI    | 4   | GLN  |
| 8   | CI    | 37  | TYR  |
| 8   | CI    | 45  | MET  |
| 8   | CI    | 47  | VAL  |
| 8   | CI    | 53  | LEU  |
| 8   | CI    | 54  | VAL  |
| 8   | CI    | 63  | TYR  |
| 8   | CI    | 71  | ILE  |
| 8   | CI    | 72  | SER  |
| 8   | CI    | 87  | MET  |
| 8   | CI    | 89  | TYR  |
| 8   | CI    | 111 | GLU  |
| 8   | CI    | 125 | GLN  |
| 8   | CI    | 126 | PHE  |
| 9   | CJ    | 11  | LYS  |
| 9   | CJ    | 15  | HIS  |
| 9   | CJ    | 59  | LYS  |
| 9   | CJ    | 63  | ASP  |
| 9   | CJ    | 67  | ILE  |
| 9   | CJ    | 69  | THR  |
| 9   | CJ    | 80  | THR  |
| 9   | CJ    | 82  | LYS  |
| 9   | CJ    | 92  | LEU  |
| 10  | CK    | 27  | ASN  |
| 10  | CK    | 45  | THR  |
| 10  | CK    | 55  | ARG  |
| 10  | CK    | 73  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | CK    | 78  | ILE  |
| 10  | CK    | 80  | ASN  |
| 10  | CK    | 81  | LEU  |
| 10  | CK    | 105 | ARG  |
| 10  | CK    | 106 | ILE  |
| 10  | CK    | 117 | HIS  |
| 11  | CL    | 5   | GLN  |
| 11  | CL    | 7   | VAL  |
| 11  | CL    | 14  | LYS  |
| 11  | CL    | 19  | ASN  |
| 11  | CL    | 28  | GLN  |
| 11  | CL    | 48  | LEU  |
| 11  | CL    | 49  | ARG  |
| 11  | CL    | 56  | LEU  |
| 11  | CL    | 62  | VAL  |
| 11  | CL    | 65  | TYR  |
| 11  | CL    | 72  | ASN  |
| 11  | CL    | 88  | ASP  |
| 11  | CL    | 107 | LYS  |
| 11  | CL    | 111 | GLN  |
| 11  | CL    | 120 | ARG  |
| 12  | CM    | 2   | ARG  |
| 12  | CM    | 7   | ASN  |
| 12  | CM    | 8   | ILE  |
| 12  | CM    | 12  | LYS  |
| 12  | CM    | 13  | HIS  |
| 12  | CM    | 24  | VAL  |
| 12  | CM    | 28  | ARG  |
| 12  | CM    | 32  | ILE  |
| 12  | CM    | 46  | GLU  |
| 12  | CM    | 53  | ASP  |
| 12  | CM    | 68  | LEU  |
| 12  | CM    | 77  | LYS  |
| 12  | CM    | 91  | ARG  |
| 12  | CM    | 92  | ARG  |
| 12  | CM    | 99  | GLN  |
| 12  | CM    | 100 | ARG  |
| 12  | CM    | 113 | LYS  |
| 13  | CN    | 3   | GLN  |
| 13  | CN    | 17  | ASP  |
| 13  | CN    | 27  | LYS  |
| 13  | CN    | 30  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | CN    | 41  | TRP  |
| 13  | CN    | 52  | ARG  |
| 13  | CN    | 53  | ASP  |
| 13  | CN    | 58  | ARG  |
| 13  | CN    | 65  | GLN  |
| 13  | CN    | 72  | PHE  |
| 13  | CN    | 96  | LYS  |
| 14  | CO    | 13  | GLU  |
| 14  | CO    | 16  | ARG  |
| 14  | CO    | 63  | ARG  |
| 14  | CO    | 80  | LEU  |
| 15  | CP    | 3   | THR  |
| 15  | CP    | 6   | LEU  |
| 15  | CP    | 19  | VAL  |
| 15  | CP    | 35  | ARG  |
| 15  | CP    | 46  | LYS  |
| 15  | CP    | 67  | ILE  |
| 16  | CQ    | 3   | LYS  |
| 16  | CQ    | 20  | ILE  |
| 16  | CQ    | 27  | PHE  |
| 16  | CQ    | 39  | ARG  |
| 16  | CQ    | 51  | GLU  |
| 16  | CQ    | 52  | CYS  |
| 16  | CQ    | 60  | ILE  |
| 16  | CQ    | 73  | THR  |
| 16  | CQ    | 75  | VAL  |
| 16  | CQ    | 80  | LYS  |
| 17  | CR    | 69  | TYR  |
| 17  | CR    | 72  | ARG  |
| 18  | CS    | 5   | LYS  |
| 18  | CS    | 10  | ILE  |
| 18  | CS    | 11  | ASP  |
| 18  | CS    | 38  | THR  |
| 18  | CS    | 43  | MET  |
| 18  | CS    | 52  | ASN  |
| 18  | CS    | 54  | ARG  |
| 18  | CS    | 55  | GLN  |
| 18  | CS    | 56  | HIS  |
| 18  | CS    | 62  | THR  |
| 18  | CS    | 79  | TYR  |
| 19  | CT    | 26  | MET  |
| 19  | CT    | 30  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | CT    | 47  | GLN  |
| 19  | CT    | 53  | MET  |
| 19  | CT    | 68  | LYS  |
| 19  | CT    | 69  | ASN  |
| 19  | CT    | 73  | ARG  |
| 19  | CT    | 77  | ASN  |
| 19  | CT    | 82  | ILE  |
| 20  | CU    | 4   | LYS  |
| 20  | CU    | 17  | ARG  |
| 20  | CU    | 18  | PHE  |
| 20  | CU    | 19  | LYS  |
| 20  | CU    | 32  | ARG  |
| 20  | CU    | 33  | ARG  |
| 20  | CU    | 37  | TYR  |
| 20  | CU    | 39  | LYS  |
| 20  | CU    | 53  | LYS  |
| 26  | DC    | 18  | VAL  |
| 26  | DC    | 23  | LEU  |
| 26  | DC    | 35  | LYS  |
| 26  | DC    | 51  | ARG  |
| 26  | DC    | 53  | ILE  |
| 26  | DC    | 57  | HIS  |
| 26  | DC    | 62  | ARG  |
| 26  | DC    | 90  | ILE  |
| 26  | DC    | 102 | TYR  |
| 26  | DC    | 124 | LYS  |
| 26  | DC    | 129 | LEU  |
| 26  | DC    | 152 | GLN  |
| 26  | DC    | 172 | THR  |
| 26  | DC    | 173 | LEU  |
| 26  | DC    | 183 | VAL  |
| 26  | DC    | 187 | CYS  |
| 26  | DC    | 188 | ARG  |
| 26  | DC    | 193 | GLU  |
| 26  | DC    | 212 | TRP  |
| 26  | DC    | 213 | ARG  |
| 26  | DC    | 220 | ARG  |
| 26  | DC    | 227 | VAL  |
| 26  | DC    | 235 | GLU  |
| 26  | DC    | 256 | THR  |
| 26  | DC    | 269 | ARG  |
| 27  | DD    | 24  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | DD    | 28  | GLU  |
| 27  | DD    | 33  | ARG  |
| 27  | DD    | 35  | THR  |
| 27  | DD    | 38  | LYS  |
| 27  | DD    | 50  | VAL  |
| 27  | DD    | 55  | LYS  |
| 27  | DD    | 62  | LYS  |
| 27  | DD    | 79  | LEU  |
| 27  | DD    | 84  | LEU  |
| 27  | DD    | 106 | LYS  |
| 27  | DD    | 121 | THR  |
| 27  | DD    | 138 | LEU  |
| 27  | DD    | 141 | ARG  |
| 27  | DD    | 148 | GLN  |
| 27  | DD    | 150 | GLN  |
| 27  | DD    | 159 | LYS  |
| 27  | DD    | 168 | GLU  |
| 27  | DD    | 189 | VAL  |
| 27  | DD    | 193 | VAL  |
| 28  | DE    | 53  | THR  |
| 28  | DE    | 57  | LYS  |
| 28  | DE    | 67  | ARG  |
| 28  | DE    | 77  | ILE  |
| 28  | DE    | 108 | ILE  |
| 28  | DE    | 117 | ARG  |
| 28  | DE    | 126 | VAL  |
| 28  | DE    | 139 | LYS  |
| 28  | DE    | 149 | ILE  |
| 28  | DE    | 157 | LEU  |
| 28  | DE    | 163 | ASN  |
| 28  | DE    | 164 | LEU  |
| 28  | DE    | 166 | LYS  |
| 29  | DF    | 13  | LYS  |
| 29  | DF    | 47  | LYS  |
| 29  | DF    | 48  | LEU  |
| 29  | DF    | 49  | LEU  |
| 29  | DF    | 76  | PHE  |
| 29  | DF    | 82  | TYR  |
| 29  | DF    | 94  | ARG  |
| 29  | DF    | 97  | GLU  |
| 29  | DF    | 109 | ARG  |
| 29  | DF    | 110 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | DF    | 111 | ARG  |
| 29  | DF    | 113 | PHE  |
| 29  | DF    | 119 | LYS  |
| 29  | DF    | 131 | VAL  |
| 29  | DF    | 133 | GLU  |
| 29  | DF    | 134 | GLN  |
| 29  | DF    | 135 | ILE  |
| 29  | DF    | 139 | GLU  |
| 29  | DF    | 142 | TYR  |
| 29  | DF    | 147 | ARG  |
| 29  | DF    | 151 | LEU  |
| 29  | DF    | 160 | LYS  |
| 29  | DF    | 166 | ARG  |
| 29  | DF    | 172 | PHE  |
| 29  | DF    | 177 | ARG  |
| 30  | DG    | 2   | ARG  |
| 30  | DG    | 18  | ILE  |
| 30  | DG    | 19  | ASN  |
| 30  | DG    | 21  | GLN  |
| 30  | DG    | 34  | ARG  |
| 30  | DG    | 35  | THR  |
| 30  | DG    | 40  | VAL  |
| 30  | DG    | 51  | PHE  |
| 30  | DG    | 72  | ASN  |
| 30  | DG    | 84  | LYS  |
| 30  | DG    | 91  | VAL  |
| 30  | DG    | 93  | TYR  |
| 30  | DG    | 120 | ILE  |
| 30  | DG    | 162 | ARG  |
| 30  | DG    | 163 | TYR  |
| 30  | DG    | 166 | GLU  |
| 30  | DG    | 176 | LYS  |
| 31  | DH    | 8   | LYS  |
| 31  | DH    | 22  | LYS  |
| 31  | DH    | 25  | TYR  |
| 31  | DH    | 27  | ARG  |
| 31  | DH    | 28  | ASN  |
| 31  | DH    | 48  | GLU  |
| 31  | DH    | 50  | ARG  |
| 31  | DH    | 57  | LYS  |
| 31  | DH    | 66  | ASN  |
| 31  | DH    | 68  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | DH    | 76  | GLU  |
| 31  | DH    | 86  | ASP  |
| 31  | DH    | 90  | LEU  |
| 31  | DH    | 91  | PHE  |
| 31  | DH    | 103 | VAL  |
| 31  | DH    | 104 | THR  |
| 31  | DH    | 109 | GLU  |
| 31  | DH    | 132 | PHE  |
| 31  | DH    | 144 | VAL  |
| 32  | DI    | 7   | TYR  |
| 32  | DI    | 9   | LYS  |
| 32  | DI    | 16  | MET  |
| 32  | DI    | 30  | GLN  |
| 32  | DI    | 58  | ILE  |
| 32  | DI    | 68  | PHE  |
| 32  | DI    | 93  | ASN  |
| 33  | DJ    | 3   | THR  |
| 33  | DJ    | 25  | LEU  |
| 33  | DJ    | 43  | GLU  |
| 33  | DJ    | 47  | HIS  |
| 33  | DJ    | 54  | ILE  |
| 33  | DJ    | 57  | LEU  |
| 33  | DJ    | 95  | ARG  |
| 33  | DJ    | 106 | LYS  |
| 33  | DJ    | 129 | GLU  |
| 33  | DJ    | 139 | VAL  |
| 34  | DK    | 3   | GLN  |
| 34  | DK    | 7   | MET  |
| 34  | DK    | 10  | VAL  |
| 34  | DK    | 13  | ASN  |
| 34  | DK    | 21  | CYS  |
| 34  | DK    | 25  | LEU  |
| 34  | DK    | 39  | ILE  |
| 34  | DK    | 41  | ILE  |
| 34  | DK    | 47  | ILE  |
| 34  | DK    | 49  | ARG  |
| 34  | DK    | 54  | LYS  |
| 34  | DK    | 87  | LEU  |
| 34  | DK    | 103 | VAL  |
| 34  | DK    | 105 | ARG  |
| 34  | DK    | 106 | GLU  |
| 34  | DK    | 107 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | DK    | 111 | LYS  |
| 34  | DK    | 114 | LYS  |
| 35  | DL    | 3   | LEU  |
| 35  | DL    | 4   | ASN  |
| 35  | DL    | 47  | ARG  |
| 35  | DL    | 79  | LEU  |
| 35  | DL    | 82  | LEU  |
| 35  | DL    | 92  | LEU  |
| 35  | DL    | 99  | ASN  |
| 35  | DL    | 103 | ILE  |
| 35  | DL    | 111 | ILE  |
| 35  | DL    | 112 | LEU  |
| 35  | DL    | 141 | LYS  |
| 35  | DL    | 143 | GLU  |
| 36  | DM    | 8   | LYS  |
| 36  | DM    | 50  | ARG  |
| 36  | DM    | 78  | LEU  |
| 36  | DM    | 96  | ILE  |
| 36  | DM    | 97  | GLN  |
| 36  | DM    | 102 | LEU  |
| 36  | DM    | 105 | MET  |
| 36  | DM    | 115 | GLU  |
| 36  | DM    | 126 | ILE  |
| 37  | DN    | 14  | SER  |
| 37  | DN    | 18  | GLN  |
| 37  | DN    | 20  | MET  |
| 37  | DN    | 29  | VAL  |
| 37  | DN    | 33  | ILE  |
| 37  | DN    | 53  | THR  |
| 37  | DN    | 54  | LEU  |
| 37  | DN    | 62  | ASN  |
| 37  | DN    | 63  | ARG  |
| 37  | DN    | 69  | ARG  |
| 37  | DN    | 81  | ASN  |
| 37  | DN    | 94  | TYR  |
| 37  | DN    | 95  | THR  |
| 37  | DN    | 98  | LEU  |
| 37  | DN    | 114 | GLU  |
| 38  | DO    | 17  | LYS  |
| 38  | DO    | 30  | ARG  |
| 38  | DO    | 31  | THR  |
| 38  | DO    | 65  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | DO    | 68  | LYS  |
| 38  | DO    | 90  | VAL  |
| 38  | DO    | 115 | LEU  |
| 38  | DO    | 117 | PHE  |
| 39  | DP    | 6   | GLN  |
| 39  | DP    | 13  | LYS  |
| 39  | DP    | 28  | LYS  |
| 39  | DP    | 31  | VAL  |
| 39  | DP    | 83  | ILE  |
| 39  | DP    | 86  | LYS  |
| 39  | DP    | 95  | LYS  |
| 39  | DP    | 101 | GLU  |
| 40  | DQ    | 3   | VAL  |
| 40  | DQ    | 10  | ARG  |
| 40  | DQ    | 12  | ARG  |
| 40  | DQ    | 35  | PHE  |
| 40  | DQ    | 50  | ARG  |
| 40  | DQ    | 54  | ARG  |
| 40  | DQ    | 57  | ARG  |
| 40  | DQ    | 63  | ARG  |
| 40  | DQ    | 69  | ARG  |
| 40  | DQ    | 79  | ILE  |
| 41  | DR    | 6   | GLN  |
| 41  | DR    | 10  | LYS  |
| 41  | DR    | 13  | ARG  |
| 41  | DR    | 37  | GLU  |
| 41  | DR    | 48  | LYS  |
| 41  | DR    | 58  | VAL  |
| 41  | DR    | 75  | VAL  |
| 41  | DR    | 80  | ARG  |
| 41  | DR    | 81  | LYS  |
| 41  | DR    | 83  | TYR  |
| 41  | DR    | 86  | GLN  |
| 41  | DR    | 90  | ARG  |
| 41  | DR    | 93  | PHE  |
| 41  | DR    | 95  | ASP  |
| 42  | DS    | 6   | LYS  |
| 42  | DS    | 22  | ASP  |
| 42  | DS    | 23  | LEU  |
| 42  | DS    | 31  | GLN  |
| 42  | DS    | 45  | VAL  |
| 42  | DS    | 46  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | DS    | 66  | ILE  |
| 42  | DS    | 70  | LYS  |
| 42  | DS    | 74  | ILE  |
| 42  | DS    | 76  | VAL  |
| 42  | DS    | 84  | ARG  |
| 42  | DS    | 85  | ILE  |
| 42  | DS    | 86  | MET  |
| 42  | DS    | 88  | ARG  |
| 43  | DT    | 9   | LYS  |
| 43  | DT    | 12  | ARG  |
| 43  | DT    | 18  | GLU  |
| 43  | DT    | 39  | THR  |
| 43  | DT    | 50  | LEU  |
| 43  | DT    | 54  | GLU  |
| 44  | DU    | 13  | LEU  |
| 44  | DU    | 14  | THR  |
| 44  | DU    | 20  | LYS  |
| 44  | DU    | 21  | ARG  |
| 44  | DU    | 40  | LEU  |
| 44  | DU    | 45  | GLN  |
| 44  | DU    | 81  | ARG  |
| 44  | DU    | 82  | VAL  |
| 44  | DU    | 85  | ARG  |
| 44  | DU    | 94  | PHE  |
| 44  | DU    | 95  | PHE  |
| 45  | DV    | 26  | PHE  |
| 45  | DV    | 40  | ILE  |
| 45  | DV    | 51  | GLN  |
| 45  | DV    | 61  | LEU  |
| 45  | DV    | 65  | VAL  |
| 45  | DV    | 69  | GLU  |
| 45  | DV    | 70  | ILE  |
| 45  | DV    | 76  | ASP  |
| 45  | DV    | 77  | VAL  |
| 45  | DV    | 90  | ASP  |
| 46  | DW    | 18  | LYS  |
| 46  | DW    | 20  | LEU  |
| 46  | DW    | 22  | VAL  |
| 46  | DW    | 23  | LYS  |
| 46  | DW    | 25  | PHE  |
| 46  | DW    | 30  | VAL  |
| 46  | DW    | 37  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | DW    | 38  | ARG  |
| 46  | DW    | 39  | GLN  |
| 46  | DW    | 40  | ARG  |
| 46  | DW    | 44  | PHE  |
| 46  | DW    | 58  | LEU  |
| 46  | DW    | 68  | PHE  |
| 46  | DW    | 76  | ARG  |
| 46  | DW    | 77  | LYS  |
| 47  | DX    | 5   | GLN  |
| 47  | DX    | 26  | ARG  |
| 47  | DX    | 31  | ASN  |
| 47  | DX    | 33  | HIS  |
| 47  | DX    | 46  | VAL  |
| 47  | DX    | 47  | THR  |
| 47  | DX    | 57  | VAL  |
| 47  | DX    | 63  | ILE  |
| 47  | DX    | 73  | ARG  |
| 48  | DY    | 1   | MET  |
| 48  | DY    | 4   | LYS  |
| 48  | DY    | 28  | LEU  |
| 49  | DZ    | 16  | LEU  |
| 49  | DZ    | 24  | LEU  |
| 49  | DZ    | 28  | LEU  |
| 49  | DZ    | 29  | ARG  |
| 49  | DZ    | 50  | VAL  |
| 49  | DZ    | 53  | MET  |
| 49  | DZ    | 55  | LYS  |
| 50  | D0    | 3   | GLN  |
| 50  | D0    | 5   | ASN  |
| 50  | D0    | 41  | HIS  |
| 50  | D0    | 42  | ILE  |
| 50  | D0    | 49  | ARG  |
| 51  | D1    | 10  | LEU  |
| 51  | D1    | 20  | TYR  |
| 51  | D1    | 35  | LEU  |
| 51  | D1    | 44  | GLN  |
| 52  | D2    | 8   | SER  |
| 52  | D2    | 22  | MET  |
| 52  | D2    | 26  | ASN  |
| 52  | D2    | 33  | ARG  |
| 53  | D3    | 12  | ARG  |
| 53  | D3    | 14  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | D3    | 27  | ASN  |
| 53  | D3    | 29  | ARG  |
| 53  | D3    | 41  | ARG  |
| 53  | D3    | 46  | LYS  |
| 53  | D3    | 48  | MET  |
| 53  | D3    | 51  | LYS  |
| 53  | D3    | 61  | LEU  |
| 54  | D4    | 2   | LYS  |
| 54  | D4    | 9   | LYS  |
| 54  | D4    | 13  | ASN  |
| 54  | D4    | 15  | LYS  |
| 54  | D4    | 17  | VAL  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (323) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AB    | 14  | HIS  |
| 1   | AB    | 17  | HIS  |
| 1   | AB    | 18  | GLN  |
| 1   | AB    | 38  | HIS  |
| 1   | AB    | 41  | ASN  |
| 1   | AB    | 57  | ASN  |
| 1   | AB    | 88  | GLN  |
| 1   | AB    | 93  | HIS  |
| 1   | AB    | 102 | ASN  |
| 1   | AB    | 108 | GLN  |
| 1   | AB    | 119 | GLN  |
| 1   | AB    | 189 | ASN  |
| 2   | AC    | 24  | ASN  |
| 2   | AC    | 68  | HIS  |
| 2   | AC    | 139 | ASN  |
| 2   | AC    | 184 | ASN  |
| 3   | AD    | 58  | GLN  |
| 3   | AD    | 73  | ASN  |
| 3   | AD    | 99  | ASN  |
| 3   | AD    | 115 | GLN  |
| 3   | AD    | 119 | HIS  |
| 3   | AD    | 135 | GLN  |
| 3   | AD    | 163 | GLN  |
| 3   | AD    | 195 | ASN  |
| 4   | AE    | 42  | ASN  |
| 4   | AE    | 69  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AE    | 72  | ASN  |
| 4   | AE    | 76  | ASN  |
| 4   | AE    | 77  | ASN  |
| 4   | AE    | 121 | ASN  |
| 4   | AE    | 145 | ASN  |
| 5   | AF    | 11  | HIS  |
| 5   | AF    | 46  | GLN  |
| 5   | AF    | 52  | ASN  |
| 5   | AF    | 68  | GLN  |
| 6   | AG    | 121 | ASN  |
| 6   | AG    | 147 | ASN  |
| 7   | AH    | 15  | ASN  |
| 7   | AH    | 117 | GLN  |
| 8   | AI    | 4   | GLN  |
| 8   | AI    | 74  | GLN  |
| 8   | AI    | 80  | HIS  |
| 8   | AI    | 125 | GLN  |
| 9   | AJ    | 15  | HIS  |
| 9   | AJ    | 20  | GLN  |
| 9   | AJ    | 35  | GLN  |
| 10  | AK    | 21  | HIS  |
| 10  | AK    | 28  | ASN  |
| 10  | AK    | 108 | ASN  |
| 10  | AK    | 118 | ASN  |
| 11  | AL    | 45  | ASN  |
| 11  | AL    | 95  | HIS  |
| 11  | AL    | 111 | GLN  |
| 13  | AN    | 34  | ASN  |
| 13  | AN    | 48  | GLN  |
| 13  | AN    | 61  | ASN  |
| 14  | AO    | 36  | ASN  |
| 14  | AO    | 37  | HIS  |
| 14  | AO    | 61  | GLN  |
| 15  | AP    | 18  | GLN  |
| 15  | AP    | 29  | ASN  |
| 16  | AQ    | 44  | HIS  |
| 17  | AR    | 30  | ASN  |
| 17  | AR    | 53  | GLN  |
| 18  | AS    | 42  | ASN  |
| 19  | AT    | 20  | ASN  |
| 19  | AT    | 60  | GLN  |
| 19  | AT    | 74  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | AT    | 77  | ASN  |
| 19  | AT    | 83  | ASN  |
| 20  | AU    | 8   | ASN  |
| 26  | BC    | 14  | HIS  |
| 26  | BC    | 20  | ASN  |
| 26  | BC    | 43  | ASN  |
| 26  | BC    | 59  | GLN  |
| 26  | BC    | 89  | ASN  |
| 26  | BC    | 114 | GLN  |
| 26  | BC    | 152 | GLN  |
| 26  | BC    | 225 | ASN  |
| 26  | BC    | 242 | HIS  |
| 26  | BC    | 250 | GLN  |
| 26  | BC    | 259 | ASN  |
| 27  | BD    | 32  | ASN  |
| 27  | BD    | 49  | GLN  |
| 27  | BD    | 126 | ASN  |
| 27  | BD    | 130 | GLN  |
| 28  | BE    | 24  | ASN  |
| 28  | BE    | 30  | GLN  |
| 28  | BE    | 62  | GLN  |
| 28  | BE    | 97  | ASN  |
| 28  | BE    | 136 | GLN  |
| 28  | BE    | 163 | ASN  |
| 29  | BF    | 22  | ASN  |
| 29  | BF    | 26  | GLN  |
| 29  | BF    | 134 | GLN  |
| 30  | BG    | 72  | ASN  |
| 30  | BG    | 114 | HIS  |
| 30  | BG    | 138 | GLN  |
| 31  | BH    | 18  | GLN  |
| 31  | BH    | 33  | GLN  |
| 31  | BH    | 43  | ASN  |
| 31  | BH    | 145 | ASN  |
| 32  | BI    | 5   | GLN  |
| 32  | BI    | 30  | GLN  |
| 32  | BI    | 110 | GLN  |
| 33  | BJ    | 40  | HIS  |
| 33  | BJ    | 58  | ASN  |
| 33  | BJ    | 76  | HIS  |
| 33  | BJ    | 77  | HIS  |
| 33  | BJ    | 128 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | BJ    | 130 | HIS  |
| 34  | BK    | 5   | GLN  |
| 34  | BK    | 88  | ASN  |
| 34  | BK    | 89  | ASN  |
| 35  | BL    | 4   | ASN  |
| 35  | BL    | 54  | GLN  |
| 35  | BL    | 93  | ASN  |
| 35  | BL    | 99  | ASN  |
| 35  | BL    | 104 | GLN  |
| 37  | BN    | 9   | GLN  |
| 37  | BN    | 11  | ASN  |
| 37  | BN    | 18  | GLN  |
| 37  | BN    | 23  | ASN  |
| 37  | BN    | 62  | ASN  |
| 37  | BN    | 73  | ASN  |
| 38  | BO    | 34  | HIS  |
| 38  | BO    | 38  | GLN  |
| 39  | BP    | 9   | GLN  |
| 39  | BP    | 74  | GLN  |
| 40  | BQ    | 13  | HIS  |
| 40  | BQ    | 51  | GLN  |
| 40  | BQ    | 65  | ASN  |
| 41  | BR    | 6   | GLN  |
| 41  | BR    | 43  | ASN  |
| 41  | BR    | 82  | HIS  |
| 42  | BS    | 9   | HIS  |
| 42  | BS    | 57  | ASN  |
| 42  | BS    | 61  | ASN  |
| 43  | BT    | 48  | GLN  |
| 43  | BT    | 70  | HIS  |
| 43  | BT    | 72  | GLN  |
| 43  | BT    | 91  | GLN  |
| 44  | BU    | 52  | ASN  |
| 44  | BU    | 65  | GLN  |
| 44  | BU    | 73  | ASN  |
| 45  | BV    | 5   | ASN  |
| 45  | BV    | 51  | GLN  |
| 45  | BV    | 80  | HIS  |
| 46  | BW    | 39  | GLN  |
| 46  | BW    | 49  | ASN  |
| 47  | BX    | 5   | GLN  |
| 47  | BX    | 22  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | BX    | 33  | HIS  |
| 48  | BY    | 15  | ASN  |
| 48  | BY    | 27  | ASN  |
| 48  | BY    | 31  | GLN  |
| 48  | BY    | 41  | HIS  |
| 52  | B2    | 13  | ASN  |
| 52  | B2    | 26  | ASN  |
| 53  | B3    | 27  | ASN  |
| 54  | B4    | 35  | GLN  |
| 1   | CB    | 14  | HIS  |
| 1   | CB    | 92  | ASN  |
| 1   | CB    | 145 | ASN  |
| 1   | CB    | 167 | HIS  |
| 1   | CB    | 176 | ASN  |
| 2   | CC    | 2   | GLN  |
| 2   | CC    | 18  | ASN  |
| 2   | CC    | 31  | ASN  |
| 2   | CC    | 122 | GLN  |
| 2   | CC    | 139 | ASN  |
| 2   | CC    | 184 | ASN  |
| 3   | CD    | 39  | GLN  |
| 3   | CD    | 84  | ASN  |
| 3   | CD    | 119 | HIS  |
| 3   | CD    | 125 | ASN  |
| 3   | CD    | 163 | GLN  |
| 4   | CE    | 11  | GLN  |
| 4   | CE    | 60  | GLN  |
| 4   | CE    | 76  | ASN  |
| 4   | CE    | 77  | ASN  |
| 4   | CE    | 88  | HIS  |
| 4   | CE    | 121 | ASN  |
| 4   | CE    | 131 | ASN  |
| 4   | CE    | 147 | ASN  |
| 5   | CF    | 11  | HIS  |
| 5   | CF    | 81  | ASN  |
| 6   | CG    | 85  | GLN  |
| 7   | CH    | 3   | GLN  |
| 7   | CH    | 15  | ASN  |
| 7   | CH    | 37  | ASN  |
| 8   | CI    | 3   | ASN  |
| 8   | CI    | 4   | GLN  |
| 8   | CI    | 24  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | CI    | 30  | ASN  |
| 8   | CI    | 49  | GLN  |
| 8   | CI    | 74  | GLN  |
| 8   | CI    | 109 | GLN  |
| 8   | CI    | 125 | GLN  |
| 9   | CJ    | 56  | HIS  |
| 9   | CJ    | 64  | GLN  |
| 9   | CJ    | 70  | HIS  |
| 10  | CK    | 21  | HIS  |
| 10  | CK    | 27  | ASN  |
| 10  | CK    | 118 | ASN  |
| 11  | CL    | 4   | ASN  |
| 11  | CL    | 19  | ASN  |
| 11  | CL    | 28  | GLN  |
| 11  | CL    | 72  | ASN  |
| 11  | CL    | 74  | GLN  |
| 11  | CL    | 95  | HIS  |
| 11  | CL    | 111 | GLN  |
| 12  | CM    | 11  | HIS  |
| 12  | CM    | 99  | GLN  |
| 12  | CM    | 104 | ASN  |
| 13  | CN    | 59  | GLN  |
| 13  | CN    | 65  | GLN  |
| 13  | CN    | 70  | HIS  |
| 14  | CO    | 27  | GLN  |
| 16  | CQ    | 49  | ASN  |
| 18  | CS    | 13  | HIS  |
| 18  | CS    | 51  | HIS  |
| 18  | CS    | 52  | ASN  |
| 19  | CT    | 12  | GLN  |
| 19  | CT    | 51  | ASN  |
| 19  | CT    | 69  | ASN  |
| 19  | CT    | 81  | GLN  |
| 26  | DC    | 14  | HIS  |
| 26  | DC    | 20  | ASN  |
| 26  | DC    | 43  | ASN  |
| 26  | DC    | 52  | HIS  |
| 26  | DC    | 57  | HIS  |
| 26  | DC    | 59  | GLN  |
| 26  | DC    | 89  | ASN  |
| 26  | DC    | 116 | GLN  |
| 26  | DC    | 133 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | DD    | 32  | ASN  |
| 27  | DD    | 36  | GLN  |
| 27  | DD    | 49  | GLN  |
| 27  | DD    | 58  | ASN  |
| 27  | DD    | 185 | ASN  |
| 28  | DE    | 30  | GLN  |
| 28  | DE    | 41  | GLN  |
| 29  | DF    | 4   | HIS  |
| 29  | DF    | 126 | ASN  |
| 29  | DF    | 134 | GLN  |
| 30  | DG    | 19  | ASN  |
| 30  | DG    | 37  | ASN  |
| 30  | DG    | 44  | HIS  |
| 30  | DG    | 103 | ASN  |
| 30  | DG    | 138 | GLN  |
| 31  | DH    | 2   | GLN  |
| 31  | DH    | 28  | ASN  |
| 31  | DH    | 43  | ASN  |
| 31  | DH    | 66  | ASN  |
| 32  | DI    | 42  | ASN  |
| 32  | DI    | 93  | ASN  |
| 32  | DI    | 106 | GLN  |
| 33  | DJ    | 40  | HIS  |
| 33  | DJ    | 138 | GLN  |
| 34  | DK    | 3   | GLN  |
| 34  | DK    | 9   | ASN  |
| 34  | DK    | 13  | ASN  |
| 34  | DK    | 89  | ASN  |
| 35  | DL    | 4   | ASN  |
| 35  | DL    | 54  | GLN  |
| 36  | DM    | 3   | GLN  |
| 36  | DM    | 13  | HIS  |
| 37  | DN    | 3   | HIS  |
| 37  | DN    | 16  | HIS  |
| 37  | DN    | 23  | ASN  |
| 37  | DN    | 31  | HIS  |
| 37  | DN    | 73  | ASN  |
| 37  | DN    | 107 | ASN  |
| 38  | DO    | 29  | HIS  |
| 39  | DP    | 6   | GLN  |
| 39  | DP    | 9   | GLN  |
| 39  | DP    | 11  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | DP    | 65  | ASN  |
| 39  | DP    | 114 | ASN  |
| 40  | DQ    | 19  | GLN  |
| 40  | DQ    | 71  | ASN  |
| 41  | DR    | 6   | GLN  |
| 41  | DR    | 12  | HIS  |
| 41  | DR    | 66  | HIS  |
| 41  | DR    | 82  | HIS  |
| 41  | DR    | 86  | GLN  |
| 41  | DR    | 87  | GLN  |
| 42  | DS    | 31  | GLN  |
| 42  | DS    | 57  | ASN  |
| 43  | DT    | 15  | HIS  |
| 43  | DT    | 48  | GLN  |
| 43  | DT    | 91  | GLN  |
| 43  | DT    | 92  | ASN  |
| 44  | DU    | 44  | HIS  |
| 44  | DU    | 45  | GLN  |
| 44  | DU    | 52  | ASN  |
| 44  | DU    | 53  | GLN  |
| 45  | DV    | 51  | GLN  |
| 45  | DV    | 78  | GLN  |
| 45  | DV    | 80  | HIS  |
| 47  | DX    | 15  | ASN  |
| 47  | DX    | 22  | ASN  |
| 47  | DX    | 31  | ASN  |
| 47  | DX    | 33  | HIS  |
| 47  | DX    | 35  | HIS  |
| 48  | DY    | 15  | ASN  |
| 48  | DY    | 20  | ASN  |
| 48  | DY    | 41  | HIS  |
| 48  | DY    | 45  | GLN  |
| 48  | DY    | 58  | ASN  |
| 49  | DZ    | 19  | HIS  |
| 50  | D0    | 18  | HIS  |
| 50  | D0    | 41  | HIS  |
| 52  | D2    | 6   | GLN  |
| 52  | D2    | 16  | HIS  |
| 52  | D2    | 26  | ASN  |
| 52  | D2    | 29  | GLN  |
| 53  | D3    | 25  | HIS  |
| 53  | D3    | 27  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | D3    | 30  | HIS  |
| 53  | D3    | 42  | HIS  |
| 54  | D4    | 37  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 21  | AA    | 1532/1533 (99%) | 465 (30%)         | 0               |
| 22  | AV    | 16/17 (94%)     | 2 (12%)           | 0               |
| 22  | AX    | 16/17 (94%)     | 2 (12%)           | 0               |
| 22  | CV    | 16/17 (94%)     | 3 (18%)           | 0               |
| 22  | CX    | 16/17 (94%)     | 2 (12%)           | 0               |
| 23  | AW    | 5/6 (83%)       | 3 (60%)           | 0               |
| 23  | CW    | 5/6 (83%)       | 1 (20%)           | 0               |
| 24  | BA    | 2850/2903 (98%) | 925 (32%)         | 0               |
| 24  | DA    | 2837/2903 (97%) | 1020 (35%)        | 0               |
| 25  | BB    | 117/118 (99%)   | 32 (27%)          | 0               |
| 55  | CA    | 1529/1530 (99%) | 516 (33%)         | 0               |
| 56  | DB    | 116/117 (99%)   | 29 (25%)          | 0               |
| All | All   | 9055/9184 (98%) | 3000 (33%)        | 0               |

All (3000) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 5   | U    |
| 21  | AA    | 6   | G    |
| 21  | AA    | 7   | A    |
| 21  | AA    | 9   | G    |
| 21  | AA    | 13  | U    |
| 21  | AA    | 14  | U    |
| 21  | AA    | 15  | G    |
| 21  | AA    | 31  | G    |
| 21  | AA    | 32  | A    |
| 21  | AA    | 33  | A    |
| 21  | AA    | 39  | G    |
| 21  | AA    | 47  | C    |
| 21  | AA    | 48  | C    |
| 21  | AA    | 50  | A    |
| 21  | AA    | 51  | A    |
| 21  | AA    | 52  | C    |
| 21  | AA    | 53  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 61  | G    |
| 21  | AA    | 65  | A    |
| 21  | AA    | 66  | A    |
| 21  | AA    | 67  | C    |
| 21  | AA    | 70  | U    |
| 21  | AA    | 71  | A    |
| 21  | AA    | 72  | A    |
| 21  | AA    | 73  | C    |
| 21  | AA    | 74  | A    |
| 21  | AA    | 75  | G    |
| 21  | AA    | 76  | G    |
| 21  | AA    | 77  | A    |
| 21  | AA    | 78  | A    |
| 21  | AA    | 79  | G    |
| 21  | AA    | 82  | G    |
| 21  | AA    | 83  | C    |
| 21  | AA    | 85  | U    |
| 21  | AA    | 86  | G    |
| 21  | AA    | 87  | C    |
| 21  | AA    | 88  | U    |
| 21  | AA    | 89  | U    |
| 21  | AA    | 90  | C    |
| 21  | AA    | 91  | U    |
| 21  | AA    | 92  | U    |
| 21  | AA    | 94  | G    |
| 21  | AA    | 95  | C    |
| 21  | AA    | 97  | G    |
| 21  | AA    | 109 | A    |
| 21  | AA    | 110 | C    |
| 21  | AA    | 111 | G    |
| 21  | AA    | 116 | A    |
| 21  | AA    | 117 | G    |
| 21  | AA    | 119 | A    |
| 21  | AA    | 120 | A    |
| 21  | AA    | 121 | U    |
| 21  | AA    | 122 | G    |
| 21  | AA    | 127 | G    |
| 21  | AA    | 129 | A    |
| 21  | AA    | 130 | A    |
| 21  | AA    | 131 | A    |
| 21  | AA    | 132 | C    |
| 21  | AA    | 141 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 143 | A    |
| 21  | AA    | 159 | G    |
| 21  | AA    | 163 | C    |
| 21  | AA    | 164 | G    |
| 21  | AA    | 174 | A    |
| 21  | AA    | 175 | C    |
| 21  | AA    | 181 | A    |
| 21  | AA    | 182 | A    |
| 21  | AA    | 184 | G    |
| 21  | AA    | 185 | U    |
| 21  | AA    | 192 | A    |
| 21  | AA    | 197 | A    |
| 21  | AA    | 198 | G    |
| 21  | AA    | 199 | A    |
| 21  | AA    | 202 | G    |
| 21  | AA    | 205 | A    |
| 21  | AA    | 207 | C    |
| 21  | AA    | 208 | U    |
| 21  | AA    | 209 | U    |
| 21  | AA    | 210 | C    |
| 21  | AA    | 211 | G    |
| 21  | AA    | 212 | G    |
| 21  | AA    | 213 | G    |
| 21  | AA    | 214 | C    |
| 21  | AA    | 240 | G    |
| 21  | AA    | 243 | A    |
| 21  | AA    | 244 | U    |
| 21  | AA    | 245 | U    |
| 21  | AA    | 246 | A    |
| 21  | AA    | 247 | G    |
| 21  | AA    | 248 | C    |
| 21  | AA    | 250 | A    |
| 21  | AA    | 251 | G    |
| 21  | AA    | 252 | U    |
| 21  | AA    | 253 | A    |
| 21  | AA    | 266 | G    |
| 21  | AA    | 267 | C    |
| 21  | AA    | 268 | U    |
| 21  | AA    | 274 | A    |
| 21  | AA    | 275 | G    |
| 21  | AA    | 276 | G    |
| 21  | AA    | 279 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 280 | C    |
| 21  | AA    | 285 | C    |
| 21  | AA    | 289 | G    |
| 21  | AA    | 305 | G    |
| 21  | AA    | 306 | A    |
| 21  | AA    | 307 | C    |
| 21  | AA    | 313 | A    |
| 21  | AA    | 315 | A    |
| 21  | AA    | 316 | C    |
| 21  | AA    | 317 | U    |
| 21  | AA    | 321 | A    |
| 21  | AA    | 327 | A    |
| 21  | AA    | 328 | C    |
| 21  | AA    | 329 | A    |
| 21  | AA    | 330 | C    |
| 21  | AA    | 331 | G    |
| 21  | AA    | 332 | G    |
| 21  | AA    | 344 | A    |
| 21  | AA    | 345 | C    |
| 21  | AA    | 346 | G    |
| 21  | AA    | 347 | G    |
| 21  | AA    | 352 | C    |
| 21  | AA    | 353 | A    |
| 21  | AA    | 354 | G    |
| 21  | AA    | 367 | U    |
| 21  | AA    | 369 | G    |
| 21  | AA    | 370 | C    |
| 21  | AA    | 373 | A    |
| 21  | AA    | 374 | A    |
| 21  | AA    | 384 | G    |
| 21  | AA    | 388 | G    |
| 21  | AA    | 389 | A    |
| 21  | AA    | 390 | U    |
| 21  | AA    | 398 | U    |
| 21  | AA    | 406 | G    |
| 21  | AA    | 411 | A    |
| 21  | AA    | 412 | A    |
| 21  | AA    | 413 | G    |
| 21  | AA    | 414 | A    |
| 21  | AA    | 415 | A    |
| 21  | AA    | 421 | U    |
| 21  | AA    | 422 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 423 | G    |
| 21  | AA    | 424 | G    |
| 21  | AA    | 428 | G    |
| 21  | AA    | 429 | U    |
| 21  | AA    | 430 | A    |
| 21  | AA    | 431 | A    |
| 21  | AA    | 441 | A    |
| 21  | AA    | 451 | A    |
| 21  | AA    | 452 | A    |
| 21  | AA    | 453 | G    |
| 21  | AA    | 454 | G    |
| 21  | AA    | 456 | A    |
| 21  | AA    | 458 | U    |
| 21  | AA    | 459 | A    |
| 21  | AA    | 461 | A    |
| 21  | AA    | 462 | G    |
| 21  | AA    | 463 | U    |
| 21  | AA    | 465 | A    |
| 21  | AA    | 466 | A    |
| 21  | AA    | 467 | U    |
| 21  | AA    | 468 | A    |
| 21  | AA    | 481 | G    |
| 21  | AA    | 484 | G    |
| 21  | AA    | 485 | U    |
| 21  | AA    | 486 | U    |
| 21  | AA    | 496 | A    |
| 21  | AA    | 497 | G    |
| 21  | AA    | 498 | A    |
| 21  | AA    | 500 | G    |
| 21  | AA    | 501 | C    |
| 21  | AA    | 505 | G    |
| 21  | AA    | 508 | U    |
| 21  | AA    | 509 | A    |
| 21  | AA    | 510 | A    |
| 21  | AA    | 511 | C    |
| 21  | AA    | 512 | U    |
| 21  | AA    | 517 | G    |
| 21  | AA    | 518 | C    |
| 21  | AA    | 519 | C    |
| 21  | AA    | 520 | A    |
| 21  | AA    | 524 | G    |
| 21  | AA    | 527 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 531 | U    |
| 21  | AA    | 532 | A    |
| 21  | AA    | 533 | A    |
| 21  | AA    | 534 | U    |
| 21  | AA    | 536 | C    |
| 21  | AA    | 537 | G    |
| 21  | AA    | 548 | G    |
| 21  | AA    | 549 | C    |
| 21  | AA    | 550 | G    |
| 21  | AA    | 556 | C    |
| 21  | AA    | 559 | A    |
| 21  | AA    | 560 | A    |
| 21  | AA    | 562 | U    |
| 21  | AA    | 563 | A    |
| 21  | AA    | 564 | C    |
| 21  | AA    | 566 | G    |
| 21  | AA    | 567 | G    |
| 21  | AA    | 568 | G    |
| 21  | AA    | 572 | A    |
| 21  | AA    | 573 | A    |
| 21  | AA    | 575 | G    |
| 21  | AA    | 576 | C    |
| 21  | AA    | 577 | G    |
| 21  | AA    | 578 | C    |
| 21  | AA    | 588 | G    |
| 21  | AA    | 595 | A    |
| 21  | AA    | 604 | G    |
| 21  | AA    | 623 | C    |
| 21  | AA    | 653 | U    |
| 21  | AA    | 654 | G    |
| 21  | AA    | 655 | A    |
| 21  | AA    | 665 | A    |
| 21  | AA    | 688 | G    |
| 21  | AA    | 689 | C    |
| 21  | AA    | 700 | G    |
| 21  | AA    | 701 | U    |
| 21  | AA    | 702 | A    |
| 21  | AA    | 703 | G    |
| 21  | AA    | 704 | A    |
| 21  | AA    | 705 | G    |
| 21  | AA    | 719 | C    |
| 21  | AA    | 721 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AA    | 722 | G    |
| 21  | AA    | 723 | U    |
| 21  | AA    | 724 | G    |
| 21  | AA    | 725 | G    |
| 21  | AA    | 731 | G    |
| 21  | AA    | 748 | G    |
| 21  | AA    | 752 | G    |
| 21  | AA    | 754 | C    |
| 21  | AA    | 755 | G    |
| 21  | AA    | 792 | A    |
| 21  | AA    | 793 | U    |
| 21  | AA    | 794 | A    |
| 21  | AA    | 795 | C    |
| 21  | AA    | 796 | C    |
| 21  | AA    | 810 | C    |
| 21  | AA    | 812 | G    |
| 21  | AA    | 813 | U    |
| 21  | AA    | 814 | A    |
| 21  | AA    | 815 | A    |
| 21  | AA    | 816 | A    |
| 21  | AA    | 817 | C    |
| 21  | AA    | 819 | A    |
| 21  | AA    | 828 | U    |
| 21  | AA    | 841 | C    |
| 21  | AA    | 843 | U    |
| 21  | AA    | 845 | A    |
| 21  | AA    | 846 | G    |
| 21  | AA    | 859 | G    |
| 21  | AA    | 871 | U    |
| 21  | AA    | 873 | A    |
| 21  | AA    | 874 | G    |
| 21  | AA    | 875 | U    |
| 21  | AA    | 876 | C    |
| 21  | AA    | 884 | U    |
| 21  | AA    | 885 | G    |
| 21  | AA    | 886 | G    |
| 21  | AA    | 887 | G    |
| 21  | AA    | 889 | A    |
| 21  | AA    | 890 | G    |
| 21  | AA    | 891 | U    |
| 21  | AA    | 892 | A    |
| 21  | AA    | 913 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 914  | A    |
| 21  | AA    | 915  | A    |
| 21  | AA    | 916  | U    |
| 21  | AA    | 926  | G    |
| 21  | AA    | 927  | G    |
| 21  | AA    | 934  | C    |
| 21  | AA    | 935  | A    |
| 21  | AA    | 936  | C    |
| 21  | AA    | 942  | G    |
| 21  | AA    | 960  | U    |
| 21  | AA    | 961  | U    |
| 21  | AA    | 962  | C    |
| 21  | AA    | 966  | G    |
| 21  | AA    | 967  | C    |
| 21  | AA    | 968  | A    |
| 21  | AA    | 969  | A    |
| 21  | AA    | 972  | C    |
| 21  | AA    | 974  | A    |
| 21  | AA    | 975  | A    |
| 21  | AA    | 976  | G    |
| 21  | AA    | 977  | A    |
| 21  | AA    | 978  | A    |
| 21  | AA    | 979  | C    |
| 21  | AA    | 982  | U    |
| 21  | AA    | 983  | A    |
| 21  | AA    | 984  | C    |
| 21  | AA    | 985  | C    |
| 21  | AA    | 991  | U    |
| 21  | AA    | 992  | U    |
| 21  | AA    | 993  | G    |
| 21  | AA    | 994  | A    |
| 21  | AA    | 995  | C    |
| 21  | AA    | 1004 | A    |
| 21  | AA    | 1008 | U    |
| 21  | AA    | 1017 | U    |
| 21  | AA    | 1022 | A    |
| 21  | AA    | 1025 | U    |
| 21  | AA    | 1029 | U    |
| 21  | AA    | 1030 | U    |
| 21  | AA    | 1031 | C    |
| 21  | AA    | 1032 | G    |
| 21  | AA    | 1033 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 1034 | G    |
| 21  | AA    | 1037 | C    |
| 21  | AA    | 1050 | G    |
| 21  | AA    | 1051 | C    |
| 21  | AA    | 1052 | U    |
| 21  | AA    | 1053 | G    |
| 21  | AA    | 1054 | C    |
| 21  | AA    | 1055 | A    |
| 21  | AA    | 1064 | G    |
| 21  | AA    | 1065 | U    |
| 21  | AA    | 1066 | C    |
| 21  | AA    | 1068 | G    |
| 21  | AA    | 1069 | C    |
| 21  | AA    | 1080 | A    |
| 21  | AA    | 1085 | U    |
| 21  | AA    | 1086 | U    |
| 21  | AA    | 1087 | G    |
| 21  | AA    | 1088 | G    |
| 21  | AA    | 1094 | G    |
| 21  | AA    | 1097 | C    |
| 21  | AA    | 1101 | A    |
| 21  | AA    | 1102 | A    |
| 21  | AA    | 1103 | C    |
| 21  | AA    | 1104 | G    |
| 21  | AA    | 1107 | C    |
| 21  | AA    | 1113 | C    |
| 21  | AA    | 1124 | G    |
| 21  | AA    | 1125 | U    |
| 21  | AA    | 1126 | U    |
| 21  | AA    | 1130 | A    |
| 21  | AA    | 1131 | G    |
| 21  | AA    | 1132 | C    |
| 21  | AA    | 1133 | G    |
| 21  | AA    | 1135 | U    |
| 21  | AA    | 1137 | C    |
| 21  | AA    | 1138 | G    |
| 21  | AA    | 1140 | C    |
| 21  | AA    | 1141 | C    |
| 21  | AA    | 1142 | G    |
| 21  | AA    | 1144 | G    |
| 21  | AA    | 1145 | A    |
| 21  | AA    | 1146 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 1154 | G    |
| 21  | AA    | 1158 | C    |
| 21  | AA    | 1159 | U    |
| 21  | AA    | 1160 | G    |
| 21  | AA    | 1161 | C    |
| 21  | AA    | 1167 | A    |
| 21  | AA    | 1168 | U    |
| 21  | AA    | 1169 | A    |
| 21  | AA    | 1170 | A    |
| 21  | AA    | 1181 | G    |
| 21  | AA    | 1183 | U    |
| 21  | AA    | 1184 | G    |
| 21  | AA    | 1185 | G    |
| 21  | AA    | 1192 | C    |
| 21  | AA    | 1193 | G    |
| 21  | AA    | 1196 | A    |
| 21  | AA    | 1197 | A    |
| 21  | AA    | 1198 | G    |
| 21  | AA    | 1200 | C    |
| 21  | AA    | 1201 | A    |
| 21  | AA    | 1202 | U    |
| 21  | AA    | 1203 | C    |
| 21  | AA    | 1212 | U    |
| 21  | AA    | 1213 | A    |
| 21  | AA    | 1214 | C    |
| 21  | AA    | 1215 | G    |
| 21  | AA    | 1216 | A    |
| 21  | AA    | 1224 | U    |
| 21  | AA    | 1225 | A    |
| 21  | AA    | 1226 | C    |
| 21  | AA    | 1227 | A    |
| 21  | AA    | 1228 | C    |
| 21  | AA    | 1229 | A    |
| 21  | AA    | 1238 | A    |
| 21  | AA    | 1240 | U    |
| 21  | AA    | 1241 | G    |
| 21  | AA    | 1242 | G    |
| 21  | AA    | 1256 | A    |
| 21  | AA    | 1257 | A    |
| 21  | AA    | 1258 | G    |
| 21  | AA    | 1259 | C    |
| 21  | AA    | 1260 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 1278 | G    |
| 21  | AA    | 1280 | A    |
| 21  | AA    | 1282 | C    |
| 21  | AA    | 1283 | U    |
| 21  | AA    | 1285 | A    |
| 21  | AA    | 1286 | U    |
| 21  | AA    | 1287 | A    |
| 21  | AA    | 1288 | A    |
| 21  | AA    | 1289 | A    |
| 21  | AA    | 1298 | U    |
| 21  | AA    | 1299 | A    |
| 21  | AA    | 1303 | C    |
| 21  | AA    | 1304 | G    |
| 21  | AA    | 1305 | G    |
| 21  | AA    | 1317 | C    |
| 21  | AA    | 1320 | C    |
| 21  | AA    | 1321 | U    |
| 21  | AA    | 1322 | C    |
| 21  | AA    | 1323 | G    |
| 21  | AA    | 1324 | A    |
| 21  | AA    | 1332 | A    |
| 21  | AA    | 1336 | C    |
| 21  | AA    | 1337 | G    |
| 21  | AA    | 1338 | G    |
| 21  | AA    | 1340 | A    |
| 21  | AA    | 1346 | A    |
| 21  | AA    | 1348 | U    |
| 21  | AA    | 1349 | A    |
| 21  | AA    | 1353 | G    |
| 21  | AA    | 1362 | A    |
| 21  | AA    | 1364 | U    |
| 21  | AA    | 1365 | G    |
| 21  | AA    | 1366 | C    |
| 21  | AA    | 1378 | C    |
| 21  | AA    | 1381 | U    |
| 21  | AA    | 1382 | C    |
| 21  | AA    | 1383 | C    |
| 21  | AA    | 1395 | C    |
| 21  | AA    | 1398 | A    |
| 21  | AA    | 1399 | C    |
| 21  | AA    | 1400 | C    |
| 21  | AA    | 1441 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 21  | AA    | 1446 | A    |
| 21  | AA    | 1447 | A    |
| 21  | AA    | 1448 | C    |
| 21  | AA    | 1449 | C    |
| 21  | AA    | 1450 | U    |
| 21  | AA    | 1451 | U    |
| 21  | AA    | 1452 | C    |
| 21  | AA    | 1453 | G    |
| 21  | AA    | 1454 | G    |
| 21  | AA    | 1455 | G    |
| 21  | AA    | 1469 | C    |
| 21  | AA    | 1475 | G    |
| 21  | AA    | 1487 | G    |
| 21  | AA    | 1492 | A    |
| 21  | AA    | 1497 | G    |
| 21  | AA    | 1499 | A    |
| 21  | AA    | 1500 | A    |
| 21  | AA    | 1502 | A    |
| 21  | AA    | 1503 | A    |
| 21  | AA    | 1505 | G    |
| 21  | AA    | 1507 | A    |
| 21  | AA    | 1508 | A    |
| 21  | AA    | 1517 | G    |
| 21  | AA    | 1520 | C    |
| 21  | AA    | 1528 | U    |
| 21  | AA    | 1529 | G    |
| 21  | AA    | 1530 | G    |
| 21  | AA    | 1531 | A    |
| 22  | AV    | 34   | G    |
| 22  | AV    | 36   | A    |
| 23  | AW    | 3    | U    |
| 23  | AW    | 5    | U    |
| 23  | AW    | 6    | U    |
| 22  | AX    | 28   | G    |
| 22  | AX    | 34   | G    |
| 24  | BA    | 10   | A    |
| 24  | BA    | 13   | A    |
| 24  | BA    | 14   | A    |
| 24  | BA    | 15   | G    |
| 24  | BA    | 28   | A    |
| 24  | BA    | 34   | U    |
| 24  | BA    | 35   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | BA    | 36  | G    |
| 24  | BA    | 40  | U    |
| 24  | BA    | 43  | G    |
| 24  | BA    | 46  | G    |
| 24  | BA    | 49  | A    |
| 24  | BA    | 50  | U    |
| 24  | BA    | 51  | G    |
| 24  | BA    | 61  | C    |
| 24  | BA    | 62  | U    |
| 24  | BA    | 63  | A    |
| 24  | BA    | 70  | G    |
| 24  | BA    | 71  | A    |
| 24  | BA    | 73  | A    |
| 24  | BA    | 74  | A    |
| 24  | BA    | 75  | G    |
| 24  | BA    | 84  | A    |
| 24  | BA    | 85  | G    |
| 24  | BA    | 86  | G    |
| 24  | BA    | 87  | U    |
| 24  | BA    | 91  | A    |
| 24  | BA    | 92  | U    |
| 24  | BA    | 93  | G    |
| 24  | BA    | 99  | U    |
| 24  | BA    | 101 | A    |
| 24  | BA    | 103 | A    |
| 24  | BA    | 118 | A    |
| 24  | BA    | 119 | A    |
| 24  | BA    | 120 | U    |
| 24  | BA    | 121 | G    |
| 24  | BA    | 122 | G    |
| 24  | BA    | 125 | A    |
| 24  | BA    | 126 | A    |
| 24  | BA    | 127 | A    |
| 24  | BA    | 128 | C    |
| 24  | BA    | 135 | U    |
| 24  | BA    | 137 | U    |
| 24  | BA    | 138 | U    |
| 24  | BA    | 139 | U    |
| 24  | BA    | 140 | C    |
| 24  | BA    | 141 | G    |
| 24  | BA    | 142 | A    |
| 24  | BA    | 143 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | BA    | 144 | A    |
| 24  | BA    | 162 | U    |
| 24  | BA    | 163 | C    |
| 24  | BA    | 164 | C    |
| 24  | BA    | 177 | G    |
| 24  | BA    | 178 | G    |
| 24  | BA    | 180 | G    |
| 24  | BA    | 182 | A    |
| 24  | BA    | 188 | G    |
| 24  | BA    | 196 | A    |
| 24  | BA    | 197 | A    |
| 24  | BA    | 199 | A    |
| 24  | BA    | 200 | U    |
| 24  | BA    | 201 | C    |
| 24  | BA    | 204 | A    |
| 24  | BA    | 205 | G    |
| 24  | BA    | 206 | U    |
| 24  | BA    | 207 | A    |
| 24  | BA    | 215 | G    |
| 24  | BA    | 216 | A    |
| 24  | BA    | 217 | A    |
| 24  | BA    | 221 | A    |
| 24  | BA    | 222 | A    |
| 24  | BA    | 223 | A    |
| 24  | BA    | 227 | A    |
| 24  | BA    | 228 | C    |
| 24  | BA    | 229 | C    |
| 24  | BA    | 230 | G    |
| 24  | BA    | 232 | G    |
| 24  | BA    | 233 | A    |
| 24  | BA    | 234 | U    |
| 24  | BA    | 241 | A    |
| 24  | BA    | 242 | G    |
| 24  | BA    | 243 | U    |
| 24  | BA    | 244 | A    |
| 24  | BA    | 248 | G    |
| 24  | BA    | 249 | C    |
| 24  | BA    | 250 | G    |
| 24  | BA    | 255 | A    |
| 24  | BA    | 265 | A    |
| 24  | BA    | 266 | G    |
| 24  | BA    | 267 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | BA    | 272 | A    |
| 24  | BA    | 273 | G    |
| 24  | BA    | 276 | U    |
| 24  | BA    | 277 | G    |
| 24  | BA    | 278 | A    |
| 24  | BA    | 279 | A    |
| 24  | BA    | 280 | U    |
| 24  | BA    | 285 | G    |
| 24  | BA    | 298 | G    |
| 24  | BA    | 299 | A    |
| 24  | BA    | 301 | G    |
| 24  | BA    | 302 | C    |
| 24  | BA    | 303 | G    |
| 24  | BA    | 310 | A    |
| 24  | BA    | 311 | A    |
| 24  | BA    | 312 | G    |
| 24  | BA    | 313 | G    |
| 24  | BA    | 322 | A    |
| 24  | BA    | 329 | G    |
| 24  | BA    | 330 | A    |
| 24  | BA    | 333 | G    |
| 24  | BA    | 334 | C    |
| 24  | BA    | 346 | A    |
| 24  | BA    | 347 | A    |
| 24  | BA    | 349 | U    |
| 24  | BA    | 352 | A    |
| 24  | BA    | 353 | C    |
| 24  | BA    | 359 | G    |
| 24  | BA    | 361 | G    |
| 24  | BA    | 362 | A    |
| 24  | BA    | 367 | G    |
| 24  | BA    | 370 | G    |
| 24  | BA    | 371 | A    |
| 24  | BA    | 372 | G    |
| 24  | BA    | 383 | C    |
| 24  | BA    | 387 | U    |
| 24  | BA    | 388 | G    |
| 24  | BA    | 390 | U    |
| 24  | BA    | 395 | U    |
| 24  | BA    | 396 | G    |
| 24  | BA    | 399 | U    |
| 24  | BA    | 404 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | BA    | 405 | U    |
| 24  | BA    | 412 | A    |
| 24  | BA    | 419 | U    |
| 24  | BA    | 422 | A    |
| 24  | BA    | 424 | G    |
| 24  | BA    | 433 | C    |
| 24  | BA    | 435 | C    |
| 24  | BA    | 436 | C    |
| 24  | BA    | 437 | U    |
| 24  | BA    | 443 | A    |
| 24  | BA    | 446 | G    |
| 24  | BA    | 447 | A    |
| 24  | BA    | 449 | A    |
| 24  | BA    | 454 | A    |
| 24  | BA    | 455 | C    |
| 24  | BA    | 459 | U    |
| 24  | BA    | 460 | A    |
| 24  | BA    | 461 | C    |
| 24  | BA    | 475 | C    |
| 24  | BA    | 476 | G    |
| 24  | BA    | 479 | A    |
| 24  | BA    | 480 | A    |
| 24  | BA    | 481 | G    |
| 24  | BA    | 482 | A    |
| 24  | BA    | 483 | A    |
| 24  | BA    | 490 | C    |
| 24  | BA    | 491 | G    |
| 24  | BA    | 492 | A    |
| 24  | BA    | 504 | A    |
| 24  | BA    | 505 | A    |
| 24  | BA    | 506 | G    |
| 24  | BA    | 507 | A    |
| 24  | BA    | 508 | A    |
| 24  | BA    | 509 | C    |
| 24  | BA    | 510 | C    |
| 24  | BA    | 512 | G    |
| 24  | BA    | 513 | A    |
| 24  | BA    | 514 | A    |
| 24  | BA    | 515 | A    |
| 24  | BA    | 528 | A    |
| 24  | BA    | 529 | A    |
| 24  | BA    | 530 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | BA    | 531 | C    |
| 24  | BA    | 532 | A    |
| 24  | BA    | 533 | G    |
| 24  | BA    | 534 | U    |
| 24  | BA    | 543 | G    |
| 24  | BA    | 544 | C    |
| 24  | BA    | 545 | U    |
| 24  | BA    | 546 | U    |
| 24  | BA    | 547 | A    |
| 24  | BA    | 548 | G    |
| 24  | BA    | 549 | G    |
| 24  | BA    | 550 | C    |
| 24  | BA    | 563 | A    |
| 24  | BA    | 566 | U    |
| 24  | BA    | 572 | A    |
| 24  | BA    | 573 | U    |
| 24  | BA    | 575 | A    |
| 24  | BA    | 586 | A    |
| 24  | BA    | 587 | C    |
| 24  | BA    | 588 | U    |
| 24  | BA    | 589 | U    |
| 24  | BA    | 603 | A    |
| 24  | BA    | 604 | G    |
| 24  | BA    | 605 | G    |
| 24  | BA    | 613 | A    |
| 24  | BA    | 614 | A    |
| 24  | BA    | 615 | U    |
| 24  | BA    | 616 | A    |
| 24  | BA    | 617 | G    |
| 24  | BA    | 621 | A    |
| 24  | BA    | 622 | G    |
| 24  | BA    | 627 | A    |
| 24  | BA    | 628 | G    |
| 24  | BA    | 631 | A    |
| 24  | BA    | 634 | C    |
| 24  | BA    | 637 | A    |
| 24  | BA    | 638 | G    |
| 24  | BA    | 639 | U    |
| 24  | BA    | 645 | C    |
| 24  | BA    | 646 | U    |
| 24  | BA    | 647 | G    |
| 24  | BA    | 653 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | BA    | 654 | A    |
| 24  | BA    | 655 | A    |
| 24  | BA    | 656 | G    |
| 24  | BA    | 657 | U    |
| 24  | BA    | 669 | G    |
| 24  | BA    | 670 | A    |
| 24  | BA    | 682 | G    |
| 24  | BA    | 684 | G    |
| 24  | BA    | 685 | A    |
| 24  | BA    | 686 | U    |
| 24  | BA    | 687 | C    |
| 24  | BA    | 688 | U    |
| 24  | BA    | 689 | A    |
| 24  | BA    | 690 | G    |
| 24  | BA    | 705 | A    |
| 24  | BA    | 713 | G    |
| 24  | BA    | 714 | U    |
| 24  | BA    | 715 | A    |
| 24  | BA    | 717 | C    |
| 24  | BA    | 727 | A    |
| 24  | BA    | 728 | G    |
| 24  | BA    | 729 | G    |
| 24  | BA    | 730 | A    |
| 24  | BA    | 738 | G    |
| 24  | BA    | 740 | C    |
| 24  | BA    | 743 | A    |
| 24  | BA    | 744 | U    |
| 24  | BA    | 747 | U    |
| 24  | BA    | 748 | G    |
| 24  | BA    | 749 | A    |
| 24  | BA    | 751 | A    |
| 24  | BA    | 753 | A    |
| 24  | BA    | 754 | U    |
| 24  | BA    | 763 | G    |
| 24  | BA    | 764 | A    |
| 24  | BA    | 765 | C    |
| 24  | BA    | 766 | U    |
| 24  | BA    | 775 | G    |
| 24  | BA    | 776 | G    |
| 24  | BA    | 777 | G    |
| 24  | BA    | 782 | A    |
| 24  | BA    | 783 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | BA    | 784 | G    |
| 24  | BA    | 785 | G    |
| 24  | BA    | 789 | A    |
| 24  | BA    | 790 | U    |
| 24  | BA    | 791 | C    |
| 24  | BA    | 792 | A    |
| 24  | BA    | 800 | A    |
| 24  | BA    | 801 | G    |
| 24  | BA    | 802 | A    |
| 24  | BA    | 803 | U    |
| 24  | BA    | 805 | G    |
| 24  | BA    | 806 | C    |
| 24  | BA    | 810 | U    |
| 24  | BA    | 811 | U    |
| 24  | BA    | 812 | C    |
| 24  | BA    | 813 | U    |
| 24  | BA    | 819 | A    |
| 24  | BA    | 827 | U    |
| 24  | BA    | 828 | U    |
| 24  | BA    | 830 | G    |
| 24  | BA    | 845 | A    |
| 24  | BA    | 846 | U    |
| 24  | BA    | 847 | U    |
| 24  | BA    | 856 | G    |
| 24  | BA    | 858 | G    |
| 24  | BA    | 859 | G    |
| 24  | BA    | 860 | U    |
| 24  | BA    | 865 | C    |
| 24  | BA    | 866 | A    |
| 24  | BA    | 867 | C    |
| 24  | BA    | 868 | U    |
| 24  | BA    | 896 | A    |
| 24  | BA    | 897 | C    |
| 24  | BA    | 900 | A    |
| 24  | BA    | 910 | A    |
| 24  | BA    | 914 | G    |
| 24  | BA    | 915 | C    |
| 24  | BA    | 916 | G    |
| 24  | BA    | 927 | A    |
| 24  | BA    | 931 | U    |
| 24  | BA    | 932 | U    |
| 24  | BA    | 933 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 934  | U    |
| 24  | BA    | 941  | A    |
| 24  | BA    | 945  | A    |
| 24  | BA    | 946  | C    |
| 24  | BA    | 947  | A    |
| 24  | BA    | 950  | G    |
| 24  | BA    | 957  | C    |
| 24  | BA    | 958  | U    |
| 24  | BA    | 959  | A    |
| 24  | BA    | 961  | C    |
| 24  | BA    | 962  | G    |
| 24  | BA    | 963  | U    |
| 24  | BA    | 973  | A    |
| 24  | BA    | 974  | G    |
| 24  | BA    | 975  | A    |
| 24  | BA    | 976  | G    |
| 24  | BA    | 983  | A    |
| 24  | BA    | 984  | A    |
| 24  | BA    | 985  | C    |
| 24  | BA    | 990  | A    |
| 24  | BA    | 991  | C    |
| 24  | BA    | 995  | C    |
| 24  | BA    | 996  | A    |
| 24  | BA    | 997  | G    |
| 24  | BA    | 1005 | C    |
| 24  | BA    | 1006 | C    |
| 24  | BA    | 1008 | A    |
| 24  | BA    | 1009 | A    |
| 24  | BA    | 1010 | A    |
| 24  | BA    | 1011 | G    |
| 24  | BA    | 1012 | U    |
| 24  | BA    | 1013 | C    |
| 24  | BA    | 1017 | G    |
| 24  | BA    | 1021 | A    |
| 24  | BA    | 1022 | G    |
| 24  | BA    | 1023 | U    |
| 24  | BA    | 1024 | G    |
| 24  | BA    | 1025 | G    |
| 24  | BA    | 1026 | G    |
| 24  | BA    | 1027 | A    |
| 24  | BA    | 1028 | A    |
| 24  | BA    | 1033 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 1034 | G    |
| 24  | BA    | 1035 | U    |
| 24  | BA    | 1045 | C    |
| 24  | BA    | 1046 | A    |
| 24  | BA    | 1047 | G    |
| 24  | BA    | 1060 | U    |
| 24  | BA    | 1061 | U    |
| 24  | BA    | 1062 | G    |
| 24  | BA    | 1063 | G    |
| 24  | BA    | 1065 | U    |
| 24  | BA    | 1066 | U    |
| 24  | BA    | 1070 | A    |
| 24  | BA    | 1071 | G    |
| 24  | BA    | 1072 | C    |
| 24  | BA    | 1073 | A    |
| 24  | BA    | 1074 | G    |
| 24  | BA    | 1078 | U    |
| 24  | BA    | 1083 | U    |
| 24  | BA    | 1084 | A    |
| 24  | BA    | 1088 | A    |
| 24  | BA    | 1091 | G    |
| 24  | BA    | 1092 | C    |
| 24  | BA    | 1098 | A    |
| 24  | BA    | 1104 | C    |
| 24  | BA    | 1110 | G    |
| 24  | BA    | 1111 | A    |
| 24  | BA    | 1112 | G    |
| 24  | BA    | 1113 | U    |
| 24  | BA    | 1126 | A    |
| 24  | BA    | 1127 | A    |
| 24  | BA    | 1128 | G    |
| 24  | BA    | 1129 | A    |
| 24  | BA    | 1130 | U    |
| 24  | BA    | 1132 | U    |
| 24  | BA    | 1133 | A    |
| 24  | BA    | 1135 | C    |
| 24  | BA    | 1136 | G    |
| 24  | BA    | 1137 | G    |
| 24  | BA    | 1139 | G    |
| 24  | BA    | 1142 | A    |
| 24  | BA    | 1144 | A    |
| 24  | BA    | 1145 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 1154 | G    |
| 24  | BA    | 1155 | A    |
| 24  | BA    | 1157 | G    |
| 24  | BA    | 1158 | C    |
| 24  | BA    | 1174 | U    |
| 24  | BA    | 1175 | A    |
| 24  | BA    | 1176 | U    |
| 24  | BA    | 1180 | U    |
| 24  | BA    | 1181 | U    |
| 24  | BA    | 1204 | A    |
| 24  | BA    | 1205 | A    |
| 24  | BA    | 1206 | G    |
| 24  | BA    | 1207 | C    |
| 24  | BA    | 1210 | G    |
| 24  | BA    | 1211 | C    |
| 24  | BA    | 1215 | G    |
| 24  | BA    | 1236 | G    |
| 24  | BA    | 1237 | A    |
| 24  | BA    | 1238 | G    |
| 24  | BA    | 1240 | U    |
| 24  | BA    | 1247 | A    |
| 24  | BA    | 1248 | G    |
| 24  | BA    | 1249 | U    |
| 24  | BA    | 1250 | G    |
| 24  | BA    | 1251 | C    |
| 24  | BA    | 1253 | A    |
| 24  | BA    | 1254 | A    |
| 24  | BA    | 1256 | G    |
| 24  | BA    | 1265 | A    |
| 24  | BA    | 1266 | G    |
| 24  | BA    | 1268 | A    |
| 24  | BA    | 1271 | G    |
| 24  | BA    | 1272 | A    |
| 24  | BA    | 1273 | U    |
| 24  | BA    | 1274 | A    |
| 24  | BA    | 1275 | A    |
| 24  | BA    | 1276 | A    |
| 24  | BA    | 1277 | G    |
| 24  | BA    | 1281 | G    |
| 24  | BA    | 1287 | A    |
| 24  | BA    | 1288 | G    |
| 24  | BA    | 1289 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 1290 | C    |
| 24  | BA    | 1300 | G    |
| 24  | BA    | 1301 | A    |
| 24  | BA    | 1303 | G    |
| 24  | BA    | 1310 | G    |
| 24  | BA    | 1320 | C    |
| 24  | BA    | 1321 | A    |
| 24  | BA    | 1324 | G    |
| 24  | BA    | 1325 | U    |
| 24  | BA    | 1326 | U    |
| 24  | BA    | 1327 | A    |
| 24  | BA    | 1329 | U    |
| 24  | BA    | 1330 | C    |
| 24  | BA    | 1332 | G    |
| 24  | BA    | 1333 | G    |
| 24  | BA    | 1334 | G    |
| 24  | BA    | 1340 | U    |
| 24  | BA    | 1341 | G    |
| 24  | BA    | 1343 | G    |
| 24  | BA    | 1344 | U    |
| 24  | BA    | 1345 | C    |
| 24  | BA    | 1352 | U    |
| 24  | BA    | 1365 | A    |
| 24  | BA    | 1368 | G    |
| 24  | BA    | 1378 | A    |
| 24  | BA    | 1379 | U    |
| 24  | BA    | 1380 | G    |
| 24  | BA    | 1383 | A    |
| 24  | BA    | 1385 | A    |
| 24  | BA    | 1386 | C    |
| 24  | BA    | 1387 | A    |
| 24  | BA    | 1396 | U    |
| 24  | BA    | 1397 | U    |
| 24  | BA    | 1398 | C    |
| 24  | BA    | 1403 | A    |
| 24  | BA    | 1416 | G    |
| 24  | BA    | 1419 | A    |
| 24  | BA    | 1420 | A    |
| 24  | BA    | 1421 | G    |
| 24  | BA    | 1427 | A    |
| 24  | BA    | 1428 | C    |
| 24  | BA    | 1429 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 1430 | G    |
| 24  | BA    | 1451 | C    |
| 24  | BA    | 1452 | G    |
| 24  | BA    | 1453 | A    |
| 24  | BA    | 1455 | G    |
| 24  | BA    | 1458 | U    |
| 24  | BA    | 1459 | G    |
| 24  | BA    | 1460 | U    |
| 24  | BA    | 1461 | C    |
| 24  | BA    | 1476 | U    |
| 24  | BA    | 1477 | A    |
| 24  | BA    | 1482 | G    |
| 24  | BA    | 1490 | A    |
| 24  | BA    | 1491 | G    |
| 24  | BA    | 1492 | G    |
| 24  | BA    | 1493 | C    |
| 24  | BA    | 1496 | A    |
| 24  | BA    | 1497 | U    |
| 24  | BA    | 1498 | C    |
| 24  | BA    | 1499 | C    |
| 24  | BA    | 1504 | A    |
| 24  | BA    | 1508 | A    |
| 24  | BA    | 1509 | A    |
| 24  | BA    | 1510 | G    |
| 24  | BA    | 1511 | G    |
| 24  | BA    | 1515 | A    |
| 24  | BA    | 1522 | A    |
| 24  | BA    | 1523 | U    |
| 24  | BA    | 1531 | C    |
| 24  | BA    | 1533 | C    |
| 24  | BA    | 1534 | U    |
| 24  | BA    | 1536 | C    |
| 24  | BA    | 1537 | G    |
| 24  | BA    | 1538 | G    |
| 24  | BA    | 1539 | U    |
| 24  | BA    | 1540 | G    |
| 24  | BA    | 1555 | G    |
| 24  | BA    | 1556 | C    |
| 24  | BA    | 1557 | C    |
| 24  | BA    | 1558 | C    |
| 24  | BA    | 1559 | U    |
| 24  | BA    | 1560 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 1561 | C    |
| 24  | BA    | 1568 | G    |
| 24  | BA    | 1569 | A    |
| 24  | BA    | 1578 | U    |
| 24  | BA    | 1581 | G    |
| 24  | BA    | 1583 | A    |
| 24  | BA    | 1584 | U    |
| 24  | BA    | 1585 | C    |
| 24  | BA    | 1602 | U    |
| 24  | BA    | 1603 | A    |
| 24  | BA    | 1604 | C    |
| 24  | BA    | 1607 | C    |
| 24  | BA    | 1608 | A    |
| 24  | BA    | 1610 | A    |
| 24  | BA    | 1611 | C    |
| 24  | BA    | 1612 | C    |
| 24  | BA    | 1616 | A    |
| 24  | BA    | 1619 | G    |
| 24  | BA    | 1625 | C    |
| 24  | BA    | 1635 | A    |
| 24  | BA    | 1647 | U    |
| 24  | BA    | 1648 | U    |
| 24  | BA    | 1649 | G    |
| 24  | BA    | 1654 | A    |
| 24  | BA    | 1655 | A    |
| 24  | BA    | 1669 | A    |
| 24  | BA    | 1670 | C    |
| 24  | BA    | 1674 | G    |
| 24  | BA    | 1675 | C    |
| 24  | BA    | 1677 | A    |
| 24  | BA    | 1682 | G    |
| 24  | BA    | 1683 | U    |
| 24  | BA    | 1694 | C    |
| 24  | BA    | 1695 | G    |
| 24  | BA    | 1696 | G    |
| 24  | BA    | 1697 | G    |
| 24  | BA    | 1698 | A    |
| 24  | BA    | 1699 | G    |
| 24  | BA    | 1700 | A    |
| 24  | BA    | 1701 | A    |
| 24  | BA    | 1706 | C    |
| 24  | BA    | 1707 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 1708 | C    |
| 24  | BA    | 1713 | A    |
| 24  | BA    | 1714 | U    |
| 24  | BA    | 1715 | G    |
| 24  | BA    | 1716 | U    |
| 24  | BA    | 1717 | A    |
| 24  | BA    | 1723 | G    |
| 24  | BA    | 1729 | U    |
| 24  | BA    | 1730 | C    |
| 24  | BA    | 1731 | G    |
| 24  | BA    | 1732 | C    |
| 24  | BA    | 1733 | G    |
| 24  | BA    | 1738 | G    |
| 24  | BA    | 1743 | G    |
| 24  | BA    | 1744 | A    |
| 24  | BA    | 1746 | A    |
| 24  | BA    | 1758 | U    |
| 24  | BA    | 1759 | A    |
| 24  | BA    | 1760 | C    |
| 24  | BA    | 1761 | C    |
| 24  | BA    | 1764 | C    |
| 24  | BA    | 1770 | G    |
| 24  | BA    | 1773 | A    |
| 24  | BA    | 1776 | G    |
| 24  | BA    | 1780 | A    |
| 24  | BA    | 1782 | U    |
| 24  | BA    | 1784 | A    |
| 24  | BA    | 1785 | A    |
| 24  | BA    | 1786 | A    |
| 24  | BA    | 1787 | A    |
| 24  | BA    | 1788 | C    |
| 24  | BA    | 1791 | A    |
| 24  | BA    | 1800 | C    |
| 24  | BA    | 1802 | A    |
| 24  | BA    | 1803 | A    |
| 24  | BA    | 1806 | C    |
| 24  | BA    | 1808 | A    |
| 24  | BA    | 1809 | A    |
| 24  | BA    | 1810 | A    |
| 24  | BA    | 1813 | G    |
| 24  | BA    | 1815 | A    |
| 24  | BA    | 1816 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 1817 | G    |
| 24  | BA    | 1818 | U    |
| 24  | BA    | 1821 | A    |
| 24  | BA    | 1822 | C    |
| 24  | BA    | 1825 | U    |
| 24  | BA    | 1828 | G    |
| 24  | BA    | 1829 | A    |
| 24  | BA    | 1830 | C    |
| 24  | BA    | 1833 | C    |
| 24  | BA    | 1838 | C    |
| 24  | BA    | 1839 | G    |
| 24  | BA    | 1847 | A    |
| 24  | BA    | 1858 | A    |
| 24  | BA    | 1859 | U    |
| 24  | BA    | 1866 | A    |
| 24  | BA    | 1867 | G    |
| 24  | BA    | 1871 | A    |
| 24  | BA    | 1872 | A    |
| 24  | BA    | 1876 | A    |
| 24  | BA    | 1884 | G    |
| 24  | BA    | 1885 | A    |
| 24  | BA    | 1900 | A    |
| 24  | BA    | 1906 | G    |
| 24  | BA    | 1913 | A    |
| 24  | BA    | 1914 | C    |
| 24  | BA    | 1915 | U    |
| 24  | BA    | 1918 | A    |
| 24  | BA    | 1919 | A    |
| 24  | BA    | 1927 | A    |
| 24  | BA    | 1929 | G    |
| 24  | BA    | 1930 | G    |
| 24  | BA    | 1931 | U    |
| 24  | BA    | 1932 | A    |
| 24  | BA    | 1937 | A    |
| 24  | BA    | 1938 | A    |
| 24  | BA    | 1941 | C    |
| 24  | BA    | 1942 | C    |
| 24  | BA    | 1943 | U    |
| 24  | BA    | 1944 | U    |
| 24  | BA    | 1945 | G    |
| 24  | BA    | 1946 | U    |
| 24  | BA    | 1955 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 1956 | U    |
| 24  | BA    | 1957 | C    |
| 24  | BA    | 1960 | A    |
| 24  | BA    | 1963 | U    |
| 24  | BA    | 1965 | C    |
| 24  | BA    | 1966 | A    |
| 24  | BA    | 1967 | C    |
| 24  | BA    | 1968 | G    |
| 24  | BA    | 1970 | A    |
| 24  | BA    | 1971 | U    |
| 24  | BA    | 1972 | G    |
| 24  | BA    | 1977 | A    |
| 24  | BA    | 1981 | A    |
| 24  | BA    | 1982 | U    |
| 24  | BA    | 1992 | G    |
| 24  | BA    | 1993 | U    |
| 24  | BA    | 1994 | C    |
| 24  | BA    | 1996 | C    |
| 24  | BA    | 1997 | C    |
| 24  | BA    | 2006 | C    |
| 24  | BA    | 2021 | C    |
| 24  | BA    | 2022 | U    |
| 24  | BA    | 2023 | C    |
| 24  | BA    | 2024 | G    |
| 24  | BA    | 2030 | A    |
| 24  | BA    | 2031 | A    |
| 24  | BA    | 2032 | G    |
| 24  | BA    | 2033 | A    |
| 24  | BA    | 2035 | G    |
| 24  | BA    | 2036 | C    |
| 24  | BA    | 2037 | A    |
| 24  | BA    | 2043 | C    |
| 24  | BA    | 2051 | A    |
| 24  | BA    | 2052 | A    |
| 24  | BA    | 2055 | C    |
| 24  | BA    | 2056 | G    |
| 24  | BA    | 2059 | A    |
| 24  | BA    | 2060 | A    |
| 24  | BA    | 2061 | G    |
| 24  | BA    | 2062 | A    |
| 24  | BA    | 2063 | C    |
| 24  | BA    | 2064 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 2068 | U    |
| 24  | BA    | 2069 | G    |
| 24  | BA    | 2072 | C    |
| 24  | BA    | 2092 | U    |
| 24  | BA    | 2093 | G    |
| 24  | BA    | 2095 | A    |
| 24  | BA    | 2104 | C    |
| 24  | BA    | 2106 | U    |
| 24  | BA    | 2107 | G    |
| 24  | BA    | 2109 | U    |
| 24  | BA    | 2110 | G    |
| 24  | BA    | 2134 | A    |
| 24  | BA    | 2135 | A    |
| 24  | BA    | 2136 | G    |
| 24  | BA    | 2137 | U    |
| 24  | BA    | 2140 | G    |
| 24  | BA    | 2143 | C    |
| 24  | BA    | 2144 | G    |
| 24  | BA    | 2145 | C    |
| 24  | BA    | 2146 | C    |
| 24  | BA    | 2147 | A    |
| 24  | BA    | 2148 | G    |
| 24  | BA    | 2149 | U    |
| 24  | BA    | 2150 | C    |
| 24  | BA    | 2151 | U    |
| 24  | BA    | 2155 | U    |
| 24  | BA    | 2156 | G    |
| 24  | BA    | 2180 | U    |
| 24  | BA    | 2181 | U    |
| 24  | BA    | 2183 | A    |
| 24  | BA    | 2184 | A    |
| 24  | BA    | 2185 | U    |
| 24  | BA    | 2187 | U    |
| 24  | BA    | 2197 | U    |
| 24  | BA    | 2198 | A    |
| 24  | BA    | 2199 | A    |
| 24  | BA    | 2200 | C    |
| 24  | BA    | 2201 | G    |
| 24  | BA    | 2204 | G    |
| 24  | BA    | 2210 | U    |
| 24  | BA    | 2211 | A    |
| 24  | BA    | 2212 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 2214 | C    |
| 24  | BA    | 2215 | C    |
| 24  | BA    | 2225 | A    |
| 24  | BA    | 2226 | C    |
| 24  | BA    | 2227 | A    |
| 24  | BA    | 2228 | G    |
| 24  | BA    | 2238 | G    |
| 24  | BA    | 2239 | G    |
| 24  | BA    | 2249 | U    |
| 24  | BA    | 2250 | G    |
| 24  | BA    | 2252 | G    |
| 24  | BA    | 2253 | G    |
| 24  | BA    | 2256 | G    |
| 24  | BA    | 2259 | U    |
| 24  | BA    | 2266 | A    |
| 24  | BA    | 2267 | A    |
| 24  | BA    | 2268 | A    |
| 24  | BA    | 2269 | G    |
| 24  | BA    | 2273 | A    |
| 24  | BA    | 2275 | C    |
| 24  | BA    | 2278 | A    |
| 24  | BA    | 2283 | C    |
| 24  | BA    | 2284 | A    |
| 24  | BA    | 2286 | G    |
| 24  | BA    | 2287 | A    |
| 24  | BA    | 2288 | A    |
| 24  | BA    | 2296 | U    |
| 24  | BA    | 2297 | A    |
| 24  | BA    | 2298 | A    |
| 24  | BA    | 2305 | U    |
| 24  | BA    | 2307 | G    |
| 24  | BA    | 2308 | G    |
| 24  | BA    | 2309 | A    |
| 24  | BA    | 2310 | C    |
| 24  | BA    | 2312 | U    |
| 24  | BA    | 2313 | C    |
| 24  | BA    | 2319 | G    |
| 24  | BA    | 2320 | U    |
| 24  | BA    | 2321 | U    |
| 24  | BA    | 2323 | G    |
| 24  | BA    | 2325 | G    |
| 24  | BA    | 2327 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 2328 | A    |
| 24  | BA    | 2333 | A    |
| 24  | BA    | 2334 | U    |
| 24  | BA    | 2335 | A    |
| 24  | BA    | 2336 | A    |
| 24  | BA    | 2337 | G    |
| 24  | BA    | 2345 | G    |
| 24  | BA    | 2347 | C    |
| 24  | BA    | 2348 | U    |
| 24  | BA    | 2350 | C    |
| 24  | BA    | 2354 | C    |
| 24  | BA    | 2361 | G    |
| 24  | BA    | 2372 | U    |
| 24  | BA    | 2382 | G    |
| 24  | BA    | 2383 | G    |
| 24  | BA    | 2384 | U    |
| 24  | BA    | 2385 | C    |
| 24  | BA    | 2386 | A    |
| 24  | BA    | 2388 | A    |
| 24  | BA    | 2389 | G    |
| 24  | BA    | 2391 | G    |
| 24  | BA    | 2392 | A    |
| 24  | BA    | 2402 | U    |
| 24  | BA    | 2406 | A    |
| 24  | BA    | 2407 | A    |
| 24  | BA    | 2423 | U    |
| 24  | BA    | 2424 | C    |
| 24  | BA    | 2425 | A    |
| 24  | BA    | 2426 | A    |
| 24  | BA    | 2427 | C    |
| 24  | BA    | 2428 | G    |
| 24  | BA    | 2429 | G    |
| 24  | BA    | 2430 | A    |
| 24  | BA    | 2431 | U    |
| 24  | BA    | 2435 | A    |
| 24  | BA    | 2439 | A    |
| 24  | BA    | 2440 | C    |
| 24  | BA    | 2441 | U    |
| 24  | BA    | 2447 | G    |
| 24  | BA    | 2448 | A    |
| 24  | BA    | 2450 | A    |
| 24  | BA    | 2459 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 2465 | C    |
| 24  | BA    | 2469 | A    |
| 24  | BA    | 2470 | G    |
| 24  | BA    | 2476 | A    |
| 24  | BA    | 2477 | U    |
| 24  | BA    | 2490 | G    |
| 24  | BA    | 2491 | U    |
| 24  | BA    | 2492 | U    |
| 24  | BA    | 2493 | U    |
| 24  | BA    | 2498 | C    |
| 24  | BA    | 2499 | C    |
| 24  | BA    | 2502 | G    |
| 24  | BA    | 2503 | A    |
| 24  | BA    | 2504 | U    |
| 24  | BA    | 2505 | G    |
| 24  | BA    | 2506 | U    |
| 24  | BA    | 2517 | C    |
| 24  | BA    | 2518 | A    |
| 24  | BA    | 2520 | C    |
| 24  | BA    | 2521 | C    |
| 24  | BA    | 2529 | G    |
| 24  | BA    | 2542 | A    |
| 24  | BA    | 2543 | G    |
| 24  | BA    | 2554 | U    |
| 24  | BA    | 2566 | A    |
| 24  | BA    | 2567 | G    |
| 24  | BA    | 2568 | U    |
| 24  | BA    | 2573 | C    |
| 24  | BA    | 2574 | G    |
| 24  | BA    | 2579 | C    |
| 24  | BA    | 2581 | G    |
| 24  | BA    | 2582 | G    |
| 24  | BA    | 2583 | G    |
| 24  | BA    | 2585 | U    |
| 24  | BA    | 2586 | U    |
| 24  | BA    | 2589 | A    |
| 24  | BA    | 2603 | G    |
| 24  | BA    | 2609 | U    |
| 24  | BA    | 2610 | C    |
| 24  | BA    | 2611 | C    |
| 24  | BA    | 2612 | C    |
| 24  | BA    | 2613 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 2614 | A    |
| 24  | BA    | 2615 | U    |
| 24  | BA    | 2630 | G    |
| 24  | BA    | 2631 | G    |
| 24  | BA    | 2639 | A    |
| 24  | BA    | 2640 | G    |
| 24  | BA    | 2646 | C    |
| 24  | BA    | 2654 | A    |
| 24  | BA    | 2655 | G    |
| 24  | BA    | 2658 | C    |
| 24  | BA    | 2663 | G    |
| 24  | BA    | 2664 | G    |
| 24  | BA    | 2668 | G    |
| 24  | BA    | 2681 | C    |
| 24  | BA    | 2682 | A    |
| 24  | BA    | 2683 | C    |
| 24  | BA    | 2689 | U    |
| 24  | BA    | 2690 | U    |
| 24  | BA    | 2691 | C    |
| 24  | BA    | 2692 | G    |
| 24  | BA    | 2714 | G    |
| 24  | BA    | 2724 | U    |
| 24  | BA    | 2727 | A    |
| 24  | BA    | 2728 | U    |
| 24  | BA    | 2729 | G    |
| 24  | BA    | 2732 | G    |
| 24  | BA    | 2733 | A    |
| 24  | BA    | 2748 | A    |
| 24  | BA    | 2750 | A    |
| 24  | BA    | 2751 | G    |
| 24  | BA    | 2753 | A    |
| 24  | BA    | 2756 | U    |
| 24  | BA    | 2757 | A    |
| 24  | BA    | 2765 | A    |
| 24  | BA    | 2769 | U    |
| 24  | BA    | 2777 | G    |
| 24  | BA    | 2778 | A    |
| 24  | BA    | 2779 | U    |
| 24  | BA    | 2781 | A    |
| 24  | BA    | 2791 | G    |
| 24  | BA    | 2792 | A    |
| 24  | BA    | 2793 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 2798 | U    |
| 24  | BA    | 2799 | A    |
| 24  | BA    | 2800 | A    |
| 24  | BA    | 2801 | G    |
| 24  | BA    | 2808 | G    |
| 24  | BA    | 2809 | A    |
| 24  | BA    | 2810 | A    |
| 24  | BA    | 2812 | G    |
| 24  | BA    | 2820 | A    |
| 24  | BA    | 2821 | A    |
| 24  | BA    | 2822 | G    |
| 24  | BA    | 2824 | C    |
| 24  | BA    | 2825 | G    |
| 24  | BA    | 2833 | U    |
| 24  | BA    | 2834 | G    |
| 24  | BA    | 2835 | A    |
| 24  | BA    | 2836 | U    |
| 24  | BA    | 2837 | A    |
| 24  | BA    | 2848 | G    |
| 24  | BA    | 2849 | U    |
| 24  | BA    | 2850 | A    |
| 24  | BA    | 2851 | A    |
| 24  | BA    | 2861 | U    |
| 24  | BA    | 2866 | U    |
| 24  | BA    | 2867 | G    |
| 24  | BA    | 2868 | A    |
| 24  | BA    | 2869 | G    |
| 24  | BA    | 2874 | C    |
| 24  | BA    | 2879 | A    |
| 24  | BA    | 2880 | C    |
| 24  | BA    | 2883 | A    |
| 24  | BA    | 2884 | U    |
| 24  | BA    | 2886 | A    |
| 24  | BA    | 2894 | G    |
| 24  | BA    | 2895 | G    |
| 24  | BA    | 2896 | C    |
| 25  | BB    | 3    | C    |
| 25  | BB    | 12   | C    |
| 25  | BB    | 13   | G    |
| 25  | BB    | 14   | U    |
| 25  | BB    | 15   | A    |
| 25  | BB    | 16   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | BB    | 24  | G    |
| 25  | BB    | 25  | U    |
| 25  | BB    | 26  | C    |
| 25  | BB    | 35  | C    |
| 25  | BB    | 37  | C    |
| 25  | BB    | 38  | C    |
| 25  | BB    | 41  | G    |
| 25  | BB    | 42  | C    |
| 25  | BB    | 43  | C    |
| 25  | BB    | 44  | G    |
| 25  | BB    | 45  | A    |
| 25  | BB    | 52  | A    |
| 25  | BB    | 53  | A    |
| 25  | BB    | 54  | G    |
| 25  | BB    | 57  | A    |
| 25  | BB    | 58  | A    |
| 25  | BB    | 66  | A    |
| 25  | BB    | 67  | G    |
| 25  | BB    | 87  | U    |
| 25  | BB    | 88  | C    |
| 25  | BB    | 89  | U    |
| 25  | BB    | 90  | C    |
| 25  | BB    | 91  | C    |
| 25  | BB    | 99  | A    |
| 25  | BB    | 108 | A    |
| 25  | BB    | 109 | A    |
| 55  | CA    | 6   | G    |
| 55  | CA    | 7   | A    |
| 55  | CA    | 8   | A    |
| 55  | CA    | 9   | G    |
| 55  | CA    | 10  | A    |
| 55  | CA    | 13  | U    |
| 55  | CA    | 14  | U    |
| 55  | CA    | 15  | G    |
| 55  | CA    | 22  | G    |
| 55  | CA    | 31  | G    |
| 55  | CA    | 32  | A    |
| 55  | CA    | 33  | A    |
| 55  | CA    | 39  | G    |
| 55  | CA    | 40  | C    |
| 55  | CA    | 47  | C    |
| 55  | CA    | 48  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | CA    | 49  | U    |
| 55  | CA    | 51  | A    |
| 55  | CA    | 52  | C    |
| 55  | CA    | 53  | A    |
| 55  | CA    | 61  | G    |
| 55  | CA    | 62  | U    |
| 55  | CA    | 64  | G    |
| 55  | CA    | 65  | A    |
| 55  | CA    | 66  | A    |
| 55  | CA    | 67  | C    |
| 55  | CA    | 70  | U    |
| 55  | CA    | 71  | A    |
| 55  | CA    | 72  | A    |
| 55  | CA    | 76  | G    |
| 55  | CA    | 77  | A    |
| 55  | CA    | 80  | A    |
| 55  | CA    | 81  | A    |
| 55  | CA    | 82  | G    |
| 55  | CA    | 83  | C    |
| 55  | CA    | 84  | U    |
| 55  | CA    | 85  | U    |
| 55  | CA    | 86  | G    |
| 55  | CA    | 87  | C    |
| 55  | CA    | 88  | U    |
| 55  | CA    | 89  | U    |
| 55  | CA    | 90  | C    |
| 55  | CA    | 91  | U    |
| 55  | CA    | 92  | U    |
| 55  | CA    | 94  | G    |
| 55  | CA    | 95  | C    |
| 55  | CA    | 96  | U    |
| 55  | CA    | 97  | G    |
| 55  | CA    | 110 | C    |
| 55  | CA    | 111 | G    |
| 55  | CA    | 116 | A    |
| 55  | CA    | 117 | G    |
| 55  | CA    | 119 | A    |
| 55  | CA    | 120 | A    |
| 55  | CA    | 121 | U    |
| 55  | CA    | 122 | G    |
| 55  | CA    | 131 | A    |
| 55  | CA    | 132 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | CA    | 133 | U    |
| 55  | CA    | 143 | A    |
| 55  | CA    | 144 | G    |
| 55  | CA    | 155 | A    |
| 55  | CA    | 159 | G    |
| 55  | CA    | 164 | G    |
| 55  | CA    | 166 | U    |
| 55  | CA    | 175 | C    |
| 55  | CA    | 178 | C    |
| 55  | CA    | 182 | A    |
| 55  | CA    | 197 | A    |
| 55  | CA    | 198 | G    |
| 55  | CA    | 199 | A    |
| 55  | CA    | 200 | G    |
| 55  | CA    | 206 | C    |
| 55  | CA    | 207 | C    |
| 55  | CA    | 208 | U    |
| 55  | CA    | 209 | U    |
| 55  | CA    | 210 | C    |
| 55  | CA    | 211 | G    |
| 55  | CA    | 212 | G    |
| 55  | CA    | 213 | G    |
| 55  | CA    | 214 | C    |
| 55  | CA    | 239 | U    |
| 55  | CA    | 240 | G    |
| 55  | CA    | 243 | A    |
| 55  | CA    | 244 | U    |
| 55  | CA    | 245 | U    |
| 55  | CA    | 247 | G    |
| 55  | CA    | 248 | C    |
| 55  | CA    | 250 | A    |
| 55  | CA    | 251 | G    |
| 55  | CA    | 252 | U    |
| 55  | CA    | 253 | A    |
| 55  | CA    | 254 | G    |
| 55  | CA    | 266 | G    |
| 55  | CA    | 267 | C    |
| 55  | CA    | 275 | G    |
| 55  | CA    | 276 | G    |
| 55  | CA    | 277 | C    |
| 55  | CA    | 280 | C    |
| 55  | CA    | 282 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | CA    | 283 | U    |
| 55  | CA    | 289 | G    |
| 55  | CA    | 306 | A    |
| 55  | CA    | 316 | C    |
| 55  | CA    | 317 | U    |
| 55  | CA    | 328 | C    |
| 55  | CA    | 329 | A    |
| 55  | CA    | 330 | C    |
| 55  | CA    | 331 | G    |
| 55  | CA    | 332 | G    |
| 55  | CA    | 338 | A    |
| 55  | CA    | 344 | A    |
| 55  | CA    | 345 | C    |
| 55  | CA    | 346 | G    |
| 55  | CA    | 347 | G    |
| 55  | CA    | 348 | G    |
| 55  | CA    | 352 | C    |
| 55  | CA    | 353 | A    |
| 55  | CA    | 354 | G    |
| 55  | CA    | 367 | U    |
| 55  | CA    | 369 | G    |
| 55  | CA    | 370 | C    |
| 55  | CA    | 372 | C    |
| 55  | CA    | 373 | A    |
| 55  | CA    | 374 | A    |
| 55  | CA    | 381 | C    |
| 55  | CA    | 383 | A    |
| 55  | CA    | 384 | G    |
| 55  | CA    | 389 | A    |
| 55  | CA    | 397 | A    |
| 55  | CA    | 398 | U    |
| 55  | CA    | 406 | G    |
| 55  | CA    | 411 | A    |
| 55  | CA    | 412 | A    |
| 55  | CA    | 413 | G    |
| 55  | CA    | 414 | A    |
| 55  | CA    | 415 | A    |
| 55  | CA    | 421 | U    |
| 55  | CA    | 422 | C    |
| 55  | CA    | 423 | G    |
| 55  | CA    | 424 | G    |
| 55  | CA    | 425 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | CA    | 428 | G    |
| 55  | CA    | 429 | U    |
| 55  | CA    | 430 | A    |
| 55  | CA    | 431 | A    |
| 55  | CA    | 436 | C    |
| 55  | CA    | 439 | U    |
| 55  | CA    | 440 | C    |
| 55  | CA    | 452 | A    |
| 55  | CA    | 453 | G    |
| 55  | CA    | 454 | G    |
| 55  | CA    | 456 | A    |
| 55  | CA    | 457 | G    |
| 55  | CA    | 458 | U    |
| 55  | CA    | 459 | A    |
| 55  | CA    | 460 | A    |
| 55  | CA    | 461 | A    |
| 55  | CA    | 462 | G    |
| 55  | CA    | 463 | U    |
| 55  | CA    | 464 | U    |
| 55  | CA    | 465 | A    |
| 55  | CA    | 466 | A    |
| 55  | CA    | 467 | U    |
| 55  | CA    | 468 | A    |
| 55  | CA    | 469 | C    |
| 55  | CA    | 474 | G    |
| 55  | CA    | 476 | U    |
| 55  | CA    | 478 | A    |
| 55  | CA    | 479 | U    |
| 55  | CA    | 481 | G    |
| 55  | CA    | 482 | A    |
| 55  | CA    | 483 | C    |
| 55  | CA    | 484 | G    |
| 55  | CA    | 485 | U    |
| 55  | CA    | 486 | U    |
| 55  | CA    | 487 | A    |
| 55  | CA    | 496 | A    |
| 55  | CA    | 497 | G    |
| 55  | CA    | 498 | A    |
| 55  | CA    | 499 | A    |
| 55  | CA    | 500 | G    |
| 55  | CA    | 501 | C    |
| 55  | CA    | 505 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | CA    | 508 | U    |
| 55  | CA    | 509 | A    |
| 55  | CA    | 510 | A    |
| 55  | CA    | 511 | C    |
| 55  | CA    | 512 | U    |
| 55  | CA    | 513 | C    |
| 55  | CA    | 514 | C    |
| 55  | CA    | 517 | G    |
| 55  | CA    | 518 | C    |
| 55  | CA    | 519 | C    |
| 55  | CA    | 520 | A    |
| 55  | CA    | 521 | G    |
| 55  | CA    | 527 | G    |
| 55  | CA    | 531 | U    |
| 55  | CA    | 532 | A    |
| 55  | CA    | 533 | A    |
| 55  | CA    | 534 | U    |
| 55  | CA    | 536 | C    |
| 55  | CA    | 537 | G    |
| 55  | CA    | 538 | G    |
| 55  | CA    | 548 | G    |
| 55  | CA    | 549 | C    |
| 55  | CA    | 559 | A    |
| 55  | CA    | 560 | A    |
| 55  | CA    | 562 | U    |
| 55  | CA    | 563 | A    |
| 55  | CA    | 564 | C    |
| 55  | CA    | 565 | U    |
| 55  | CA    | 566 | G    |
| 55  | CA    | 567 | G    |
| 55  | CA    | 568 | G    |
| 55  | CA    | 572 | A    |
| 55  | CA    | 573 | A    |
| 55  | CA    | 575 | G    |
| 55  | CA    | 576 | C    |
| 55  | CA    | 577 | G    |
| 55  | CA    | 578 | C    |
| 55  | CA    | 596 | A    |
| 55  | CA    | 597 | G    |
| 55  | CA    | 611 | C    |
| 55  | CA    | 617 | G    |
| 55  | CA    | 642 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | CA    | 643 | C    |
| 55  | CA    | 644 | U    |
| 55  | CA    | 653 | U    |
| 55  | CA    | 654 | G    |
| 55  | CA    | 655 | A    |
| 55  | CA    | 665 | A    |
| 55  | CA    | 666 | G    |
| 55  | CA    | 688 | G    |
| 55  | CA    | 689 | C    |
| 55  | CA    | 693 | G    |
| 55  | CA    | 694 | A    |
| 55  | CA    | 695 | A    |
| 55  | CA    | 699 | C    |
| 55  | CA    | 700 | G    |
| 55  | CA    | 701 | U    |
| 55  | CA    | 702 | A    |
| 55  | CA    | 703 | G    |
| 55  | CA    | 704 | A    |
| 55  | CA    | 705 | G    |
| 55  | CA    | 718 | A    |
| 55  | CA    | 721 | G    |
| 55  | CA    | 722 | G    |
| 55  | CA    | 723 | U    |
| 55  | CA    | 724 | G    |
| 55  | CA    | 725 | G    |
| 55  | CA    | 731 | G    |
| 55  | CA    | 733 | G    |
| 55  | CA    | 734 | G    |
| 55  | CA    | 735 | C    |
| 55  | CA    | 736 | C    |
| 55  | CA    | 748 | G    |
| 55  | CA    | 753 | A    |
| 55  | CA    | 754 | C    |
| 55  | CA    | 755 | G    |
| 55  | CA    | 756 | C    |
| 55  | CA    | 777 | A    |
| 55  | CA    | 781 | A    |
| 55  | CA    | 782 | A    |
| 55  | CA    | 784 | A    |
| 55  | CA    | 785 | G    |
| 55  | CA    | 787 | A    |
| 55  | CA    | 792 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | CA    | 793 | U    |
| 55  | CA    | 794 | A    |
| 55  | CA    | 795 | C    |
| 55  | CA    | 799 | G    |
| 55  | CA    | 803 | G    |
| 55  | CA    | 804 | U    |
| 55  | CA    | 810 | C    |
| 55  | CA    | 812 | G    |
| 55  | CA    | 814 | A    |
| 55  | CA    | 815 | A    |
| 55  | CA    | 816 | A    |
| 55  | CA    | 817 | C    |
| 55  | CA    | 818 | G    |
| 55  | CA    | 819 | A    |
| 55  | CA    | 820 | U    |
| 55  | CA    | 821 | G    |
| 55  | CA    | 822 | U    |
| 55  | CA    | 828 | U    |
| 55  | CA    | 829 | G    |
| 55  | CA    | 841 | C    |
| 55  | CA    | 842 | U    |
| 55  | CA    | 843 | U    |
| 55  | CA    | 844 | G    |
| 55  | CA    | 845 | A    |
| 55  | CA    | 846 | G    |
| 55  | CA    | 849 | G    |
| 55  | CA    | 871 | U    |
| 55  | CA    | 874 | G    |
| 55  | CA    | 875 | U    |
| 55  | CA    | 876 | C    |
| 55  | CA    | 880 | C    |
| 55  | CA    | 885 | G    |
| 55  | CA    | 886 | G    |
| 55  | CA    | 889 | A    |
| 55  | CA    | 890 | G    |
| 55  | CA    | 891 | U    |
| 55  | CA    | 892 | A    |
| 55  | CA    | 914 | A    |
| 55  | CA    | 915 | A    |
| 55  | CA    | 926 | G    |
| 55  | CA    | 927 | G    |
| 55  | CA    | 934 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 55  | CA    | 935  | A    |
| 55  | CA    | 936  | C    |
| 55  | CA    | 939  | G    |
| 55  | CA    | 942  | G    |
| 55  | CA    | 945  | G    |
| 55  | CA    | 960  | U    |
| 55  | CA    | 961  | U    |
| 55  | CA    | 962  | C    |
| 55  | CA    | 966  | G    |
| 55  | CA    | 968  | A    |
| 55  | CA    | 969  | A    |
| 55  | CA    | 970  | C    |
| 55  | CA    | 971  | G    |
| 55  | CA    | 972  | C    |
| 55  | CA    | 975  | A    |
| 55  | CA    | 976  | G    |
| 55  | CA    | 977  | A    |
| 55  | CA    | 978  | A    |
| 55  | CA    | 982  | U    |
| 55  | CA    | 983  | A    |
| 55  | CA    | 984  | C    |
| 55  | CA    | 990  | C    |
| 55  | CA    | 992  | U    |
| 55  | CA    | 993  | G    |
| 55  | CA    | 995  | C    |
| 55  | CA    | 996  | A    |
| 55  | CA    | 1000 | A    |
| 55  | CA    | 1004 | A    |
| 55  | CA    | 1019 | A    |
| 55  | CA    | 1020 | G    |
| 55  | CA    | 1022 | A    |
| 55  | CA    | 1029 | U    |
| 55  | CA    | 1031 | C    |
| 55  | CA    | 1032 | G    |
| 55  | CA    | 1036 | A    |
| 55  | CA    | 1037 | C    |
| 55  | CA    | 1044 | A    |
| 55  | CA    | 1045 | C    |
| 55  | CA    | 1046 | A    |
| 55  | CA    | 1049 | U    |
| 55  | CA    | 1050 | G    |
| 55  | CA    | 1051 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 55  | CA    | 1052 | U    |
| 55  | CA    | 1053 | G    |
| 55  | CA    | 1054 | C    |
| 55  | CA    | 1055 | A    |
| 55  | CA    | 1056 | U    |
| 55  | CA    | 1064 | G    |
| 55  | CA    | 1065 | U    |
| 55  | CA    | 1066 | C    |
| 55  | CA    | 1068 | G    |
| 55  | CA    | 1069 | C    |
| 55  | CA    | 1070 | U    |
| 55  | CA    | 1085 | U    |
| 55  | CA    | 1086 | U    |
| 55  | CA    | 1087 | G    |
| 55  | CA    | 1094 | G    |
| 55  | CA    | 1095 | U    |
| 55  | CA    | 1101 | A    |
| 55  | CA    | 1102 | A    |
| 55  | CA    | 1103 | C    |
| 55  | CA    | 1113 | C    |
| 55  | CA    | 1125 | U    |
| 55  | CA    | 1127 | G    |
| 55  | CA    | 1128 | C    |
| 55  | CA    | 1129 | C    |
| 55  | CA    | 1130 | A    |
| 55  | CA    | 1137 | C    |
| 55  | CA    | 1138 | G    |
| 55  | CA    | 1139 | G    |
| 55  | CA    | 1140 | C    |
| 55  | CA    | 1141 | C    |
| 55  | CA    | 1142 | G    |
| 55  | CA    | 1143 | G    |
| 55  | CA    | 1145 | A    |
| 55  | CA    | 1146 | A    |
| 55  | CA    | 1152 | A    |
| 55  | CA    | 1157 | A    |
| 55  | CA    | 1158 | C    |
| 55  | CA    | 1159 | U    |
| 55  | CA    | 1160 | G    |
| 55  | CA    | 1161 | C    |
| 55  | CA    | 1162 | C    |
| 55  | CA    | 1169 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 55  | CA    | 1178 | G    |
| 55  | CA    | 1179 | A    |
| 55  | CA    | 1181 | G    |
| 55  | CA    | 1183 | U    |
| 55  | CA    | 1184 | G    |
| 55  | CA    | 1185 | G    |
| 55  | CA    | 1196 | A    |
| 55  | CA    | 1197 | A    |
| 55  | CA    | 1200 | C    |
| 55  | CA    | 1201 | A    |
| 55  | CA    | 1202 | U    |
| 55  | CA    | 1203 | C    |
| 55  | CA    | 1212 | U    |
| 55  | CA    | 1213 | A    |
| 55  | CA    | 1214 | C    |
| 55  | CA    | 1215 | G    |
| 55  | CA    | 1216 | A    |
| 55  | CA    | 1219 | A    |
| 55  | CA    | 1222 | G    |
| 55  | CA    | 1224 | U    |
| 55  | CA    | 1225 | A    |
| 55  | CA    | 1226 | C    |
| 55  | CA    | 1228 | C    |
| 55  | CA    | 1229 | A    |
| 55  | CA    | 1230 | C    |
| 55  | CA    | 1238 | A    |
| 55  | CA    | 1239 | A    |
| 55  | CA    | 1240 | U    |
| 55  | CA    | 1241 | G    |
| 55  | CA    | 1242 | G    |
| 55  | CA    | 1243 | C    |
| 55  | CA    | 1250 | A    |
| 55  | CA    | 1251 | A    |
| 55  | CA    | 1256 | A    |
| 55  | CA    | 1257 | A    |
| 55  | CA    | 1263 | C    |
| 55  | CA    | 1266 | G    |
| 55  | CA    | 1270 | G    |
| 55  | CA    | 1278 | G    |
| 55  | CA    | 1279 | G    |
| 55  | CA    | 1280 | A    |
| 55  | CA    | 1281 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 55  | CA    | 1282 | C    |
| 55  | CA    | 1283 | U    |
| 55  | CA    | 1284 | C    |
| 55  | CA    | 1285 | A    |
| 55  | CA    | 1286 | U    |
| 55  | CA    | 1287 | A    |
| 55  | CA    | 1288 | A    |
| 55  | CA    | 1289 | A    |
| 55  | CA    | 1290 | G    |
| 55  | CA    | 1294 | G    |
| 55  | CA    | 1297 | G    |
| 55  | CA    | 1299 | A    |
| 55  | CA    | 1300 | G    |
| 55  | CA    | 1301 | U    |
| 55  | CA    | 1302 | C    |
| 55  | CA    | 1303 | C    |
| 55  | CA    | 1305 | G    |
| 55  | CA    | 1312 | G    |
| 55  | CA    | 1316 | G    |
| 55  | CA    | 1317 | C    |
| 55  | CA    | 1319 | A    |
| 55  | CA    | 1320 | C    |
| 55  | CA    | 1322 | C    |
| 55  | CA    | 1323 | G    |
| 55  | CA    | 1324 | A    |
| 55  | CA    | 1325 | C    |
| 55  | CA    | 1338 | G    |
| 55  | CA    | 1346 | A    |
| 55  | CA    | 1348 | U    |
| 55  | CA    | 1349 | A    |
| 55  | CA    | 1353 | G    |
| 55  | CA    | 1362 | A    |
| 55  | CA    | 1364 | U    |
| 55  | CA    | 1365 | G    |
| 55  | CA    | 1366 | C    |
| 55  | CA    | 1370 | G    |
| 55  | CA    | 1379 | G    |
| 55  | CA    | 1381 | U    |
| 55  | CA    | 1382 | C    |
| 55  | CA    | 1383 | C    |
| 55  | CA    | 1394 | A    |
| 55  | CA    | 1395 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 55  | CA    | 1396 | A    |
| 55  | CA    | 1398 | A    |
| 55  | CA    | 1400 | C    |
| 55  | CA    | 1411 | C    |
| 55  | CA    | 1419 | G    |
| 55  | CA    | 1429 | A    |
| 55  | CA    | 1432 | G    |
| 55  | CA    | 1441 | A    |
| 55  | CA    | 1442 | G    |
| 55  | CA    | 1443 | C    |
| 55  | CA    | 1446 | A    |
| 55  | CA    | 1447 | A    |
| 55  | CA    | 1448 | C    |
| 55  | CA    | 1449 | C    |
| 55  | CA    | 1451 | U    |
| 55  | CA    | 1452 | C    |
| 55  | CA    | 1453 | G    |
| 55  | CA    | 1454 | G    |
| 55  | CA    | 1455 | G    |
| 55  | CA    | 1456 | A    |
| 55  | CA    | 1492 | A    |
| 55  | CA    | 1494 | G    |
| 55  | CA    | 1497 | G    |
| 55  | CA    | 1498 | U    |
| 55  | CA    | 1499 | A    |
| 55  | CA    | 1500 | A    |
| 55  | CA    | 1502 | A    |
| 55  | CA    | 1503 | A    |
| 55  | CA    | 1505 | G    |
| 55  | CA    | 1507 | A    |
| 55  | CA    | 1508 | A    |
| 55  | CA    | 1517 | G    |
| 55  | CA    | 1519 | A    |
| 55  | CA    | 1520 | C    |
| 55  | CA    | 1529 | G    |
| 55  | CA    | 1530 | G    |
| 55  | CA    | 1531 | A    |
| 55  | CA    | 1534 | A    |
| 22  | CV    | 28   | G    |
| 22  | CV    | 34   | G    |
| 22  | CV    | 36   | A    |
| 23  | CW    | 5    | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | CX    | 34  | G    |
| 22  | CX    | 36  | A    |
| 24  | DA    | 10  | A    |
| 24  | DA    | 12  | U    |
| 24  | DA    | 14  | A    |
| 24  | DA    | 15  | G    |
| 24  | DA    | 16  | C    |
| 24  | DA    | 34  | U    |
| 24  | DA    | 35  | G    |
| 24  | DA    | 36  | G    |
| 24  | DA    | 37  | C    |
| 24  | DA    | 39  | G    |
| 24  | DA    | 40  | U    |
| 24  | DA    | 46  | G    |
| 24  | DA    | 49  | A    |
| 24  | DA    | 50  | U    |
| 24  | DA    | 51  | G    |
| 24  | DA    | 52  | A    |
| 24  | DA    | 53  | A    |
| 24  | DA    | 60  | G    |
| 24  | DA    | 61  | C    |
| 24  | DA    | 62  | U    |
| 24  | DA    | 70  | G    |
| 24  | DA    | 71  | A    |
| 24  | DA    | 73  | A    |
| 24  | DA    | 74  | A    |
| 24  | DA    | 75  | G    |
| 24  | DA    | 76  | C    |
| 24  | DA    | 77  | G    |
| 24  | DA    | 79  | C    |
| 24  | DA    | 83  | A    |
| 24  | DA    | 84  | A    |
| 24  | DA    | 85  | G    |
| 24  | DA    | 86  | G    |
| 24  | DA    | 87  | U    |
| 24  | DA    | 91  | A    |
| 24  | DA    | 92  | U    |
| 24  | DA    | 93  | G    |
| 24  | DA    | 100 | U    |
| 24  | DA    | 101 | A    |
| 24  | DA    | 102 | U    |
| 24  | DA    | 103 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | DA    | 104 | A    |
| 24  | DA    | 118 | A    |
| 24  | DA    | 119 | A    |
| 24  | DA    | 120 | U    |
| 24  | DA    | 121 | G    |
| 24  | DA    | 122 | G    |
| 24  | DA    | 126 | A    |
| 24  | DA    | 128 | C    |
| 24  | DA    | 129 | C    |
| 24  | DA    | 134 | G    |
| 24  | DA    | 139 | U    |
| 24  | DA    | 140 | C    |
| 24  | DA    | 141 | G    |
| 24  | DA    | 142 | A    |
| 24  | DA    | 143 | C    |
| 24  | DA    | 144 | A    |
| 24  | DA    | 155 | A    |
| 24  | DA    | 156 | A    |
| 24  | DA    | 160 | A    |
| 24  | DA    | 162 | U    |
| 24  | DA    | 164 | C    |
| 24  | DA    | 165 | A    |
| 24  | DA    | 171 | U    |
| 24  | DA    | 180 | G    |
| 24  | DA    | 181 | A    |
| 24  | DA    | 193 | U    |
| 24  | DA    | 196 | A    |
| 24  | DA    | 197 | A    |
| 24  | DA    | 198 | C    |
| 24  | DA    | 199 | A    |
| 24  | DA    | 204 | A    |
| 24  | DA    | 205 | G    |
| 24  | DA    | 206 | U    |
| 24  | DA    | 207 | A    |
| 24  | DA    | 216 | A    |
| 24  | DA    | 217 | A    |
| 24  | DA    | 218 | A    |
| 24  | DA    | 221 | A    |
| 24  | DA    | 222 | A    |
| 24  | DA    | 223 | A    |
| 24  | DA    | 224 | U    |
| 24  | DA    | 225 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | DA    | 226 | A    |
| 24  | DA    | 227 | A    |
| 24  | DA    | 228 | C    |
| 24  | DA    | 229 | C    |
| 24  | DA    | 230 | G    |
| 24  | DA    | 231 | A    |
| 24  | DA    | 233 | A    |
| 24  | DA    | 234 | U    |
| 24  | DA    | 235 | U    |
| 24  | DA    | 241 | A    |
| 24  | DA    | 242 | G    |
| 24  | DA    | 243 | U    |
| 24  | DA    | 244 | A    |
| 24  | DA    | 245 | G    |
| 24  | DA    | 248 | G    |
| 24  | DA    | 249 | C    |
| 24  | DA    | 250 | G    |
| 24  | DA    | 251 | A    |
| 24  | DA    | 252 | G    |
| 24  | DA    | 255 | A    |
| 24  | DA    | 264 | C    |
| 24  | DA    | 265 | A    |
| 24  | DA    | 266 | G    |
| 24  | DA    | 271 | G    |
| 24  | DA    | 272 | A    |
| 24  | DA    | 273 | G    |
| 24  | DA    | 277 | G    |
| 24  | DA    | 281 | C    |
| 24  | DA    | 284 | U    |
| 24  | DA    | 285 | G    |
| 24  | DA    | 295 | G    |
| 24  | DA    | 299 | A    |
| 24  | DA    | 301 | G    |
| 24  | DA    | 302 | C    |
| 24  | DA    | 303 | G    |
| 24  | DA    | 311 | A    |
| 24  | DA    | 312 | G    |
| 24  | DA    | 314 | C    |
| 24  | DA    | 315 | G    |
| 24  | DA    | 322 | A    |
| 24  | DA    | 323 | C    |
| 24  | DA    | 324 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | DA    | 325 | G    |
| 24  | DA    | 326 | G    |
| 24  | DA    | 329 | G    |
| 24  | DA    | 330 | A    |
| 24  | DA    | 334 | C    |
| 24  | DA    | 335 | C    |
| 24  | DA    | 343 | C    |
| 24  | DA    | 351 | C    |
| 24  | DA    | 353 | C    |
| 24  | DA    | 362 | A    |
| 24  | DA    | 363 | G    |
| 24  | DA    | 364 | C    |
| 24  | DA    | 365 | U    |
| 24  | DA    | 367 | G    |
| 24  | DA    | 370 | G    |
| 24  | DA    | 371 | A    |
| 24  | DA    | 372 | G    |
| 24  | DA    | 374 | A    |
| 24  | DA    | 375 | G    |
| 24  | DA    | 383 | C    |
| 24  | DA    | 386 | G    |
| 24  | DA    | 387 | U    |
| 24  | DA    | 388 | G    |
| 24  | DA    | 389 | G    |
| 24  | DA    | 390 | U    |
| 24  | DA    | 391 | A    |
| 24  | DA    | 392 | U    |
| 24  | DA    | 396 | G    |
| 24  | DA    | 397 | U    |
| 24  | DA    | 398 | C    |
| 24  | DA    | 399 | U    |
| 24  | DA    | 404 | A    |
| 24  | DA    | 405 | U    |
| 24  | DA    | 406 | G    |
| 24  | DA    | 407 | G    |
| 24  | DA    | 411 | G    |
| 24  | DA    | 412 | A    |
| 24  | DA    | 413 | C    |
| 24  | DA    | 421 | C    |
| 24  | DA    | 422 | A    |
| 24  | DA    | 423 | A    |
| 24  | DA    | 424 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | DA    | 430 | A    |
| 24  | DA    | 437 | U    |
| 24  | DA    | 442 | G    |
| 24  | DA    | 443 | A    |
| 24  | DA    | 444 | C    |
| 24  | DA    | 445 | C    |
| 24  | DA    | 446 | G    |
| 24  | DA    | 447 | A    |
| 24  | DA    | 449 | A    |
| 24  | DA    | 450 | G    |
| 24  | DA    | 451 | U    |
| 24  | DA    | 452 | G    |
| 24  | DA    | 455 | C    |
| 24  | DA    | 457 | A    |
| 24  | DA    | 459 | U    |
| 24  | DA    | 460 | A    |
| 24  | DA    | 461 | C    |
| 24  | DA    | 462 | C    |
| 24  | DA    | 475 | C    |
| 24  | DA    | 476 | G    |
| 24  | DA    | 477 | A    |
| 24  | DA    | 479 | A    |
| 24  | DA    | 480 | A    |
| 24  | DA    | 481 | G    |
| 24  | DA    | 482 | A    |
| 24  | DA    | 489 | G    |
| 24  | DA    | 490 | C    |
| 24  | DA    | 491 | G    |
| 24  | DA    | 492 | A    |
| 24  | DA    | 498 | G    |
| 24  | DA    | 502 | A    |
| 24  | DA    | 503 | A    |
| 24  | DA    | 504 | A    |
| 24  | DA    | 505 | A    |
| 24  | DA    | 506 | G    |
| 24  | DA    | 507 | A    |
| 24  | DA    | 509 | C    |
| 24  | DA    | 510 | C    |
| 24  | DA    | 511 | U    |
| 24  | DA    | 512 | G    |
| 24  | DA    | 527 | C    |
| 24  | DA    | 528 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | DA    | 529 | A    |
| 24  | DA    | 530 | G    |
| 24  | DA    | 531 | C    |
| 24  | DA    | 532 | A    |
| 24  | DA    | 533 | G    |
| 24  | DA    | 534 | U    |
| 24  | DA    | 544 | C    |
| 24  | DA    | 546 | U    |
| 24  | DA    | 547 | A    |
| 24  | DA    | 548 | G    |
| 24  | DA    | 549 | G    |
| 24  | DA    | 550 | C    |
| 24  | DA    | 556 | A    |
| 24  | DA    | 563 | A    |
| 24  | DA    | 571 | U    |
| 24  | DA    | 572 | A    |
| 24  | DA    | 573 | U    |
| 24  | DA    | 575 | A    |
| 24  | DA    | 576 | U    |
| 24  | DA    | 586 | A    |
| 24  | DA    | 587 | C    |
| 24  | DA    | 589 | U    |
| 24  | DA    | 590 | A    |
| 24  | DA    | 603 | A    |
| 24  | DA    | 604 | G    |
| 24  | DA    | 605 | G    |
| 24  | DA    | 613 | A    |
| 24  | DA    | 614 | A    |
| 24  | DA    | 615 | U    |
| 24  | DA    | 616 | A    |
| 24  | DA    | 617 | G    |
| 24  | DA    | 620 | G    |
| 24  | DA    | 621 | A    |
| 24  | DA    | 622 | G    |
| 24  | DA    | 627 | A    |
| 24  | DA    | 638 | G    |
| 24  | DA    | 639 | U    |
| 24  | DA    | 645 | C    |
| 24  | DA    | 647 | G    |
| 24  | DA    | 648 | G    |
| 24  | DA    | 654 | A    |
| 24  | DA    | 655 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | DA    | 656 | G    |
| 24  | DA    | 657 | U    |
| 24  | DA    | 658 | U    |
| 24  | DA    | 662 | G    |
| 24  | DA    | 669 | G    |
| 24  | DA    | 670 | A    |
| 24  | DA    | 671 | C    |
| 24  | DA    | 672 | C    |
| 24  | DA    | 673 | C    |
| 24  | DA    | 686 | U    |
| 24  | DA    | 687 | C    |
| 24  | DA    | 688 | U    |
| 24  | DA    | 699 | A    |
| 24  | DA    | 717 | C    |
| 24  | DA    | 718 | A    |
| 24  | DA    | 727 | A    |
| 24  | DA    | 728 | G    |
| 24  | DA    | 729 | G    |
| 24  | DA    | 730 | A    |
| 24  | DA    | 740 | C    |
| 24  | DA    | 741 | U    |
| 24  | DA    | 746 | U    |
| 24  | DA    | 747 | U    |
| 24  | DA    | 748 | G    |
| 24  | DA    | 752 | A    |
| 24  | DA    | 753 | A    |
| 24  | DA    | 754 | U    |
| 24  | DA    | 755 | U    |
| 24  | DA    | 757 | G    |
| 24  | DA    | 763 | G    |
| 24  | DA    | 764 | A    |
| 24  | DA    | 765 | C    |
| 24  | DA    | 766 | U    |
| 24  | DA    | 775 | G    |
| 24  | DA    | 776 | G    |
| 24  | DA    | 777 | G    |
| 24  | DA    | 778 | G    |
| 24  | DA    | 779 | U    |
| 24  | DA    | 781 | A    |
| 24  | DA    | 782 | A    |
| 24  | DA    | 783 | A    |
| 24  | DA    | 784 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | DA    | 785 | G    |
| 24  | DA    | 789 | A    |
| 24  | DA    | 790 | U    |
| 24  | DA    | 791 | C    |
| 24  | DA    | 792 | A    |
| 24  | DA    | 793 | A    |
| 24  | DA    | 794 | A    |
| 24  | DA    | 795 | C    |
| 24  | DA    | 800 | A    |
| 24  | DA    | 801 | G    |
| 24  | DA    | 802 | A    |
| 24  | DA    | 803 | U    |
| 24  | DA    | 805 | G    |
| 24  | DA    | 806 | C    |
| 24  | DA    | 812 | C    |
| 24  | DA    | 819 | A    |
| 24  | DA    | 827 | U    |
| 24  | DA    | 828 | U    |
| 24  | DA    | 830 | G    |
| 24  | DA    | 831 | G    |
| 24  | DA    | 832 | U    |
| 24  | DA    | 846 | U    |
| 24  | DA    | 847 | U    |
| 24  | DA    | 858 | G    |
| 24  | DA    | 859 | G    |
| 24  | DA    | 861 | A    |
| 24  | DA    | 866 | A    |
| 24  | DA    | 867 | C    |
| 24  | DA    | 868 | U    |
| 24  | DA    | 874 | G    |
| 24  | DA    | 875 | G    |
| 24  | DA    | 877 | A    |
| 24  | DA    | 878 | A    |
| 24  | DA    | 902 | C    |
| 24  | DA    | 910 | A    |
| 24  | DA    | 912 | C    |
| 24  | DA    | 914 | G    |
| 24  | DA    | 915 | C    |
| 24  | DA    | 916 | G    |
| 24  | DA    | 921 | C    |
| 24  | DA    | 922 | C    |
| 24  | DA    | 932 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 933  | A    |
| 24  | DA    | 934  | U    |
| 24  | DA    | 941  | A    |
| 24  | DA    | 944  | C    |
| 24  | DA    | 946  | C    |
| 24  | DA    | 947  | A    |
| 24  | DA    | 958  | U    |
| 24  | DA    | 959  | A    |
| 24  | DA    | 960  | A    |
| 24  | DA    | 961  | C    |
| 24  | DA    | 962  | G    |
| 24  | DA    | 964  | C    |
| 24  | DA    | 973  | A    |
| 24  | DA    | 974  | G    |
| 24  | DA    | 975  | A    |
| 24  | DA    | 976  | G    |
| 24  | DA    | 983  | A    |
| 24  | DA    | 985  | C    |
| 24  | DA    | 990  | A    |
| 24  | DA    | 991  | C    |
| 24  | DA    | 995  | C    |
| 24  | DA    | 996  | A    |
| 24  | DA    | 1008 | A    |
| 24  | DA    | 1009 | A    |
| 24  | DA    | 1010 | A    |
| 24  | DA    | 1011 | G    |
| 24  | DA    | 1012 | U    |
| 24  | DA    | 1013 | C    |
| 24  | DA    | 1014 | A    |
| 24  | DA    | 1020 | A    |
| 24  | DA    | 1021 | A    |
| 24  | DA    | 1022 | G    |
| 24  | DA    | 1023 | U    |
| 24  | DA    | 1024 | G    |
| 24  | DA    | 1025 | G    |
| 24  | DA    | 1026 | G    |
| 24  | DA    | 1027 | A    |
| 24  | DA    | 1033 | U    |
| 24  | DA    | 1034 | G    |
| 24  | DA    | 1035 | U    |
| 24  | DA    | 1036 | G    |
| 24  | DA    | 1044 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 1045 | C    |
| 24  | DA    | 1046 | A    |
| 24  | DA    | 1047 | G    |
| 24  | DA    | 1049 | C    |
| 24  | DA    | 1050 | A    |
| 24  | DA    | 1056 | G    |
| 24  | DA    | 1057 | A    |
| 24  | DA    | 1060 | U    |
| 24  | DA    | 1061 | U    |
| 24  | DA    | 1062 | G    |
| 24  | DA    | 1063 | G    |
| 24  | DA    | 1064 | C    |
| 24  | DA    | 1066 | U    |
| 24  | DA    | 1068 | G    |
| 24  | DA    | 1070 | A    |
| 24  | DA    | 1071 | G    |
| 24  | DA    | 1072 | C    |
| 24  | DA    | 1073 | A    |
| 24  | DA    | 1074 | G    |
| 24  | DA    | 1075 | C    |
| 24  | DA    | 1076 | C    |
| 24  | DA    | 1079 | C    |
| 24  | DA    | 1080 | A    |
| 24  | DA    | 1083 | U    |
| 24  | DA    | 1086 | A    |
| 24  | DA    | 1088 | A    |
| 24  | DA    | 1089 | A    |
| 24  | DA    | 1090 | A    |
| 24  | DA    | 1091 | G    |
| 24  | DA    | 1097 | U    |
| 24  | DA    | 1100 | C    |
| 24  | DA    | 1111 | A    |
| 24  | DA    | 1112 | G    |
| 24  | DA    | 1113 | U    |
| 24  | DA    | 1114 | C    |
| 24  | DA    | 1115 | G    |
| 24  | DA    | 1126 | A    |
| 24  | DA    | 1127 | A    |
| 24  | DA    | 1128 | G    |
| 24  | DA    | 1129 | A    |
| 24  | DA    | 1130 | U    |
| 24  | DA    | 1131 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 1132 | U    |
| 24  | DA    | 1133 | A    |
| 24  | DA    | 1135 | C    |
| 24  | DA    | 1136 | G    |
| 24  | DA    | 1137 | G    |
| 24  | DA    | 1142 | A    |
| 24  | DA    | 1144 | A    |
| 24  | DA    | 1145 | C    |
| 24  | DA    | 1155 | A    |
| 24  | DA    | 1157 | G    |
| 24  | DA    | 1158 | C    |
| 24  | DA    | 1159 | U    |
| 24  | DA    | 1169 | A    |
| 24  | DA    | 1171 | G    |
| 24  | DA    | 1172 | C    |
| 24  | DA    | 1174 | U    |
| 24  | DA    | 1176 | U    |
| 24  | DA    | 1204 | A    |
| 24  | DA    | 1205 | A    |
| 24  | DA    | 1206 | G    |
| 24  | DA    | 1207 | C    |
| 24  | DA    | 1211 | C    |
| 24  | DA    | 1213 | A    |
| 24  | DA    | 1214 | A    |
| 24  | DA    | 1227 | G    |
| 24  | DA    | 1235 | G    |
| 24  | DA    | 1236 | G    |
| 24  | DA    | 1237 | A    |
| 24  | DA    | 1241 | A    |
| 24  | DA    | 1242 | U    |
| 24  | DA    | 1247 | A    |
| 24  | DA    | 1248 | G    |
| 24  | DA    | 1253 | A    |
| 24  | DA    | 1255 | U    |
| 24  | DA    | 1256 | G    |
| 24  | DA    | 1262 | A    |
| 24  | DA    | 1265 | A    |
| 24  | DA    | 1266 | G    |
| 24  | DA    | 1267 | U    |
| 24  | DA    | 1268 | A    |
| 24  | DA    | 1271 | G    |
| 24  | DA    | 1272 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 1273 | U    |
| 24  | DA    | 1274 | A    |
| 24  | DA    | 1275 | A    |
| 24  | DA    | 1276 | A    |
| 24  | DA    | 1277 | G    |
| 24  | DA    | 1278 | C    |
| 24  | DA    | 1286 | A    |
| 24  | DA    | 1290 | C    |
| 24  | DA    | 1291 | C    |
| 24  | DA    | 1300 | G    |
| 24  | DA    | 1301 | A    |
| 24  | DA    | 1303 | G    |
| 24  | DA    | 1304 | A    |
| 24  | DA    | 1311 | G    |
| 24  | DA    | 1313 | U    |
| 24  | DA    | 1314 | C    |
| 24  | DA    | 1315 | C    |
| 24  | DA    | 1321 | A    |
| 24  | DA    | 1324 | G    |
| 24  | DA    | 1325 | U    |
| 24  | DA    | 1326 | U    |
| 24  | DA    | 1327 | A    |
| 24  | DA    | 1328 | A    |
| 24  | DA    | 1329 | U    |
| 24  | DA    | 1330 | C    |
| 24  | DA    | 1331 | G    |
| 24  | DA    | 1332 | G    |
| 24  | DA    | 1333 | G    |
| 24  | DA    | 1334 | G    |
| 24  | DA    | 1336 | A    |
| 24  | DA    | 1337 | G    |
| 24  | DA    | 1340 | U    |
| 24  | DA    | 1341 | G    |
| 24  | DA    | 1342 | A    |
| 24  | DA    | 1345 | C    |
| 24  | DA    | 1349 | C    |
| 24  | DA    | 1365 | A    |
| 24  | DA    | 1374 | G    |
| 24  | DA    | 1376 | C    |
| 24  | DA    | 1379 | U    |
| 24  | DA    | 1381 | G    |
| 24  | DA    | 1382 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 1385 | A    |
| 24  | DA    | 1386 | C    |
| 24  | DA    | 1387 | A    |
| 24  | DA    | 1397 | U    |
| 24  | DA    | 1398 | C    |
| 24  | DA    | 1399 | C    |
| 24  | DA    | 1400 | U    |
| 24  | DA    | 1401 | G    |
| 24  | DA    | 1403 | A    |
| 24  | DA    | 1404 | C    |
| 24  | DA    | 1416 | G    |
| 24  | DA    | 1419 | A    |
| 24  | DA    | 1421 | G    |
| 24  | DA    | 1426 | G    |
| 24  | DA    | 1428 | C    |
| 24  | DA    | 1430 | G    |
| 24  | DA    | 1434 | A    |
| 24  | DA    | 1438 | U    |
| 24  | DA    | 1440 | U    |
| 24  | DA    | 1452 | G    |
| 24  | DA    | 1453 | A    |
| 24  | DA    | 1454 | C    |
| 24  | DA    | 1455 | G    |
| 24  | DA    | 1456 | G    |
| 24  | DA    | 1459 | G    |
| 24  | DA    | 1460 | U    |
| 24  | DA    | 1461 | C    |
| 24  | DA    | 1462 | C    |
| 24  | DA    | 1463 | C    |
| 24  | DA    | 1470 | A    |
| 24  | DA    | 1475 | G    |
| 24  | DA    | 1476 | U    |
| 24  | DA    | 1477 | A    |
| 24  | DA    | 1478 | G    |
| 24  | DA    | 1479 | G    |
| 24  | DA    | 1482 | G    |
| 24  | DA    | 1483 | G    |
| 24  | DA    | 1490 | A    |
| 24  | DA    | 1493 | C    |
| 24  | DA    | 1494 | A    |
| 24  | DA    | 1497 | U    |
| 24  | DA    | 1498 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 1499 | C    |
| 24  | DA    | 1501 | G    |
| 24  | DA    | 1507 | C    |
| 24  | DA    | 1508 | A    |
| 24  | DA    | 1509 | A    |
| 24  | DA    | 1510 | G    |
| 24  | DA    | 1511 | G    |
| 24  | DA    | 1512 | C    |
| 24  | DA    | 1520 | U    |
| 24  | DA    | 1522 | A    |
| 24  | DA    | 1523 | U    |
| 24  | DA    | 1524 | G    |
| 24  | DA    | 1528 | A    |
| 24  | DA    | 1531 | C    |
| 24  | DA    | 1532 | A    |
| 24  | DA    | 1534 | U    |
| 24  | DA    | 1535 | A    |
| 24  | DA    | 1536 | C    |
| 24  | DA    | 1537 | G    |
| 24  | DA    | 1538 | G    |
| 24  | DA    | 1539 | U    |
| 24  | DA    | 1540 | G    |
| 24  | DA    | 1555 | G    |
| 24  | DA    | 1556 | C    |
| 24  | DA    | 1558 | C    |
| 24  | DA    | 1559 | U    |
| 24  | DA    | 1560 | G    |
| 24  | DA    | 1561 | C    |
| 24  | DA    | 1562 | U    |
| 24  | DA    | 1565 | C    |
| 24  | DA    | 1566 | A    |
| 24  | DA    | 1567 | G    |
| 24  | DA    | 1569 | A    |
| 24  | DA    | 1583 | A    |
| 24  | DA    | 1584 | U    |
| 24  | DA    | 1585 | C    |
| 24  | DA    | 1586 | A    |
| 24  | DA    | 1598 | A    |
| 24  | DA    | 1600 | C    |
| 24  | DA    | 1603 | A    |
| 24  | DA    | 1607 | C    |
| 24  | DA    | 1608 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 1610 | A    |
| 24  | DA    | 1611 | C    |
| 24  | DA    | 1612 | C    |
| 24  | DA    | 1613 | G    |
| 24  | DA    | 1616 | A    |
| 24  | DA    | 1617 | C    |
| 24  | DA    | 1620 | G    |
| 24  | DA    | 1622 | G    |
| 24  | DA    | 1626 | A    |
| 24  | DA    | 1634 | A    |
| 24  | DA    | 1635 | A    |
| 24  | DA    | 1636 | U    |
| 24  | DA    | 1640 | A    |
| 24  | DA    | 1646 | C    |
| 24  | DA    | 1647 | U    |
| 24  | DA    | 1648 | U    |
| 24  | DA    | 1649 | G    |
| 24  | DA    | 1650 | A    |
| 24  | DA    | 1654 | A    |
| 24  | DA    | 1655 | A    |
| 24  | DA    | 1663 | G    |
| 24  | DA    | 1667 | G    |
| 24  | DA    | 1668 | A    |
| 24  | DA    | 1669 | A    |
| 24  | DA    | 1670 | C    |
| 24  | DA    | 1674 | G    |
| 24  | DA    | 1675 | C    |
| 24  | DA    | 1676 | A    |
| 24  | DA    | 1677 | A    |
| 24  | DA    | 1680 | U    |
| 24  | DA    | 1682 | G    |
| 24  | DA    | 1683 | U    |
| 24  | DA    | 1684 | G    |
| 24  | DA    | 1694 | C    |
| 24  | DA    | 1695 | G    |
| 24  | DA    | 1696 | G    |
| 24  | DA    | 1697 | G    |
| 24  | DA    | 1698 | A    |
| 24  | DA    | 1699 | G    |
| 24  | DA    | 1700 | A    |
| 24  | DA    | 1701 | A    |
| 24  | DA    | 1706 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 1707 | G    |
| 24  | DA    | 1713 | A    |
| 24  | DA    | 1714 | U    |
| 24  | DA    | 1715 | G    |
| 24  | DA    | 1716 | U    |
| 24  | DA    | 1717 | A    |
| 24  | DA    | 1718 | G    |
| 24  | DA    | 1722 | A    |
| 24  | DA    | 1723 | G    |
| 24  | DA    | 1728 | C    |
| 24  | DA    | 1729 | U    |
| 24  | DA    | 1730 | C    |
| 24  | DA    | 1731 | G    |
| 24  | DA    | 1732 | C    |
| 24  | DA    | 1733 | G    |
| 24  | DA    | 1734 | G    |
| 24  | DA    | 1735 | A    |
| 24  | DA    | 1739 | A    |
| 24  | DA    | 1740 | G    |
| 24  | DA    | 1758 | U    |
| 24  | DA    | 1759 | A    |
| 24  | DA    | 1760 | C    |
| 24  | DA    | 1761 | C    |
| 24  | DA    | 1764 | C    |
| 24  | DA    | 1773 | A    |
| 24  | DA    | 1774 | C    |
| 24  | DA    | 1776 | G    |
| 24  | DA    | 1780 | A    |
| 24  | DA    | 1781 | U    |
| 24  | DA    | 1782 | U    |
| 24  | DA    | 1783 | A    |
| 24  | DA    | 1784 | A    |
| 24  | DA    | 1785 | A    |
| 24  | DA    | 1786 | A    |
| 24  | DA    | 1788 | C    |
| 24  | DA    | 1789 | A    |
| 24  | DA    | 1800 | C    |
| 24  | DA    | 1802 | A    |
| 24  | DA    | 1808 | A    |
| 24  | DA    | 1809 | A    |
| 24  | DA    | 1810 | A    |
| 24  | DA    | 1811 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 1815 | A    |
| 24  | DA    | 1816 | C    |
| 24  | DA    | 1817 | G    |
| 24  | DA    | 1819 | A    |
| 24  | DA    | 1820 | U    |
| 24  | DA    | 1821 | A    |
| 24  | DA    | 1822 | C    |
| 24  | DA    | 1829 | A    |
| 24  | DA    | 1832 | C    |
| 24  | DA    | 1833 | C    |
| 24  | DA    | 1835 | G    |
| 24  | DA    | 1839 | G    |
| 24  | DA    | 1840 | G    |
| 24  | DA    | 1847 | A    |
| 24  | DA    | 1848 | A    |
| 24  | DA    | 1857 | G    |
| 24  | DA    | 1866 | A    |
| 24  | DA    | 1869 | G    |
| 24  | DA    | 1870 | C    |
| 24  | DA    | 1873 | G    |
| 24  | DA    | 1875 | G    |
| 24  | DA    | 1877 | A    |
| 24  | DA    | 1884 | G    |
| 24  | DA    | 1886 | U    |
| 24  | DA    | 1889 | A    |
| 24  | DA    | 1906 | G    |
| 24  | DA    | 1912 | A    |
| 24  | DA    | 1914 | C    |
| 24  | DA    | 1915 | U    |
| 24  | DA    | 1916 | A    |
| 24  | DA    | 1917 | U    |
| 24  | DA    | 1919 | A    |
| 24  | DA    | 1920 | C    |
| 24  | DA    | 1927 | A    |
| 24  | DA    | 1929 | G    |
| 24  | DA    | 1930 | G    |
| 24  | DA    | 1931 | U    |
| 24  | DA    | 1932 | A    |
| 24  | DA    | 1937 | A    |
| 24  | DA    | 1938 | A    |
| 24  | DA    | 1939 | U    |
| 24  | DA    | 1941 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 1942 | C    |
| 24  | DA    | 1943 | U    |
| 24  | DA    | 1944 | U    |
| 24  | DA    | 1945 | G    |
| 24  | DA    | 1946 | U    |
| 24  | DA    | 1954 | G    |
| 24  | DA    | 1955 | U    |
| 24  | DA    | 1956 | U    |
| 24  | DA    | 1957 | C    |
| 24  | DA    | 1963 | U    |
| 24  | DA    | 1964 | G    |
| 24  | DA    | 1965 | C    |
| 24  | DA    | 1966 | A    |
| 24  | DA    | 1967 | C    |
| 24  | DA    | 1968 | G    |
| 24  | DA    | 1970 | A    |
| 24  | DA    | 1971 | U    |
| 24  | DA    | 1972 | G    |
| 24  | DA    | 1980 | G    |
| 24  | DA    | 1981 | A    |
| 24  | DA    | 1982 | U    |
| 24  | DA    | 1983 | G    |
| 24  | DA    | 1991 | U    |
| 24  | DA    | 1993 | U    |
| 24  | DA    | 1994 | C    |
| 24  | DA    | 1996 | C    |
| 24  | DA    | 1997 | C    |
| 24  | DA    | 1998 | A    |
| 24  | DA    | 2018 | G    |
| 24  | DA    | 2020 | A    |
| 24  | DA    | 2022 | U    |
| 24  | DA    | 2023 | C    |
| 24  | DA    | 2024 | G    |
| 24  | DA    | 2030 | A    |
| 24  | DA    | 2031 | A    |
| 24  | DA    | 2032 | G    |
| 24  | DA    | 2033 | A    |
| 24  | DA    | 2034 | U    |
| 24  | DA    | 2035 | G    |
| 24  | DA    | 2036 | C    |
| 24  | DA    | 2037 | A    |
| 24  | DA    | 2038 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 2043 | C    |
| 24  | DA    | 2050 | C    |
| 24  | DA    | 2051 | A    |
| 24  | DA    | 2052 | A    |
| 24  | DA    | 2055 | C    |
| 24  | DA    | 2056 | G    |
| 24  | DA    | 2060 | A    |
| 24  | DA    | 2061 | G    |
| 24  | DA    | 2062 | A    |
| 24  | DA    | 2063 | C    |
| 24  | DA    | 2064 | C    |
| 24  | DA    | 2068 | U    |
| 24  | DA    | 2069 | G    |
| 24  | DA    | 2070 | A    |
| 24  | DA    | 2072 | C    |
| 24  | DA    | 2080 | A    |
| 24  | DA    | 2092 | U    |
| 24  | DA    | 2093 | G    |
| 24  | DA    | 2094 | A    |
| 24  | DA    | 2100 | G    |
| 24  | DA    | 2104 | C    |
| 24  | DA    | 2105 | U    |
| 24  | DA    | 2107 | G    |
| 24  | DA    | 2108 | A    |
| 24  | DA    | 2109 | U    |
| 24  | DA    | 2110 | G    |
| 24  | DA    | 2134 | A    |
| 24  | DA    | 2135 | A    |
| 24  | DA    | 2136 | G    |
| 24  | DA    | 2138 | G    |
| 24  | DA    | 2143 | C    |
| 24  | DA    | 2144 | G    |
| 24  | DA    | 2145 | C    |
| 24  | DA    | 2147 | A    |
| 24  | DA    | 2148 | G    |
| 24  | DA    | 2149 | U    |
| 24  | DA    | 2152 | G    |
| 24  | DA    | 2153 | C    |
| 24  | DA    | 2154 | A    |
| 24  | DA    | 2155 | U    |
| 24  | DA    | 2156 | G    |
| 24  | DA    | 2157 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 2180 | U    |
| 24  | DA    | 2181 | U    |
| 24  | DA    | 2183 | A    |
| 24  | DA    | 2187 | U    |
| 24  | DA    | 2190 | G    |
| 24  | DA    | 2191 | A    |
| 24  | DA    | 2192 | U    |
| 24  | DA    | 2198 | A    |
| 24  | DA    | 2199 | A    |
| 24  | DA    | 2200 | C    |
| 24  | DA    | 2204 | G    |
| 24  | DA    | 2210 | U    |
| 24  | DA    | 2211 | A    |
| 24  | DA    | 2212 | A    |
| 24  | DA    | 2213 | U    |
| 24  | DA    | 2214 | C    |
| 24  | DA    | 2215 | C    |
| 24  | DA    | 2216 | G    |
| 24  | DA    | 2226 | C    |
| 24  | DA    | 2227 | A    |
| 24  | DA    | 2238 | G    |
| 24  | DA    | 2239 | G    |
| 24  | DA    | 2240 | U    |
| 24  | DA    | 2241 | A    |
| 24  | DA    | 2249 | U    |
| 24  | DA    | 2250 | G    |
| 24  | DA    | 2251 | G    |
| 24  | DA    | 2252 | G    |
| 24  | DA    | 2259 | U    |
| 24  | DA    | 2260 | C    |
| 24  | DA    | 2261 | C    |
| 24  | DA    | 2266 | A    |
| 24  | DA    | 2267 | A    |
| 24  | DA    | 2268 | A    |
| 24  | DA    | 2275 | C    |
| 24  | DA    | 2279 | G    |
| 24  | DA    | 2283 | C    |
| 24  | DA    | 2284 | A    |
| 24  | DA    | 2286 | G    |
| 24  | DA    | 2288 | A    |
| 24  | DA    | 2289 | G    |
| 24  | DA    | 2290 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 2297 | A    |
| 24  | DA    | 2298 | A    |
| 24  | DA    | 2305 | U    |
| 24  | DA    | 2308 | G    |
| 24  | DA    | 2309 | A    |
| 24  | DA    | 2310 | C    |
| 24  | DA    | 2311 | A    |
| 24  | DA    | 2312 | U    |
| 24  | DA    | 2313 | C    |
| 24  | DA    | 2314 | A    |
| 24  | DA    | 2320 | U    |
| 24  | DA    | 2321 | U    |
| 24  | DA    | 2322 | A    |
| 24  | DA    | 2323 | G    |
| 24  | DA    | 2325 | G    |
| 24  | DA    | 2334 | U    |
| 24  | DA    | 2335 | A    |
| 24  | DA    | 2337 | G    |
| 24  | DA    | 2338 | C    |
| 24  | DA    | 2339 | C    |
| 24  | DA    | 2345 | G    |
| 24  | DA    | 2347 | C    |
| 24  | DA    | 2348 | U    |
| 24  | DA    | 2357 | G    |
| 24  | DA    | 2358 | A    |
| 24  | DA    | 2361 | G    |
| 24  | DA    | 2379 | G    |
| 24  | DA    | 2382 | G    |
| 24  | DA    | 2383 | G    |
| 24  | DA    | 2384 | U    |
| 24  | DA    | 2385 | C    |
| 24  | DA    | 2386 | A    |
| 24  | DA    | 2387 | U    |
| 24  | DA    | 2392 | A    |
| 24  | DA    | 2399 | G    |
| 24  | DA    | 2401 | U    |
| 24  | DA    | 2402 | U    |
| 24  | DA    | 2403 | C    |
| 24  | DA    | 2405 | G    |
| 24  | DA    | 2406 | A    |
| 24  | DA    | 2407 | A    |
| 24  | DA    | 2408 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 2409 | G    |
| 24  | DA    | 2410 | G    |
| 24  | DA    | 2424 | C    |
| 24  | DA    | 2425 | A    |
| 24  | DA    | 2426 | A    |
| 24  | DA    | 2427 | C    |
| 24  | DA    | 2428 | G    |
| 24  | DA    | 2429 | G    |
| 24  | DA    | 2430 | A    |
| 24  | DA    | 2431 | U    |
| 24  | DA    | 2435 | A    |
| 24  | DA    | 2439 | A    |
| 24  | DA    | 2440 | C    |
| 24  | DA    | 2441 | U    |
| 24  | DA    | 2447 | G    |
| 24  | DA    | 2448 | A    |
| 24  | DA    | 2450 | A    |
| 24  | DA    | 2457 | U    |
| 24  | DA    | 2459 | A    |
| 24  | DA    | 2460 | U    |
| 24  | DA    | 2461 | A    |
| 24  | DA    | 2468 | A    |
| 24  | DA    | 2475 | C    |
| 24  | DA    | 2476 | A    |
| 24  | DA    | 2490 | G    |
| 24  | DA    | 2491 | U    |
| 24  | DA    | 2492 | U    |
| 24  | DA    | 2493 | U    |
| 24  | DA    | 2494 | G    |
| 24  | DA    | 2498 | C    |
| 24  | DA    | 2499 | C    |
| 24  | DA    | 2500 | U    |
| 24  | DA    | 2502 | G    |
| 24  | DA    | 2503 | A    |
| 24  | DA    | 2504 | U    |
| 24  | DA    | 2505 | G    |
| 24  | DA    | 2506 | U    |
| 24  | DA    | 2517 | C    |
| 24  | DA    | 2518 | A    |
| 24  | DA    | 2519 | U    |
| 24  | DA    | 2520 | C    |
| 24  | DA    | 2521 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 2522 | U    |
| 24  | DA    | 2529 | G    |
| 24  | DA    | 2534 | A    |
| 24  | DA    | 2543 | G    |
| 24  | DA    | 2544 | G    |
| 24  | DA    | 2547 | A    |
| 24  | DA    | 2554 | U    |
| 24  | DA    | 2566 | A    |
| 24  | DA    | 2567 | G    |
| 24  | DA    | 2573 | C    |
| 24  | DA    | 2574 | G    |
| 24  | DA    | 2576 | G    |
| 24  | DA    | 2578 | G    |
| 24  | DA    | 2582 | G    |
| 24  | DA    | 2583 | G    |
| 24  | DA    | 2585 | U    |
| 24  | DA    | 2586 | U    |
| 24  | DA    | 2602 | A    |
| 24  | DA    | 2603 | G    |
| 24  | DA    | 2604 | U    |
| 24  | DA    | 2609 | U    |
| 24  | DA    | 2610 | C    |
| 24  | DA    | 2611 | C    |
| 24  | DA    | 2612 | C    |
| 24  | DA    | 2613 | U    |
| 24  | DA    | 2614 | A    |
| 24  | DA    | 2615 | U    |
| 24  | DA    | 2616 | C    |
| 24  | DA    | 2617 | U    |
| 24  | DA    | 2629 | U    |
| 24  | DA    | 2630 | G    |
| 24  | DA    | 2631 | G    |
| 24  | DA    | 2632 | A    |
| 24  | DA    | 2645 | G    |
| 24  | DA    | 2646 | C    |
| 24  | DA    | 2654 | A    |
| 24  | DA    | 2655 | G    |
| 24  | DA    | 2656 | U    |
| 24  | DA    | 2657 | A    |
| 24  | DA    | 2667 | C    |
| 24  | DA    | 2682 | A    |
| 24  | DA    | 2683 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 2689 | U    |
| 24  | DA    | 2690 | U    |
| 24  | DA    | 2691 | C    |
| 24  | DA    | 2692 | G    |
| 24  | DA    | 2713 | U    |
| 24  | DA    | 2714 | G    |
| 24  | DA    | 2715 | C    |
| 24  | DA    | 2718 | G    |
| 24  | DA    | 2726 | A    |
| 24  | DA    | 2727 | A    |
| 24  | DA    | 2728 | U    |
| 24  | DA    | 2739 | U    |
| 24  | DA    | 2748 | A    |
| 24  | DA    | 2751 | G    |
| 24  | DA    | 2752 | C    |
| 24  | DA    | 2753 | A    |
| 24  | DA    | 2756 | U    |
| 24  | DA    | 2757 | A    |
| 24  | DA    | 2758 | A    |
| 24  | DA    | 2760 | C    |
| 24  | DA    | 2765 | A    |
| 24  | DA    | 2766 | A    |
| 24  | DA    | 2777 | G    |
| 24  | DA    | 2778 | A    |
| 24  | DA    | 2779 | U    |
| 24  | DA    | 2781 | A    |
| 24  | DA    | 2782 | G    |
| 24  | DA    | 2791 | G    |
| 24  | DA    | 2796 | U    |
| 24  | DA    | 2799 | A    |
| 24  | DA    | 2800 | A    |
| 24  | DA    | 2801 | G    |
| 24  | DA    | 2808 | G    |
| 24  | DA    | 2820 | A    |
| 24  | DA    | 2826 | A    |
| 24  | DA    | 2833 | U    |
| 24  | DA    | 2834 | G    |
| 24  | DA    | 2835 | A    |
| 24  | DA    | 2836 | U    |
| 24  | DA    | 2837 | A    |
| 24  | DA    | 2838 | G    |
| 24  | DA    | 2848 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 2850 | A    |
| 24  | DA    | 2851 | A    |
| 24  | DA    | 2861 | U    |
| 24  | DA    | 2866 | U    |
| 24  | DA    | 2867 | G    |
| 24  | DA    | 2872 | A    |
| 24  | DA    | 2874 | C    |
| 24  | DA    | 2875 | C    |
| 24  | DA    | 2879 | A    |
| 24  | DA    | 2883 | A    |
| 24  | DA    | 2894 | G    |
| 24  | DA    | 2895 | G    |
| 24  | DA    | 2896 | C    |
| 24  | DA    | 2902 | C    |
| 56  | DB    | 12   | C    |
| 56  | DB    | 13   | G    |
| 56  | DB    | 15   | A    |
| 56  | DB    | 16   | G    |
| 56  | DB    | 17   | C    |
| 56  | DB    | 18   | G    |
| 56  | DB    | 24   | G    |
| 56  | DB    | 30   | C    |
| 56  | DB    | 35   | C    |
| 56  | DB    | 36   | C    |
| 56  | DB    | 40   | U    |
| 56  | DB    | 41   | G    |
| 56  | DB    | 42   | C    |
| 56  | DB    | 43   | C    |
| 56  | DB    | 44   | G    |
| 56  | DB    | 45   | A    |
| 56  | DB    | 46   | A    |
| 56  | DB    | 48   | U    |
| 56  | DB    | 57   | A    |
| 56  | DB    | 58   | A    |
| 56  | DB    | 63   | C    |
| 56  | DB    | 64   | G    |
| 56  | DB    | 87   | U    |
| 56  | DB    | 88   | C    |
| 56  | DB    | 89   | U    |
| 56  | DB    | 90   | C    |
| 56  | DB    | 91   | C    |
| 56  | DB    | 99   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | DB    | 109 | A    |

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 365 ligands modelled in this entry, 365 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1   | AB    | 218/241 (90%) | 2.00   | 82 (37%) 0 1  | 170, 274, 284, 290    | 0     |
| 1   | CB    | 218/241 (90%) | 0.79   | 36 (16%) 2 2  | 159, 222, 233, 241    | 0     |
| 2   | AC    | 206/233 (88%) | 0.43   | 11 (5%) 27 20 | 133, 162, 187, 202    | 0     |
| 2   | CC    | 206/233 (88%) | 0.59   | 16 (7%) 14 10 | 140, 172, 212, 228    | 0     |
| 3   | AD    | 205/206 (99%) | 0.26   | 11 (5%) 26 20 | 122, 157, 195, 218    | 0     |
| 3   | CD    | 205/206 (99%) | -0.27  | 0 100 100     | 112, 131, 152, 165    | 0     |
| 4   | AE    | 150/167 (89%) | 2.91   | 84 (56%) 0 1  | 108, 211, 223, 227    | 0     |
| 4   | CE    | 150/167 (89%) | 0.50   | 14 (9%) 9 8   | 100, 156, 171, 176    | 0     |
| 5   | AF    | 100/135 (74%) | 0.30   | 7 (7%) 17 12  | 197, 229, 250, 260    | 0     |
| 5   | CF    | 100/135 (74%) | 0.85   | 18 (18%) 2 2  | 164, 186, 203, 209    | 0     |
| 6   | AG    | 151/179 (84%) | 0.34   | 17 (11%) 6 6  | 158, 192, 220, 237    | 0     |
| 6   | CG    | 150/179 (83%) | 0.34   | 20 (13%) 4 4  | 142, 194, 228, 244    | 0     |
| 7   | AH    | 129/130 (99%) | 0.34   | 11 (8%) 11 10 | 127, 155, 181, 193    | 0     |
| 7   | CH    | 129/130 (99%) | 0.81   | 23 (17%) 2 2  | 152, 177, 195, 203    | 0     |
| 8   | AI    | 127/130 (97%) | 0.71   | 18 (14%) 3 3  | 142, 193, 220, 233    | 0     |
| 8   | CI    | 127/130 (97%) | 0.52   | 14 (11%) 6 6  | 155, 195, 223, 232    | 0     |
| 9   | AJ    | 98/103 (95%)  | 0.31   | 6 (6%) 22 16  | 135, 181, 216, 239    | 0     |
| 9   | CJ    | 98/103 (95%)  | 0.83   | 14 (14%) 3 3  | 155, 196, 230, 240    | 0     |
| 10  | AK    | 117/129 (90%) | 0.74   | 14 (11%) 5 5  | 132, 195, 243, 254    | 0     |
| 10  | CK    | 117/129 (90%) | 0.31   | 6 (5%) 29 22  | 125, 155, 181, 196    | 0     |
| 11  | AL    | 123/124 (99%) | 0.15   | 4 (3%) 47 36  | 89, 106, 131, 150     | 0     |
| 11  | CL    | 123/124 (99%) | 0.68   | 13 (10%) 7 6  | 117, 139, 155, 161    | 0     |
| 12  | AM    | 114/118 (96%) | 0.61   | 14 (12%) 5 5  | 157, 219, 252, 264    | 0     |
| 12  | CM    | 113/118 (95%) | 0.71   | 15 (13%) 4 4  | 195, 269, 309, 322    | 0     |

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| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|----------------|-----------------------|-------|
| 13  | AN    | 96/101 (95%)     | 0.28   | 5 (5%) 28 21   | 142, 165, 217, 227    | 0     |
| 13  | CN    | 95/101 (94%)     | 1.05   | 15 (15%) 2 2   | 155, 207, 265, 284    | 0     |
| 14  | AO    | 88/89 (98%)      | -0.20  | 0 100 100      | 138, 168, 199, 219    | 0     |
| 14  | CO    | 88/89 (98%)      | -0.06  | 1 (1%) 80 70   | 142, 174, 193, 201    | 0     |
| 15  | AP    | 82/82 (100%)     | 0.79   | 11 (13%) 4 4   | 117, 144, 178, 192    | 0     |
| 15  | CP    | 80/82 (97%)      | 1.48   | 23 (28%) 1 1   | 151, 180, 203, 207    | 0     |
| 16  | AQ    | 80/84 (95%)      | 0.64   | 5 (6%) 21 14   | 90, 113, 135, 144     | 0     |
| 16  | CQ    | 80/84 (95%)      | 1.11   | 16 (20%) 1 1   | 99, 123, 145, 163     | 0     |
| 17  | AR    | 55/75 (73%)      | 0.81   | 8 (14%) 3 3    | 175, 198, 219, 234    | 0     |
| 17  | CR    | 55/75 (73%)      | 0.24   | 3 (5%) 26 19   | 148, 165, 180, 187    | 0     |
| 18  | AS    | 79/92 (85%)      | 1.49   | 27 (34%) 0 1   | 171, 203, 244, 257    | 0     |
| 18  | CS    | 79/92 (85%)      | 1.53   | 26 (32%) 0 1   | 223, 265, 319, 334    | 0     |
| 19  | AT    | 85/87 (97%)      | 0.12   | 3 (3%) 44 34   | 114, 141, 164, 180    | 0     |
| 19  | CT    | 85/87 (97%)      | 1.16   | 25 (29%) 1 1   | 194, 242, 275, 283    | 0     |
| 20  | AU    | 51/71 (71%)      | 0.76   | 6 (11%) 5 5    | 133, 168, 248, 252    | 0     |
| 20  | CU    | 51/71 (71%)      | 0.19   | 2 (3%) 40 30   | 126, 150, 183, 193    | 0     |
| 21  | AA    | 1533/1533 (100%) | -0.47  | 13 (0%) 86 77  | 76, 150, 233, 282     | 0     |
| 22  | AV    | 17/17 (100%)     | 0.18   | 1 (5%) 23 16   | 142, 154, 182, 203    | 0     |
| 22  | AX    | 17/17 (100%)     | -0.25  | 1 (5%) 23 16   | 139, 144, 186, 195    | 0     |
| 22  | CV    | 17/17 (100%)     | 0.05   | 1 (5%) 23 16   | 158, 162, 193, 208    | 0     |
| 22  | CX    | 17/17 (100%)     | 2.35   | 8 (47%) 0 1    | 187, 193, 221, 222    | 0     |
| 23  | AW    | 6/6 (100%)       | 0.13   | 0 100 100      | 136, 138, 143, 152    | 0     |
| 23  | CW    | 6/6 (100%)       | 0.47   | 0 100 100      | 160, 160, 168, 179    | 0     |
| 24  | BA    | 2854/2903 (98%)  | -0.38  | 39 (1%) 75 64  | 52, 81, 194, 355      | 0     |
| 24  | DA    | 2841/2903 (97%)  | 0.27   | 139 (4%) 30 23 | 132, 200, 303, 402    | 0     |
| 25  | BB    | 118/118 (100%)   | -0.62  | 0 100 100      | 66, 101, 133, 171     | 0     |
| 26  | BC    | 271/273 (99%)    | -0.08  | 3 (1%) 80 70   | 60, 99, 129, 161      | 0     |
| 26  | DC    | 271/273 (99%)    | 0.60   | 25 (9%) 10 8   | 133, 157, 179, 190    | 0     |
| 27  | BD    | 209/209 (100%)   | -0.18  | 2 (0%) 82 72   | 55, 75, 114, 129      | 0     |
| 27  | DD    | 209/209 (100%)   | 1.42   | 67 (32%) 0 1   | 147, 200, 232, 242    | 0     |
| 28  | BE    | 201/201 (100%)   | -0.17  | 2 (0%) 82 72   | 56, 96, 129, 157      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 28  | DE    | 201/201 (100%) | 1.26   | 47 (23%) 1 1 | 154, 282, 335, 351    | 0     |
| 29  | BF    | 177/179 (98%)  | 1.04   | 32 (18%) 1 2 | 120, 166, 201, 215    | 0     |
| 29  | DF    | 178/179 (99%)  | 2.08   | 77 (43%) 0 1 | 307, 314, 321, 323    | 0     |
| 30  | BG    | 176/177 (99%)  | 0.09   | 3 (1%) 70 59 | 83, 108, 134, 152     | 0     |
| 30  | DG    | 176/177 (99%)  | 1.59   | 55 (31%) 0 1 | 186, 221, 245, 259    | 0     |
| 31  | BH    | 149/149 (100%) | 2.05   | 57 (38%) 0 1 | 110, 239, 259, 264    | 0     |
| 31  | DH    | 149/149 (100%) | 1.54   | 42 (28%) 1 1 | 186, 240, 256, 260    | 0     |
| 32  | BI    | 141/142 (99%)  | 2.13   | 59 (41%) 0 1 | 243, 307, 359, 366    | 0     |
| 32  | DI    | 141/142 (99%)  | 3.16   | 87 (61%) 0 0 | 367, 394, 412, 419    | 0     |
| 33  | BJ    | 142/142 (100%) | -0.30  | 0 100 100    | 59, 76, 102, 132      | 0     |
| 33  | DJ    | 142/142 (100%) | 1.24   | 35 (24%) 1 1 | 161, 201, 223, 233    | 0     |
| 34  | BK    | 122/123 (99%)  | -0.09  | 1 (0%) 86 77 | 55, 73, 113, 169      | 0     |
| 34  | DK    | 122/123 (99%)  | 1.23   | 36 (29%) 1 1 | 151, 171, 189, 198    | 0     |
| 35  | BL    | 143/144 (99%)  | -0.27  | 1 (0%) 87 80 | 55, 93, 124, 136      | 0     |
| 35  | DL    | 143/144 (99%)  | 1.19   | 38 (26%) 1 1 | 166, 240, 288, 297    | 0     |
| 36  | BM    | 136/136 (100%) | -0.08  | 1 (0%) 87 80 | 58, 81, 111, 138      | 0     |
| 36  | DM    | 136/136 (100%) | 1.76   | 55 (40%) 0 1 | 144, 181, 210, 232    | 0     |
| 37  | BN    | 120/127 (94%)  | -0.07  | 0 100 100    | 61, 76, 96, 141       | 0     |
| 37  | DN    | 120/127 (94%)  | 2.05   | 52 (43%) 0 1 | 183, 222, 252, 266    | 0     |
| 38  | BO    | 116/117 (99%)  | -0.05  | 1 (0%) 84 74 | 96, 105, 123, 147     | 0     |
| 38  | DO    | 116/117 (99%)  | 2.44   | 56 (48%) 0 1 | 286, 293, 297, 303    | 0     |
| 39  | BP    | 114/115 (99%)  | -0.07  | 0 100 100    | 64, 81, 119, 134      | 0     |
| 39  | DP    | 114/115 (99%)  | 1.40   | 33 (28%) 1 1 | 179, 203, 220, 230    | 0     |
| 40  | BQ    | 117/118 (99%)  | -0.47  | 0 100 100    | 56, 77, 99, 120       | 0     |
| 40  | DQ    | 117/118 (99%)  | 1.13   | 26 (22%) 1 1 | 184, 211, 240, 247    | 0     |
| 41  | BR    | 103/103 (100%) | -0.22  | 0 100 100    | 55, 87, 114, 131      | 0     |
| 41  | DR    | 103/103 (100%) | 2.21   | 45 (43%) 0 1 | 173, 249, 271, 277    | 0     |
| 42  | BS    | 110/110 (100%) | -0.34  | 0 100 100    | 55, 70, 105, 159      | 0     |
| 42  | DS    | 110/110 (100%) | 1.74   | 39 (35%) 0 1 | 159, 223, 269, 278    | 0     |
| 43  | BT    | 93/100 (93%)   | 0.11   | 2 (2%) 62 50 | 65, 105, 142, 151     | 0     |
| 43  | DT    | 93/100 (93%)   | 2.27   | 47 (50%) 0 1 | 206, 253, 285, 294    | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44  | BU    | 102/104 (98%)     | 0.32   | 5 (4%) 30 23   | 89, 114, 136, 158     | 0     |
| 44  | DU    | 102/104 (98%)     | 3.17   | 60 (58%) 0 1   | 272, 312, 355, 358    | 0     |
| 45  | BV    | 94/94 (100%)      | -0.15  | 0 100 100      | 71, 90, 116, 126      | 0     |
| 45  | DV    | 94/94 (100%)      | 1.19   | 23 (24%) 1 1   | 228, 241, 252, 254    | 0     |
| 46  | BW    | 79/85 (92%)       | -0.02  | 2 (2%) 58 46   | 68, 86, 136, 156      | 0     |
| 46  | DW    | 79/85 (92%)       | 3.13   | 54 (68%) 0 0   | 156, 216, 233, 252    | 0     |
| 47  | BX    | 77/78 (98%)       | -0.20  | 0 100 100      | 65, 101, 124, 137     | 0     |
| 47  | DX    | 77/78 (98%)       | 0.78   | 10 (12%) 4 4   | 157, 185, 209, 224    | 0     |
| 48  | BY    | 63/63 (100%)      | -0.02  | 3 (4%) 31 23   | 101, 123, 149, 159    | 0     |
| 48  | DY    | 63/63 (100%)      | 1.20   | 16 (25%) 1 1   | 264, 288, 316, 329    | 0     |
| 49  | BZ    | 58/59 (98%)       | 0.14   | 1 (1%) 70 59   | 64, 74, 111, 141      | 0     |
| 49  | DZ    | 58/59 (98%)       | 1.12   | 12 (20%) 1 1   | 188, 215, 238, 248    | 0     |
| 50  | B0    | 56/57 (98%)       | -0.52  | 0 100 100      | 54, 77, 113, 132      | 0     |
| 50  | D0    | 56/57 (98%)       | 1.32   | 11 (19%) 1 1   | 157, 230, 260, 265    | 0     |
| 51  | B1    | 50/55 (90%)       | 0.58   | 4 (8%) 13 10   | 76, 100, 118, 132     | 0     |
| 51  | D1    | 50/55 (90%)       | 1.67   | 18 (36%) 0 1   | 174, 207, 228, 238    | 0     |
| 52  | B2    | 46/46 (100%)      | -0.27  | 0 100 100      | 62, 75, 103, 137      | 0     |
| 52  | D2    | 46/46 (100%)      | 0.69   | 4 (8%) 11 9    | 155, 182, 198, 202    | 0     |
| 53  | B3    | 64/65 (98%)       | -0.30  | 0 100 100      | 58, 73, 96, 120       | 0     |
| 53  | D3    | 64/65 (98%)       | 1.23   | 14 (21%) 1 1   | 180, 194, 211, 215    | 0     |
| 54  | B4    | 38/38 (100%)      | -0.03  | 0 100 100      | 69, 84, 110, 120      | 0     |
| 54  | D4    | 38/38 (100%)      | 1.23   | 11 (28%) 1 1   | 171, 187, 198, 203    | 0     |
| 55  | CA    | 1530/1530 (100%)  | -0.14  | 34 (2%) 62 50  | 109, 171, 272, 362    | 0     |
| 56  | DB    | 117/117 (100%)    | 0.07   | 2 (1%) 70 59   | 219, 294, 300, 302    | 0     |
| All | All   | 20511/21154 (96%) | 0.38   | 2156 (10%) 7 6 | 52, 166, 293, 419     | 0     |

All (2156) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | AB    | 194  | GLY  | 17.7 |
| 31  | BH    | 87   | GLU  | 14.7 |
| 4   | AE    | 145  | ASN  | 14.0 |
| 29  | DF    | 129  | MET  | 13.7 |
| 24  | BA    | 2179 | C    | 13.7 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 32  | BI    | 1    | ALA  | 13.7 |
| 4   | AE    | 50   | GLY  | 13.5 |
| 31  | DH    | 124  | THR  | 13.3 |
| 55  | CA    | 209  | U    | 12.7 |
| 4   | AE    | 147  | ASN  | 12.7 |
| 4   | AE    | 106  | ALA  | 12.6 |
| 31  | DH    | 92   | GLY  | 12.5 |
| 24  | BA    | 2154 | A    | 12.1 |
| 24  | DA    | 2799 | A    | 12.0 |
| 24  | BA    | 2180 | U    | 11.9 |
| 31  | BH    | 85   | GLY  | 11.2 |
| 44  | DU    | 35   | VAL  | 11.2 |
| 4   | AE    | 86   | GLY  | 11.1 |
| 31  | BH    | 88   | GLY  | 11.0 |
| 32  | BI    | 2    | LYS  | 10.9 |
| 24  | BA    | 2147 | A    | 10.9 |
| 38  | DO    | 24   | THR  | 10.8 |
| 31  | BH    | 84   | ALA  | 10.7 |
| 4   | AE    | 74   | ALA  | 10.7 |
| 31  | BH    | 86   | ASP  | 10.6 |
| 32  | DI    | 67   | THR  | 10.6 |
| 31  | BH    | 79   | THR  | 10.5 |
| 31  | BH    | 93   | SER  | 10.2 |
| 24  | BA    | 2146 | C    | 10.1 |
| 44  | DU    | 12   | VAL  | 10.1 |
| 38  | DO    | 25   | ARG  | 10.0 |
| 29  | DF    | 105  | ILE  | 9.9  |
| 38  | DO    | 28   | VAL  | 9.8  |
| 31  | BH    | 118  | PRO  | 9.6  |
| 44  | DU    | 37   | GLY  | 9.6  |
| 38  | DO    | 41   | ALA  | 9.6  |
| 46  | DW    | 21   | GLY  | 9.6  |
| 43  | DT    | 75   | GLY  | 9.4  |
| 38  | DO    | 40   | ILE  | 9.4  |
| 28  | DE    | 42   | GLY  | 9.3  |
| 24  | BA    | 2143 | C    | 9.2  |
| 24  | BA    | 2155 | U    | 9.2  |
| 1   | AB    | 35   | ASN  | 9.2  |
| 32  | DI    | 3    | LYS  | 9.1  |
| 31  | BH    | 92   | GLY  | 9.1  |
| 38  | DO    | 52   | SER  | 9.0  |
| 38  | DO    | 23   | ALA  | 9.0  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 27         | DD           | 25         | THR         | 8.9         |
| 43         | DT           | 35         | ALA         | 8.8         |
| 31         | DH           | 79         | THR         | 8.7         |
| 32         | DI           | 120        | ASP         | 8.7         |
| 29         | DF           | 153        | ILE         | 8.7         |
| 44         | DU           | 24         | VAL         | 8.6         |
| 4          | AE           | 105        | ILE         | 8.6         |
| 43         | DT           | 34         | VAL         | 8.6         |
| 1          | AB           | 17         | HIS         | 8.6         |
| 31         | DH           | 125        | THR         | 8.6         |
| 55         | CA           | 86         | G           | 8.5         |
| 46         | DW           | 84         | GLU         | 8.5         |
| 1          | AB           | 59         | ILE         | 8.5         |
| 46         | DW           | 51         | GLY         | 8.4         |
| 32         | DI           | 1          | ALA         | 8.3         |
| 1          | AB           | 18         | GLN         | 8.3         |
| 31         | BH           | 89         | LYS         | 8.3         |
| 11         | AL           | 123        | ALA         | 8.3         |
| 44         | DU           | 39         | ASN         | 8.3         |
| 44         | DU           | 80         | ASP         | 8.2         |
| 37         | DN           | 29         | VAL         | 8.2         |
| 29         | BF           | 75         | GLY         | 8.1         |
| 29         | DF           | 9          | ASP         | 8.1         |
| 44         | DU           | 79         | ALA         | 8.1         |
| 4          | AE           | 137        | ARG         | 8.1         |
| 32         | DI           | 59         | THR         | 8.1         |
| 41         | DR           | 19         | THR         | 8.1         |
| 4          | AE           | 42         | ASN         | 8.0         |
| 29         | BF           | 79         | ARG         | 8.0         |
| 1          | AB           | 74         | ALA         | 8.0         |
| 44         | DU           | 41         | VAL         | 8.0         |
| 1          | CB           | 15         | PHE         | 8.0         |
| 1          | AB           | 166        | ASP         | 8.0         |
| 44         | DU           | 36         | GLU         | 8.0         |
| 1          | AB           | 106        | VAL         | 8.0         |
| 37         | DN           | 63         | ARG         | 8.0         |
| 24         | DA           | 1172       | C           | 7.9         |
| 44         | DU           | 87         | GLU         | 7.9         |
| 32         | BI           | 3          | LYS         | 7.9         |
| 32         | DI           | 50         | LYS         | 7.9         |
| 24         | BA           | 2138       | G           | 7.8         |
| 32         | DI           | 51         | GLY         | 7.6         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 4          | AE           | 114        | LEU         | 7.6         |
| 37         | DN           | 100        | CYS         | 7.5         |
| 37         | DN           | 78         | LYS         | 7.5         |
| 4          | AE           | 141        | ASP         | 7.5         |
| 32         | DI           | 15         | GLY         | 7.4         |
| 32         | BI           | 52         | LEU         | 7.4         |
| 29         | DF           | 66         | ILE         | 7.4         |
| 29         | BF           | 115        | GLY         | 7.3         |
| 32         | DI           | 2          | LYS         | 7.3         |
| 31         | BH           | 149        | GLU         | 7.3         |
| 32         | BI           | 86         | LYS         | 7.3         |
| 29         | BF           | 77         | LYS         | 7.3         |
| 4          | AE           | 72         | ASN         | 7.3         |
| 28         | DE           | 143        | LEU         | 7.3         |
| 13         | CN           | 33         | VAL         | 7.2         |
| 42         | DS           | 94         | ASP         | 7.2         |
| 28         | DE           | 90         | GLN         | 7.2         |
| 44         | DU           | 11         | ILE         | 7.2         |
| 31         | BH           | 105        | ALA         | 7.2         |
| 31         | DH           | 123        | ARG         | 7.1         |
| 27         | DD           | 201        | LEU         | 7.1         |
| 46         | DW           | 39         | GLN         | 7.1         |
| 32         | DI           | 141        | ASP         | 7.1         |
| 32         | DI           | 96         | LYS         | 7.1         |
| 44         | DU           | 77         | GLY         | 7.0         |
| 32         | BI           | 113        | ALA         | 7.0         |
| 22         | CX           | 27         | G           | 7.0         |
| 24         | BA           | 2145       | C           | 7.0         |
| 32         | DI           | 93         | ASN         | 7.0         |
| 31         | BH           | 117        | LEU         | 7.0         |
| 44         | DU           | 38         | ILE         | 7.0         |
| 32         | DI           | 122        | GLU         | 7.0         |
| 18         | CS           | 79         | TYR         | 7.0         |
| 46         | DW           | 52         | CYS         | 6.9         |
| 41         | DR           | 52         | PRO         | 6.9         |
| 8          | CI           | 42         | THR         | 6.9         |
| 4          | AE           | 12         | GLU         | 6.8         |
| 46         | DW           | 34         | SER         | 6.8         |
| 31         | DH           | 98         | ASP         | 6.8         |
| 29         | DF           | 128        | SER         | 6.8         |
| 46         | DW           | 53         | GLY         | 6.8         |
| 39         | DP           | 33         | GLU         | 6.8         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | DH    | 126  | GLY  | 6.8  |
| 29  | DF    | 10   | GLU  | 6.8  |
| 31  | DH    | 82   | SER  | 6.8  |
| 1   | AB    | 189  | ASN  | 6.7  |
| 1   | AB    | 34   | ARG  | 6.7  |
| 32  | DI    | 63   | ASP  | 6.7  |
| 1   | AB    | 27   | LYS  | 6.7  |
| 4   | AE    | 144  | GLU  | 6.7  |
| 1   | AB    | 225  | SER  | 6.7  |
| 4   | AE    | 85   | LYS  | 6.7  |
| 27  | DD    | 24   | VAL  | 6.7  |
| 44  | DU    | 76   | THR  | 6.7  |
| 4   | AE    | 49   | TYR  | 6.6  |
| 21  | AA    | 86   | G    | 6.6  |
| 4   | AE    | 110  | MET  | 6.6  |
| 4   | AE    | 99   | SER  | 6.6  |
| 32  | BI    | 82   | ALA  | 6.6  |
| 29  | BF    | 116  | LEU  | 6.6  |
| 24  | DA    | 33   | C    | 6.6  |
| 35  | DL    | 74   | THR  | 6.6  |
| 29  | DF    | 22   | ASN  | 6.6  |
| 24  | BA    | 546  | U    | 6.5  |
| 30  | DG    | 6    | ALA  | 6.5  |
| 31  | DH    | 127  | GLU  | 6.5  |
| 34  | DK    | 75   | SER  | 6.5  |
| 4   | AE    | 68   | ARG  | 6.5  |
| 31  | DH    | 88   | GLY  | 6.5  |
| 46  | DW    | 79   | ILE  | 6.5  |
| 1   | AB    | 161  | PHE  | 6.5  |
| 53  | D3    | 22   | LYS  | 6.5  |
| 18  | CS    | 80   | ARG  | 6.5  |
| 27  | DD    | 26   | VAL  | 6.5  |
| 44  | DU    | 70   | ALA  | 6.5  |
| 8   | AI    | 50   | PRO  | 6.5  |
| 29  | DF    | 155  | ILE  | 6.4  |
| 24  | BA    | 2144 | G    | 6.4  |
| 15  | AP    | 82   | ALA  | 6.4  |
| 28  | DE    | 86   | ALA  | 6.4  |
| 50  | D0    | 56   | LYS  | 6.4  |
| 55  | CA    | 210  | C    | 6.3  |
| 32  | DI    | 8    | VAL  | 6.3  |
| 37  | DN    | 111  | ALA  | 6.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 38  | DO    | 51   | ALA  | 6.3  |
| 15  | CP    | 17   | TYR  | 6.3  |
| 32  | DI    | 95   | ASP  | 6.2  |
| 32  | DI    | 48   | ILE  | 6.2  |
| 1   | AB    | 81   | ASP  | 6.2  |
| 41  | DR    | 12   | HIS  | 6.2  |
| 39  | DP    | 109  | ILE  | 6.2  |
| 44  | DU    | 31   | GLY  | 6.2  |
| 17  | AR    | 19   | GLU  | 6.2  |
| 8   | AI    | 42   | THR  | 6.2  |
| 41  | DR    | 6    | GLN  | 6.2  |
| 42  | DS    | 110  | ARG  | 6.2  |
| 44  | DU    | 82   | VAL  | 6.2  |
| 11  | CL    | 123  | ALA  | 6.2  |
| 45  | DV    | 81   | PRO  | 6.1  |
| 32  | DI    | 4    | VAL  | 6.1  |
| 24  | DA    | 1536 | C    | 6.1  |
| 29  | DF    | 125  | GLY  | 6.1  |
| 29  | DF    | 104  | THR  | 6.1  |
| 41  | DR    | 59   | ILE  | 6.1  |
| 15  | CP    | 16   | PHE  | 6.1  |
| 44  | DU    | 34   | ILE  | 6.1  |
| 36  | DM    | 136  | MET  | 6.1  |
| 31  | BH    | 119  | ASN  | 6.1  |
| 31  | BH    | 123  | ARG  | 6.1  |
| 44  | DU    | 19   | GLY  | 6.1  |
| 12  | AM    | 114  | PRO  | 6.1  |
| 48  | DY    | 24   | GLU  | 6.1  |
| 36  | DM    | 135  | VAL  | 6.1  |
| 18  | CS    | 10   | ILE  | 6.0  |
| 31  | BH    | 116  | ARG  | 6.0  |
| 31  | BH    | 112  | LYS  | 6.0  |
| 36  | DM    | 61   | GLY  | 6.0  |
| 15  | CP    | 38   | PHE  | 6.0  |
| 6   | AG    | 84   | TYR  | 6.0  |
| 31  | BH    | 90   | LEU  | 6.0  |
| 33  | DJ    | 142  | ILE  | 6.0  |
| 46  | DW    | 58   | LEU  | 6.0  |
| 22  | CX    | 43   | C    | 6.0  |
| 32  | BI    | 114  | ALA  | 6.0  |
| 43  | DT    | 3    | ARG  | 6.0  |
| 32  | DI    | 60   | VAL  | 6.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 32  | BI    | 132  | ALA  | 6.0  |
| 24  | DA    | 1173 | U    | 6.0  |
| 42  | DS    | 70   | LYS  | 5.9  |
| 18  | AS    | 68   | HIS  | 5.9  |
| 46  | DW    | 50   | VAL  | 5.9  |
| 6   | CG    | 150  | PHE  | 5.9  |
| 29  | BF    | 78   | ILE  | 5.9  |
| 28  | DE    | 119  | ILE  | 5.9  |
| 32  | BI    | 33   | ASN  | 5.9  |
| 31  | DH    | 105  | ALA  | 5.9  |
| 32  | DI    | 65   | SER  | 5.8  |
| 4   | AE    | 133  | ILE  | 5.8  |
| 31  | DH    | 89   | LYS  | 5.8  |
| 30  | DG    | 113  | ASP  | 5.8  |
| 24  | DA    | 1171 | G    | 5.8  |
| 6   | CG    | 151  | ALA  | 5.8  |
| 19  | CT    | 60   | GLN  | 5.8  |
| 32  | DI    | 47   | SER  | 5.8  |
| 18  | CS    | 43   | MET  | 5.8  |
| 37  | DN    | 118  | ARG  | 5.8  |
| 1   | AB    | 217  | ALA  | 5.8  |
| 1   | AB    | 19   | THR  | 5.8  |
| 31  | BH    | 91   | PHE  | 5.7  |
| 37  | DN    | 28   | LEU  | 5.7  |
| 44  | DU    | 78   | LYS  | 5.7  |
| 27  | DD    | 6    | GLY  | 5.7  |
| 31  | BH    | 129  | GLU  | 5.7  |
| 32  | BI    | 10   | LEU  | 5.7  |
| 4   | AE    | 124  | ALA  | 5.7  |
| 41  | DR    | 20   | VAL  | 5.7  |
| 1   | CB    | 17   | HIS  | 5.7  |
| 32  | DI    | 66   | PHE  | 5.7  |
| 41  | DR    | 88   | GLY  | 5.7  |
| 29  | DF    | 77   | LYS  | 5.6  |
| 50  | D0    | 41   | HIS  | 5.6  |
| 45  | DV    | 42   | LEU  | 5.6  |
| 48  | DY    | 63   | ALA  | 5.6  |
| 18  | CS    | 12   | LEU  | 5.6  |
| 32  | DI    | 22   | PRO  | 5.6  |
| 38  | DO    | 29   | HIS  | 5.6  |
| 4   | AE    | 146  | MET  | 5.6  |
| 34  | DK    | 101  | GLY  | 5.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 18  | CS    | 3    | SER  | 5.5  |
| 4   | AE    | 75   | LEU  | 5.5  |
| 28  | DE    | 87   | ALA  | 5.5  |
| 18  | CS    | 23   | GLU  | 5.5  |
| 24  | DA    | 1583 | A    | 5.5  |
| 46  | DW    | 63   | ASP  | 5.5  |
| 29  | DF    | 30   | VAL  | 5.5  |
| 43  | DT    | 9    | LYS  | 5.5  |
| 1   | AB    | 103  | TRP  | 5.5  |
| 24  | DA    | 1535 | A    | 5.5  |
| 27  | DD    | 14   | ILE  | 5.5  |
| 55  | CA    | 1534 | A    | 5.5  |
| 36  | DM    | 125  | PRO  | 5.5  |
| 40  | DQ    | 94   | LEU  | 5.5  |
| 31  | DH    | 93   | SER  | 5.5  |
| 42  | DS    | 68   | ASP  | 5.4  |
| 38  | DO    | 112  | GLU  | 5.4  |
| 43  | DT    | 70   | HIS  | 5.4  |
| 29  | BF    | 152  | ASP  | 5.4  |
| 46  | DW    | 45   | HIS  | 5.4  |
| 29  | DF    | 151  | LEU  | 5.4  |
| 37  | DN    | 25   | ALA  | 5.4  |
| 51  | D1    | 52   | LYS  | 5.4  |
| 36  | DM    | 90   | GLU  | 5.4  |
| 44  | DU    | 8    | ASP  | 5.4  |
| 24  | BA    | 2136 | G    | 5.4  |
| 24  | BA    | 2148 | G    | 5.4  |
| 46  | DW    | 73   | PRO  | 5.4  |
| 32  | BI    | 80   | LYS  | 5.4  |
| 32  | DI    | 55   | PRO  | 5.4  |
| 48  | DY    | 62   | GLY  | 5.4  |
| 31  | BH    | 98   | ASP  | 5.4  |
| 4   | AE    | 84   | VAL  | 5.4  |
| 36  | DM    | 72   | PRO  | 5.4  |
| 38  | DO    | 26   | LEU  | 5.3  |
| 37  | DN    | 30   | ARG  | 5.3  |
| 30  | DG    | 166  | GLU  | 5.3  |
| 48  | DY    | 13   | GLU  | 5.3  |
| 53  | D3    | 35   | LYS  | 5.3  |
| 32  | DI    | 58   | ILE  | 5.3  |
| 45  | DV    | 54   | ALA  | 5.3  |
| 43  | DT    | 37   | ASP  | 5.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 29  | DF    | 154  | THR  | 5.3  |
| 30  | DG    | 165  | ASP  | 5.3  |
| 36  | DM    | 89   | VAL  | 5.3  |
| 29  | BF    | 76   | PHE  | 5.3  |
| 24  | DA    | 1175 | A    | 5.2  |
| 29  | DF    | 130  | GLY  | 5.2  |
| 32  | DI    | 123  | ALA  | 5.2  |
| 29  | DF    | 157  | THR  | 5.2  |
| 4   | AE    | 151  | MET  | 5.2  |
| 29  | DF    | 152  | ASP  | 5.2  |
| 4   | AE    | 148  | SER  | 5.2  |
| 32  | BI    | 139  | VAL  | 5.2  |
| 46  | DW    | 29   | SER  | 5.2  |
| 45  | DV    | 47   | VAL  | 5.2  |
| 29  | DF    | 173  | ASP  | 5.2  |
| 32  | DI    | 23   | VAL  | 5.2  |
| 46  | DW    | 42   | THR  | 5.2  |
| 38  | DO    | 92   | PHE  | 5.2  |
| 21  | AA    | 1534 | A    | 5.2  |
| 22  | CX    | 42   | C    | 5.2  |
| 24  | DA    | 645  | C    | 5.2  |
| 37  | DN    | 24   | MET  | 5.2  |
| 43  | DT    | 42   | GLU  | 5.2  |
| 30  | DG    | 168  | VAL  | 5.2  |
| 32  | DI    | 119  | ALA  | 5.2  |
| 32  | BI    | 4    | VAL  | 5.1  |
| 38  | DO    | 61   | GLN  | 5.1  |
| 55  | CA    | 85   | U    | 5.1  |
| 46  | DW    | 72   | GLY  | 5.1  |
| 27  | DD    | 202  | ILE  | 5.1  |
| 43  | DT    | 43   | ILE  | 5.1  |
| 30  | DG    | 51   | PHE  | 5.1  |
| 51  | D1    | 32   | LYS  | 5.1  |
| 29  | DF    | 114  | ARG  | 5.1  |
| 45  | DV    | 57   | TYR  | 5.1  |
| 39  | DP    | 114  | ASN  | 5.1  |
| 44  | DU    | 32   | LYS  | 5.1  |
| 31  | DH    | 128  | HIS  | 5.1  |
| 33  | DJ    | 74   | TYR  | 5.0  |
| 27  | DD    | 10   | GLY  | 5.0  |
| 4   | AE    | 150  | GLU  | 5.0  |
| 48  | DY    | 21   | LEU  | 5.0  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 24         | DA           | 137        | U           | 5.0         |
| 1          | AB           | 206        | ILE         | 5.0         |
| 38         | DO           | 47         | VAL         | 5.0         |
| 51         | D1           | 22         | THR         | 5.0         |
| 37         | DN           | 23         | ASN         | 5.0         |
| 38         | DO           | 117        | PHE         | 5.0         |
| 32         | BI           | 78         | LEU         | 5.0         |
| 24         | DA           | 1174       | U           | 5.0         |
| 35         | DL           | 71         | ALA         | 5.0         |
| 1          | AB           | 8          | MET         | 5.0         |
| 22         | CV           | 27         | G           | 5.0         |
| 22         | CX           | 30         | G           | 5.0         |
| 36         | DM           | 129        | THR         | 5.0         |
| 37         | DN           | 70         | THR         | 5.0         |
| 38         | DO           | 53         | THR         | 5.0         |
| 15         | AP           | 81         | ALA         | 5.0         |
| 32         | DI           | 83         | ALA         | 5.0         |
| 28         | DE           | 175        | ILE         | 5.0         |
| 44         | DU           | 21         | ARG         | 5.0         |
| 38         | DO           | 50         | ALA         | 5.0         |
| 4          | AE           | 113        | VAL         | 4.9         |
| 18         | AS           | 37         | SER         | 4.9         |
| 50         | D0           | 27         | LEU         | 4.9         |
| 42         | DS           | 38         | TYR         | 4.9         |
| 28         | DE           | 144        | GLU         | 4.9         |
| 37         | DN           | 98         | LEU         | 4.9         |
| 1          | AB           | 73         | ARG         | 4.9         |
| 32         | DI           | 25         | PRO         | 4.9         |
| 18         | AS           | 38         | THR         | 4.9         |
| 28         | DE           | 89         | PRO         | 4.9         |
| 36         | DM           | 110        | GLU         | 4.9         |
| 46         | DW           | 59         | PHE         | 4.9         |
| 15         | CP           | 39         | PHE         | 4.9         |
| 39         | DP           | 8          | GLU         | 4.9         |
| 4          | AE           | 140        | ILE         | 4.9         |
| 32         | DI           | 99         | LYS         | 4.8         |
| 15         | CP           | 49         | GLY         | 4.8         |
| 45         | DV           | 94         | ALA         | 4.8         |
| 24         | DA           | 613        | A           | 4.8         |
| 37         | DN           | 26         | GLY         | 4.8         |
| 31         | DH           | 91         | PHE         | 4.8         |
| 38         | DO           | 113        | ALA         | 4.8         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 42         | DS           | 13         | SER         | 4.8         |
| 48         | DY           | 1          | MET         | 4.8         |
| 1          | AB           | 205        | ALA         | 4.8         |
| 1          | AB           | 36         | LYS         | 4.8         |
| 43         | DT           | 36         | LYS         | 4.8         |
| 49         | DZ           | 55         | LYS         | 4.8         |
| 46         | DW           | 54         | ARG         | 4.8         |
| 44         | DU           | 13         | LEU         | 4.8         |
| 24         | DA           | 587        | C           | 4.8         |
| 22         | AV           | 27         | G           | 4.8         |
| 7          | CH           | 1          | SER         | 4.8         |
| 18         | AS           | 63         | ASP         | 4.8         |
| 18         | CS           | 11         | ASP         | 4.8         |
| 21         | AA           | 78         | A           | 4.8         |
| 31         | DH           | 129        | GLU         | 4.8         |
| 32         | BI           | 67         | THR         | 4.8         |
| 24         | BA           | 2110       | G           | 4.8         |
| 31         | BH           | 73         | ASN         | 4.8         |
| 34         | DK           | 73         | ASP         | 4.8         |
| 32         | BI           | 5          | GLN         | 4.7         |
| 42         | DS           | 91         | GLY         | 4.7         |
| 24         | BA           | 2149       | U           | 4.7         |
| 44         | DU           | 26         | ASN         | 4.7         |
| 1          | AB           | 42         | LEU         | 4.7         |
| 32         | DI           | 62         | ALA         | 4.7         |
| 41         | DR           | 27         | ILE         | 4.7         |
| 11         | AL           | 122        | LYS         | 4.7         |
| 30         | DG           | 55         | ASP         | 4.7         |
| 41         | DR           | 75         | VAL         | 4.7         |
| 4          | AE           | 51         | LYS         | 4.7         |
| 39         | DP           | 111        | GLU         | 4.7         |
| 30         | DG           | 85         | LYS         | 4.7         |
| 1          | CB           | 205        | ALA         | 4.7         |
| 36         | DM           | 34         | LYS         | 4.7         |
| 51         | D1           | 35         | LEU         | 4.7         |
| 1          | AB           | 43         | GLU         | 4.7         |
| 32         | BI           | 81         | LYS         | 4.7         |
| 37         | DN           | 62         | ASN         | 4.7         |
| 46         | DW           | 80         | SER         | 4.7         |
| 1          | AB           | 204        | ASP         | 4.6         |
| 28         | DE           | 24         | ASN         | 4.6         |
| 27         | DD           | 186        | LEU         | 4.6         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 24         | BA           | 138        | U           | 4.6         |
| 18         | AS           | 69         | LYS         | 4.6         |
| 43         | DT           | 69         | ARG         | 4.6         |
| 29         | DF           | 90         | LEU         | 4.6         |
| 41         | DR           | 5          | PHE         | 4.6         |
| 29         | DF           | 127        | TYR         | 4.6         |
| 28         | DE           | 44         | ARG         | 4.6         |
| 4          | AE           | 83         | PRO         | 4.6         |
| 31         | DH           | 145        | ASN         | 4.6         |
| 32         | DI           | 92         | PRO         | 4.6         |
| 24         | BA           | 2309       | A           | 4.6         |
| 39         | DP           | 11         | GLN         | 4.6         |
| 5          | AF           | 84         | VAL         | 4.6         |
| 4          | CE           | 106        | ALA         | 4.6         |
| 44         | DU           | 73         | ASN         | 4.6         |
| 32         | BI           | 11         | GLN         | 4.6         |
| 30         | DG           | 110        | HIS         | 4.6         |
| 32         | BI           | 68         | PHE         | 4.6         |
| 41         | DR           | 29         | THR         | 4.5         |
| 24         | DA           | 1217       | U           | 4.5         |
| 28         | DE           | 188        | MET         | 4.5         |
| 51         | D1           | 21         | THR         | 4.5         |
| 1          | AB           | 195        | VAL         | 4.5         |
| 32         | BI           | 12         | VAL         | 4.5         |
| 24         | BA           | 2137       | U           | 4.5         |
| 43         | DT           | 15         | HIS         | 4.5         |
| 41         | DR           | 87         | GLN         | 4.5         |
| 43         | DT           | 83         | ALA         | 4.5         |
| 2          | CC           | 74         | ILE         | 4.5         |
| 33         | DJ           | 23         | LYS         | 4.5         |
| 32         | DI           | 31         | GLY         | 4.5         |
| 4          | AE           | 138        | ALA         | 4.5         |
| 29         | DF           | 35         | LEU         | 4.5         |
| 39         | DP           | 71         | ARG         | 4.5         |
| 32         | DI           | 121        | ILE         | 4.5         |
| 24         | DA           | 2402       | U           | 4.5         |
| 30         | DG           | 170        | THR         | 4.5         |
| 31         | BH           | 113        | SER         | 4.5         |
| 36         | DM           | 6          | ARG         | 4.5         |
| 1          | AB           | 78         | ALA         | 4.5         |
| 1          | AB           | 167        | HIS         | 4.5         |
| 36         | DM           | 124        | LEU         | 4.5         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 15  | AP    | 80  | LYS  | 4.5  |
| 32  | DI    | 39  | LYS  | 4.5  |
| 27  | DD    | 21  | SER  | 4.5  |
| 31  | BH    | 128 | HIS  | 4.4  |
| 49  | DZ    | 36  | GLU  | 4.4  |
| 27  | DD    | 30  | GLU  | 4.4  |
| 21  | AA    | 87  | C    | 4.4  |
| 33  | DJ    | 54  | ILE  | 4.4  |
| 38  | DO    | 109 | ALA  | 4.4  |
| 44  | DU    | 20  | LYS  | 4.4  |
| 42  | DS    | 47  | VAL  | 4.4  |
| 36  | DM    | 88  | ASN  | 4.4  |
| 32  | DI    | 43  | ALA  | 4.4  |
| 4   | AE    | 82  | HIS  | 4.4  |
| 32  | BI    | 37  | PHE  | 4.4  |
| 55  | CA    | 87  | C    | 4.4  |
| 33  | DJ    | 118 | MET  | 4.4  |
| 18  | CS    | 41  | PRO  | 4.4  |
| 32  | DI    | 12  | VAL  | 4.4  |
| 1   | AB    | 26  | MET  | 4.4  |
| 32  | DI    | 68  | PHE  | 4.4  |
| 1   | AB    | 93  | HIS  | 4.4  |
| 31  | BH    | 131 | SER  | 4.4  |
| 37  | DN    | 113 | ILE  | 4.3  |
| 36  | DM    | 99  | GLY  | 4.3  |
| 44  | DU    | 17  | ASP  | 4.3  |
| 29  | DF    | 83  | PRO  | 4.3  |
| 8   | AI    | 39  | GLY  | 4.3  |
| 41  | DR    | 26  | ASP  | 4.3  |
| 37  | DN    | 112 | TYR  | 4.3  |
| 1   | AB    | 68  | PHE  | 4.3  |
| 21  | AA    | 88  | U    | 4.3  |
| 32  | DI    | 133 | ARG  | 4.3  |
| 43  | DT    | 12  | ARG  | 4.3  |
| 43  | DT    | 80  | TRP  | 4.3  |
| 48  | DY    | 37  | LEU  | 4.3  |
| 6   | AG    | 83  | THR  | 4.3  |
| 44  | DU    | 59  | GLU  | 4.3  |
| 35  | DL    | 70  | LYS  | 4.3  |
| 1   | CB    | 209 | VAL  | 4.3  |
| 29  | DF    | 37  | MET  | 4.3  |
| 15  | CP    | 52  | LEU  | 4.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 27  | DD    | 59  | ARG  | 4.3  |
| 38  | DO    | 44  | GLY  | 4.3  |
| 7   | CH    | 92  | PRO  | 4.3  |
| 26  | DC    | 1   | ALA  | 4.3  |
| 37  | DN    | 22  | ARG  | 4.3  |
| 46  | DW    | 78  | PHE  | 4.2  |
| 10  | AK    | 20  | ALA  | 4.2  |
| 29  | DF    | 17  | THR  | 4.2  |
| 32  | DI    | 20  | SER  | 4.2  |
| 38  | DO    | 22  | GLY  | 4.2  |
| 33  | DJ    | 63  | ALA  | 4.2  |
| 41  | DR    | 46  | GLU  | 4.2  |
| 27  | DD    | 197 | THR  | 4.2  |
| 32  | DI    | 32  | VAL  | 4.2  |
| 29  | BF    | 106 | ALA  | 4.2  |
| 32  | DI    | 17  | ALA  | 4.2  |
| 38  | DO    | 76  | LYS  | 4.2  |
| 32  | DI    | 49  | GLU  | 4.2  |
| 16  | CQ    | 72  | TRP  | 4.2  |
| 43  | DT    | 10  | VAL  | 4.2  |
| 4   | AE    | 88  | HIS  | 4.2  |
| 43  | DT    | 33  | LYS  | 4.2  |
| 6   | CG    | 149 | ALA  | 4.2  |
| 9   | AJ    | 89  | ARG  | 4.2  |
| 24  | DA    | 236 | C    | 4.2  |
| 1   | AB    | 16  | GLY  | 4.2  |
| 29  | BF    | 105 | ILE  | 4.2  |
| 34  | DK    | 77  | ILE  | 4.2  |
| 37  | DN    | 82  | GLU  | 4.2  |
| 9   | CJ    | 6   | ILE  | 4.2  |
| 7   | CH    | 59  | GLU  | 4.2  |
| 1   | AB    | 85  | SER  | 4.2  |
| 4   | AE    | 123 | LEU  | 4.2  |
| 28  | DE    | 200 | LEU  | 4.2  |
| 18  | CS    | 40  | PHE  | 4.2  |
| 1   | AB    | 218 | ALA  | 4.2  |
| 24  | DA    | 62  | U    | 4.2  |
| 4   | CE    | 72  | ASN  | 4.2  |
| 55  | CA    | 81  | A    | 4.2  |
| 16  | AQ    | 82  | VAL  | 4.1  |
| 10  | AK    | 29  | THR  | 4.1  |
| 31  | BH    | 147 | VAL  | 4.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 35         | DL           | 107        | PHE         | 4.1         |
| 32         | DI           | 54         | ILE         | 4.1         |
| 37         | DN           | 43         | GLU         | 4.1         |
| 38         | DO           | 108        | ASP         | 4.1         |
| 30         | DG           | 56         | GLY         | 4.1         |
| 40         | DQ           | 70         | GLN         | 4.1         |
| 15         | CP           | 7          | ALA         | 4.1         |
| 29         | DF           | 150        | GLY         | 4.1         |
| 21         | AA           | 412        | A           | 4.1         |
| 29         | DF           | 18         | GLU         | 4.1         |
| 32         | BI           | 87         | SER         | 4.1         |
| 40         | DQ           | 79         | ILE         | 4.1         |
| 48         | DY           | 36         | GLN         | 4.1         |
| 43         | DT           | 81         | LYS         | 4.1         |
| 42         | DS           | 69         | LEU         | 4.1         |
| 6          | AG           | 79         | VAL         | 4.1         |
| 42         | DS           | 34         | ASP         | 4.1         |
| 51         | D1           | 20         | TYR         | 4.1         |
| 24         | DA           | 1170       | C           | 4.1         |
| 34         | DK           | 104        | THR         | 4.1         |
| 39         | DP           | 59         | THR         | 4.1         |
| 12         | AM           | 4          | ALA         | 4.1         |
| 32         | DI           | 10         | LEU         | 4.1         |
| 37         | DN           | 79         | LEU         | 4.1         |
| 8          | AI           | 16         | ALA         | 4.1         |
| 31         | DH           | 104        | THR         | 4.1         |
| 32         | BI           | 51         | GLY         | 4.1         |
| 30         | DG           | 83         | THR         | 4.1         |
| 27         | DD           | 9          | VAL         | 4.1         |
| 32         | DI           | 24         | GLY         | 4.1         |
| 30         | DG           | 164        | ALA         | 4.1         |
| 1          | AB           | 53         | LEU         | 4.1         |
| 53         | D3           | 47         | ALA         | 4.1         |
| 1          | AB           | 158        | ASP         | 4.1         |
| 8          | CI           | 38         | PHE         | 4.1         |
| 27         | DD           | 1          | MET         | 4.1         |
| 24         | BA           | 2139       | U           | 4.0         |
| 46         | DW           | 35         | ILE         | 4.0         |
| 36         | DM           | 41         | LEU         | 4.0         |
| 46         | DW           | 15         | SER         | 4.0         |
| 4          | AE           | 154        | ALA         | 4.0         |
| 32         | BI           | 111        | THR         | 4.0         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 47  | DX    | 12   | VAL  | 4.0  |
| 44  | DU    | 50   | ALA  | 4.0  |
| 53  | D3    | 48   | MET  | 4.0  |
| 2   | CC    | 85   | LYS  | 4.0  |
| 1   | CB    | 163  | ILE  | 4.0  |
| 7   | CH    | 60   | LEU  | 4.0  |
| 37  | DN    | 39   | PRO  | 4.0  |
| 35  | DL    | 124  | GLY  | 4.0  |
| 54  | D4    | 8    | LYS  | 4.0  |
| 53  | D3    | 13   | PHE  | 4.0  |
| 43  | DT    | 61   | LEU  | 4.0  |
| 43  | DT    | 72   | GLN  | 4.0  |
| 36  | DM    | 103  | TYR  | 4.0  |
| 46  | DW    | 49   | ASN  | 4.0  |
| 3   | AD    | 28   | ASP  | 4.0  |
| 38  | DO    | 105  | ALA  | 4.0  |
| 41  | DR    | 4    | VAL  | 4.0  |
| 43  | DT    | 74   | ILE  | 4.0  |
| 31  | BH    | 146  | VAL  | 4.0  |
| 45  | DV    | 74   | ALA  | 4.0  |
| 24  | DA    | 1067 | A    | 4.0  |
| 34  | DK    | 76   | VAL  | 4.0  |
| 32  | DI    | 118  | GLY  | 4.0  |
| 37  | DN    | 76   | VAL  | 4.0  |
| 21  | AA    | 85   | U    | 4.0  |
| 4   | AE    | 136  | VAL  | 4.0  |
| 27  | DD    | 166  | GLY  | 4.0  |
| 27  | DD    | 15   | PHE  | 4.0  |
| 38  | DO    | 62   | LEU  | 3.9  |
| 28  | DE    | 177  | PRO  | 3.9  |
| 32  | DI    | 18   | ASN  | 3.9  |
| 26  | DC    | 126  | GLY  | 3.9  |
| 29  | BF    | 110  | ILE  | 3.9  |
| 31  | DH    | 113  | SER  | 3.9  |
| 19  | CT    | 12   | GLN  | 3.9  |
| 26  | DC    | 91   | ALA  | 3.9  |
| 44  | DU    | 27   | VAL  | 3.9  |
| 30  | DG    | 125  | PRO  | 3.9  |
| 30  | DG    | 173  | ALA  | 3.9  |
| 32  | BI    | 13   | ALA  | 3.9  |
| 18  | CS    | 29   | PRO  | 3.9  |
| 47  | DX    | 13   | THR  | 3.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 13  | CN    | 32  | ASP  | 3.9  |
| 31  | BH    | 134 | VAL  | 3.9  |
| 32  | DI    | 21  | PRO  | 3.9  |
| 43  | DT    | 5   | GLU  | 3.9  |
| 45  | DV    | 6   | ALA  | 3.9  |
| 35  | DL    | 89  | VAL  | 3.9  |
| 7   | CH    | 102 | VAL  | 3.9  |
| 31  | BH    | 148 | ALA  | 3.9  |
| 31  | BH    | 77  | THR  | 3.9  |
| 1   | AB    | 163 | ILE  | 3.9  |
| 43  | DT    | 2   | ILE  | 3.9  |
| 36  | DM    | 71  | LYS  | 3.9  |
| 31  | DH    | 77  | THR  | 3.9  |
| 24  | DA    | 139 | U    | 3.9  |
| 42  | DS    | 97  | LEU  | 3.9  |
| 46  | DW    | 56  | HIS  | 3.9  |
| 53  | D3    | 14  | LYS  | 3.9  |
| 32  | DI    | 5   | GLN  | 3.9  |
| 27  | DD    | 4   | LEU  | 3.9  |
| 32  | BI    | 137 | LEU  | 3.9  |
| 27  | DD    | 192 | ALA  | 3.9  |
| 44  | DU    | 86  | PHE  | 3.9  |
| 15  | CP    | 45  | GLU  | 3.8  |
| 24  | DA    | 947 | A    | 3.8  |
| 38  | DO    | 39  | VAL  | 3.8  |
| 41  | DR    | 96  | VAL  | 3.8  |
| 4   | AE    | 57  | ALA  | 3.8  |
| 20  | AU    | 42  | THR  | 3.8  |
| 24  | DA    | 588 | U    | 3.8  |
| 4   | AE    | 109 | ALA  | 3.8  |
| 41  | DR    | 13  | ARG  | 3.8  |
| 20  | AU    | 23  | GLU  | 3.8  |
| 38  | DO    | 46  | GLU  | 3.8  |
| 30  | DG    | 130 | ILE  | 3.8  |
| 31  | BH    | 144 | VAL  | 3.8  |
| 32  | BI    | 98  | GLY  | 3.8  |
| 28  | DE    | 43  | THR  | 3.8  |
| 31  | BH    | 80  | ILE  | 3.8  |
| 31  | BH    | 124 | THR  | 3.8  |
| 30  | DG    | 147 | LEU  | 3.8  |
| 29  | BF    | 132 | ARG  | 3.8  |
| 18  | AS    | 67  | GLY  | 3.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | CF    | 58   | HIS  | 3.8  |
| 4   | AE    | 95   | MET  | 3.8  |
| 32  | DI    | 16   | MET  | 3.8  |
| 38  | DO    | 60   | GLU  | 3.8  |
| 1   | CB    | 206  | ILE  | 3.8  |
| 53  | D3    | 60   | CYS  | 3.8  |
| 29  | BF    | 112  | ASP  | 3.8  |
| 40  | DQ    | 13   | HIS  | 3.8  |
| 43  | DT    | 31   | VAL  | 3.8  |
| 27  | DD    | 55   | LYS  | 3.8  |
| 30  | DG    | 53   | PRO  | 3.8  |
| 24  | DA    | 1537 | G    | 3.8  |
| 9   | CJ    | 66   | GLU  | 3.8  |
| 35  | DL    | 31   | GLY  | 3.8  |
| 45  | DV    | 58   | SER  | 3.8  |
| 31  | BH    | 99   | ILE  | 3.8  |
| 38  | DO    | 27   | VAL  | 3.8  |
| 34  | DK    | 68   | GLY  | 3.8  |
| 34  | DK    | 64   | ARG  | 3.8  |
| 18  | CS    | 67   | GLY  | 3.8  |
| 41  | DR    | 71   | LYS  | 3.8  |
| 46  | DW    | 57   | THR  | 3.7  |
| 28  | DE    | 180  | LEU  | 3.7  |
| 44  | DU    | 93   | ARG  | 3.7  |
| 47  | DX    | 45   | PHE  | 3.7  |
| 21  | AA    | 461  | A    | 3.7  |
| 40  | DQ    | 90   | ASP  | 3.7  |
| 44  | DU    | 18   | LYS  | 3.7  |
| 45  | DV    | 69   | GLU  | 3.7  |
| 19  | CT    | 74   | HIS  | 3.7  |
| 44  | DU    | 74   | ALA  | 3.7  |
| 32  | DI    | 98   | GLY  | 3.7  |
| 32  | BI    | 97   | VAL  | 3.7  |
| 46  | DW    | 43   | LYS  | 3.7  |
| 33  | DJ    | 55   | ILE  | 3.7  |
| 33  | DJ    | 95   | ARG  | 3.7  |
| 4   | AE    | 52   | ALA  | 3.7  |
| 32  | DI    | 75   | ALA  | 3.7  |
| 12  | AM    | 113  | LYS  | 3.7  |
| 27  | DD    | 5    | VAL  | 3.7  |
| 51  | D1    | 43   | ARG  | 3.7  |
| 26  | DC    | 47   | ARG  | 3.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | CL    | 81   | ILE  | 3.7  |
| 24  | DA    | 1169 | A    | 3.7  |
| 30  | DG    | 102  | ILE  | 3.7  |
| 1   | AB    | 92   | ASN  | 3.7  |
| 29  | DF    | 51   | ASN  | 3.7  |
| 31  | BH    | 106  | ALA  | 3.7  |
| 46  | BW    | 45   | HIS  | 3.7  |
| 29  | DF    | 141  | ASP  | 3.7  |
| 46  | DW    | 14   | ASP  | 3.7  |
| 30  | DG    | 61   | TRP  | 3.7  |
| 36  | DM    | 5    | LYS  | 3.7  |
| 6   | CG    | 121  | ASN  | 3.7  |
| 31  | DH    | 122  | LEU  | 3.7  |
| 4   | CE    | 157  | GLY  | 3.7  |
| 24  | DA    | 34   | U    | 3.7  |
| 46  | DW    | 44   | PHE  | 3.7  |
| 35  | DL    | 42   | SER  | 3.7  |
| 38  | DO    | 116  | GLN  | 3.7  |
| 41  | DR    | 28   | ALA  | 3.7  |
| 51  | D1    | 34   | GLU  | 3.7  |
| 1   | AB    | 214  | GLY  | 3.7  |
| 27  | DD    | 176  | ASP  | 3.7  |
| 44  | DU    | 6    | ARG  | 3.7  |
| 37  | DN    | 21   | PHE  | 3.7  |
| 46  | DW    | 68   | PHE  | 3.7  |
| 15  | CP    | 51   | ARG  | 3.7  |
| 18  | CS    | 70   | LEU  | 3.7  |
| 39  | DP    | 91   | VAL  | 3.7  |
| 7   | CH    | 127  | TYR  | 3.7  |
| 29  | DF    | 6    | TYR  | 3.7  |
| 18  | AS    | 39   | ILE  | 3.7  |
| 6   | AG    | 4    | ARG  | 3.7  |
| 31  | BH    | 127  | GLU  | 3.7  |
| 49  | DZ    | 7    | THR  | 3.7  |
| 40  | DQ    | 72   | GLY  | 3.6  |
| 27  | DD    | 20   | VAL  | 3.6  |
| 39  | DP    | 73   | PHE  | 3.6  |
| 46  | DW    | 67   | LYS  | 3.6  |
| 4   | AE    | 10   | LEU  | 3.6  |
| 31  | DH    | 38   | PRO  | 3.6  |
| 42  | DS    | 5    | ALA  | 3.6  |
| 29  | BF    | 139  | GLU  | 3.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | DJ    | 9    | GLU  | 3.6  |
| 34  | DK    | 82   | ASN  | 3.6  |
| 28  | DE    | 34   | ALA  | 3.6  |
| 9   | AJ    | 24   | GLU  | 3.6  |
| 44  | DU    | 94   | PHE  | 3.6  |
| 38  | DO    | 42   | PRO  | 3.6  |
| 43  | DT    | 84   | TYR  | 3.6  |
| 46  | DW    | 69   | GLU  | 3.6  |
| 6   | CG    | 76   | SER  | 3.6  |
| 43  | DT    | 59   | ASN  | 3.6  |
| 1   | CB    | 16   | GLY  | 3.6  |
| 24  | BA    | 2142 | A    | 3.6  |
| 35  | DL    | 122  | VAL  | 3.6  |
| 51  | D1    | 49   | LYS  | 3.6  |
| 15  | AP    | 3    | THR  | 3.6  |
| 1   | CB    | 32   | GLY  | 3.6  |
| 16  | CQ    | 20   | ILE  | 3.6  |
| 29  | BF    | 175  | PRO  | 3.6  |
| 5   | CF    | 10   | VAL  | 3.6  |
| 13  | CN    | 51   | PRO  | 3.6  |
| 48  | DY    | 7    | ARG  | 3.6  |
| 32  | DI    | 44   | LYS  | 3.6  |
| 41  | DR    | 2    | TYR  | 3.6  |
| 1   | AB    | 169  | HIS  | 3.6  |
| 6   | CG    | 7    | GLY  | 3.6  |
| 1   | AB    | 183  | PHE  | 3.6  |
| 4   | AE    | 87   | VAL  | 3.6  |
| 33  | DJ    | 98   | GLU  | 3.6  |
| 39  | DP    | 96   | LEU  | 3.6  |
| 24  | BA    | 1065 | U    | 3.6  |
| 1   | CB    | 135  | MET  | 3.6  |
| 49  | DZ    | 1    | ALA  | 3.6  |
| 4   | AE    | 43   | GLY  | 3.6  |
| 13  | CN    | 91   | GLU  | 3.6  |
| 18  | AS    | 58   | PRO  | 3.6  |
| 35  | DL    | 5    | THR  | 3.6  |
| 41  | DR    | 32   | THR  | 3.6  |
| 1   | AB    | 20   | ARG  | 3.6  |
| 37  | DN    | 66   | ALA  | 3.6  |
| 1   | AB    | 56   | LEU  | 3.6  |
| 8   | AI    | 9    | GLY  | 3.6  |
| 15  | CP    | 50   | THR  | 3.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 37         | DN           | 27         | SER         | 3.6         |
| 3          | AD           | 146        | GLU         | 3.6         |
| 18         | AS           | 64         | GLU         | 3.6         |
| 22         | CX           | 31         | A           | 3.6         |
| 31         | DH           | 121        | VAL         | 3.6         |
| 33         | DJ           | 89         | PHE         | 3.6         |
| 26         | DC           | 103        | ILE         | 3.6         |
| 44         | DU           | 62         | ALA         | 3.6         |
| 13         | CN           | 50         | LEU         | 3.6         |
| 13         | CN           | 22         | LYS         | 3.5         |
| 19         | CT           | 63         | LYS         | 3.5         |
| 38         | DO           | 63         | LYS         | 3.5         |
| 1          | AB           | 109        | SER         | 3.5         |
| 42         | DS           | 4          | ILE         | 3.5         |
| 29         | DF           | 33         | ILE         | 3.5         |
| 42         | DS           | 105        | VAL         | 3.5         |
| 36         | DM           | 40         | ARG         | 3.5         |
| 45         | DV           | 79         | ARG         | 3.5         |
| 35         | DL           | 101        | ILE         | 3.5         |
| 19         | AT           | 60         | GLN         | 3.5         |
| 28         | DE           | 46         | GLN         | 3.5         |
| 50         | D0           | 34         | GLY         | 3.5         |
| 27         | DD           | 8          | LYS         | 3.5         |
| 27         | DD           | 75         | ALA         | 3.5         |
| 44         | DU           | 40         | LEU         | 3.5         |
| 8          | CI           | 4          | GLN         | 3.5         |
| 55         | CA           | 175        | C           | 3.5         |
| 43         | DT           | 60         | THR         | 3.5         |
| 39         | DP           | 72         | VAL         | 3.5         |
| 46         | DW           | 22         | VAL         | 3.5         |
| 1          | AB           | 134        | LEU         | 3.5         |
| 22         | CX           | 40         | C           | 3.5         |
| 31         | BH           | 143        | ILE         | 3.5         |
| 24         | BA           | 2182       | U           | 3.5         |
| 29         | BF           | 150        | GLY         | 3.5         |
| 37         | DN           | 99         | LYS         | 3.5         |
| 46         | DW           | 71         | LYS         | 3.5         |
| 6          | CG           | 70         | PRO         | 3.5         |
| 41         | DR           | 18         | GLN         | 3.5         |
| 7          | CH           | 91         | LEU         | 3.5         |
| 41         | DR           | 73         | LYS         | 3.5         |
| 41         | DR           | 33         | VAL         | 3.5         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 43  | DT    | 62  | VAL  | 3.5  |
| 17  | AR    | 28  | LEU  | 3.5  |
| 4   | AE    | 98  | ALA  | 3.5  |
| 27  | DD    | 91  | THR  | 3.5  |
| 32  | BI    | 59  | THR  | 3.5  |
| 46  | DW    | 41  | GLY  | 3.5  |
| 46  | DW    | 19  | ARG  | 3.5  |
| 46  | DW    | 28  | GLU  | 3.5  |
| 27  | DD    | 23  | PRO  | 3.5  |
| 27  | DD    | 19  | GLY  | 3.5  |
| 1   | CB    | 161 | PHE  | 3.5  |
| 40  | DQ    | 87  | VAL  | 3.5  |
| 18  | AS    | 70  | LEU  | 3.5  |
| 29  | DF    | 78  | ILE  | 3.5  |
| 30  | DG    | 116 | LEU  | 3.5  |
| 1   | AB    | 135 | MET  | 3.5  |
| 40  | DQ    | 28  | SER  | 3.5  |
| 27  | DD    | 205 | PRO  | 3.5  |
| 30  | DG    | 33  | THR  | 3.5  |
| 29  | DF    | 171 | ALA  | 3.5  |
| 46  | DW    | 62  | ALA  | 3.5  |
| 27  | DD    | 113 | SER  | 3.5  |
| 28  | DE    | 186 | VAL  | 3.5  |
| 29  | BF    | 74  | ALA  | 3.4  |
| 15  | CP    | 47  | GLU  | 3.4  |
| 31  | BH    | 78  | VAL  | 3.4  |
| 9   | CJ    | 17  | LEU  | 3.4  |
| 34  | DK    | 33  | ALA  | 3.4  |
| 32  | DI    | 30  | GLN  | 3.4  |
| 53  | D3    | 46  | LYS  | 3.4  |
| 55  | CA    | 205 | A    | 3.4  |
| 8   | AI    | 129 | ARG  | 3.4  |
| 29  | DF    | 85  | GLY  | 3.4  |
| 22  | AX    | 27  | G    | 3.4  |
| 24  | DA    | 345 | A    | 3.4  |
| 34  | DK    | 83  | ALA  | 3.4  |
| 34  | DK    | 102 | PRO  | 3.4  |
| 1   | AB    | 66  | ILE  | 3.4  |
| 4   | AE    | 65  | LYS  | 3.4  |
| 19  | CT    | 24  | ARG  | 3.4  |
| 19  | CT    | 86  | ALA  | 3.4  |
| 33  | DJ    | 56  | VAL  | 3.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | CH    | 101  | ALA  | 3.4  |
| 53  | D3    | 21   | PHE  | 3.4  |
| 2   | CC    | 52   | SER  | 3.4  |
| 42  | DS    | 22   | ASP  | 3.4  |
| 1   | AB    | 176  | ASN  | 3.4  |
| 36  | DM    | 93   | VAL  | 3.4  |
| 41  | DR    | 72   | VAL  | 3.4  |
| 46  | DW    | 76   | ARG  | 3.4  |
| 32  | BI    | 16   | MET  | 3.4  |
| 27  | DD    | 203  | VAL  | 3.4  |
| 18  | AS    | 62   | THR  | 3.4  |
| 29  | DF    | 58   | ALA  | 3.4  |
| 13  | CN    | 19   | TYR  | 3.4  |
| 43  | DT    | 7    | LEU  | 3.4  |
| 4   | AE    | 15   | ILE  | 3.4  |
| 4   | AE    | 54   | GLU  | 3.4  |
| 29  | DF    | 76   | PHE  | 3.4  |
| 35  | DL    | 75   | ALA  | 3.4  |
| 24  | DA    | 446  | G    | 3.4  |
| 24  | BA    | 1066 | U    | 3.4  |
| 27  | DD    | 191  | GLY  | 3.4  |
| 18  | AS    | 73   | PHE  | 3.4  |
| 43  | DT    | 6    | ARG  | 3.4  |
| 24  | DA    | 1216 | G    | 3.4  |
| 24  | DA    | 1530 | G    | 3.4  |
| 39  | DP    | 29   | VAL  | 3.4  |
| 15  | CP    | 18   | GLN  | 3.4  |
| 27  | DD    | 97   | SER  | 3.4  |
| 31  | DH    | 86   | ASP  | 3.4  |
| 44  | DU    | 71   | ILE  | 3.4  |
| 16  | CQ    | 35   | LYS  | 3.3  |
| 15  | AP    | 22   | ALA  | 3.3  |
| 30  | DG    | 115  | GLN  | 3.3  |
| 30  | DG    | 123  | GLU  | 3.3  |
| 28  | DE    | 118  | LEU  | 3.3  |
| 24  | BA    | 2150 | C    | 3.3  |
| 28  | DE    | 104  | ALA  | 3.3  |
| 35  | DL    | 8    | PRO  | 3.3  |
| 32  | DI    | 129  | GLU  | 3.3  |
| 11  | CL    | 80   | LEU  | 3.3  |
| 33  | DJ    | 36   | LEU  | 3.3  |
| 44  | DU    | 2    | ALA  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | AE    | 39   | GLY  | 3.3  |
| 26  | DC    | 46   | GLY  | 3.3  |
| 13  | CN    | 95   | LEU  | 3.3  |
| 28  | DE    | 57   | LYS  | 3.3  |
| 24  | DA    | 2157 | G    | 3.3  |
| 32  | DI    | 13   | ALA  | 3.3  |
| 44  | DU    | 4    | ILE  | 3.3  |
| 39  | DP    | 70   | GLU  | 3.3  |
| 51  | D1    | 36   | LYS  | 3.3  |
| 33  | DJ    | 128  | ASN  | 3.3  |
| 1   | CB    | 217  | ALA  | 3.3  |
| 1   | CB    | 218  | ALA  | 3.3  |
| 20  | AU    | 3    | ILE  | 3.3  |
| 8   | AI    | 78   | ILE  | 3.3  |
| 4   | AE    | 108  | GLY  | 3.3  |
| 28  | DE    | 22   | ASP  | 3.3  |
| 49  | DZ    | 8    | GLN  | 3.3  |
| 19  | CT    | 43   | LYS  | 3.3  |
| 31  | BH    | 94   | ILE  | 3.3  |
| 43  | DT    | 20   | ALA  | 3.3  |
| 26  | BC    | 242  | HIS  | 3.3  |
| 31  | BH    | 126  | GLY  | 3.3  |
| 45  | DV    | 82   | TYR  | 3.3  |
| 53  | D3    | 20   | GLY  | 3.3  |
| 36  | DM    | 77   | PRO  | 3.3  |
| 26  | DC    | 11   | GLY  | 3.3  |
| 30  | DG    | 114  | HIS  | 3.3  |
| 6   | CG    | 85   | GLN  | 3.3  |
| 10  | AK    | 109  | ILE  | 3.3  |
| 45  | DV    | 37   | PRO  | 3.3  |
| 27  | DD    | 13   | ARG  | 3.3  |
| 44  | DU    | 25   | LYS  | 3.3  |
| 33  | DJ    | 62   | VAL  | 3.3  |
| 41  | DR    | 74   | ILE  | 3.3  |
| 13  | CN    | 94   | GLY  | 3.3  |
| 34  | DK    | 99   | ILE  | 3.3  |
| 39  | DP    | 74   | GLN  | 3.3  |
| 27  | DD    | 168  | GLU  | 3.3  |
| 31  | BH    | 76   | GLU  | 3.3  |
| 34  | DK    | 74   | GLY  | 3.3  |
| 44  | DU    | 85   | ARG  | 3.3  |
| 36  | DM    | 17   | ASN  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 18  | AS    | 65   | MET  | 3.3  |
| 27  | DD    | 2    | ILE  | 3.3  |
| 8   | CI    | 107  | ALA  | 3.2  |
| 4   | AE    | 71   | ILE  | 3.2  |
| 41  | DR    | 53   | PHE  | 3.2  |
| 31  | BH    | 71   | LYS  | 3.2  |
| 1   | AB    | 49   | PHE  | 3.2  |
| 5   | CF    | 8    | PHE  | 3.2  |
| 46  | DW    | 82   | GLU  | 3.2  |
| 29  | DF    | 39   | VAL  | 3.2  |
| 44  | DU    | 69   | VAL  | 3.2  |
| 34  | DK    | 103  | VAL  | 3.2  |
| 35  | DL    | 90   | VAL  | 3.2  |
| 31  | DH    | 146  | VAL  | 3.2  |
| 32  | BI    | 57   | VAL  | 3.2  |
| 16  | CQ    | 60   | ILE  | 3.2  |
| 4   | AE    | 158  | LYS  | 3.2  |
| 29  | DF    | 55   | ASP  | 3.2  |
| 31  | BH    | 100  | ALA  | 3.2  |
| 24  | DA    | 88   | G    | 3.2  |
| 38  | DO    | 49   | VAL  | 3.2  |
| 45  | DV    | 65   | VAL  | 3.2  |
| 1   | AB    | 170  | ILE  | 3.2  |
| 10  | CK    | 51   | PHE  | 3.2  |
| 11  | CL    | 84   | GLY  | 3.2  |
| 35  | DL    | 88   | GLY  | 3.2  |
| 44  | DU    | 83   | GLY  | 3.2  |
| 47  | DX    | 34   | SER  | 3.2  |
| 31  | BH    | 125  | THR  | 3.2  |
| 36  | DM    | 74   | THR  | 3.2  |
| 37  | DN    | 75   | ILE  | 3.2  |
| 38  | DO    | 3    | LYS  | 3.2  |
| 8   | AI    | 10   | ARG  | 3.2  |
| 24  | DA    | 1078 | U    | 3.2  |
| 4   | AE    | 76   | ASN  | 3.2  |
| 30  | DG    | 124  | CYS  | 3.2  |
| 37  | DN    | 32   | GLU  | 3.2  |
| 4   | AE    | 153  | ALA  | 3.2  |
| 55  | CA    | 1227 | A    | 3.2  |
| 8   | AI    | 77   | ALA  | 3.2  |
| 32  | DI    | 94   | LYS  | 3.2  |
| 2   | AC    | 184  | ASN  | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | CL    | 28   | GLN  | 3.2  |
| 1   | AB    | 21   | TYR  | 3.2  |
| 24  | DA    | 138  | U    | 3.2  |
| 41  | DR    | 38   | VAL  | 3.2  |
| 4   | AE    | 78   | GLY  | 3.2  |
| 32  | DI    | 97   | VAL  | 3.2  |
| 35  | DL    | 91   | ASP  | 3.2  |
| 36  | DM    | 60   | GLN  | 3.2  |
| 44  | DU    | 7    | ASP  | 3.2  |
| 28  | DE    | 135  | ALA  | 3.2  |
| 29  | DF    | 172  | PHE  | 3.2  |
| 32  | BI    | 66   | PHE  | 3.2  |
| 2   | CC    | 184  | ASN  | 3.2  |
| 3   | AD    | 26   | ALA  | 3.2  |
| 3   | AD    | 35   | GLN  | 3.2  |
| 4   | AE    | 48   | GLY  | 3.2  |
| 49  | DZ    | 43   | ILE  | 3.1  |
| 2   | CC    | 53   | ARG  | 3.1  |
| 30  | DG    | 81   | GLY  | 3.1  |
| 36  | DM    | 73   | ILE  | 3.1  |
| 1   | AB    | 29   | PHE  | 3.1  |
| 50  | D0    | 42   | ILE  | 3.1  |
| 19  | CT    | 42   | ASP  | 3.1  |
| 30  | DG    | 176  | LYS  | 3.1  |
| 37  | DN    | 96   | ARG  | 3.1  |
| 8   | CI    | 39   | GLY  | 3.1  |
| 38  | DO    | 87   | ILE  | 3.1  |
| 30  | DG    | 104  | LEU  | 3.1  |
| 15  | CP    | 48   | GLU  | 3.1  |
| 16  | CQ    | 5    | ARG  | 3.1  |
| 18  | CS    | 2    | ARG  | 3.1  |
| 42  | DS    | 108  | SER  | 3.1  |
| 42  | DS    | 93   | ALA  | 3.1  |
| 19  | CT    | 64   | GLY  | 3.1  |
| 44  | DU    | 10   | VAL  | 3.1  |
| 24  | DA    | 1278 | C    | 3.1  |
| 7   | CH    | 129  | ALA  | 3.1  |
| 21  | AA    | 79   | G    | 3.1  |
| 24  | DA    | 1460 | U    | 3.1  |
| 12  | AM    | 112  | ARG  | 3.1  |
| 29  | BF    | 131  | VAL  | 3.1  |
| 32  | DI    | 53   | PRO  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 21  | AA    | 81  | A    | 3.1  |
| 55  | CA    | 461 | A    | 3.1  |
| 1   | AB    | 82  | ALA  | 3.1  |
| 41  | DR    | 3   | ALA  | 3.1  |
| 44  | DU    | 75  | ALA  | 3.1  |
| 4   | AE    | 9   | GLU  | 3.1  |
| 30  | DG    | 100 | ASN  | 3.1  |
| 36  | DM    | 131 | VAL  | 3.1  |
| 42  | DS    | 40  | ASN  | 3.1  |
| 54  | D4    | 1   | MET  | 3.1  |
| 24  | DA    | 431 | U    | 3.1  |
| 51  | D1    | 30  | PRO  | 3.1  |
| 4   | AE    | 112 | ALA  | 3.1  |
| 15  | AP    | 2   | VAL  | 3.1  |
| 19  | CT    | 61  | ALA  | 3.1  |
| 51  | D1    | 38  | PHE  | 3.1  |
| 12  | AM    | 104 | ASN  | 3.1  |
| 27  | DD    | 56  | LYS  | 3.1  |
| 49  | DZ    | 33  | HIS  | 3.1  |
| 51  | D1    | 24  | LYS  | 3.1  |
| 24  | DA    | 805 | G    | 3.1  |
| 24  | DA    | 654 | A    | 3.1  |
| 28  | DE    | 88  | ARG  | 3.1  |
| 33  | DJ    | 35  | ARG  | 3.1  |
| 39  | DP    | 27  | VAL  | 3.1  |
| 6   | AG    | 20  | GLU  | 3.1  |
| 11  | AL    | 24  | GLU  | 3.1  |
| 24  | DA    | 318 | C    | 3.1  |
| 32  | BI    | 22  | PRO  | 3.1  |
| 32  | DI    | 61  | TYR  | 3.1  |
| 35  | DL    | 82  | LEU  | 3.1  |
| 26  | BC    | 239 | PHE  | 3.1  |
| 8   | CI    | 50  | PRO  | 3.1  |
| 30  | DG    | 101 | VAL  | 3.1  |
| 32  | DI    | 112 | LYS  | 3.1  |
| 19  | CT    | 58  | ASP  | 3.1  |
| 34  | DK    | 69  | VAL  | 3.1  |
| 28  | DE    | 48  | THR  | 3.1  |
| 43  | DT    | 1   | MET  | 3.1  |
| 34  | DK    | 2   | ILE  | 3.1  |
| 9   | CJ    | 96  | VAL  | 3.0  |
| 28  | DE    | 41  | GLN  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 27  | DD    | 190  | LYS  | 3.0  |
| 29  | BF    | 38   | GLY  | 3.0  |
| 48  | BY    | 63   | ALA  | 3.0  |
| 42  | DS    | 59   | GLU  | 3.0  |
| 9   | CJ    | 8    | ILE  | 3.0  |
| 46  | DW    | 16   | GLU  | 3.0  |
| 46  | DW    | 75   | ASN  | 3.0  |
| 1   | AB    | 171  | ALA  | 3.0  |
| 50  | D0    | 44   | ALA  | 3.0  |
| 42  | DS    | 67   | ASP  | 3.0  |
| 18  | AS    | 40   | PHE  | 3.0  |
| 9   | CJ    | 34   | ALA  | 3.0  |
| 24  | DA    | 1077 | A    | 3.0  |
| 30  | DG    | 163  | TYR  | 3.0  |
| 31  | BH    | 120  | GLY  | 3.0  |
| 29  | DF    | 110  | ILE  | 3.0  |
| 24  | DA    | 2021 | C    | 3.0  |
| 8   | CI    | 3    | ASN  | 3.0  |
| 31  | BH    | 74   | ALA  | 3.0  |
| 5   | CF    | 90   | MET  | 3.0  |
| 9   | CJ    | 74   | VAL  | 3.0  |
| 24  | DA    | 546  | U    | 3.0  |
| 42  | DS    | 17   | VAL  | 3.0  |
| 34  | DK    | 14   | SER  | 3.0  |
| 36  | DM    | 56   | ALA  | 3.0  |
| 24  | BA    | 2885 | G    | 3.0  |
| 48  | DY    | 56   | LEU  | 3.0  |
| 1   | CB    | 127  | LYS  | 3.0  |
| 24  | BA    | 2153 | C    | 3.0  |
| 44  | DU    | 72   | PHE  | 3.0  |
| 39  | DP    | 32   | VAL  | 3.0  |
| 55  | CA    | 206  | C    | 3.0  |
| 55  | CA    | 88   | U    | 3.0  |
| 24  | DA    | 1420 | A    | 3.0  |
| 39  | DP    | 58   | PHE  | 3.0  |
| 41  | DR    | 90   | ARG  | 3.0  |
| 32  | BI    | 7    | TYR  | 3.0  |
| 40  | DQ    | 20   | ALA  | 3.0  |
| 1   | CB    | 46   | VAL  | 3.0  |
| 55  | CA    | 208  | U    | 3.0  |
| 38  | DO    | 106  | LEU  | 3.0  |
| 45  | DV    | 55   | GLU  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 18  | AS    | 29   | PRO  | 3.0  |
| 5   | AF    | 66   | ALA  | 3.0  |
| 22  | CX    | 41   | C    | 3.0  |
| 1   | AB    | 192  | PRO  | 3.0  |
| 32  | DI    | 82   | ALA  | 3.0  |
| 32  | DI    | 57   | VAL  | 3.0  |
| 1   | CB    | 31   | PHE  | 3.0  |
| 1   | AB    | 69   | VAL  | 3.0  |
| 30  | DG    | 42   | VAL  | 3.0  |
| 1   | AB    | 141  | GLU  | 3.0  |
| 4   | AE    | 64   | GLU  | 3.0  |
| 6   | CG    | 145  | GLU  | 3.0  |
| 27  | DD    | 7    | LYS  | 3.0  |
| 32  | BI    | 40   | ALA  | 3.0  |
| 32  | BI    | 60   | VAL  | 3.0  |
| 40  | DQ    | 71   | ASN  | 3.0  |
| 24  | DA    | 790  | U    | 3.0  |
| 30  | DG    | 57   | TYR  | 3.0  |
| 55  | CA    | 121  | U    | 3.0  |
| 17  | AR    | 39   | VAL  | 2.9  |
| 46  | DW    | 6    | GLY  | 2.9  |
| 7   | AH    | 60   | LEU  | 2.9  |
| 26  | BC    | 241  | LYS  | 2.9  |
| 46  | DW    | 77   | LYS  | 2.9  |
| 54  | D4    | 35   | GLN  | 2.9  |
| 33  | DJ    | 93   | ILE  | 2.9  |
| 42  | DS    | 66   | ILE  | 2.9  |
| 1   | CB    | 99   | MET  | 2.9  |
| 29  | DF    | 34   | THR  | 2.9  |
| 39  | DP    | 37   | LYS  | 2.9  |
| 16  | CQ    | 58   | VAL  | 2.9  |
| 19  | CT    | 2    | ASN  | 2.9  |
| 24  | DA    | 1075 | C    | 2.9  |
| 29  | DF    | 131  | VAL  | 2.9  |
| 31  | BH    | 145  | ASN  | 2.9  |
| 21  | AA    | 1362 | A    | 2.9  |
| 26  | DC    | 222  | THR  | 2.9  |
| 1   | AB    | 33   | ALA  | 2.9  |
| 2   | CC    | 179  | ALA  | 2.9  |
| 24  | DA    | 810  | U    | 2.9  |
| 26  | DC    | 45   | ASN  | 2.9  |
| 35  | DL    | 38   | GLN  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 42  | DS    | 39   | THR  | 2.9  |
| 24  | DA    | 136  | G    | 2.9  |
| 24  | DA    | 1095 | A    | 2.9  |
| 51  | B1    | 52   | LYS  | 2.9  |
| 36  | DM    | 111  | GLU  | 2.9  |
| 41  | DR    | 62   | GLU  | 2.9  |
| 45  | DV    | 84   | PRO  | 2.9  |
| 8   | AI    | 20   | ILE  | 2.9  |
| 36  | DM    | 10   | ARG  | 2.9  |
| 9   | CJ    | 91   | ASP  | 2.9  |
| 21  | AA    | 80   | A    | 2.9  |
| 26  | DC    | 63   | ILE  | 2.9  |
| 32  | BI    | 58   | ILE  | 2.9  |
| 32  | DI    | 45   | THR  | 2.9  |
| 2   | AC    | 102  | ILE  | 2.9  |
| 15  | AP    | 4    | ILE  | 2.9  |
| 30  | BG    | 120  | ILE  | 2.9  |
| 30  | DG    | 169  | ARG  | 2.9  |
| 26  | DC    | 121  | ALA  | 2.9  |
| 31  | DH    | 97   | ARG  | 2.9  |
| 48  | DY    | 59   | GLU  | 2.9  |
| 27  | DD    | 188  | LEU  | 2.9  |
| 1   | AB    | 210  | THR  | 2.9  |
| 4   | AE    | 119  | VAL  | 2.9  |
| 37  | DN    | 74   | GLU  | 2.9  |
| 13  | AN    | 45   | LEU  | 2.9  |
| 28  | DE    | 103  | GLY  | 2.9  |
| 4   | AE    | 41   | GLY  | 2.9  |
| 19  | CT    | 41   | GLY  | 2.9  |
| 4   | AE    | 70   | MET  | 2.9  |
| 6   | AG    | 77   | ARG  | 2.9  |
| 36  | DM    | 132  | THR  | 2.9  |
| 32  | BI    | 32   | VAL  | 2.9  |
| 51  | D1    | 31   | GLU  | 2.9  |
| 15  | CP    | 35   | ARG  | 2.9  |
| 37  | DN    | 46   | ARG  | 2.9  |
| 51  | B1    | 16   | THR  | 2.9  |
| 1   | CB    | 53   | LEU  | 2.9  |
| 16  | CQ    | 7    | LEU  | 2.9  |
| 24  | DA    | 846  | U    | 2.9  |
| 34  | DK    | 80   | ASP  | 2.9  |
| 52  | D2    | 18   | PHE  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 55  | CA    | 971  | G    | 2.9  |
| 55  | CA    | 250  | A    | 2.8  |
| 15  | CP    | 4    | ILE  | 2.8  |
| 12  | AM    | 95   | PRO  | 2.8  |
| 38  | DO    | 15   | ARG  | 2.8  |
| 47  | DX    | 17   | ARG  | 2.8  |
| 12  | AM    | 94   | LEU  | 2.8  |
| 24  | DA    | 1731 | G    | 2.8  |
| 39  | DP    | 54   | LEU  | 2.8  |
| 33  | DJ    | 123  | LYS  | 2.8  |
| 44  | BU    | 52   | ASN  | 2.8  |
| 28  | DE    | 138  | LEU  | 2.8  |
| 10  | AK    | 128  | VAL  | 2.8  |
| 32  | DI    | 14   | ALA  | 2.8  |
| 32  | DI    | 40   | ALA  | 2.8  |
| 12  | CM    | 111  | PRO  | 2.8  |
| 18  | CS    | 38   | THR  | 2.8  |
| 24  | DA    | 1434 | A    | 2.8  |
| 24  | DA    | 2376 | A    | 2.8  |
| 19  | CT    | 54   | GLN  | 2.8  |
| 1   | AB    | 100  | LEU  | 2.8  |
| 2   | AC    | 110  | LEU  | 2.8  |
| 16  | CQ    | 79   | GLU  | 2.8  |
| 8   | AI    | 38   | PHE  | 2.8  |
| 29  | BF    | 151  | LEU  | 2.8  |
| 34  | DK    | 79   | PHE  | 2.8  |
| 38  | BO    | 58   | ILE  | 2.8  |
| 29  | BF    | 118  | ALA  | 2.8  |
| 31  | DH    | 120  | GLY  | 2.8  |
| 34  | DK    | 105  | ARG  | 2.8  |
| 38  | DO    | 111  | ARG  | 2.8  |
| 30  | DG    | 84   | LYS  | 2.8  |
| 48  | DY    | 5    | GLU  | 2.8  |
| 51  | D1    | 8    | ILE  | 2.8  |
| 55  | CA    | 1362 | A    | 2.8  |
| 24  | BA    | 2402 | U    | 2.8  |
| 32  | DI    | 70   | THR  | 2.8  |
| 32  | DI    | 72   | THR  | 2.8  |
| 1   | CB    | 109  | SER  | 2.8  |
| 13  | CN    | 55   | SER  | 2.8  |
| 15  | CP    | 9    | HIS  | 2.8  |
| 1   | AB    | 67   | LEU  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | AE    | 40   | ASP  | 2.8  |
| 36  | DM    | 70   | ASP  | 2.8  |
| 7   | CH    | 24   | VAL  | 2.8  |
| 34  | DK    | 19   | VAL  | 2.8  |
| 41  | DR    | 58   | VAL  | 2.8  |
| 37  | DN    | 95   | THR  | 2.8  |
| 24  | DA    | 2618 | G    | 2.8  |
| 55  | CA    | 213  | G    | 2.8  |
| 27  | DD    | 11   | MET  | 2.8  |
| 13  | AN    | 28   | ALA  | 2.8  |
| 32  | BI    | 19   | PRO  | 2.8  |
| 47  | DX    | 44   | ARG  | 2.8  |
| 39  | DP    | 110  | LYS  | 2.8  |
| 28  | DE    | 147  | LEU  | 2.8  |
| 42  | DS    | 23   | LEU  | 2.8  |
| 7   | CH    | 124  | ILE  | 2.8  |
| 29  | DF    | 79   | ARG  | 2.8  |
| 24  | BA    | 1175 | A    | 2.8  |
| 21  | AA    | 1032 | G    | 2.8  |
| 29  | DF    | 65   | LEU  | 2.8  |
| 5   | CF    | 40   | GLU  | 2.8  |
| 5   | CF    | 62   | MET  | 2.8  |
| 8   | AI    | 18   | VAL  | 2.8  |
| 37  | DN    | 42   | LYS  | 2.8  |
| 5   | CF    | 9    | MET  | 2.8  |
| 37  | DN    | 81   | ASN  | 2.8  |
| 1   | AB    | 190  | SER  | 2.8  |
| 1   | AB    | 77   | GLU  | 2.8  |
| 5   | AF    | 9    | MET  | 2.8  |
| 34  | DK    | 65   | THR  | 2.8  |
| 36  | DM    | 128  | THR  | 2.8  |
| 30  | DG    | 171  | LYS  | 2.8  |
| 32  | BI    | 61   | TYR  | 2.8  |
| 43  | DT    | 73   | ARG  | 2.8  |
| 6   | AG    | 80   | GLY  | 2.8  |
| 24  | BA    | 2306 | C    | 2.8  |
| 24  | DA    | 183  | C    | 2.8  |
| 32  | DI    | 73   | PRO  | 2.8  |
| 44  | DU    | 28   | LEU  | 2.8  |
| 18  | CS    | 6    | LYS  | 2.8  |
| 16  | CQ    | 45   | VAL  | 2.8  |
| 27  | DD    | 22   | ILE  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 32  | DI    | 19   | PRO  | 2.8  |
| 10  | AK    | 58   | THR  | 2.8  |
| 37  | DN    | 68   | ALA  | 2.8  |
| 35  | DL    | 142  | ILE  | 2.7  |
| 24  | BA    | 2151 | U    | 2.7  |
| 24  | DA    | 2310 | C    | 2.7  |
| 32  | DI    | 56   | VAL  | 2.7  |
| 55  | CA    | 214  | C    | 2.7  |
| 37  | DN    | 20   | MET  | 2.7  |
| 1   | AB    | 215  | ALA  | 2.7  |
| 48  | DY    | 61   | ALA  | 2.7  |
| 10  | AK    | 95   | THR  | 2.7  |
| 18  | AS    | 48   | ILE  | 2.7  |
| 18  | CS    | 78   | THR  | 2.7  |
| 4   | CE    | 110  | MET  | 2.7  |
| 12  | CM    | 71   | GLU  | 2.7  |
| 24  | BA    | 1093 | G    | 2.7  |
| 24  | DA    | 2145 | C    | 2.7  |
| 1   | AB    | 131  | LYS  | 2.7  |
| 6   | AG    | 78   | ARG  | 2.7  |
| 32  | BI    | 138  | VAL  | 2.7  |
| 54  | D4    | 19   | ARG  | 2.7  |
| 15  | CP    | 29   | ASN  | 2.7  |
| 42  | DS    | 101  | SER  | 2.7  |
| 18  | AS    | 8    | PRO  | 2.7  |
| 30  | DG    | 82   | PHE  | 2.7  |
| 38  | DO    | 89   | ASP  | 2.7  |
| 2   | AC    | 167  | TYR  | 2.7  |
| 16  | CQ    | 6    | THR  | 2.7  |
| 29  | DF    | 86   | CYS  | 2.7  |
| 19  | CT    | 67   | HIS  | 2.7  |
| 6   | AG    | 7    | GLY  | 2.7  |
| 39  | DP    | 31   | VAL  | 2.7  |
| 50  | D0    | 3    | GLN  | 2.7  |
| 12  | AM    | 82   | LEU  | 2.7  |
| 33  | DJ    | 47   | HIS  | 2.7  |
| 31  | DH    | 138  | VAL  | 2.7  |
| 36  | DM    | 11   | LYS  | 2.7  |
| 55  | CA    | 1286 | U    | 2.7  |
| 3   | AD    | 65   | GLY  | 2.7  |
| 36  | DM    | 92   | TRP  | 2.7  |
| 41  | DR    | 51   | VAL  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 48  | DY    | 35   | GLY  | 2.7  |
| 24  | DA    | 341  | C    | 2.7  |
| 35  | DL    | 121  | THR  | 2.7  |
| 1   | AB    | 41   | ASN  | 2.7  |
| 27  | DD    | 70   | LYS  | 2.7  |
| 32  | BI    | 35   | MET  | 2.7  |
| 39  | DP    | 108  | ARG  | 2.7  |
| 7   | AH    | 121  | GLY  | 2.7  |
| 7   | AH    | 129  | ALA  | 2.7  |
| 18  | AS    | 10   | ILE  | 2.7  |
| 36  | DM    | 69   | PRO  | 2.7  |
| 5   | CF    | 74   | LEU  | 2.7  |
| 35  | DL    | 125  | LEU  | 2.7  |
| 55  | CA    | 211  | G    | 2.7  |
| 15  | CP    | 80   | LYS  | 2.7  |
| 48  | DY    | 29   | ARG  | 2.7  |
| 4   | AE    | 157  | GLY  | 2.7  |
| 29  | DF    | 44   | ALA  | 2.7  |
| 30  | DG    | 1    | SER  | 2.7  |
| 32  | BI    | 83   | ALA  | 2.7  |
| 32  | DI    | 46   | ASP  | 2.7  |
| 29  | DF    | 64   | PRO  | 2.7  |
| 26  | DC    | 62   | ARG  | 2.7  |
| 33  | DJ    | 44   | TYR  | 2.7  |
| 24  | DA    | 2146 | C    | 2.7  |
| 36  | DM    | 120  | ALA  | 2.7  |
| 3   | AD    | 143  | SER  | 2.7  |
| 24  | DA    | 2152 | G    | 2.7  |
| 30  | DG    | 126  | THR  | 2.7  |
| 55  | CA    | 412  | A    | 2.7  |
| 15  | CP    | 8    | ARG  | 2.7  |
| 29  | BF    | 84   | ILE  | 2.7  |
| 12  | CM    | 67   | ASP  | 2.7  |
| 27  | DD    | 145  | SER  | 2.7  |
| 28  | DE    | 179  | SER  | 2.7  |
| 30  | DG    | 128  | THR  | 2.7  |
| 32  | DI    | 81   | LYS  | 2.7  |
| 37  | DN    | 83   | LEU  | 2.7  |
| 42  | DS    | 98   | LYS  | 2.7  |
| 24  | DA    | 1615 | C    | 2.7  |
| 33  | DJ    | 20   | ALA  | 2.7  |
| 6   | CG    | 87   | PRO  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 28  | DE    | 134  | LEU  | 2.7  |
| 29  | BF    | 101  | ARG  | 2.7  |
| 19  | AT    | 58   | ASP  | 2.7  |
| 27  | DD    | 43   | ASP  | 2.7  |
| 32  | BI    | 77   | VAL  | 2.7  |
| 42  | DS    | 71   | VAL  | 2.7  |
| 24  | DA    | 1590 | A    | 2.7  |
| 24  | DA    | 549  | G    | 2.7  |
| 24  | DA    | 1168 | G    | 2.7  |
| 46  | DW    | 60   | ALA  | 2.7  |
| 46  | DW    | 61   | LYS  | 2.7  |
| 34  | BK    | 71   | ARG  | 2.6  |
| 26  | DC    | 48   | ILE  | 2.6  |
| 42  | DS    | 43   | ALA  | 2.6  |
| 42  | DS    | 73   | LYS  | 2.6  |
| 24  | BA    | 140  | C    | 2.6  |
| 24  | DA    | 1066 | U    | 2.6  |
| 29  | DF    | 149  | ARG  | 2.6  |
| 38  | DO    | 7    | ARG  | 2.6  |
| 1   | CB    | 195  | VAL  | 2.6  |
| 29  | DF    | 36   | ASN  | 2.6  |
| 31  | DH    | 142  | VAL  | 2.6  |
| 1   | AB    | 191  | ASP  | 2.6  |
| 37  | DN    | 72   | ASP  | 2.6  |
| 24  | DA    | 1277 | G    | 2.6  |
| 24  | DA    | 1459 | G    | 2.6  |
| 5   | CF    | 61   | LEU  | 2.6  |
| 35  | DL    | 92   | LEU  | 2.6  |
| 41  | DR    | 14   | VAL  | 2.6  |
| 8   | AI    | 89   | TYR  | 2.6  |
| 24  | DA    | 1325 | U    | 2.6  |
| 12  | AM    | 3    | ILE  | 2.6  |
| 11  | CL    | 30   | ARG  | 2.6  |
| 29  | DF    | 159  | ALA  | 2.6  |
| 34  | DK    | 100  | PHE  | 2.6  |
| 35  | DL    | 37   | GLY  | 2.6  |
| 24  | BA    | 2108 | A    | 2.6  |
| 35  | DL    | 126  | ARG  | 2.6  |
| 4   | AE    | 100  | GLU  | 2.6  |
| 29  | BF    | 82   | TYR  | 2.6  |
| 31  | DH    | 87   | GLU  | 2.6  |
| 30  | DG    | 133  | LYS  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | DJ    | 53   | TYR  | 2.6  |
| 43  | DT    | 14   | PRO  | 2.6  |
| 1   | CB    | 56   | LEU  | 2.6  |
| 36  | DM    | 38   | ARG  | 2.6  |
| 37  | DN    | 41   | ALA  | 2.6  |
| 40  | DQ    | 29   | ARG  | 2.6  |
| 46  | DW    | 31   | LEU  | 2.6  |
| 22  | CX    | 39   | U    | 2.6  |
| 6   | AG    | 73   | GLU  | 2.6  |
| 27  | DD    | 12   | THR  | 2.6  |
| 51  | D1    | 6    | GLU  | 2.6  |
| 24  | DA    | 586  | A    | 2.6  |
| 34  | DK    | 78   | ARG  | 2.6  |
| 40  | DQ    | 36   | GLN  | 2.6  |
| 12  | CM    | 15   | VAL  | 2.6  |
| 33  | DJ    | 125  | TYR  | 2.6  |
| 42  | DS    | 3    | THR  | 2.6  |
| 13  | CN    | 52   | ARG  | 2.6  |
| 18  | AS    | 50   | VAL  | 2.6  |
| 28  | DE    | 30   | GLN  | 2.6  |
| 27  | DD    | 199  | SER  | 2.6  |
| 46  | DW    | 70   | VAL  | 2.6  |
| 28  | DE    | 127  | GLU  | 2.6  |
| 4   | AE    | 126  | ALA  | 2.6  |
| 50  | D0    | 50   | GLY  | 2.6  |
| 5   | CF    | 64   | VAL  | 2.6  |
| 1   | CB    | 125  | PHE  | 2.6  |
| 9   | AJ    | 63   | ASP  | 2.6  |
| 29  | BF    | 111  | ARG  | 2.6  |
| 33  | DJ    | 99   | ARG  | 2.6  |
| 50  | D0    | 45   | ASP  | 2.6  |
| 8   | AI    | 47   | VAL  | 2.6  |
| 16  | CQ    | 33   | TYR  | 2.6  |
| 32  | DI    | 89   | SER  | 2.6  |
| 11  | CL    | 29   | LYS  | 2.6  |
| 26  | DC    | 241  | LYS  | 2.6  |
| 35  | DL    | 144  | GLU  | 2.6  |
| 38  | DO    | 80   | GLU  | 2.6  |
| 49  | BZ    | 58   | GLU  | 2.6  |
| 54  | D4    | 10   | LEU  | 2.6  |
| 19  | CT    | 70   | LYS  | 2.6  |
| 24  | DA    | 1032 | A    | 2.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 31         | BH           | 83         | LYS         | 2.6         |
| 32         | BI           | 141        | ASP         | 2.6         |
| 42         | DS           | 106        | VAL         | 2.6         |
| 29         | BF           | 39         | VAL         | 2.6         |
| 29         | DF           | 178        | LYS         | 2.6         |
| 41         | DR           | 54         | VAL         | 2.6         |
| 19         | CT           | 23         | ARG         | 2.6         |
| 33         | DJ           | 96         | ARG         | 2.6         |
| 34         | DK           | 72         | PRO         | 2.6         |
| 38         | DO           | 30         | ARG         | 2.6         |
| 40         | DQ           | 63         | ARG         | 2.6         |
| 12         | CM           | 16         | ILE         | 2.6         |
| 4          | AE           | 20         | VAL         | 2.6         |
| 26         | DC           | 127        | ASN         | 2.6         |
| 32         | BI           | 75         | ALA         | 2.6         |
| 6          | CG           | 71         | THR         | 2.6         |
| 30         | DG           | 129        | GLU         | 2.6         |
| 3          | AD           | 24         | VAL         | 2.6         |
| 7          | CH           | 32         | LYS         | 2.6         |
| 31         | DH           | 90         | LEU         | 2.6         |
| 12         | CM           | 5          | GLY         | 2.6         |
| 5          | CF           | 81         | ASN         | 2.6         |
| 33         | DJ           | 119        | PHE         | 2.6         |
| 46         | BW           | 40         | ARG         | 2.6         |
| 4          | CE           | 82         | HIS         | 2.6         |
| 24         | DA           | 914        | G           | 2.6         |
| 13         | AN           | 35         | ALA         | 2.6         |
| 32         | BI           | 15         | GLY         | 2.6         |
| 43         | DT           | 46         | ALA         | 2.6         |
| 29         | BF           | 37         | MET         | 2.5         |
| 29         | BF           | 143        | ASP         | 2.5         |
| 36         | DM           | 98         | PRO         | 2.5         |
| 45         | DV           | 44         | HIS         | 2.5         |
| 6          | CG           | 18         | GLY         | 2.5         |
| 10         | CK           | 29         | THR         | 2.5         |
| 12         | CM           | 83         | GLY         | 2.5         |
| 31         | BH           | 122        | LEU         | 2.5         |
| 42         | DS           | 12         | SER         | 2.5         |
| 18         | AS           | 57         | VAL         | 2.5         |
| 27         | DD           | 185        | ASN         | 2.5         |
| 34         | DK           | 9          | ASN         | 2.5         |
| 43         | DT           | 64         | LYS         | 2.5         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | CF    | 60   | VAL  | 2.5  |
| 32  | DI    | 140  | GLU  | 2.5  |
| 55  | CA    | 1441 | A    | 2.5  |
| 15  | AP    | 37   | GLY  | 2.5  |
| 43  | DT    | 39   | THR  | 2.5  |
| 40  | DQ    | 89   | ILE  | 2.5  |
| 4   | AE    | 93   | VAL  | 2.5  |
| 4   | AE    | 129  | SER  | 2.5  |
| 7   | CH    | 126  | CYS  | 2.5  |
| 10  | AK    | 55   | ARG  | 2.5  |
| 14  | CO    | 85   | GLY  | 2.5  |
| 24  | BA    | 139  | U    | 2.5  |
| 18  | CS    | 48   | ILE  | 2.5  |
| 44  | BU    | 51   | LEU  | 2.5  |
| 4   | CE    | 86   | GLY  | 2.5  |
| 26  | DC    | 239  | PHE  | 2.5  |
| 47  | DX    | 14   | GLY  | 2.5  |
| 34  | DK    | 39   | ILE  | 2.5  |
| 28  | DE    | 31   | VAL  | 2.5  |
| 3   | AD    | 23   | GLY  | 2.5  |
| 7   | AH    | 68   | LYS  | 2.5  |
| 28  | DE    | 76   | PRO  | 2.5  |
| 37  | DN    | 77   | ALA  | 2.5  |
| 4   | AE    | 120  | HIS  | 2.5  |
| 27  | DD    | 96   | ILE  | 2.5  |
| 36  | DM    | 80   | VAL  | 2.5  |
| 45  | DV    | 43   | ASP  | 2.5  |
| 35  | DL    | 123  | ARG  | 2.5  |
| 2   | AC    | 157  | GLY  | 2.5  |
| 32  | DI    | 103  | ALA  | 2.5  |
| 36  | DM    | 109  | PRO  | 2.5  |
| 2   | AC    | 181  | ILE  | 2.5  |
| 27  | DD    | 27   | ILE  | 2.5  |
| 31  | BH    | 121  | VAL  | 2.5  |
| 39  | DP    | 69   | VAL  | 2.5  |
| 12  | AM    | 106  | ARG  | 2.5  |
| 20  | CU    | 35   | GLU  | 2.5  |
| 49  | DZ    | 39   | ASP  | 2.5  |
| 7   | AH    | 122  | GLY  | 2.5  |
| 24  | DA    | 671  | C    | 2.5  |
| 1   | CB    | 128  | LEU  | 2.5  |
| 11  | AL    | 47   | ALA  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 39  | DP    | 34   | GLY  | 2.5  |
| 28  | DE    | 12   | LEU  | 2.5  |
| 31  | BH    | 141  | LYS  | 2.5  |
| 24  | DA    | 356  | G    | 2.5  |
| 34  | DK    | 81   | GLY  | 2.5  |
| 39  | DP    | 39   | LEU  | 2.5  |
| 24  | DA    | 983  | A    | 2.5  |
| 31  | DH    | 141  | LYS  | 2.5  |
| 40  | DQ    | 31   | TYR  | 2.5  |
| 33  | DJ    | 94   | ALA  | 2.5  |
| 41  | DR    | 50   | GLY  | 2.5  |
| 43  | DT    | 65   | GLY  | 2.5  |
| 4   | CE    | 84   | VAL  | 2.5  |
| 4   | CE    | 158  | LYS  | 2.5  |
| 43  | DT    | 40   | LYS  | 2.5  |
| 40  | DQ    | 105  | PHE  | 2.5  |
| 15  | CP    | 21   | VAL  | 2.5  |
| 37  | DN    | 34   | ILE  | 2.5  |
| 51  | B1    | 51   | ALA  | 2.5  |
| 38  | DO    | 88   | LYS  | 2.5  |
| 4   | CE    | 49   | TYR  | 2.5  |
| 12  | AM    | 62   | PHE  | 2.5  |
| 4   | AE    | 26   | GLY  | 2.5  |
| 6   | CG    | 74   | VAL  | 2.5  |
| 12  | CM    | 81   | ASP  | 2.5  |
| 13  | AN    | 23   | ARG  | 2.5  |
| 32  | DI    | 9    | LYS  | 2.5  |
| 35  | DL    | 36   | LYS  | 2.5  |
| 16  | AQ    | 19   | SER  | 2.5  |
| 29  | DF    | 41   | GLU  | 2.5  |
| 35  | DL    | 68   | SER  | 2.5  |
| 24  | DA    | 1090 | A    | 2.5  |
| 41  | DR    | 68   | ARG  | 2.5  |
| 50  | D0    | 36   | LYS  | 2.5  |
| 24  | DA    | 653  | U    | 2.5  |
| 24  | DA    | 2259 | U    | 2.5  |
| 24  | DA    | 2798 | U    | 2.5  |
| 18  | CS    | 19   | GLU  | 2.5  |
| 18  | CS    | 64   | GLU  | 2.5  |
| 29  | DF    | 175  | PRO  | 2.5  |
| 35  | DL    | 143  | GLU  | 2.5  |
| 49  | DZ    | 40   | THR  | 2.5  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 37         | DN           | 119        | SER         | 2.5         |
| 40         | DQ           | 86         | SER         | 2.5         |
| 8          | AI           | 128        | LYS         | 2.5         |
| 32         | DI           | 26         | ALA         | 2.5         |
| 53         | D3           | 23         | HIS         | 2.5         |
| 18         | AS           | 14         | LEU         | 2.4         |
| 18         | CS           | 8          | PRO         | 2.4         |
| 7          | CH           | 74         | ILE         | 2.4         |
| 12         | CM           | 11         | HIS         | 2.4         |
| 32         | BI           | 41         | PHE         | 2.4         |
| 27         | DD           | 200        | ASP         | 2.4         |
| 2          | AC           | 7          | ASN         | 2.4         |
| 16         | CQ           | 10         | ARG         | 2.4         |
| 18         | CS           | 7          | GLY         | 2.4         |
| 24         | DA           | 580        | U           | 2.4         |
| 24         | DA           | 2052       | A           | 2.4         |
| 55         | CA           | 79         | G           | 2.4         |
| 4          | AE           | 73         | VAL         | 2.4         |
| 26         | DC           | 101        | ARG         | 2.4         |
| 29         | BF           | 109        | ARG         | 2.4         |
| 1          | CB           | 159        | ALA         | 2.4         |
| 4          | AE           | 77         | ASN         | 2.4         |
| 7          | AH           | 67         | GLY         | 2.4         |
| 1          | AB           | 222        | GLU         | 2.4         |
| 44         | DU           | 51         | LEU         | 2.4         |
| 7          | AH           | 102        | VAL         | 2.4         |
| 42         | DS           | 24         | ILE         | 2.4         |
| 24         | DA           | 470        | A           | 2.4         |
| 24         | DA           | 1764       | C           | 2.4         |
| 24         | DA           | 2743       | U           | 2.4         |
| 51         | D1           | 51         | ALA         | 2.4         |
| 24         | DA           | 971        | G           | 2.4         |
| 31         | DH           | 73         | ASN         | 2.4         |
| 6          | CG           | 35         | LYS         | 2.4         |
| 27         | DD           | 89         | GLU         | 2.4         |
| 28         | DE           | 35         | TYR         | 2.4         |
| 43         | DT           | 11         | LEU         | 2.4         |
| 30         | DG           | 16         | VAL         | 2.4         |
| 5          | AF           | 83         | ALA         | 2.4         |
| 38         | DO           | 56         | LYS         | 2.4         |
| 18         | AS           | 55         | GLN         | 2.4         |
| 1          | CB           | 225        | SER         | 2.4         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 4          | CE           | 137        | ARG         | 2.4         |
| 43         | DT           | 16         | VAL         | 2.4         |
| 43         | DT           | 55         | VAL         | 2.4         |
| 44         | DU           | 52         | ASN         | 2.4         |
| 52         | D2           | 33         | ARG         | 2.4         |
| 45         | DV           | 33         | GLY         | 2.4         |
| 46         | DW           | 47         | GLY         | 2.4         |
| 24         | BA           | 2305       | U           | 2.4         |
| 29         | DF           | 108        | PRO         | 2.4         |
| 8          | CI           | 47         | VAL         | 2.4         |
| 9          | CJ           | 92         | LEU         | 2.4         |
| 24         | DA           | 2000       | C           | 2.4         |
| 49         | DZ           | 54         | VAL         | 2.4         |
| 2          | CC           | 36         | PHE         | 2.4         |
| 24         | DA           | 1538       | G           | 2.4         |
| 35         | DL           | 45         | GLY         | 2.4         |
| 4          | CE           | 113        | VAL         | 2.4         |
| 42         | DS           | 20         | VAL         | 2.4         |
| 12         | CM           | 40         | GLU         | 2.4         |
| 11         | CL           | 31         | GLY         | 2.4         |
| 2          | CC           | 23         | ALA         | 2.4         |
| 24         | DA           | 2616       | C           | 2.4         |
| 10         | AK           | 33         | ILE         | 2.4         |
| 10         | CK           | 92         | ARG         | 2.4         |
| 28         | DE           | 201        | ALA         | 2.4         |
| 11         | CL           | 92         | VAL         | 2.4         |
| 24         | DA           | 1083       | U           | 2.4         |
| 24         | DA           | 2106       | U           | 2.4         |
| 8          | CI           | 89         | TYR         | 2.4         |
| 33         | DJ           | 77         | HIS         | 2.4         |
| 39         | DP           | 42         | PHE         | 2.4         |
| 9          | AJ           | 101        | SER         | 2.4         |
| 15         | CP           | 24         | SER         | 2.4         |
| 19         | CT           | 21         | ALA         | 2.4         |
| 24         | DA           | 1640       | A           | 2.4         |
| 32         | BI           | 20         | SER         | 2.4         |
| 30         | DG           | 45         | ALA         | 2.4         |
| 38         | DO           | 2          | ASP         | 2.4         |
| 31         | BH           | 75         | LEU         | 2.4         |
| 40         | DQ           | 67         | ALA         | 2.4         |
| 40         | DQ           | 91         | ARG         | 2.4         |
| 6          | AG           | 74         | VAL         | 2.4         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 6   | CG    | 5    | VAL  | 2.4  |
| 26  | DC    | 238  | ASN  | 2.4  |
| 54  | D4    | 25   | VAL  | 2.4  |
| 17  | AR    | 73   | HIS  | 2.4  |
| 29  | DF    | 138  | PRO  | 2.4  |
| 1   | CB    | 36   | LYS  | 2.4  |
| 7   | CH    | 44   | PHE  | 2.4  |
| 15  | AP    | 39   | PHE  | 2.4  |
| 15  | AP    | 45   | GLU  | 2.4  |
| 32  | BI    | 100  | ILE  | 2.4  |
| 33  | DJ    | 101  | ILE  | 2.4  |
| 35  | DL    | 106  | GLU  | 2.4  |
| 33  | DJ    | 22   | GLY  | 2.4  |
| 4   | CE    | 109  | ALA  | 2.4  |
| 8   | CI    | 90   | ASP  | 2.4  |
| 9   | CJ    | 98   | VAL  | 2.4  |
| 27  | DD    | 181  | ASP  | 2.4  |
| 28  | DE    | 164  | LEU  | 2.4  |
| 38  | DO    | 77   | ALA  | 2.4  |
| 31  | BH    | 130  | VAL  | 2.4  |
| 46  | DW    | 66   | VAL  | 2.4  |
| 29  | DF    | 59   | ILE  | 2.4  |
| 32  | BI    | 53   | PRO  | 2.4  |
| 32  | BI    | 54   | ILE  | 2.4  |
| 2   | CC    | 106  | ARG  | 2.4  |
| 1   | AB    | 110  | ILE  | 2.4  |
| 28  | DE    | 198  | GLU  | 2.4  |
| 29  | BF    | 41   | GLU  | 2.4  |
| 43  | BT    | 70   | HIS  | 2.4  |
| 1   | CB    | 184  | ALA  | 2.4  |
| 17  | CR    | 39   | VAL  | 2.4  |
| 29  | DF    | 23   | SER  | 2.4  |
| 4   | AE    | 130  | THR  | 2.4  |
| 8   | CI    | 91   | GLU  | 2.3  |
| 10  | CK    | 67   | GLU  | 2.3  |
| 39  | DP    | 10   | GLU  | 2.3  |
| 24  | DA    | 589  | U    | 2.3  |
| 5   | CF    | 97   | THR  | 2.3  |
| 24  | DA    | 2308 | G    | 2.3  |
| 43  | DT    | 54   | GLU  | 2.3  |
| 1   | AB    | 178  | LEU  | 2.3  |
| 6   | CG    | 86   | VAL  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 12  | AM    | 90   | HIS  | 2.3  |
| 29  | DF    | 1    | ALA  | 2.3  |
| 32  | DI    | 124  | MET  | 2.3  |
| 30  | DG    | 172  | GLU  | 2.3  |
| 26  | DC    | 30   | ALA  | 2.3  |
| 27  | DD    | 104  | VAL  | 2.3  |
| 40  | DQ    | 97   | ILE  | 2.3  |
| 2   | AC    | 204  | GLY  | 2.3  |
| 34  | DK    | 107  | LEU  | 2.3  |
| 12  | CM    | 1    | ALA  | 2.3  |
| 24  | DA    | 566  | U    | 2.3  |
| 24  | DA    | 1065 | U    | 2.3  |
| 36  | DM    | 45   | GLN  | 2.3  |
| 39  | DP    | 90   | ALA  | 2.3  |
| 45  | DV    | 51   | GLN  | 2.3  |
| 55  | CA    | 83   | C    | 2.3  |
| 55  | CA    | 970  | C    | 2.3  |
| 29  | BF    | 71   | LYS  | 2.3  |
| 28  | BE    | 124  | PHE  | 2.3  |
| 9   | CJ    | 65   | TYR  | 2.3  |
| 42  | DS    | 84   | ARG  | 2.3  |
| 44  | DU    | 68   | ASN  | 2.3  |
| 27  | DD    | 29   | VAL  | 2.3  |
| 29  | DF    | 158  | THR  | 2.3  |
| 31  | DH    | 118  | PRO  | 2.3  |
| 40  | DQ    | 111  | LYS  | 2.3  |
| 50  | D0    | 22   | THR  | 2.3  |
| 24  | DA    | 808  | G    | 2.3  |
| 35  | DL    | 77   | ILE  | 2.3  |
| 24  | DA    | 1161 | C    | 2.3  |
| 31  | DH    | 70   | GLU  | 2.3  |
| 35  | BL    | 144  | GLU  | 2.3  |
| 40  | DQ    | 82   | LEU  | 2.3  |
| 7   | CH    | 9    | MET  | 2.3  |
| 54  | D4    | 37   | GLN  | 2.3  |
| 5   | AF    | 71   | ILE  | 2.3  |
| 17  | AR    | 22   | TYR  | 2.3  |
| 18  | AS    | 2    | ARG  | 2.3  |
| 20  | CU    | 23   | GLU  | 2.3  |
| 4   | AE    | 69   | ASN  | 2.3  |
| 36  | DM    | 97   | GLN  | 2.3  |
| 38  | DO    | 38   | GLN  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 55  | CA    | 1447 | A    | 2.3  |
| 44  | BU    | 59   | GLU  | 2.3  |
| 1   | AB    | 57   | ASN  | 2.3  |
| 8   | CI    | 129  | ARG  | 2.3  |
| 10  | AK    | 30   | ILE  | 2.3  |
| 19  | CT    | 59   | ARG  | 2.3  |
| 28  | DE    | 50   | ALA  | 2.3  |
| 17  | AR    | 31   | TYR  | 2.3  |
| 32  | BI    | 107  | GLU  | 2.3  |
| 33  | DJ    | 76   | HIS  | 2.3  |
| 34  | DK    | 36   | GLY  | 2.3  |
| 55  | CA    | 80   | A    | 2.3  |
| 24  | DA    | 1163 | G    | 2.3  |
| 27  | DD    | 182  | ALA  | 2.3  |
| 28  | BE    | 148  | ILE  | 2.3  |
| 6   | CG    | 73   | GLU  | 2.3  |
| 30  | DG    | 112  | VAL  | 2.3  |
| 36  | DM    | 24   | THR  | 2.3  |
| 4   | AE    | 44   | ARG  | 2.3  |
| 6   | CG    | 77   | ARG  | 2.3  |
| 11  | CL    | 16   | ALA  | 2.3  |
| 11  | CL    | 93   | ARG  | 2.3  |
| 18  | CS    | 77   | ARG  | 2.3  |
| 24  | DA    | 1224 | U    | 2.3  |
| 34  | DK    | 60   | ALA  | 2.3  |
| 30  | DG    | 109  | SER  | 2.3  |
| 32  | DI    | 27   | LEU  | 2.3  |
| 37  | DN    | 38   | LEU  | 2.3  |
| 41  | DR    | 7    | SER  | 2.3  |
| 24  | DA    | 61   | C    | 2.3  |
| 33  | DJ    | 141  | ASP  | 2.3  |
| 34  | DK    | 7    | MET  | 2.3  |
| 36  | DM    | 31   | PHE  | 2.3  |
| 24  | DA    | 1661 | G    | 2.3  |
| 24  | DA    | 1743 | G    | 2.3  |
| 1   | AB    | 72   | LYS  | 2.3  |
| 29  | DF    | 11   | VAL  | 2.3  |
| 46  | DW    | 20   | LEU  | 2.3  |
| 2   | AC    | 205  | GLU  | 2.3  |
| 6   | AG    | 1    | PRO  | 2.3  |
| 24  | DA    | 1130 | U    | 2.3  |
| 53  | D3    | 27   | ASN  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 36  | DM    | 39   | GLY  | 2.3  |
| 30  | DG    | 79   | THR  | 2.3  |
| 9   | CJ    | 25   | ILE  | 2.3  |
| 29  | DF    | 47   | LYS  | 2.3  |
| 36  | DM    | 96   | ILE  | 2.3  |
| 7   | CH    | 85   | TYR  | 2.3  |
| 24  | DA    | 456  | C    | 2.3  |
| 54  | D4    | 7    | VAL  | 2.3  |
| 55  | CA    | 972  | C    | 2.3  |
| 33  | DJ    | 102  | GLU  | 2.3  |
| 29  | DF    | 61   | GLY  | 2.3  |
| 7   | CH    | 23   | ALA  | 2.3  |
| 19  | CT    | 66   | ILE  | 2.3  |
| 46  | DW    | 81   | ILE  | 2.3  |
| 46  | DW    | 83   | ALA  | 2.3  |
| 47  | DX    | 2    | ARG  | 2.3  |
| 1   | AB    | 145  | ASN  | 2.3  |
| 18  | CS    | 42   | ASN  | 2.3  |
| 24  | DA    | 89   | A    | 2.3  |
| 24  | DA    | 344  | A    | 2.3  |
| 27  | BD    | 48   | ILE  | 2.3  |
| 32  | BI    | 62   | ALA  | 2.3  |
| 1   | CB    | 45   | THR  | 2.3  |
| 7   | CH    | 4    | ASP  | 2.3  |
| 32  | DI    | 105  | LEU  | 2.3  |
| 29  | DF    | 82   | TYR  | 2.3  |
| 51  | D1    | 23   | THR  | 2.3  |
| 31  | BH    | 70   | GLU  | 2.2  |
| 1   | CB    | 106  | VAL  | 2.2  |
| 53  | D3    | 57   | VAL  | 2.2  |
| 10  | AK    | 92   | ARG  | 2.2  |
| 44  | DU    | 14   | THR  | 2.2  |
| 4   | AE    | 60   | GLN  | 2.2  |
| 13  | CN    | 70   | HIS  | 2.2  |
| 5   | CF    | 66   | ALA  | 2.2  |
| 24  | DA    | 565  | C    | 2.2  |
| 26  | DC    | 232  | GLY  | 2.2  |
| 27  | DD    | 31   | ALA  | 2.2  |
| 31  | DH    | 143  | ILE  | 2.2  |
| 36  | DM    | 30   | SER  | 2.2  |
| 24  | BA    | 2181 | U    | 2.2  |
| 54  | D4    | 24   | ARG  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | AD    | 178  | GLU  | 2.2  |
| 8   | CI    | 56   | MET  | 2.2  |
| 31  | BH    | 142  | VAL  | 2.2  |
| 39  | DP    | 18   | SER  | 2.2  |
| 27  | DD    | 165  | MET  | 2.2  |
| 32  | BI    | 25   | PRO  | 2.2  |
| 41  | DR    | 36   | ALA  | 2.2  |
| 41  | DR    | 21   | ARG  | 2.2  |
| 2   | CC    | 205  | GLU  | 2.2  |
| 16  | AQ    | 15   | LYS  | 2.2  |
| 6   | AG    | 5    | VAL  | 2.2  |
| 8   | CI    | 106  | ASP  | 2.2  |
| 30  | DG    | 32   | LEU  | 2.2  |
| 30  | DG    | 160  | GLY  | 2.2  |
| 9   | CJ    | 12   | ALA  | 2.2  |
| 12  | AM    | 105  | ALA  | 2.2  |
| 24  | DA    | 1073 | A    | 2.2  |
| 31  | BH    | 18   | GLN  | 2.2  |
| 37  | DN    | 67   | PHE  | 2.2  |
| 5   | AF    | 52   | ASN  | 2.2  |
| 10  | AK    | 99   | LEU  | 2.2  |
| 34  | DK    | 8    | LEU  | 2.2  |
| 38  | DO    | 107  | ALA  | 2.2  |
| 45  | DV    | 48   | MET  | 2.2  |
| 4   | AE    | 53   | ARG  | 2.2  |
| 15  | AP    | 35   | ARG  | 2.2  |
| 29  | DF    | 109  | ARG  | 2.2  |
| 1   | AB    | 151  | LYS  | 2.2  |
| 24  | DA    | 1125 | G    | 2.2  |
| 26  | DC    | 70   | LYS  | 2.2  |
| 41  | DR    | 76   | LYS  | 2.2  |
| 1   | AB    | 180  | ILE  | 2.2  |
| 1   | CB    | 30   | ILE  | 2.2  |
| 16  | CQ    | 22   | VAL  | 2.2  |
| 1   | CB    | 158  | ASP  | 2.2  |
| 4   | AE    | 94   | PHE  | 2.2  |
| 20  | AU    | 11   | PHE  | 2.2  |
| 36  | DM    | 122  | ALA  | 2.2  |
| 54  | D4    | 36   | ARG  | 2.2  |
| 16  | CQ    | 52   | CYS  | 2.2  |
| 9   | AJ    | 76   | ILE  | 2.2  |
| 36  | DM    | 126  | ILE  | 2.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 38         | DO           | 78         | VAL         | 2.2         |
| 40         | DQ           | 73         | ILE         | 2.2         |
| 26         | DC           | 100        | ARG         | 2.2         |
| 31         | BH           | 132        | PHE         | 2.2         |
| 33         | DJ           | 97         | PRO         | 2.2         |
| 56         | DB           | 85         | G           | 2.2         |
| 24         | DA           | 1321       | A           | 2.2         |
| 24         | DA           | 1614       | A           | 2.2         |
| 15         | CP           | 10         | GLY         | 2.2         |
| 27         | DD           | 187        | LEU         | 2.2         |
| 43         | DT           | 58         | VAL         | 2.2         |
| 13         | CN           | 69         | PRO         | 2.2         |
| 1          | AB           | 64         | GLY         | 2.2         |
| 1          | CB           | 147        | LEU         | 2.2         |
| 2          | AC           | 67         | ILE         | 2.2         |
| 10         | AK           | 31         | VAL         | 2.2         |
| 29         | DF           | 117        | SER         | 2.2         |
| 32         | BI           | 65         | SER         | 2.2         |
| 35         | DL           | 33         | ARG         | 2.2         |
| 36         | DM           | 55         | ARG         | 2.2         |
| 8          | AI           | 15         | ALA         | 2.2         |
| 24         | DA           | 1383       | A           | 2.2         |
| 31         | DH           | 106        | ALA         | 2.2         |
| 56         | DB           | 86         | G           | 2.2         |
| 2          | CC           | 199        | VAL         | 2.2         |
| 24         | DA           | 343        | C           | 2.2         |
| 24         | DA           | 394        | C           | 2.2         |
| 26         | DC           | 7          | PRO         | 2.2         |
| 1          | AB           | 89         | PHE         | 2.2         |
| 10         | CK           | 20         | ALA         | 2.2         |
| 31         | DH           | 74         | ALA         | 2.2         |
| 35         | DL           | 108        | ALA         | 2.2         |
| 32         | DI           | 7          | TYR         | 2.2         |
| 7          | AH           | 103        | VAL         | 2.2         |
| 7          | CH           | 103        | VAL         | 2.2         |
| 3          | AD           | 27         | ILE         | 2.2         |
| 6          | AG           | 25         | PHE         | 2.2         |
| 37         | DN           | 40         | LYS         | 2.2         |
| 38         | DO           | 75         | GLY         | 2.2         |
| 12         | CM           | 20         | SER         | 2.2         |
| 29         | DF           | 106        | ALA         | 2.2         |
| 5          | CF           | 39         | LEU         | 2.2         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 18         | AS           | 31         | ARG         | 2.2         |
| 18         | AS           | 46         | LEU         | 2.2         |
| 19         | CT           | 65         | LEU         | 2.2         |
| 20         | AU           | 19         | LYS         | 2.2         |
| 36         | DM           | 112        | LEU         | 2.2         |
| 12         | AM           | 83         | GLY         | 2.2         |
| 27         | DD           | 47         | ALA         | 2.2         |
| 44         | DU           | 88         | ASP         | 2.2         |
| 44         | DU           | 97         | SER         | 2.2         |
| 2          | CC           | 11         | LEU         | 2.2         |
| 4          | AE           | 67         | ARG         | 2.2         |
| 26         | DC           | 64         | VAL         | 2.2         |
| 44         | BU           | 46         | LYS         | 2.2         |
| 30         | DG           | 155        | PRO         | 2.2         |
| 37         | DN           | 101        | GLY         | 2.2         |
| 24         | DA           | 254        | G           | 2.2         |
| 24         | DA           | 329        | G           | 2.2         |
| 32         | DI           | 42         | ASN         | 2.2         |
| 37         | DN           | 37         | THR         | 2.2         |
| 38         | DO           | 12         | THR         | 2.2         |
| 52         | D2           | 26         | ASN         | 2.2         |
| 30         | DG           | 131        | VAL         | 2.2         |
| 41         | DR           | 47         | VAL         | 2.2         |
| 42         | DS           | 46         | LEU         | 2.2         |
| 6          | AG           | 6          | ILE         | 2.2         |
| 40         | DQ           | 98         | ALA         | 2.1         |
| 1          | CB           | 84         | LEU         | 2.1         |
| 2          | CC           | 86         | LEU         | 2.1         |
| 18         | AS           | 32         | THR         | 2.1         |
| 27         | DD           | 45         | TYR         | 2.1         |
| 28         | DE           | 84         | THR         | 2.1         |
| 29         | DF           | 71         | LYS         | 2.1         |
| 48         | BY           | 5          | GLU         | 2.1         |
| 7          | CH           | 10         | LEU         | 2.1         |
| 24         | DA           | 235        | U           | 2.1         |
| 27         | DD           | 189        | VAL         | 2.1         |
| 28         | DE           | 121        | VAL         | 2.1         |
| 1          | CB           | 210        | THR         | 2.1         |
| 5          | CF           | 37         | HIS         | 2.1         |
| 7          | AH           | 104        | SER         | 2.1         |
| 35         | DL           | 81         | ASP         | 2.1         |
| 46         | DW           | 7          | GLY         | 2.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 24  | DA    | 2062 | A    | 2.1  |
| 29  | DF    | 16   | MET  | 2.1  |
| 31  | DH    | 147  | VAL  | 2.1  |
| 4   | AE    | 134  | ASN  | 2.1  |
| 36  | DM    | 37   | GLY  | 2.1  |
| 37  | DN    | 18   | GLN  | 2.1  |
| 2   | CC    | 133  | MET  | 2.1  |
| 6   | AG    | 15   | PRO  | 2.1  |
| 31  | DH    | 81   | ALA  | 2.1  |
| 8   | AI    | 11   | ARG  | 2.1  |
| 17  | CR    | 22   | TYR  | 2.1  |
| 1   | CB    | 129  | THR  | 2.1  |
| 24  | DA    | 126  | A    | 2.1  |
| 24  | DA    | 2147 | A    | 2.1  |
| 16  | AQ    | 14   | ASP  | 2.1  |
| 27  | DD    | 110  | THR  | 2.1  |
| 31  | DH    | 102  | ALA  | 2.1  |
| 32  | BI    | 96   | LYS  | 2.1  |
| 32  | DI    | 38   | CYS  | 2.1  |
| 42  | DS    | 107  | VAL  | 2.1  |
| 24  | DA    | 99   | U    | 2.1  |
| 24  | DA    | 75   | G    | 2.1  |
| 37  | DN    | 49   | GLU  | 2.1  |
| 11  | CL    | 122  | LYS  | 2.1  |
| 1   | AB    | 102  | ASN  | 2.1  |
| 26  | DC    | 122  | ALA  | 2.1  |
| 29  | DF    | 42   | ALA  | 2.1  |
| 47  | DX    | 10   | ARG  | 2.1  |
| 48  | DY    | 28   | LEU  | 2.1  |
| 49  | DZ    | 37   | ARG  | 2.1  |
| 11  | CL    | 94   | TYR  | 2.1  |
| 24  | DA    | 677  | A    | 2.1  |
| 47  | DX    | 11   | PRO  | 2.1  |
| 42  | DS    | 35   | ILE  | 2.1  |
| 4   | AE    | 107  | GLY  | 2.1  |
| 17  | CR    | 19   | GLU  | 2.1  |
| 43  | DT    | 4    | GLU  | 2.1  |
| 55  | CA    | 1031 | C    | 2.1  |
| 18  | CS    | 59   | VAL  | 2.1  |
| 39  | DP    | 107  | ALA  | 2.1  |
| 6   | AG    | 61   | PHE  | 2.1  |
| 24  | DA    | 1131 | G    | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 24  | DA    | 1715 | G    | 2.1  |
| 37  | DN    | 97   | ILE  | 2.1  |
| 39  | DP    | 30   | TRP  | 2.1  |
| 48  | BY    | 13   | GLU  | 2.1  |
| 19  | CT    | 57   | VAL  | 2.1  |
| 43  | DT    | 47   | VAL  | 2.1  |
| 52  | D2    | 42   | LEU  | 2.1  |
| 16  | CQ    | 36   | PHE  | 2.1  |
| 2   | CC    | 108  | PRO  | 2.1  |
| 5   | CF    | 6    | ILE  | 2.1  |
| 55  | CA    | 472  | U    | 2.1  |
| 19  | CT    | 84   | LYS  | 2.1  |
| 13  | CN    | 23   | ARG  | 2.1  |
| 13  | CN    | 40   | ARG  | 2.1  |
| 29  | DF    | 31   | GLU  | 2.1  |
| 36  | BM    | 104  | GLU  | 2.1  |
| 7   | CH    | 26   | MET  | 2.1  |
| 38  | DO    | 72   | ALA  | 2.1  |
| 4   | AE    | 155  | LYS  | 2.1  |
| 8   | AI    | 27   | ILE  | 2.1  |
| 16  | AQ    | 13   | SER  | 2.1  |
| 41  | DR    | 11   | GLN  | 2.1  |
| 42  | DS    | 31   | GLN  | 2.1  |
| 24  | BA    | 2308 | G    | 2.1  |
| 29  | DF    | 13   | LYS  | 2.1  |
| 32  | BI    | 21   | PRO  | 2.1  |
| 41  | DR    | 55   | ASP  | 2.1  |
| 20  | AU    | 20   | ARG  | 2.1  |
| 32  | DI    | 138  | VAL  | 2.1  |
| 5   | AF    | 8    | PHE  | 2.1  |
| 6   | CG    | 16   | LYS  | 2.1  |
| 30  | DG    | 150  | TYR  | 2.1  |
| 9   | AJ    | 91   | ASP  | 2.1  |
| 10  | AK    | 91   | GLY  | 2.1  |
| 29  | DF    | 93   | GLU  | 2.1  |
| 30  | BG    | 37   | ASN  | 2.1  |
| 45  | DV    | 59   | GLU  | 2.1  |
| 27  | DD    | 101  | PHE  | 2.1  |
| 35  | DL    | 72   | ALA  | 2.1  |
| 2   | AC    | 99   | GLN  | 2.1  |
| 24  | DA    | 2502 | G    | 2.1  |
| 27  | DD    | 114  | LYS  | 2.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 44         | DU           | 23         | LYS         | 2.1         |
| 55         | CA           | 202        | G           | 2.1         |
| 19         | AT           | 67         | HIS         | 2.1         |
| 24         | DA           | 135        | U           | 2.1         |
| 24         | DA           | 975        | A           | 2.1         |
| 31         | DH           | 27         | ARG         | 2.1         |
| 53         | D3           | 44         | ARG         | 2.1         |
| 1          | AB           | 37         | VAL         | 2.1         |
| 1          | CB           | 214        | GLY         | 2.1         |
| 33         | DJ           | 15         | TRP         | 2.1         |
| 35         | DL           | 19         | LEU         | 2.1         |
| 44         | DU           | 22         | GLY         | 2.1         |
| 4          | AE           | 47         | PHE         | 2.1         |
| 44         | DU           | 64         | ILE         | 2.1         |
| 12         | CM           | 78         | ARG         | 2.1         |
| 4          | CE           | 107        | GLY         | 2.1         |
| 18         | AS           | 15         | LEU         | 2.1         |
| 29         | DF           | 100        | GLU         | 2.1         |
| 37         | DN           | 115        | LEU         | 2.1         |
| 43         | DT           | 56         | GLU         | 2.1         |
| 54         | D4           | 38         | GLY         | 2.1         |
| 29         | BF           | 176        | PHE         | 2.1         |
| 24         | DA           | 508        | A           | 2.1         |
| 38         | DO           | 59         | ALA         | 2.1         |
| 1          | AB           | 94         | ARG         | 2.1         |
| 34         | DK           | 108        | ARG         | 2.1         |
| 1          | CB           | 13         | VAL         | 2.1         |
| 38         | DO           | 97         | PHE         | 2.1         |
| 45         | DV           | 32         | GLY         | 2.1         |
| 19         | CT           | 68         | LYS         | 2.1         |
| 9          | CJ           | 67         | ILE         | 2.1         |
| 12         | CM           | 38         | ILE         | 2.1         |
| 41         | DR           | 1          | MET         | 2.1         |
| 44         | BU           | 21         | ARG         | 2.1         |
| 34         | DK           | 10         | VAL         | 2.1         |
| 24         | DA           | 38         | A           | 2.0         |
| 24         | BA           | 2156       | G           | 2.0         |
| 24         | DA           | 1116       | G           | 2.0         |
| 24         | DA           | 1311       | G           | 2.0         |
| 27         | BD           | 1          | MET         | 2.0         |
| 38         | DO           | 11         | ALA         | 2.0         |
| 49         | DZ           | 9          | THR         | 2.0         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 27  | DD    | 167  | ASN  | 2.0  |
| 29  | DF    | 14   | LYS  | 2.0  |
| 35  | DL    | 51   | GLU  | 2.0  |
| 39  | DP    | 28   | LYS  | 2.0  |
| 15  | CP    | 67   | ILE  | 2.0  |
| 24  | DA    | 573  | U    | 2.0  |
| 12  | CM    | 19   | THR  | 2.0  |
| 27  | DD    | 77   | ARG  | 2.0  |
| 17  | AR    | 67   | LEU  | 2.0  |
| 18  | CS    | 30   | LEU  | 2.0  |
| 43  | BT    | 16   | VAL  | 2.0  |
| 4   | CE    | 48   | GLY  | 2.0  |
| 30  | BG    | 31   | GLU  | 2.0  |
| 30  | DG    | 31   | GLU  | 2.0  |
| 46  | DW    | 18   | LYS  | 2.0  |
| 24  | BA    | 2152 | G    | 2.0  |
| 24  | DA    | 1475 | G    | 2.0  |
| 24  | DA    | 246  | C    | 2.0  |
| 40  | DQ    | 64   | ILE  | 2.0  |
| 7   | CH    | 77   | VAL  | 2.0  |
| 28  | DE    | 13   | THR  | 2.0  |
| 6   | CG    | 8    | GLN  | 2.0  |
| 13  | AN    | 25   | GLU  | 2.0  |
| 24  | DA    | 12   | U    | 2.0  |
| 24  | DA    | 2022 | U    | 2.0  |
| 28  | DE    | 23   | PHE  | 2.0  |
| 29  | DF    | 84   | ILE  | 2.0  |
| 38  | DO    | 45   | SER  | 2.0  |
| 1   | AB    | 45   | THR  | 2.0  |
| 29  | DF    | 156  | THR  | 2.0  |
| 36  | DM    | 106  | ASP  | 2.0  |
| 36  | DM    | 46   | ILE  | 2.0  |
| 3   | AD    | 57   | LYS  | 2.0  |
| 5   | CF    | 35   | LYS  | 2.0  |
| 10  | CK    | 128  | VAL  | 2.0  |
| 16  | CQ    | 74   | LEU  | 2.0  |
| 19  | CT    | 19   | HIS  | 2.0  |
| 36  | DM    | 130  | PHE  | 2.0  |
| 1   | AB    | 152  | ASP  | 2.0  |
| 2   | CC    | 54   | ILE  | 2.0  |
| 51  | B1    | 8    | ILE  | 2.0  |
| 55  | CA    | 1021 | A    | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 17  | AR    | 63   | TYR  | 2.0  |
| 28  | DE    | 72   | SER  | 2.0  |
| 24  | DA    | 1248 | G    | 2.0  |
| 10  | AK    | 111  | ASP  | 2.0  |
| 40  | DQ    | 85   | ALA  | 2.0  |
| 7   | AH    | 127  | TYR  | 2.0  |
| 7   | AH    | 59   | GLU  | 2.0  |
| 24  | DA    | 514  | A    | 2.0  |
| 24  | DA    | 2778 | A    | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|-------|----------------------------|-------|
| 57  | MG   | DA    | 3002 | 1/1   | -0.26 | 1.16 | 37.12 | 212,212,212,212            | 0     |
| 57  | MG   | DA    | 3060 | 1/1   | 0.72  | 0.78 | 35.59 | 132,132,132,132            | 0     |
| 57  | MG   | CA    | 1628 | 1/1   | 0.91  | 1.01 | 19.97 | 99,99,99,99                | 0     |
| 57  | MG   | DA    | 3076 | 1/1   | 0.82  | 1.12 | 19.84 | 145,145,145,145            | 0     |
| 57  | MG   | CA    | 1625 | 1/1   | 0.85  | 0.49 | 17.93 | 127,127,127,127            | 0     |
| 57  | MG   | BA    | 3124 | 1/1   | 0.85  | 0.96 | 16.07 | 59,59,59,59                | 0     |
| 57  | MG   | AA    | 1641 | 1/1   | 0.82  | 0.43 | 15.38 | 108,108,108,108            | 0     |
| 57  | MG   | BA    | 3058 | 1/1   | 0.93  | 0.49 | 14.37 | 63,63,63,63                | 0     |
| 57  | MG   | BA    | 3136 | 1/1   | 0.98  | 0.37 | 13.60 | 64,64,64,64                | 0     |
| 57  | MG   | DA    | 3108 | 1/1   | 0.45  | 0.65 | 13.28 | 172,172,172,172            | 0     |
| 57  | MG   | BA    | 3002 | 1/1   | 0.94  | 0.36 | 12.80 | 61,61,61,61                | 0     |
| 57  | MG   | DA    | 3075 | 1/1   | 0.78  | 0.97 | 12.28 | 155,155,155,155            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57  | MG   | CA    | 1640 | 1/1   | 0.86 | 0.59 | 11.77 | 118,118,118,118             | 0     |
| 57  | MG   | BA    | 3060 | 1/1   | 0.91 | 0.36 | 9.07  | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3072 | 1/1   | 0.72 | 0.43 | 8.77  | 182,182,182,182             | 0     |
| 57  | MG   | AA    | 1607 | 1/1   | 0.86 | 0.45 | 8.30  | 113,113,113,113             | 0     |
| 57  | MG   | BA    | 3072 | 1/1   | 0.97 | 0.32 | 7.40  | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3028 | 1/1   | 0.82 | 0.33 | 6.56  | 57,57,57,57                 | 0     |
| 57  | MG   | CA    | 1610 | 1/1   | 0.39 | 0.22 | 6.56  | 181,181,181,181             | 0     |
| 57  | MG   | AA    | 1625 | 1/1   | 0.83 | 0.32 | 5.95  | 114,114,114,114             | 0     |
| 57  | MG   | BA    | 3084 | 1/1   | 0.96 | 0.22 | 5.53  | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3056 | 1/1   | 0.88 | 0.30 | 5.22  | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3041 | 1/1   | 0.98 | 0.23 | 3.85  | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3124 | 1/1   | 0.79 | 0.35 | 3.81  | 168,168,168,168             | 0     |
| 57  | MG   | CA    | 1637 | 1/1   | 0.92 | 0.28 | 3.78  | 112,112,112,112             | 0     |
| 57  | MG   | BA    | 3022 | 1/1   | 0.96 | 0.23 | 3.77  | 55,55,55,55                 | 0     |
| 57  | MG   | AA    | 1642 | 1/1   | 0.94 | 0.26 | 3.76  | 90,90,90,90                 | 0     |
| 57  | MG   | DA    | 3106 | 1/1   | 0.57 | 0.34 | 3.50  | 228,228,228,228             | 0     |
| 57  | MG   | DA    | 3084 | 1/1   | 0.78 | 0.35 | 3.43  | 214,214,214,214             | 0     |
| 57  | MG   | DA    | 3104 | 1/1   | 0.94 | 0.27 | 3.09  | 142,142,142,142             | 0     |
| 57  | MG   | DA    | 3065 | 1/1   | 0.93 | 0.38 | 3.06  | 152,152,152,152             | 0     |
| 57  | MG   | DA    | 3128 | 1/1   | 0.60 | 0.65 | 2.95  | 132,132,132,132             | 0     |
| 57  | MG   | AA    | 1629 | 1/1   | 0.92 | 0.21 | 2.48  | 161,161,161,161             | 0     |
| 57  | MG   | DA    | 3068 | 1/1   | 0.68 | 0.33 | 2.11  | 143,143,143,143             | 0     |
| 57  | MG   | DA    | 3069 | 1/1   | 0.68 | 0.52 | 2.10  | 139,139,139,139             | 0     |
| 57  | MG   | BA    | 3048 | 1/1   | 0.94 | 0.22 | 2.02  | 91,91,91,91                 | 0     |
| 57  | MG   | BA    | 3109 | 1/1   | 0.98 | 0.21 | 1.97  | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3005 | 1/1   | 0.94 | 0.15 | 1.55  | 91,91,91,91                 | 0     |
| 57  | MG   | DA    | 3100 | 1/1   | 0.90 | 0.31 | 1.21  | 150,150,150,150             | 0     |
| 57  | MG   | AA    | 1611 | 1/1   | 0.91 | 0.23 | 1.17  | 126,126,126,126             | 0     |
| 57  | MG   | CA    | 1618 | 1/1   | 0.93 | 0.28 | 1.17  | 148,148,148,148             | 0     |
| 57  | MG   | BD    | 301  | 1/1   | 0.94 | 0.20 | 1.10  | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3018 | 1/1   | 0.64 | 0.40 | 1.09  | 248,248,248,248             | 0     |
| 57  | MG   | CA    | 1607 | 1/1   | 0.62 | 0.22 | 1.07  | 134,134,134,134             | 0     |
| 57  | MG   | CA    | 1631 | 1/1   | 0.94 | 0.22 | 1.04  | 130,130,130,130             | 0     |
| 57  | MG   | DA    | 3051 | 1/1   | 0.75 | 0.23 | 0.94  | 160,160,160,160             | 0     |
| 57  | MG   | AA    | 1633 | 1/1   | 0.82 | 0.16 | 0.89  | 128,128,128,128             | 0     |
| 57  | MG   | BA    | 3108 | 1/1   | 0.98 | 0.18 | 0.85  | 58,58,58,58                 | 0     |
| 57  | MG   | AA    | 1617 | 1/1   | 0.69 | 0.29 | 0.70  | 150,150,150,150             | 0     |
| 57  | MG   | DA    | 3132 | 1/1   | 0.25 | 0.26 | 0.55  | 198,198,198,198             | 0     |
| 57  | MG   | BA    | 3116 | 1/1   | 0.97 | 0.17 | 0.53  | 55,55,55,55                 | 0     |
| 57  | MG   | AA    | 1616 | 1/1   | 0.95 | 0.27 | 0.42  | 161,161,161,161             | 0     |
| 57  | MG   | AA    | 1631 | 1/1   | 0.93 | 0.20 | 0.40  | 114,114,114,114             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57  | MG   | CA    | 1616 | 1/1   | 0.75 | 0.33 | 0.35  | 199,199,199,199             | 0     |
| 57  | MG   | DA    | 3039 | 1/1   | 0.72 | 0.27 | 0.32  | 186,186,186,186             | 0     |
| 57  | MG   | BA    | 3132 | 1/1   | 0.96 | 0.27 | 0.27  | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3042 | 1/1   | 0.90 | 0.26 | 0.26  | 179,179,179,179             | 0     |
| 57  | MG   | CA    | 1617 | 1/1   | 0.66 | 0.27 | 0.22  | 183,183,183,183             | 0     |
| 57  | MG   | DA    | 3057 | 1/1   | 0.92 | 0.28 | 0.22  | 133,133,133,133             | 0     |
| 57  | MG   | DA    | 3044 | 1/1   | 0.67 | 0.24 | 0.21  | 210,210,210,210             | 0     |
| 57  | MG   | BA    | 3080 | 1/1   | 0.96 | 0.15 | 0.03  | 93,93,93,93                 | 0     |
| 57  | MG   | BB    | 202  | 1/1   | 0.91 | 0.14 | 0.01  | 127,127,127,127             | 0     |
| 57  | MG   | BA    | 3074 | 1/1   | 0.98 | 0.16 | -0.02 | 54,54,54,54                 | 0     |
| 57  | MG   | CA    | 1633 | 1/1   | 0.83 | 0.14 | -0.04 | 123,123,123,123             | 0     |
| 57  | MG   | DA    | 3040 | 1/1   | 0.87 | 0.26 | -0.07 | 171,171,171,171             | 0     |
| 57  | MG   | DA    | 3037 | 1/1   | 0.72 | 0.20 | -0.20 | 204,204,204,204             | 0     |
| 57  | MG   | CA    | 1641 | 1/1   | 0.87 | 0.17 | -0.24 | 151,151,151,151             | 0     |
| 57  | MG   | BA    | 3130 | 1/1   | 0.98 | 0.16 | -0.34 | 68,68,68,68                 | 0     |
| 57  | MG   | DA    | 3023 | 1/1   | 0.87 | 0.23 | -0.44 | 148,148,148,148             | 0     |
| 57  | MG   | CA    | 1629 | 1/1   | 0.80 | 0.24 | -0.48 | 157,157,157,157             | 0     |
| 57  | MG   | BA    | 3107 | 1/1   | 0.92 | 0.18 | -0.58 | 67,67,67,67                 | 0     |
| 57  | MG   | BA    | 3105 | 1/1   | 0.91 | 0.18 | -0.59 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3104 | 1/1   | 0.94 | 0.17 | -0.72 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3012 | 1/1   | 0.95 | 0.32 | -0.77 | 168,168,168,168             | 0     |
| 57  | MG   | DA    | 3110 | 1/1   | 0.75 | 0.17 | -0.89 | 219,219,219,219             | 0     |
| 57  | MG   | BA    | 3050 | 1/1   | 0.98 | 0.14 | -0.91 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3013 | 1/1   | 0.97 | 0.17 | -1.00 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3095 | 1/1   | 0.71 | 0.19 | -1.01 | 152,152,152,152             | 0     |
| 57  | MG   | BA    | 3024 | 1/1   | 0.94 | 0.15 | -1.03 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3050 | 1/1   | 0.86 | 0.23 | -1.15 | 180,180,180,180             | 0     |
| 57  | MG   | BA    | 3120 | 1/1   | 0.96 | 0.17 | -1.18 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3066 | 1/1   | 0.97 | 0.13 | -1.20 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3114 | 1/1   | 0.95 | 0.11 | -1.23 | 88,88,88,88                 | 0     |
| 57  | MG   | DA    | 3017 | 1/1   | 0.84 | 0.19 | -1.25 | 187,187,187,187             | 0     |
| 57  | MG   | CA    | 1609 | 1/1   | 0.92 | 0.15 | -1.38 | 131,131,131,131             | 0     |
| 57  | MG   | DA    | 3079 | 1/1   | 0.80 | 0.22 | -1.41 | 148,148,148,148             | 0     |
| 57  | MG   | AA    | 1634 | 1/1   | 0.88 | 0.12 | -1.43 | 121,121,121,121             | 0     |
| 58  | ZN   | D4    | 102  | 1/1   | 0.96 | 0.07 | -1.44 | 99,99,99,99                 | 0     |
| 57  | MG   | DA    | 3130 | 1/1   | 0.88 | 0.17 | -1.46 | 170,170,170,170             | 0     |
| 57  | MG   | DA    | 3024 | 1/1   | 0.93 | 0.17 | -1.46 | 162,162,162,162             | 0     |
| 57  | MG   | DA    | 3035 | 1/1   | 0.93 | 0.11 | -1.48 | 155,155,155,155             | 0     |
| 57  | MG   | DA    | 3083 | 1/1   | 0.40 | 0.08 | -1.60 | 303,303,303,303             | 0     |
| 57  | MG   | BB    | 203  | 1/1   | 0.99 | 0.10 | -1.60 | 69,69,69,69                 | 0     |
| 57  | MG   | AA    | 1618 | 1/1   | 0.98 | 0.16 | -1.66 | 131,131,131,131             | 0     |
| 57  | MG   | CA    | 1642 | 1/1   | 0.81 | 0.12 | -1.67 | 170,170,170,170             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57  | MG   | AA    | 1609 | 1/1   | 0.82 | 0.14 | -1.79 | 118,118,118,118             | 0     |
| 57  | MG   | CA    | 1612 | 1/1   | 0.87 | 0.17 | -1.81 | 124,124,124,124             | 0     |
| 57  | MG   | DA    | 3105 | 1/1   | 0.97 | 0.12 | -1.84 | 159,159,159,159             | 0     |
| 58  | ZN   | B4    | 101  | 1/1   | 0.99 | 0.09 | -1.91 | 99,99,99,99                 | 0     |
| 57  | MG   | AA    | 1604 | 1/1   | 0.82 | 0.08 | -1.92 | 157,157,157,157             | 0     |
| 57  | MG   | BA    | 3134 | 1/1   | 0.97 | 0.15 | -1.94 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3112 | 1/1   | 0.97 | 0.14 | -1.97 | 143,143,143,143             | 0     |
| 57  | MG   | DA    | 3101 | 1/1   | 0.80 | 0.17 | -1.99 | 155,155,155,155             | 0     |
| 57  | MG   | AA    | 1613 | 1/1   | 0.94 | 0.11 | -2.00 | 95,95,95,95                 | 0     |
| 57  | MG   | CA    | 1621 | 1/1   | 0.98 | 0.14 | -2.07 | 115,115,115,115             | 0     |
| 57  | MG   | AA    | 1622 | 1/1   | 0.98 | 0.10 | -2.10 | 113,113,113,113             | 0     |
| 57  | MG   | BA    | 3012 | 1/1   | 0.98 | 0.13 | -2.17 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3101 | 1/1   | 0.81 | 0.14 | -2.17 | 54,54,54,54                 | 0     |
| 57  | MG   | AA    | 1606 | 1/1   | 0.96 | 0.12 | -2.19 | 119,119,119,119             | 0     |
| 57  | MG   | BA    | 3008 | 1/1   | 0.96 | 0.13 | -2.22 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3061 | 1/1   | 0.96 | 0.11 | -2.27 | 134,134,134,134             | 0     |
| 57  | MG   | CA    | 1613 | 1/1   | 0.88 | 0.11 | -2.30 | 121,121,121,121             | 0     |
| 57  | MG   | DA    | 3052 | 1/1   | 0.93 | 0.12 | -2.31 | 144,144,144,144             | 0     |
| 57  | MG   | BA    | 3094 | 1/1   | 0.95 | 0.12 | -2.32 | 92,92,92,92                 | 0     |
| 57  | MG   | CA    | 1634 | 1/1   | 0.75 | 0.11 | -2.39 | 153,153,153,153             | 0     |
| 57  | MG   | BA    | 3017 | 1/1   | 0.98 | 0.12 | -2.71 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3018 | 1/1   | 0.94 | 0.08 | -2.72 | 80,80,80,80                 | 0     |
| 57  | MG   | DA    | 3025 | 1/1   | 0.81 | 0.09 | -2.73 | 135,135,135,135             | 0     |
| 57  | MG   | DA    | 3066 | 1/1   | 0.88 | 0.12 | -2.83 | 150,150,150,150             | 0     |
| 57  | MG   | BA    | 3063 | 1/1   | 0.95 | 0.12 | -2.95 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3023 | 1/1   | 0.99 | 0.14 | -2.96 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3102 | 1/1   | 0.88 | 0.15 | -2.98 | 141,141,141,141             | 0     |
| 57  | MG   | AA    | 1643 | 1/1   | 0.94 | 0.11 | -3.06 | 101,101,101,101             | 0     |
| 57  | MG   | CA    | 1639 | 1/1   | 0.83 | 0.12 | -3.09 | 266,266,266,266             | 0     |
| 57  | MG   | DA    | 3055 | 1/1   | 0.91 | 0.13 | -3.13 | 136,136,136,136             | 0     |
| 57  | MG   | DA    | 3103 | 1/1   | 0.90 | 0.15 | -3.13 | 150,150,150,150             | 0     |
| 57  | MG   | CA    | 1604 | 1/1   | 0.94 | 0.04 | -3.22 | 117,117,117,117             | 0     |
| 57  | MG   | BA    | 3025 | 1/1   | 0.97 | 0.10 | -3.26 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3048 | 1/1   | 0.79 | 0.14 | -3.47 | 203,203,203,203             | 0     |
| 57  | MG   | BA    | 3039 | 1/1   | 0.98 | 0.13 | -3.50 | 57,57,57,57                 | 0     |
| 57  | MG   | AA    | 1612 | 1/1   | 0.95 | 0.09 | -3.70 | 106,106,106,106             | 0     |
| 57  | MG   | BA    | 3064 | 1/1   | 0.96 | 0.07 | -4.03 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3059 | 1/1   | 0.95 | 0.09 | -4.23 | 69,69,69,69                 | 0     |
| 57  | MG   | BA    | 3097 | 1/1   | 0.97 | 0.08 | -4.48 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3129 | 1/1   | 0.98 | 0.10 | -6.19 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3054 | 1/1   | 0.98 | 0.07 | -6.39 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3118 | 1/1   | 0.90 | 0.09 | -6.82 | 60,60,60,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF   | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 57  | MG   | BA    | 3110 | 1/1   | 0.97 | 0.09 | -7.10  | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3036 | 1/1   | 0.94 | 0.09 | -7.31  | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3029 | 1/1   | 0.96 | 0.07 | -10.40 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3096 | 1/1   | 0.98 | 0.22 | -      | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3085 | 1/1   | 0.92 | 0.42 | -      | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3053 | 1/1   | 0.94 | 0.16 | -      | 144,144,144,144             | 0     |
| 57  | MG   | BA    | 3075 | 1/1   | 0.82 | 0.32 | -      | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3062 | 1/1   | 0.81 | 1.23 | -      | 160,160,160,160             | 0     |
| 57  | MG   | AA    | 1626 | 1/1   | 0.96 | 0.30 | -      | 136,136,136,136             | 0     |
| 57  | MG   | BA    | 3015 | 1/1   | 0.85 | 0.60 | -      | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3032 | 1/1   | 0.83 | 0.15 | -      | 161,161,161,161             | 0     |
| 57  | MG   | DA    | 3109 | 1/1   | 0.37 | 0.90 | -      | 145,145,145,145             | 0     |
| 57  | MG   | DA    | 3030 | 1/1   | 0.79 | 0.30 | -      | 164,164,164,164             | 0     |
| 57  | MG   | BA    | 3079 | 1/1   | 0.89 | 0.06 | -      | 110,110,110,110             | 0     |
| 57  | MG   | DA    | 3010 | 1/1   | 0.71 | 0.26 | -      | 210,210,210,210             | 0     |
| 57  | MG   | BA    | 3103 | 1/1   | 0.92 | 0.07 | -      | 81,81,81,81                 | 0     |
| 57  | MG   | CA    | 1614 | 1/1   | 0.78 | 0.56 | -      | 146,146,146,146             | 0     |
| 57  | MG   | DA    | 3120 | 1/1   | 0.84 | 0.22 | -      | 159,159,159,159             | 0     |
| 57  | MG   | BA    | 3033 | 1/1   | 0.99 | 0.17 | -      | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3020 | 1/1   | 0.15 | 2.44 | -      | 229,229,229,229             | 0     |
| 57  | MG   | DA    | 3028 | 1/1   | 0.85 | 0.47 | -      | 165,165,165,165             | 0     |
| 57  | MG   | BA    | 3047 | 1/1   | 0.87 | 0.19 | -      | 78,78,78,78                 | 0     |
| 57  | MG   | BA    | 3034 | 1/1   | 0.99 | 0.17 | -      | 57,57,57,57                 | 0     |
| 57  | MG   | CA    | 1626 | 1/1   | 0.98 | 0.31 | -      | 139,139,139,139             | 0     |
| 57  | MG   | CA    | 1606 | 1/1   | 0.66 | 0.14 | -      | 124,124,124,124             | 0     |
| 57  | MG   | BA    | 3131 | 1/1   | 0.86 | 0.59 | -      | 68,68,68,68                 | 0     |
| 57  | MG   | CA    | 1608 | 1/1   | 0.89 | 0.19 | -      | 121,121,121,121             | 0     |
| 57  | MG   | AA    | 1632 | 1/1   | 0.86 | 0.10 | -      | 117,117,117,117             | 0     |
| 57  | MG   | BA    | 3044 | 1/1   | 0.92 | 0.08 | -      | 88,88,88,88                 | 0     |
| 57  | MG   | BA    | 3069 | 1/1   | 0.94 | 0.11 | -      | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3026 | 1/1   | 0.85 | 0.44 | -      | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3013 | 1/1   | 0.74 | 0.29 | -      | 165,165,165,165             | 0     |
| 57  | MG   | DA    | 3074 | 1/1   | 0.83 | 1.74 | -      | 187,187,187,187             | 0     |
| 57  | MG   | AA    | 1601 | 1/1   | 0.87 | 0.12 | -      | 133,133,133,133             | 0     |
| 57  | MG   | BA    | 3051 | 1/1   | 0.91 | 0.14 | -      | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3067 | 1/1   | 0.97 | 0.17 | -      | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3093 | 1/1   | 0.91 | 0.30 | -      | 104,104,104,104             | 0     |
| 57  | MG   | DA    | 3093 | 1/1   | 0.75 | 0.14 | -      | 208,208,208,208             | 0     |
| 57  | MG   | DA    | 3125 | 1/1   | 0.53 | 0.31 | -      | 187,187,187,187             | 0     |
| 57  | MG   | BA    | 3127 | 1/1   | 0.92 | 0.10 | -      | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3053 | 1/1   | 0.95 | 0.08 | -      | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3111 | 1/1   | 0.95 | 0.09 | -      | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3047 | 1/1   | 0.82  | 0.25 | -    | 208,208,208,208             | 0     |
| 57  | MG   | BA    | 3073 | 1/1   | 0.97  | 0.09 | -    | 61,61,61,61                 | 0     |
| 57  | MG   | CA    | 1630 | 1/1   | 0.92  | 0.19 | -    | 99,99,99,99                 | 0     |
| 57  | MG   | DA    | 3115 | 1/1   | 0.88  | 0.15 | -    | 154,154,154,154             | 0     |
| 57  | MG   | DA    | 3033 | 1/1   | 0.76  | 0.14 | -    | 162,162,162,162             | 0     |
| 57  | MG   | DA    | 3006 | 1/1   | 0.58  | 0.17 | -    | 296,296,296,296             | 0     |
| 57  | MG   | BA    | 3031 | 1/1   | 0.99  | 0.22 | -    | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3127 | 1/1   | 0.93  | 0.80 | -    | 138,138,138,138             | 0     |
| 57  | MG   | AA    | 1603 | 1/1   | 0.92  | 0.09 | -    | 93,93,93,93                 | 0     |
| 57  | MG   | BA    | 3003 | 1/1   | 0.96  | 0.07 | -    | 90,90,90,90                 | 0     |
| 57  | MG   | DA    | 3064 | 1/1   | 0.55  | 0.51 | -    | 157,157,157,157             | 0     |
| 57  | MG   | AA    | 1610 | 1/1   | 0.75  | 0.12 | -    | 155,155,155,155             | 0     |
| 57  | MG   | DA    | 3082 | 1/1   | 0.69  | 0.41 | -    | 220,220,220,220             | 0     |
| 57  | MG   | BA    | 3068 | 1/1   | 0.96  | 0.17 | -    | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3008 | 1/1   | 0.78  | 0.13 | -    | 198,198,198,198             | 0     |
| 57  | MG   | BA    | 3135 | 1/1   | 0.95  | 0.34 | -    | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3014 | 1/1   | 0.88  | 0.26 | -    | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3095 | 1/1   | 0.81  | 0.21 | -    | 92,92,92,92                 | 0     |
| 57  | MG   | BA    | 3099 | 1/1   | 0.93  | 0.09 | -    | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3059 | 1/1   | 0.69  | 0.28 | -    | 136,136,136,136             | 0     |
| 57  | MG   | DA    | 3009 | 1/1   | 0.93  | 0.22 | -    | 199,199,199,199             | 0     |
| 57  | MG   | BA    | 3122 | 1/1   | 0.94  | 0.22 | -    | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3091 | 1/1   | 0.84  | 0.94 | -    | 174,174,174,174             | 0     |
| 57  | MG   | BA    | 3030 | 1/1   | 0.90  | 0.40 | -    | 58,58,58,58                 | 0     |
| 57  | MG   | AA    | 1605 | 1/1   | 0.90  | 0.21 | -    | 124,124,124,124             | 0     |
| 57  | MG   | DJ    | 201  | 1/1   | 0.41  | 0.55 | -    | 183,183,183,183             | 0     |
| 57  | MG   | BA    | 3019 | 1/1   | 0.88  | 0.12 | -    | 86,86,86,86                 | 0     |
| 57  | MG   | BA    | 3102 | 1/1   | 0.94  | 0.20 | -    | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3040 | 1/1   | 0.97  | 0.17 | -    | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3007 | 1/1   | 0.86  | 0.18 | -    | 111,111,111,111             | 0     |
| 57  | MG   | BA    | 3089 | 1/1   | 0.97  | 0.18 | -    | 66,66,66,66                 | 0     |
| 57  | MG   | AA    | 1620 | 1/1   | 0.90  | 0.17 | -    | 186,186,186,186             | 0     |
| 57  | MG   | DA    | 3126 | 1/1   | 0.97  | 0.17 | -    | 199,199,199,199             | 0     |
| 57  | MG   | DA    | 3113 | 1/1   | 0.73  | 0.19 | -    | 182,182,182,182             | 0     |
| 57  | MG   | D4    | 101  | 1/1   | 0.45  | 1.38 | -    | 183,183,183,183             | 0     |
| 57  | MG   | CA    | 1615 | 1/1   | 0.89  | 0.21 | -    | 156,156,156,156             | 0     |
| 57  | MG   | BA    | 3042 | 1/1   | 0.97  | 0.11 | -    | 68,68,68,68                 | 0     |
| 57  | MG   | DA    | 3073 | 1/1   | -0.04 | 0.20 | -    | 312,312,312,312             | 0     |
| 57  | MG   | BA    | 3078 | 1/1   | 0.96  | 0.07 | -    | 100,100,100,100             | 0     |
| 57  | MG   | DA    | 3036 | 1/1   | 0.80  | 0.48 | -    | 212,212,212,212             | 0     |
| 57  | MG   | DA    | 3019 | 1/1   | 0.81  | 0.19 | -    | 245,245,245,245             | 0     |
| 57  | MG   | BA    | 3133 | 1/1   | 0.84  | 0.58 | -    | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3010 | 1/1   | 0.95 | 0.13 | -    | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3112 | 1/1   | 0.90 | 0.22 | -    | 64,64,64,64                 | 0     |
| 57  | MG   | DA    | 3114 | 1/1   | 0.94 | 0.26 | -    | 135,135,135,135             | 0     |
| 57  | MG   | DA    | 3070 | 1/1   | 0.76 | 0.09 | -    | 147,147,147,147             | 0     |
| 57  | MG   | BA    | 3027 | 1/1   | 0.96 | 0.08 | -    | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3088 | 1/1   | 0.93 | 0.12 | -    | 77,77,77,77                 | 0     |
| 57  | MG   | BA    | 3016 | 1/1   | 0.96 | 0.26 | -    | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3004 | 1/1   | 0.92 | 0.21 | -    | 206,206,206,206             | 0     |
| 57  | MG   | BA    | 3009 | 1/1   | 0.95 | 0.10 | -    | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3111 | 1/1   | 0.80 | 0.31 | -    | 160,160,160,160             | 0     |
| 57  | MG   | DA    | 3049 | 1/1   | 0.58 | 0.10 | -    | 249,249,249,249             | 0     |
| 57  | MG   | BA    | 3057 | 1/1   | 0.95 | 0.35 | -    | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3122 | 1/1   | 0.94 | 0.28 | -    | 146,146,146,146             | 0     |
| 57  | MG   | BA    | 3123 | 1/1   | 0.93 | 0.12 | -    | 79,79,79,79                 | 0     |
| 57  | MG   | DA    | 3085 | 1/1   | 0.84 | 0.23 | -    | 167,167,167,167             | 0     |
| 57  | MG   | AA    | 1602 | 1/1   | 0.93 | 0.37 | -    | 97,97,97,97                 | 0     |
| 57  | MG   | AA    | 1619 | 1/1   | 0.57 | 0.48 | -    | 162,162,162,162             | 0     |
| 57  | MG   | BA    | 3006 | 1/1   | 0.98 | 0.06 | -    | 101,101,101,101             | 0     |
| 57  | MG   | AA    | 1627 | 1/1   | 0.82 | 1.48 | -    | 142,142,142,142             | 0     |
| 57  | MG   | CA    | 1624 | 1/1   | 0.78 | 0.29 | -    | 99,99,99,99                 | 0     |
| 57  | MG   | DA    | 3007 | 1/1   | 0.86 | 0.47 | -    | 250,250,250,250             | 0     |
| 57  | MG   | DA    | 3098 | 1/1   | 0.86 | 0.33 | -    | 170,170,170,170             | 0     |
| 57  | MG   | CA    | 1603 | 1/1   | 0.69 | 0.17 | -    | 141,141,141,141             | 0     |
| 57  | MG   | AA    | 1639 | 1/1   | 0.96 | 0.08 | -    | 143,143,143,143             | 0     |
| 57  | MG   | CA    | 1635 | 1/1   | 0.89 | 0.10 | -    | 142,142,142,142             | 0     |
| 57  | MG   | DA    | 3021 | 1/1   | 0.93 | 0.36 | -    | 151,151,151,151             | 0     |
| 57  | MG   | CA    | 1632 | 1/1   | 0.80 | 0.15 | -    | 210,210,210,210             | 0     |
| 57  | MG   | BA    | 3081 | 1/1   | 0.90 | 0.10 | -    | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3037 | 1/1   | 0.88 | 0.23 | -    | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3001 | 1/1   | 0.79 | 0.29 | -    | 206,206,206,206             | 0     |
| 57  | MG   | BA    | 3004 | 1/1   | 0.87 | 0.23 | -    | 86,86,86,86                 | 0     |
| 57  | MG   | DA    | 3090 | 1/1   | 0.90 | 0.09 | -    | 200,200,200,200             | 0     |
| 57  | MG   | BA    | 3077 | 1/1   | 0.89 | 0.15 | -    | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3077 | 1/1   | 0.94 | 0.12 | -    | 162,162,162,162             | 0     |
| 57  | MG   | BA    | 3115 | 1/1   | 0.78 | 0.53 | -    | 65,65,65,65                 | 0     |
| 57  | MG   | AA    | 1615 | 1/1   | 0.98 | 0.12 | -    | 153,153,153,153             | 0     |
| 57  | MG   | BA    | 3049 | 1/1   | 0.96 | 0.07 | -    | 61,61,61,61                 | 0     |
| 57  | MG   | AA    | 1624 | 1/1   | 0.56 | 0.17 | -    | 131,131,131,131             | 0     |
| 57  | MG   | AA    | 1630 | 1/1   | 0.70 | 0.28 | -    | 99,99,99,99                 | 0     |
| 57  | MG   | AA    | 1628 | 1/1   | 0.81 | 0.28 | -    | 134,134,134,134             | 0     |
| 57  | MG   | AA    | 1637 | 1/1   | 0.79 | 0.58 | -    | 118,118,118,118             | 0     |
| 57  | MG   | BA    | 3125 | 1/1   | 0.95 | 0.24 | -    | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3052 | 1/1   | 0.91 | 0.11 | -    | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3106 | 1/1   | 0.98 | 0.15 | -    | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3071 | 1/1   | 0.51 | 0.30 | -    | 184,184,184,184             | 0     |
| 57  | MG   | BA    | 3032 | 1/1   | 0.86 | 0.13 | -    | 57,57,57,57                 | 0     |
| 57  | MG   | AA    | 1621 | 1/1   | 0.91 | 0.27 | -    | 80,80,80,80                 | 0     |
| 57  | MG   | BA    | 3035 | 1/1   | 0.93 | 0.28 | -    | 72,72,72,72                 | 0     |
| 57  | MG   | DA    | 3054 | 1/1   | 0.78 | 0.34 | -    | 155,155,155,155             | 0     |
| 57  | MG   | BA    | 3128 | 1/1   | 0.97 | 0.14 | -    | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3061 | 1/1   | 0.95 | 0.38 | -    | 56,56,56,56                 | 0     |
| 57  | MG   | CA    | 1638 | 1/1   | 0.95 | 0.10 | -    | 226,226,226,226             | 0     |
| 57  | MG   | BA    | 3113 | 1/1   | 0.96 | 0.12 | -    | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3046 | 1/1   | 0.94 | 0.25 | -    | 172,172,172,172             | 0     |
| 57  | MG   | CA    | 1622 | 1/1   | 0.58 | 0.09 | -    | 216,216,216,216             | 0     |
| 57  | MG   | CA    | 1602 | 1/1   | 0.42 | 0.16 | -    | 177,177,177,177             | 0     |
| 57  | MG   | DA    | 3129 | 1/1   | 0.70 | 1.36 | -    | 132,132,132,132             | 0     |
| 57  | MG   | AA    | 1638 | 1/1   | 0.92 | 0.19 | -    | 107,107,107,107             | 0     |
| 57  | MG   | BA    | 3055 | 1/1   | 0.96 | 0.11 | -    | 62,62,62,62                 | 0     |
| 57  | MG   | DB    | 201  | 1/1   | 0.78 | 0.16 | -    | 224,224,224,224             | 0     |
| 57  | MG   | DA    | 3056 | 1/1   | 0.91 | 0.19 | -    | 141,141,141,141             | 0     |
| 57  | MG   | CA    | 1611 | 1/1   | 0.80 | 0.29 | -    | 132,132,132,132             | 0     |
| 57  | MG   | BA    | 3062 | 1/1   | 0.90 | 0.68 | -    | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3100 | 1/1   | 0.97 | 0.15 | -    | 74,74,74,74                 | 0     |
| 57  | MG   | BA    | 3092 | 1/1   | 0.82 | 0.08 | -    | 127,127,127,127             | 0     |
| 57  | MG   | DA    | 3041 | 1/1   | 0.77 | 0.40 | -    | 176,176,176,176             | 0     |
| 57  | MG   | DA    | 3027 | 1/1   | 0.89 | 0.14 | -    | 171,171,171,171             | 0     |
| 57  | MG   | BA    | 3043 | 1/1   | 0.94 | 0.19 | -    | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3086 | 1/1   | 0.87 | 0.12 | -    | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3080 | 1/1   | 0.88 | 0.12 | -    | 134,134,134,134             | 0     |
| 57  | MG   | DA    | 3099 | 1/1   | 0.88 | 0.19 | -    | 211,211,211,211             | 0     |
| 57  | MG   | DA    | 3005 | 1/1   | 0.77 | 1.12 | -    | 197,197,197,197             | 0     |
| 57  | MG   | BA    | 3020 | 1/1   | 0.95 | 0.36 | -    | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3063 | 1/1   | 0.35 | 1.56 | -    | 157,157,157,157             | 0     |
| 57  | MG   | BA    | 3087 | 1/1   | 0.98 | 0.14 | -    | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3011 | 1/1   | 0.82 | 0.99 | -    | 184,184,184,184             | 0     |
| 57  | MG   | BA    | 3083 | 1/1   | 0.94 | 0.06 | -    | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3119 | 1/1   | 0.96 | 0.41 | -    | 68,68,68,68                 | 0     |
| 57  | MG   | CA    | 1636 | 1/1   | 0.83 | 1.55 | -    | 120,120,120,120             | 0     |
| 57  | MG   | DA    | 3089 | 1/1   | 0.93 | 0.44 | -    | 179,179,179,179             | 0     |
| 57  | MG   | CA    | 1605 | 1/1   | 0.97 | 0.12 | -    | 115,115,115,115             | 0     |
| 57  | MG   | DA    | 3058 | 1/1   | 0.64 | 0.93 | -    | 162,162,162,162             | 0     |
| 57  | MG   | BA    | 3117 | 1/1   | 0.99 | 0.15 | -    | 67,67,67,67                 | 0     |
| 57  | MG   | BA    | 3091 | 1/1   | 0.97 | 0.13 | -    | 88,88,88,88                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3126 | 1/1   | 0.96 | 0.24 | -    | 70,70,70,70                 | 0     |
| 57  | MG   | BA    | 3038 | 1/1   | 0.98 | 0.13 | -    | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3038 | 1/1   | 0.79 | 0.43 | -    | 197,197,197,197             | 0     |
| 57  | MG   | AA    | 1614 | 1/1   | 0.78 | 0.18 | -    | 150,150,150,150             | 0     |
| 57  | MG   | DA    | 3045 | 1/1   | 0.23 | 0.24 | -    | 188,188,188,188             | 0     |
| 57  | MG   | DA    | 3119 | 1/1   | 0.78 | 0.13 | -    | 147,147,147,147             | 0     |
| 57  | MG   | BA    | 3098 | 1/1   | 0.78 | 0.37 | -    | 72,72,72,72                 | 0     |
| 57  | MG   | BA    | 3001 | 1/1   | 0.98 | 0.06 | -    | 61,61,61,61                 | 0     |
| 57  | MG   | AA    | 1635 | 1/1   | 0.84 | 0.17 | -    | 148,148,148,148             | 0     |
| 57  | MG   | DA    | 3016 | 1/1   | 0.59 | 1.31 | -    | 175,175,175,175             | 0     |
| 57  | MG   | BA    | 3071 | 1/1   | 0.94 | 0.33 | -    | 55,55,55,55                 | 0     |
| 57  | MG   | CA    | 1627 | 1/1   | 0.44 | 0.35 | -    | 136,136,136,136             | 0     |
| 57  | MG   | DA    | 3088 | 1/1   | 0.82 | 0.30 | -    | 180,180,180,180             | 0     |
| 57  | MG   | DC    | 302  | 1/1   | 0.84 | 0.20 | -    | 140,140,140,140             | 0     |
| 57  | MG   | DA    | 3081 | 1/1   | 0.78 | 0.22 | -    | 182,182,182,182             | 0     |
| 57  | MG   | CA    | 1619 | 1/1   | 0.62 | 0.92 | -    | 135,135,135,135             | 0     |
| 57  | MG   | DA    | 3121 | 1/1   | 0.71 | 0.45 | -    | 206,206,206,206             | 0     |
| 57  | MG   | BA    | 3046 | 1/1   | 0.82 | 0.19 | -    | 77,77,77,77                 | 0     |
| 57  | MG   | DA    | 3078 | 1/1   | 0.63 | 0.64 | -    | 144,144,144,144             | 0     |
| 57  | MG   | DA    | 3029 | 1/1   | 0.70 | 0.62 | -    | 179,179,179,179             | 0     |
| 57  | MG   | DA    | 3043 | 1/1   | 0.83 | 0.16 | -    | 208,208,208,208             | 0     |
| 57  | MG   | DA    | 3026 | 1/1   | 0.86 | 1.01 | -    | 160,160,160,160             | 0     |
| 57  | MG   | DA    | 3118 | 1/1   | 0.90 | 0.25 | -    | 181,181,181,181             | 0     |
| 57  | MG   | DA    | 3096 | 1/1   | 0.80 | 0.32 | -    | 190,190,190,190             | 0     |
| 57  | MG   | DA    | 3107 | 1/1   | 0.75 | 0.14 | -    | 137,137,137,137             | 0     |
| 57  | MG   | DA    | 3092 | 1/1   | 0.60 | 0.26 | -    | 198,198,198,198             | 0     |
| 57  | MG   | DA    | 3087 | 1/1   | 0.65 | 0.16 | -    | 208,208,208,208             | 0     |
| 57  | MG   | DA    | 3117 | 1/1   | 0.87 | 0.45 | -    | 170,170,170,170             | 0     |
| 57  | MG   | AA    | 1608 | 1/1   | 0.94 | 0.23 | -    | 105,105,105,105             | 0     |
| 57  | MG   | AA    | 1636 | 1/1   | 0.72 | 0.35 | -    | 154,154,154,154             | 0     |
| 57  | MG   | AA    | 1640 | 1/1   | 0.94 | 0.07 | -    | 160,160,160,160             | 0     |
| 57  | MG   | BA    | 3082 | 1/1   | 0.98 | 0.12 | -    | 55,55,55,55                 | 0     |
| 57  | MG   | CA    | 1620 | 1/1   | 0.61 | 0.49 | -    | 150,150,150,150             | 0     |
| 57  | MG   | BA    | 3065 | 1/1   | 0.97 | 0.06 | -    | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3116 | 1/1   | 0.94 | 0.14 | -    | 133,133,133,133             | 0     |
| 57  | MG   | DC    | 301  | 1/1   | 0.80 | 0.18 | -    | 135,135,135,135             | 0     |
| 57  | MG   | DA    | 3015 | 1/1   | 0.46 | 1.27 | -    | 164,164,164,164             | 0     |
| 57  | MG   | BA    | 3021 | 1/1   | 0.99 | 0.31 | -    | 59,59,59,59                 | 0     |
| 57  | MG   | BB    | 204  | 1/1   | 0.93 | 0.09 | -    | 74,74,74,74                 | 0     |
| 57  | MG   | BA    | 3090 | 1/1   | 0.88 | 0.11 | -    | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3086 | 1/1   | 0.92 | 0.26 | -    | 196,196,196,196             | 0     |
| 57  | MG   | DA    | 3003 | 1/1   | 0.37 | 1.43 | -    | 229,229,229,229             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3031 | 1/1   | 0.92 | 0.16 | -    | 159,159,159,159             | 0     |
| 57  | MG   | DA    | 3014 | 1/1   | 0.86 | 0.28 | -    | 162,162,162,162             | 0     |
| 57  | MG   | DA    | 3131 | 1/1   | 0.82 | 0.44 | -    | 181,181,181,181             | 0     |
| 57  | MG   | CA    | 1601 | 1/1   | 0.94 | 0.13 | -    | 224,224,224,224             | 0     |
| 57  | MG   | BA    | 3121 | 1/1   | 0.91 | 0.11 | -    | 64,64,64,64                 | 0     |
| 57  | MG   | DA    | 3123 | 1/1   | 0.87 | 0.20 | -    | 225,225,225,225             | 0     |
| 57  | MG   | BA    | 3070 | 1/1   | 0.51 | 0.17 | -    | 158,158,158,158             | 0     |
| 57  | MG   | DA    | 3094 | 1/1   | 0.67 | 0.69 | -    | 173,173,173,173             | 0     |
| 57  | MG   | DA    | 3022 | 1/1   | 0.73 | 0.78 | -    | 152,152,152,152             | 0     |
| 57  | MG   | DA    | 3034 | 1/1   | 0.92 | 0.15 | -    | 158,158,158,158             | 0     |
| 57  | MG   | BA    | 3076 | 1/1   | 0.95 | 0.18 | -    | 62,62,62,62                 | 0     |
| 57  | MG   | AA    | 1623 | 1/1   | 0.93 | 0.11 | -    | 129,129,129,129             | 0     |
| 57  | MG   | DA    | 3097 | 1/1   | 0.74 | 0.34 | -    | 156,156,156,156             | 0     |
| 57  | MG   | CA    | 1623 | 1/1   | 0.95 | 0.30 | -    | 123,123,123,123             | 0     |
| 57  | MG   | BA    | 3011 | 1/1   | 0.87 | 0.30 | -    | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3067 | 1/1   | 0.90 | 0.15 | -    | 147,147,147,147             | 0     |
| 57  | MG   | BA    | 3045 | 1/1   | 0.96 | 0.32 | -    | 80,80,80,80                 | 0     |
| 57  | MG   | BB    | 201  | 1/1   | 0.89 | 0.49 | -    | 118,118,118,118             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.