



## wwPDB EM Map/Model Validation Report ⓘ

Jul 19, 2016 – 02:45 PM EDT

PDB ID : 3JCS  
EMDB ID: : EMD-6583  
Title : 2.8 Angstrom cryo-EM structure of the large ribosomal subunit from the eukaryotic parasite Leishmania  
Authors : Shalev-Benami, M.; Zhang, Y.; Matzov, D.; Halfon, Y.; Zackay, A.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Jaffe, C.L.; Yonath, A.; Skiniotis, G.  
Deposited on : 2016-01-21  
Resolution : 2.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027790

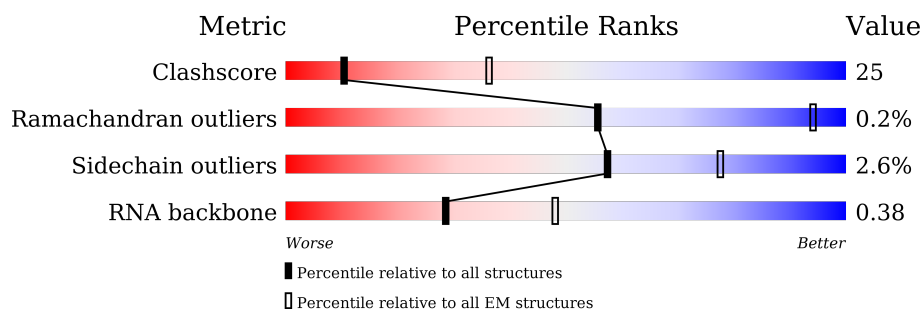
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 Å.

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







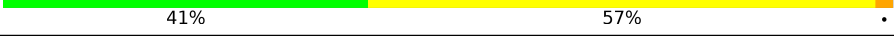
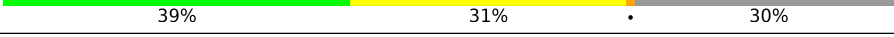
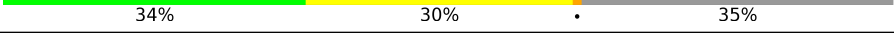

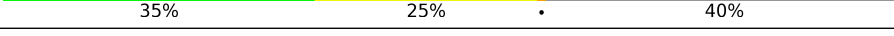

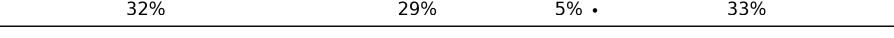
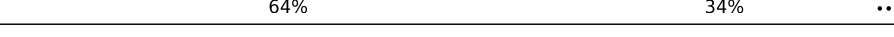

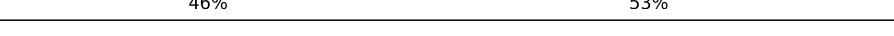


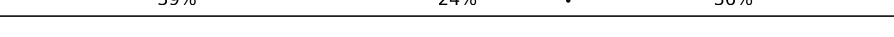

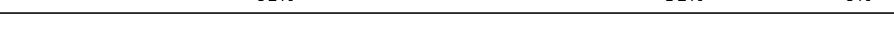






| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 114402                      | 924                         |
| Ramachandran outliers | 111179                      | 726                         |
| Sidechain outliers    | 111093                      | 686                         |
| RNA backbone          | 3027                        | 244                         |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|-------------------|
| 1   | 1     | 1782   | 25% 38% 22% • 13% |
| 2   | 2     | 1527   | 21% 34% 18% 27%   |
| 3   | 3     | 213    | 22% 38% 26% 14%   |
| 4   | 4     | 183    | 28% 35% 19% 19%   |
| 5   | 5     | 133    | 16% 28% 15% • 40% |
| 6   | 6     | 76     | • 20% 53% 5% 20%  |
| 7   | 7     | 171    | 28% 44% 16% • 10% |
| 8   | 8     | 121    | 13% 46% 39% •     |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 9   | A     | 260    |    |
| 10  | B     | 419    |    |
| 11  | C     | 373    |    |
| 12  | D     | 188    |    |
| 13  | E     | 190    |    |
| 14  | F     | 195    |    |
| 15  | G     | 348    |    |
| 16  | H     | 222    |    |
| 17  | I     | 220    |    |
| 18  | J     | 139    |    |
| 19  | K     | 233    |    |
| 20  | L     | 145    |   |
| 21  | M     | 204    |  |
| 22  | N     | 213    |  |
| 23  | O     | 305    |  |
| 24  | P     | 198    |  |
| 25  | Q     | 245    |  |
| 26  | R     | 179    |  |
| 27  | S     | 159    |  |
| 28  | T     | 166    |  |
| 29  | U     | 129    |  |
| 30  | V     | 145    |  |
| 31  | W     | 143    |  |
| 32  | X     | 124    |  |
| 33  | Y     | 134    |  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 34  | Z     | 147    |    |
| 35  | a     | 127    |    |
| 36  | b     | 70     |    |
| 37  | c     | 252    |    |
| 38  | d     | 104    |    |
| 39  | e     | 183    |    |
| 40  | f     | 133    |    |
| 41  | g     | 144    |    |
| 42  | h     | 168    |    |
| 43  | i     | 105    |    |
| 44  | j     | 83     |    |
| 45  | k     | 83     |    |
| 46  | l     | 51     |  |
| 47  | m     | 92     |  |
| 48  | n     | 106    |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 1   | OMU  | 1     | 36   | -         | -        | X       | -                |
| 1   | OMG  | 1     | 959  | -         | -        | X       | -                |
| 2   | OMU  | 2     | 1078 | -         | -        | X       | -                |
| 2   | OMG  | 2     | 1079 | -         | -        | X       | -                |
| 2   | OMG  | 2     | 1254 | -         | -        | X       | -                |
| 2   | OMC  | 2     | 1318 | -         | -        | X       | -                |
| 2   | OMC  | 2     | 443  | -         | -        | X       | -                |
| 2   | A2M  | 2     | 527  | -         | -        | X       | -                |
| 2   | OMG  | 2     | 71   | -         | -        | X       | -                |
| 7   | OMU  | 7     | 7    | -         | -        | X       | -                |

## 2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 117257 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 26S alpha ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | 1     | 1554     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 33313 | 14886 | 6081 | 10792 | 1554 |         |       |

- Molecule 2 is a RNA chain called 26S delta ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |      |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|------|---------|-------|
| 2   | 2     | 1119     | Total | C     | N    | O    | P    | 0       | 0     |
|     |       |          | 23926 | 10702 | 4308 | 7797 | 1119 |         |       |

- Molecule 3 is a RNA chain called 26S gamma ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 3   | 3     | 184      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3893  | 1740 | 662 | 1307 | 184 |         |       |

- Molecule 4 is a RNA chain called 26S delta ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 4   | 4     | 149      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3177  | 1418 | 570 | 1040 | 149 |         |       |

- Molecule 5 is a RNA chain called 26S epsilon ribosomal RNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 5   | 5     | 80       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1708  | 763 | 310 | 555 | 80 |         |       |

- Molecule 6 is a RNA chain called 26S zeta ribosomal RNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6   | 6     | 61       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1288  | 577 | 225 | 425 | 61 |         |       |

- Molecule 7 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 7   | 7     | 154      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3280  | 1469 | 584 | 1074 | 153 |         |       |

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 8   | 8     | 119      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2531  | 1132 | 450 | 830 | 119 |         |       |

- Molecule 9 is a protein called ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | A     | 245      | Total | C    | N   | O   | S  | 2       | 0     |
|     |       |          | 1859  | 1158 | 384 | 307 | 10 |         |       |

- Molecule 10 is a protein called ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | B     | 396      | Total | C    | N   | O   | S  | 2       | 0     |
|     |       |          | 3020  | 1908 | 592 | 508 | 12 |         |       |

- Molecule 11 is a protein called ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | C     | 301      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2237  | 1413 | 428 | 384 | 12 |         |       |

- Molecule 12 is a protein called ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 12  | D     | 161      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 799   | 476 | 161 | 162 |         |       |

- Molecule 13 is a protein called ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | E     | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1509  | 953 | 276 | 272 | 8 |         |       |

- Molecule 14 is a protein called ribosomal protein L6e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | F     | 137      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1002  | 641 | 192 | 167 | 2 |         |       |

- Molecule 15 is a protein called ribosomal protein L8e.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | G     | 226      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1772  | 1113 | 353 | 299 | 7 |         |       |

- Molecule 16 is a protein called ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | H     | 202      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1596  | 1019 | 307 | 263 | 7 |         |       |

- Molecule 17 is a protein called ribosomal protein L13e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | I     | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1061  | 666 | 221 | 169 | 5 |         |       |

- Molecule 18 is a protein called ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | J     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 924   | 588 | 171 | 160 | 5 |         |       |

- Molecule 19 is a protein called ribosomal protein L14e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | K     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1061  | 661 | 212 | 184 | 4 |         |       |

- Molecule 20 is a protein called ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | L     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1096  | 691 | 223 | 177 | 5 |         |       |

- Molecule 21 is a protein called ribosomal protein L15e.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21  | M     | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1714  | 1080 | 362 | 264 | 8 |         |       |

- Molecule 22 is a protein called ribosomal protein L16.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22  | N     | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1714  | 1077 | 340 | 281 | 16 |         |       |

- Molecule 23 is a protein called ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | O     | 235      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1557  | 986 | 300 | 268 | 3 |         |       |

- Molecule 24 is a protein called ribosomal protein L18e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | P     | 195      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1494  | 942 | 299 | 247 | 6 |         |       |

- Molecule 25 is a protein called ribosomal protein L19e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Q     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 730 | 243 | 186 | 3 |         |       |

- Molecule 26 is a protein called ribosomal protein L20e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | R     | 131      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1019  | 651 | 197 | 167 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| R     | 158     | ILE      | LEU    | VARIANT | UNP E9BRT7 |

- Molecule 27 is a protein called ribosomal protein L21e.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | S     | 149      | Total | C   | N   | O   | S | 2       | 0     |
|     |       |          | 1112  | 704 | 218 | 187 | 3 |         |       |

- Molecule 28 is a protein called ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 28  | T     | 154      | Total | C   | N   | O   | S  | 2       | 0     |
|     |       |          | 1221  | 763 | 241 | 206 | 11 |         |       |

- Molecule 29 is a protein called ribosomal protein L22e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | U     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 541   | 331 | 101 | 109 |   |         |       |

- Molecule 30 is a protein called ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | V     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 892   | 566 | 171 | 153 | 2 |         |       |

- Molecule 31 is a protein called ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | W     | 117      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 896   | 562 | 187 | 144 | 3 |         |       |

- Molecule 32 is a protein called ribosomal protein L24e.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32  | X     | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 508   | 333 | 96 | 76 | 3 |         |       |

- Molecule 33 is a protein called ribosomal protein L27e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | Y     | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 914   | 589 | 174 | 151 |   |         |       |

- Molecule 34 is a protein called ribosomal protein L28e.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 34  | Z     | 79       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 538   | 329 | 111 | 95 | 3 |         |       |

- Molecule 35 is a protein called ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | a     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 982   | 613 | 203 | 163 | 3 |         |       |

- Molecule 36 is a protein called ribosomal protein L29e.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 36  | b     | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 503   | 309 | 113 | 80 | 1 |         |       |

- Molecule 37 is a protein called ribosomal protein L30.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 37  | c     | 222      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1732  | 1105 | 327 | 289 | 11 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| c     | 49      | ALA      | GLY    | VARIANT | UNP E9BI29 |

- Molecule 38 is a protein called ribosomal protein L30e.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 38  | d     | 75       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 518   | 325 | 93 | 97 | 3 |         |       |

- Molecule 39 is a protein called ribosomal protein L31e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | e     | 112      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 824   | 531 | 155 | 136 | 2 |         |       |

- Molecule 40 is a protein called ribosomal protein L32e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | f     | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 982   | 616 | 195 | 167 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| f     | 105     | LYS      | THR    | VARIANT | UNP E9BFJ5 |

- Molecule 41 is a protein called ribosomal protein L33e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | g     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 983   | 612 | 205 | 161 | 5 |         |       |

- Molecule 42 is a protein called ribosomal protein L34e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | h     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 856   | 529 | 182 | 140 | 5 |         |       |

- Molecule 43 is a protein called ribosomal protein L36e.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 43  | i     | 63       | Total | C   | N   | O  | S | 1       | 0     |
|     |       |          | 494   | 316 | 100 | 76 | 2 |         |       |

- Molecule 44 is a protein called ribosomal protein L37e.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 44  | j     | 78       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 639   | 385 | 149 | 99 | 6 |         |       |

- Molecule 45 is a protein called ribosomal protein L38e.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 45  | k     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 373   | 234 | 71 | 66 | 2 |         |       |

- Molecule 46 is a protein called ribosomal protein L39e.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 46  | l     | 50       | Total | C   | N  | O  | S | 1       | 0     |
|     |       |          | 457   | 294 | 98 | 64 | 1 |         |       |

- Molecule 47 is a protein called ribosomal protein L43e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | m     | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 668   | 414 | 135 | 113 | 6 |         |       |

- Molecule 48 is a protein called ribosomal protein L44e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | n     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 659   | 418 | 129 | 110 | 2 |         |       |

- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 49  | g     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 49  | j     | 4        | Total | Mg | 0       |
|     |       |          | 4     | 4  |         |
| 49  | l     | 51       | Total | Mg | 0       |
|     |       |          | 51    | 51 |         |
| 49  | K     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 49  | h     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 49  | C     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 49  | V     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 49  | 7     | 9        | Total | Mg | 0       |
|     |       |          | 9     | 9  |         |
| 49  | a     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 49  | 4     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 49  | 5     | 4        | Total | Mg | 0       |
|     |       |          | 4     | 4  |         |
| 49  | 2     | 25       | Total | Mg | 0       |
|     |       |          | 25    | 25 |         |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 49  | 3     | 3        | Total<br>3 | Mg<br>3 | 0       |
| 49  | f     | 2        | Total<br>2 | Mg<br>2 | 0       |
| 49  | M     | 3        | Total<br>3 | Mg<br>3 | 0       |

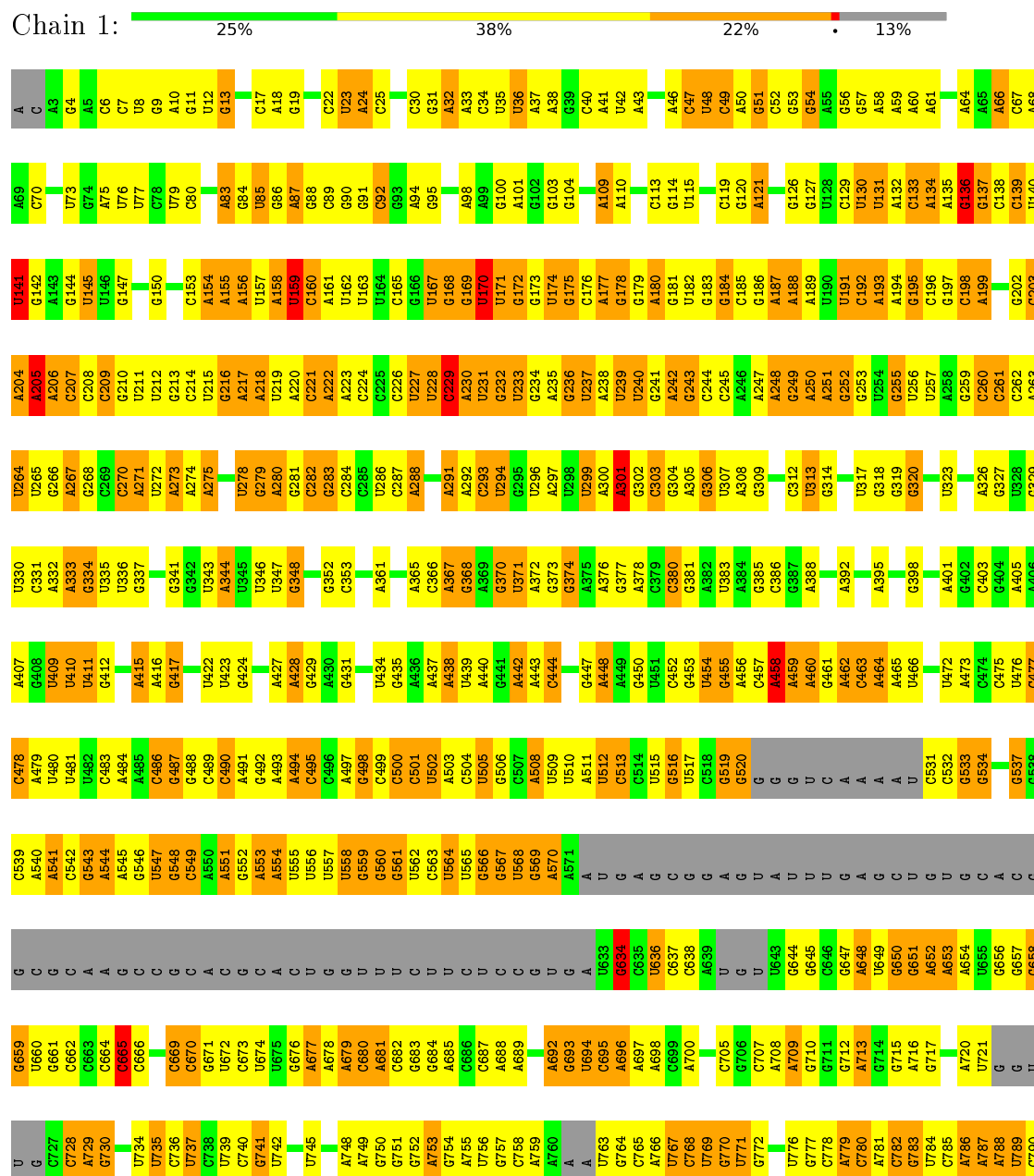
- Molecule 50 is water.

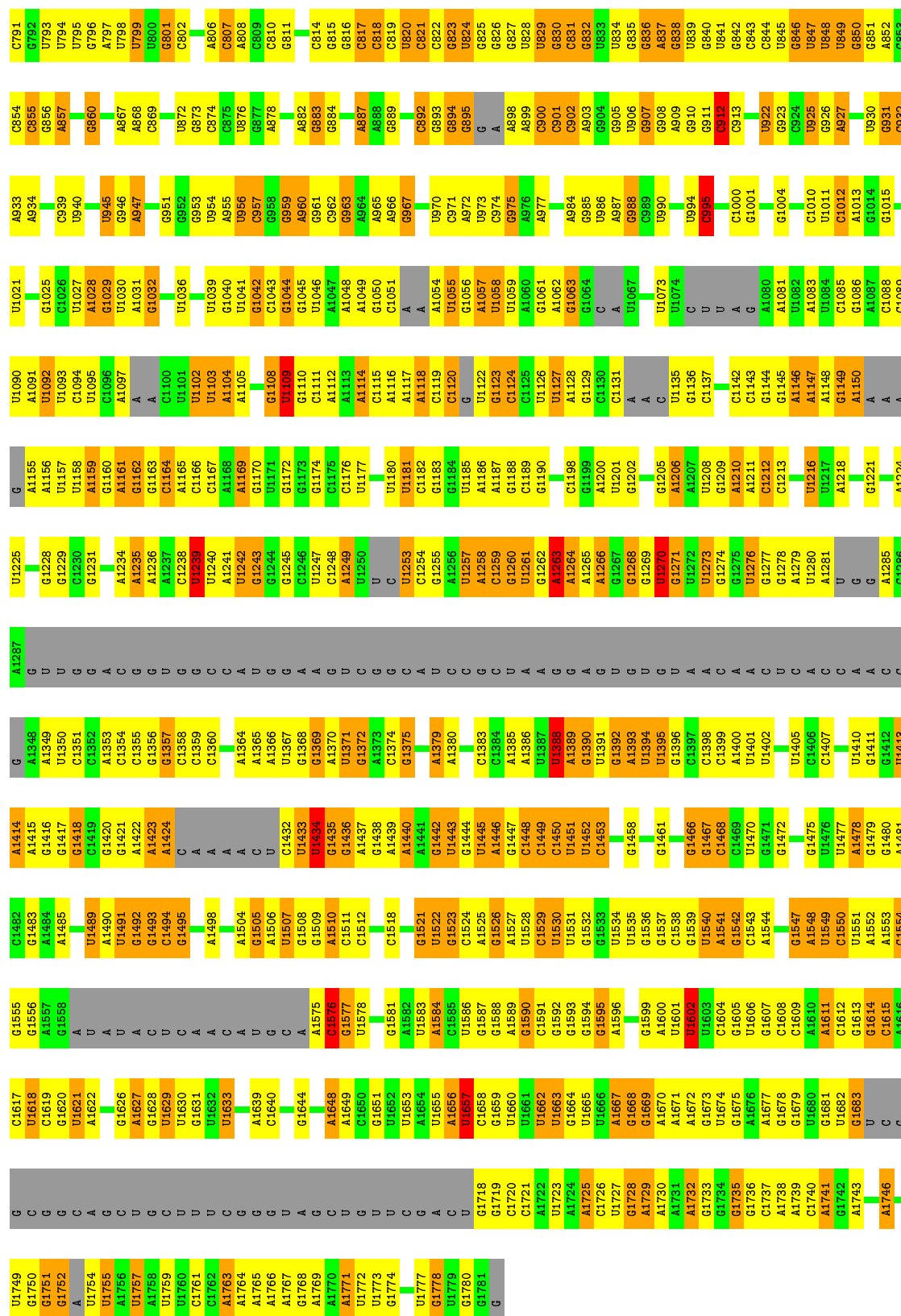
| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 50  | 1     | 72       | Total<br>72 | O<br>72 | 0       |
| 50  | 2     | 40       | Total<br>40 | O<br>40 | 0       |
| 50  | 4     | 4        | Total<br>4  | O<br>4  | 0       |
| 50  | 5     | 4        | Total<br>4  | O<br>4  | 0       |
| 50  | 7     | 16       | Total<br>16 | O<br>16 | 0       |
| 50  | 8     | 1        | Total<br>1  | O<br>1  | 0       |
| 50  | A     | 2        | Total<br>2  | O<br>2  | 0       |
| 50  | G     | 1        | Total<br>1  | O<br>1  | 0       |
| 50  | M     | 2        | Total<br>2  | O<br>2  | 0       |
| 50  | i     | 1        | Total<br>1  | O<br>1  | 0       |
| 50  | j     | 1        | Total<br>1  | O<br>1  | 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 26S alpha ribosomal RNA





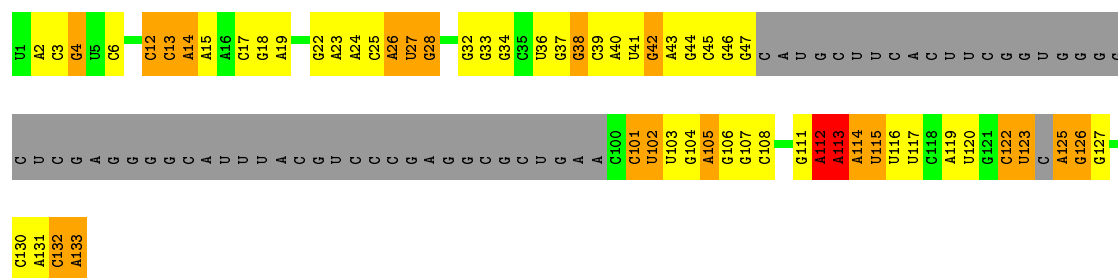
• Molecule 2: 26S delta ribosomal RNA

Chain 2: 21% 34% 18% 27%



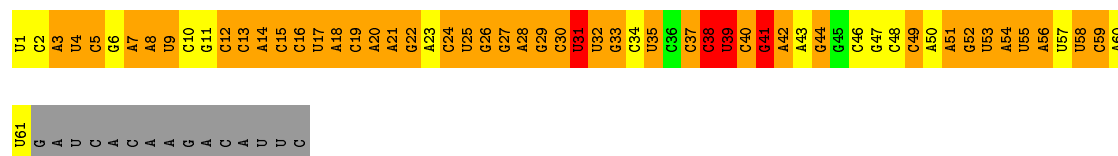




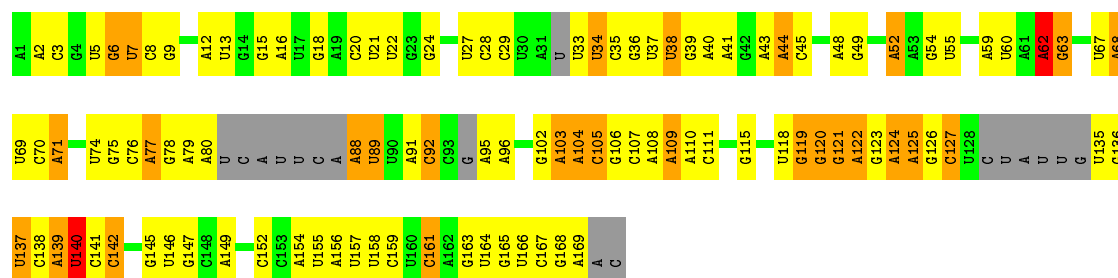
• Molecule 6: 26S zeta ribosomal RNA

Chain 6: 20% 53% 5% 20%



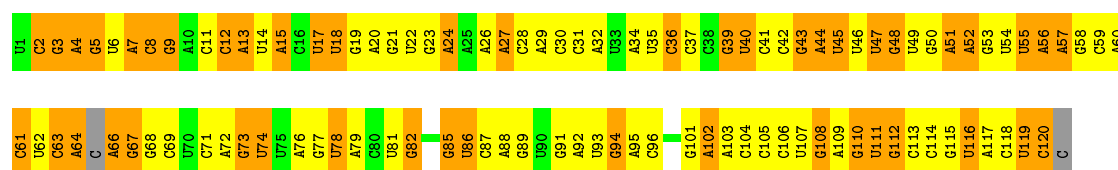
• Molecule 7: 5.8S ribosomal RNA

Chain 7: 28% 44% 16% 10%



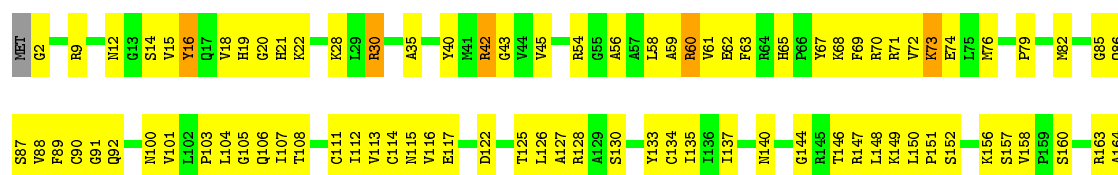
• Molecule 8: 5S ribosomal RNA

Chain 8: 13% 46% 39%



• Molecule 9: ribosomal protein L2

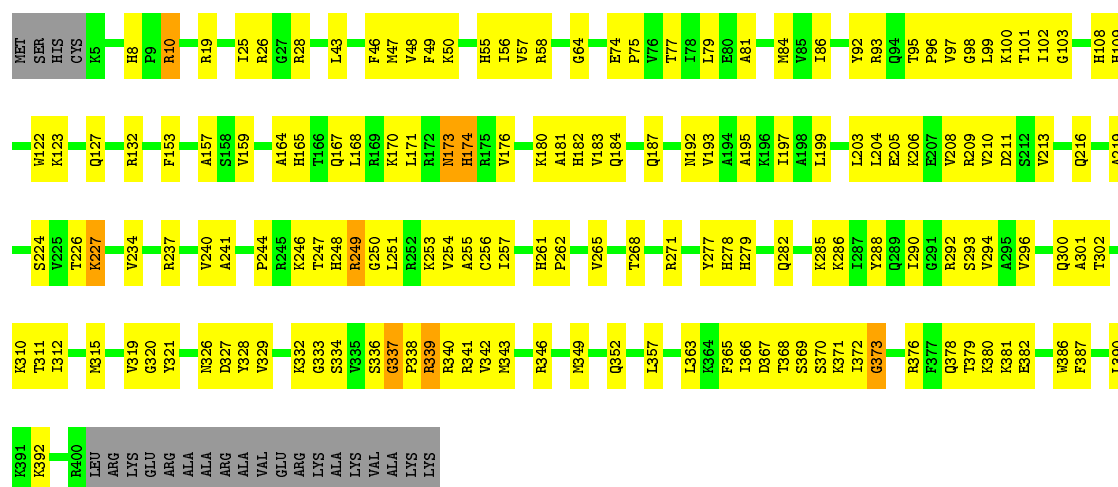
Chain A: 47% 45% 6%





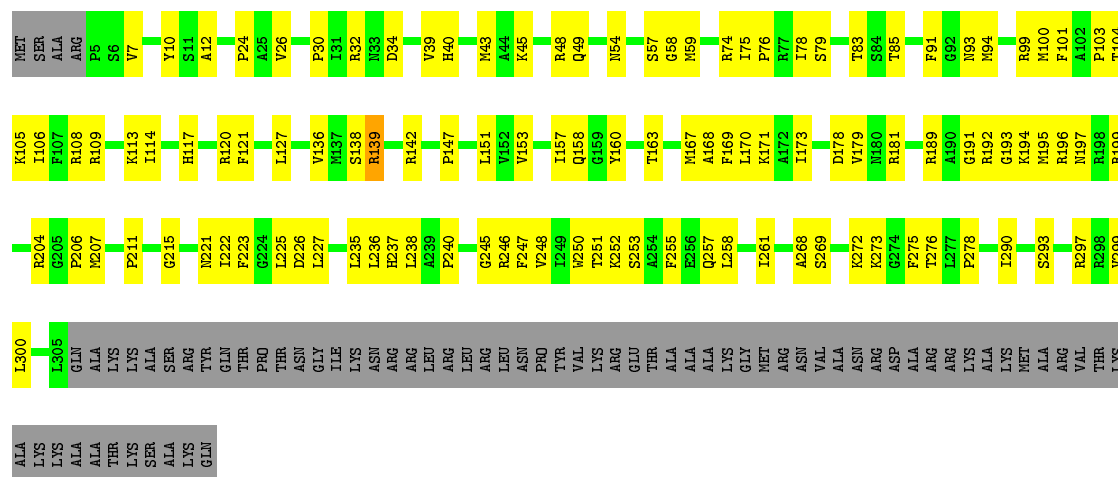
• Molecule 10: ribosomal protein L3

Chain B: 56% 36% 5%



• Molecule 11: ribosomal protein L4

Chain C: 51% 30% 19%




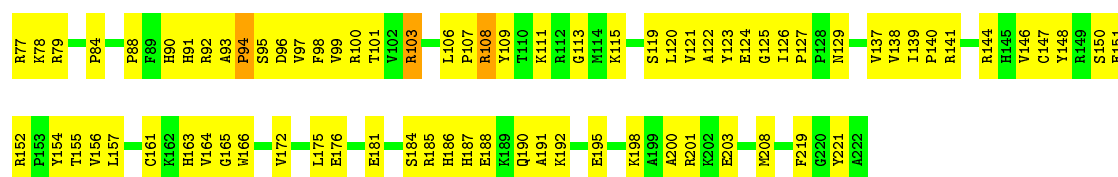
• Molecule 12: ribosomal protein L5

Chain D: 81% 5% 14%



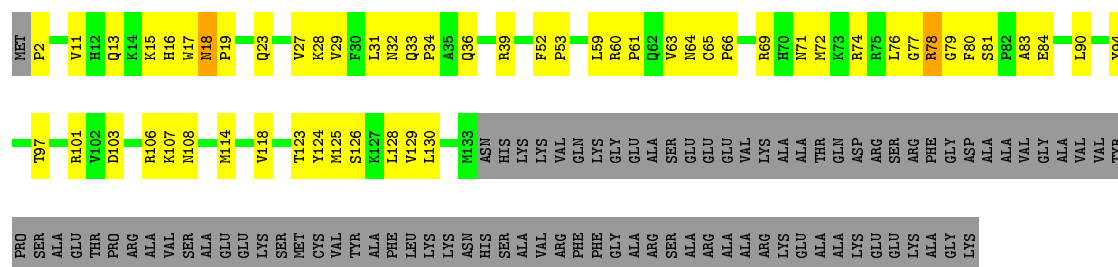
• Molecule 13: ribosomal protein L6

Chain H: 



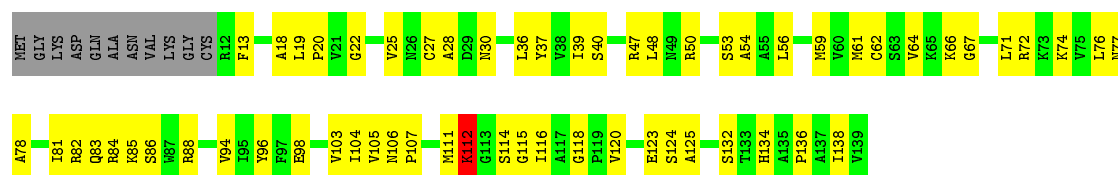
• Molecule 17: ribosomal protein L13e

Chain I: 35% 25% 40%



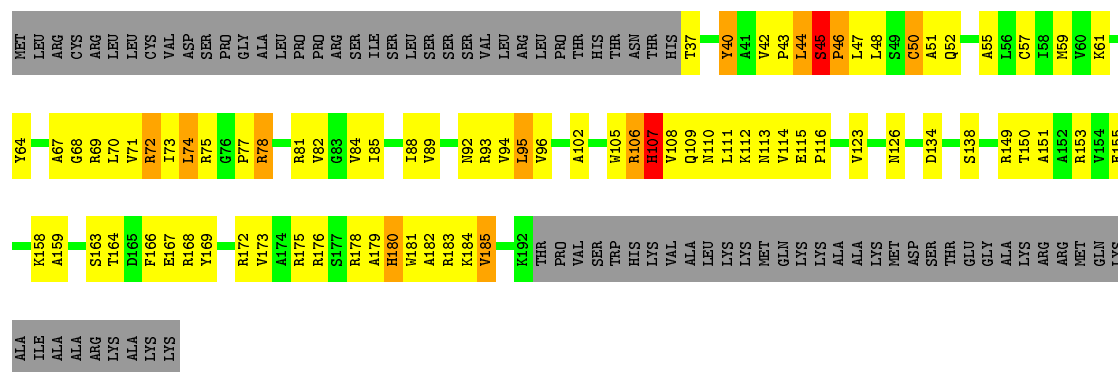
• Molecule 18: ribosomal protein L14

Chain J: 49% 42% 8%



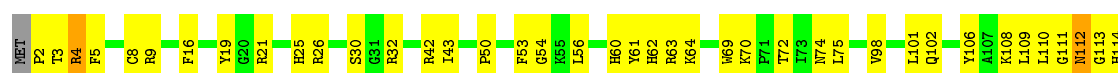
• Molecule 19: ribosomal protein L14e

Chain K: 32% 29% 5% 33%



• Molecule 20: ribosomal protein L15

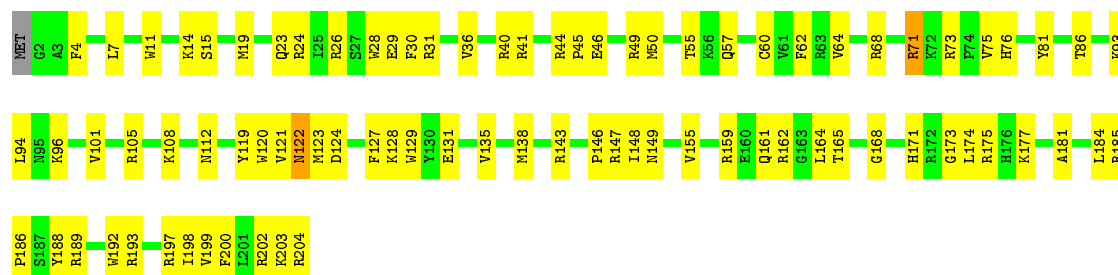
Chain L: 64% 34%





- Molecule 21: ribosomal protein L15e

Chain M: 58% 40%



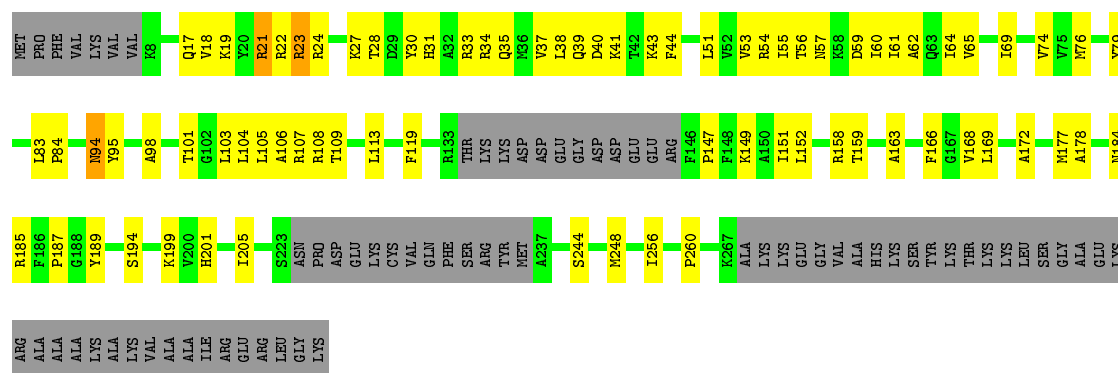
- Molecule 22: ribosomal protein L16

Chain N: 46% 53%



- Molecule 23: ribosomal protein L18

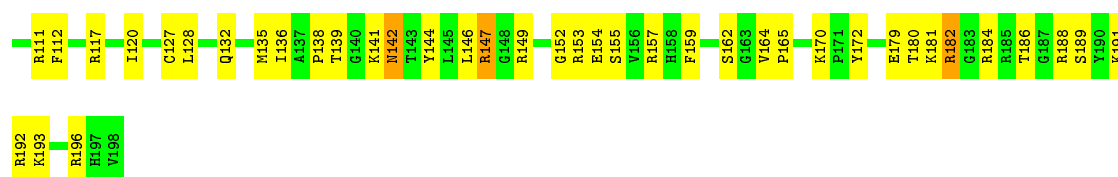
Chain O: 52% 24% 23%



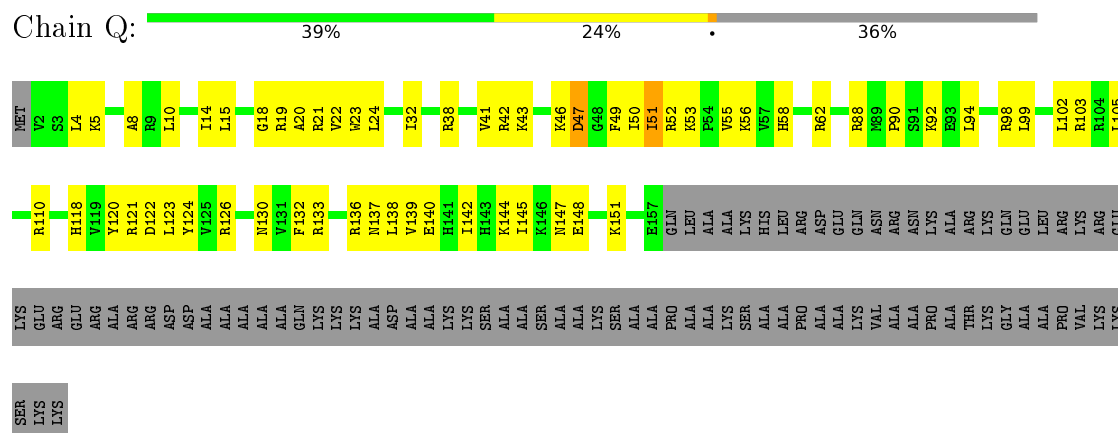
- Molecule 24: ribosomal protein L18e

Chain P: 61% 36%

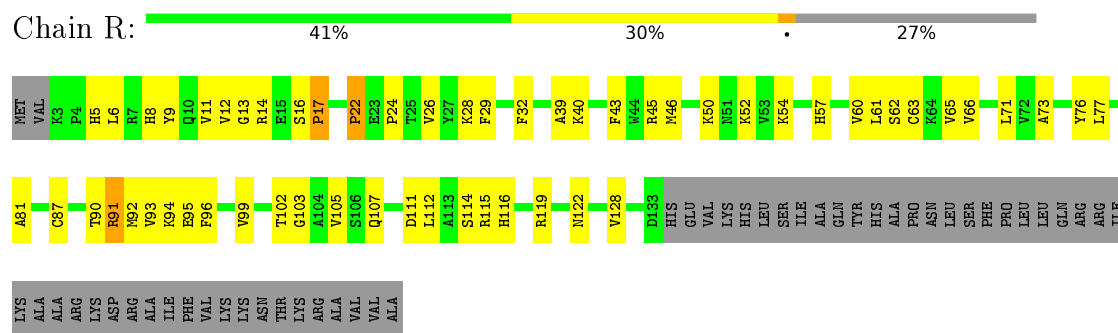




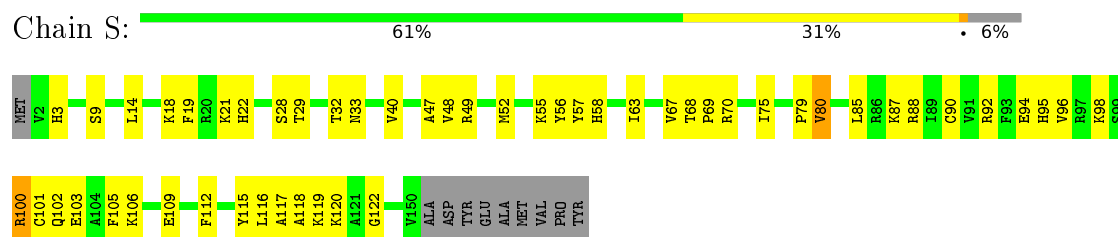
- Molecule 25: ribosomal protein L19e



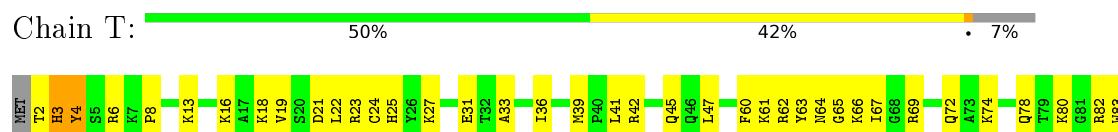
- Molecule 26: ribosomal protein L20e



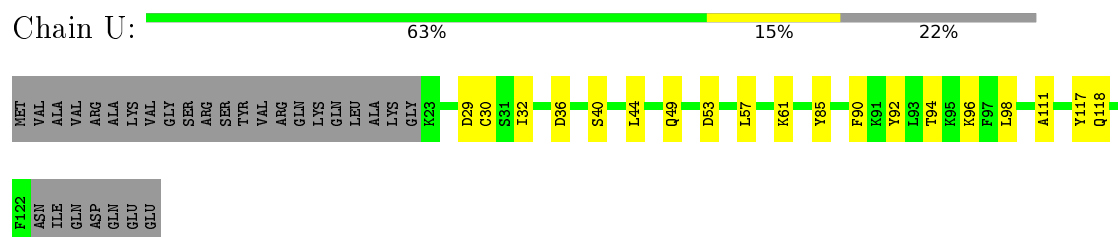
- Molecule 27: ribosomal protein L21e



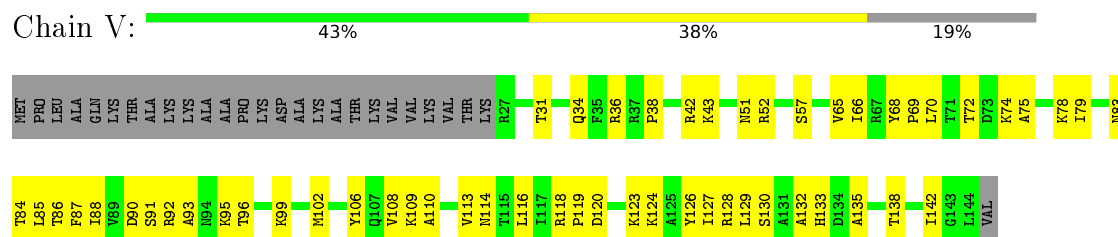
- Molecule 28: ribosomal protein L22



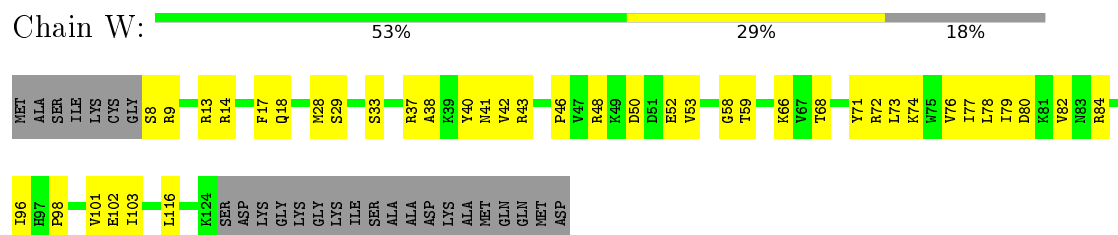
- Molecule 29: ribosomal protein L22e



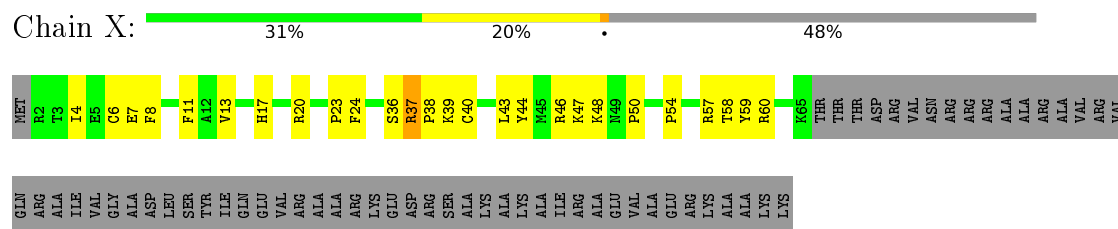
- Molecule 30: ribosomal protein L23



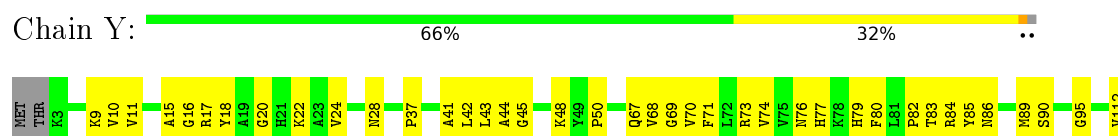
- Molecule 31: ribosomal protein L24



- Molecule 32: ribosomal protein L24e



- Molecule 33: ribosomal protein L27e






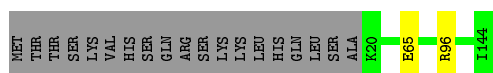


Chain f:  92% • 5%



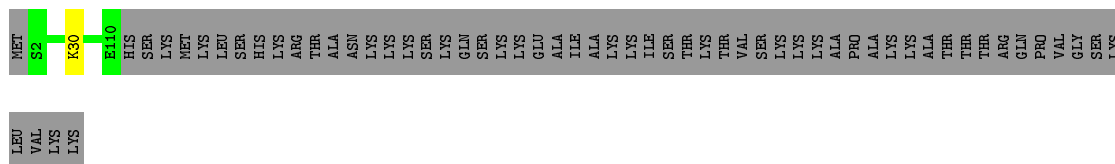
- Molecule 41: ribosomal protein L33e

Chain g:  85% • 13%



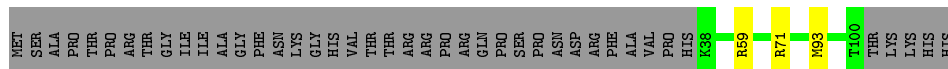
- Molecule 42: ribosomal protein L34e

Chain h:  64% • 35%




- Molecule 43: ribosomal protein L36e

Chain i:  57% • 40%



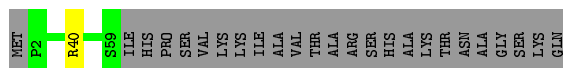
- Molecule 44: ribosomal protein L37e

Chain j:  90% • 6%



- Molecule 45: ribosomal protein L38e

Chain k:  69% • 30%

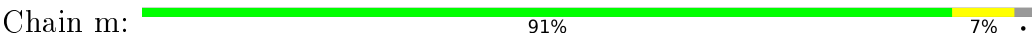


- Molecule 46: ribosomal protein L39e

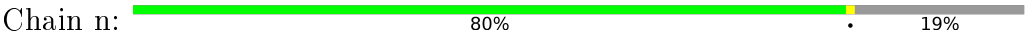
Chain l:  92% • 6%



- Molecule 47: ribosomal protein L43e



• Molecule 48: ribosomal protein L44e



## 4 Experimental information

| Property                             | Value                              | Source    |
|--------------------------------------|------------------------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE                    | Depositor |
| Imposed symmetry                     | POINT, Not provided                | Depositor |
| Number of particles used             | 107134                             | Depositor |
| Resolution determination method      | FSC 0.143                          | Depositor |
| CTF correction method                | Not provided                       | Depositor |
| Microscope                           | FEI TITAN KRIOS                    | Depositor |
| Voltage (kV)                         | 300                                | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 30                                 | Depositor |
| Minimum defocus (nm)                 | 600                                | Depositor |
| Maximum defocus (nm)                 | 2500                               | Depositor |
| Magnification                        | 29000                              | Depositor |
| Image detector                       | K2 Summit direct electron detector | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, MG, OMG, H2U, OMU, A2M

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 2$    | RMSZ        | $\# Z  > 2$     |
| 1   | 1     | 0.75         | 8/36881 (0.0%) | 0.90        | 48/57466 (0.1%) |
| 10  | B     | 0.44         | 0/3086         | 0.55        | 0/4176          |
| 11  | C     | 0.45         | 0/2284         | 0.60        | 0/3092          |
| 12  | D     | 0.25         | 0/800          | 0.49        | 0/1111          |
| 13  | E     | 0.29         | 0/1529         | 0.56        | 0/2056          |
| 14  | F     | 0.40         | 0/1023         | 0.56        | 0/1390          |
| 15  | G     | 0.38         | 0/1798         | 0.59        | 1/2423 (0.0%)   |
| 16  | H     | 0.42         | 0/1628         | 0.60        | 0/2194          |
| 17  | I     | 0.40         | 0/1084         | 0.57        | 0/1454          |
| 18  | J     | 0.39         | 0/941          | 0.61        | 2/1277 (0.2%)   |
| 19  | K     | 0.27         | 0/1077         | 0.59        | 1/1475 (0.1%)   |
| 2   | 2     | 0.60         | 0/26109        | 0.86        | 28/40668 (0.1%) |
| 20  | L     | 0.43         | 0/1123         | 0.56        | 0/1505          |
| 21  | M     | 0.49         | 0/1754         | 0.57        | 0/2342          |
| 22  | N     | 0.27         | 0/1747         | 0.54        | 0/2338          |
| 23  | O     | 0.32         | 0/1583         | 0.50        | 0/2157          |
| 24  | P     | 0.42         | 0/1519         | 0.57        | 0/2040          |
| 25  | Q     | 0.35         | 0/1179         | 0.53        | 0/1588          |
| 26  | R     | 0.42         | 0/1044         | 0.59        | 1/1415 (0.1%)   |
| 27  | S     | 0.43         | 0/1142         | 0.60        | 0/1547          |
| 28  | T     | 0.45         | 0/1249         | 0.65        | 1/1679 (0.1%)   |
| 29  | U     | 0.26         | 0/545          | 0.49        | 0/754           |
| 3   | 3     | 0.48         | 0/4337         | 0.84        | 1/6734 (0.0%)   |
| 30  | V     | 0.42         | 0/907          | 0.51        | 0/1227          |
| 31  | W     | 0.37         | 0/910          | 0.56        | 0/1224          |
| 32  | X     | 0.40         | 0/527          | 0.53        | 0/716           |
| 33  | Y     | 0.37         | 0/934          | 0.51        | 0/1274          |
| 34  | Z     | 0.28         | 0/545          | 0.52        | 0/739           |
| 35  | a     | 0.32         | 0/992          | 0.53        | 0/1326          |
| 36  | b     | 0.34         | 0/514          | 0.50        | 0/690           |
| 37  | c     | 0.42         | 0/1763         | 0.52        | 0/2374          |
| 38  | d     | 0.31         | 0/525          | 0.50        | 0/719           |

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | # Z  >2          | RMSZ        | # Z  >2          |
| 39  | e     | 0.37         | 0/838            | 0.57        | 0/1131           |
| 4   | 4     | 0.69         | 0/3549           | 0.88        | 3/5525 (0.1%)    |
| 40  | f     | 0.46         | 0/1002           | 0.55        | 0/1346           |
| 41  | g     | 0.49         | 0/1003           | 0.53        | 0/1352           |
| 42  | h     | 0.38         | 0/868            | 0.55        | 0/1160           |
| 43  | i     | 0.38         | 0/499            | 0.56        | 0/662            |
| 44  | j     | 0.50         | 0/651            | 0.61        | 0/869            |
| 45  | k     | 0.30         | 0/378            | 0.57        | 0/518            |
| 46  | l     | 0.43         | 0/470            | 0.51        | 0/627            |
| 47  | m     | 0.43         | 0/680            | 0.53        | 0/913            |
| 48  | n     | 0.34         | 0/667            | 0.56        | 0/889            |
| 5   | 5     | 0.69         | 0/1908           | 0.91        | 3/2967 (0.1%)    |
| 6   | 6     | 0.39         | 2/1437 (0.1%)    | 0.79        | 4/2234 (0.2%)    |
| 7   | 7     | 0.76         | 0/3615           | 0.87        | 2/5622 (0.0%)    |
| 8   | 8     | 0.47         | 0/2828           | 0.82        | 0/4401           |
| 9   | A     | 0.47         | 0/1903           | 0.56        | 0/2559           |
| All | All   | 0.59         | 10/125375 (0.0%) | 0.79        | 95/185945 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 10  | B     | 0                   | 2                   |
| 13  | E     | 0                   | 1                   |
| 15  | G     | 0                   | 1                   |
| 16  | H     | 0                   | 1                   |
| 19  | K     | 0                   | 3                   |
| 26  | R     | 0                   | 1                   |
| 27  | S     | 0                   | 1                   |
| 28  | T     | 0                   | 1                   |
| 40  | f     | 0                   | 1                   |
| 9   | A     | 0                   | 1                   |
| All | All   | 0                   | 13                  |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | 1     | 634 | G    | C1'-N9 | -6.69 | 1.37        | 1.46     |
| 1   | 1     | 159 | U    | C1'-N1 | 6.17  | 1.58        | 1.48     |
| 1   | 1     | 568 | U    | C1'-N1 | 6.06  | 1.57        | 1.48     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | 1     | 564 | U    | C1'-N1 | 5.95  | 1.57        | 1.48     |
| 1   | 1     | 565 | U    | C1'-N1 | 5.91  | 1.57        | 1.48     |
| 1   | 1     | 562 | U    | C1'-N1 | 5.88  | 1.57        | 1.48     |
| 6   | 6     | 31  | U    | C1'-N1 | 5.28  | 1.56        | 1.48     |
| 1   | 1     | 692 | A    | N9-C4  | -5.23 | 1.34        | 1.37     |
| 6   | 6     | 39  | U    | C1'-N1 | 5.16  | 1.56        | 1.48     |
| 1   | 1     | 170 | U    | C1'-N1 | 5.09  | 1.56        | 1.48     |

All (95) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 19  | K     | 45   | SER  | C-N-CD    | -11.87 | 94.48       | 120.60   |
| 1   | 1     | 1575 | A    | OP1-P-O3' | -11.81 | 79.22       | 105.20   |
| 1   | 1     | 1757 | U    | C2-N1-C1' | 8.96   | 128.45      | 117.70   |
| 2   | 2     | 776  | C    | N1-C2-O2  | 8.91   | 124.25      | 118.90   |
| 2   | 2     | 776  | C    | C2-N1-C1' | 8.72   | 128.39      | 118.80   |
| 2   | 2     | 24   | C    | C2-N1-C1' | 8.09   | 127.70      | 118.80   |
| 1   | 1     | 1575 | A    | OP2-P-O3' | -8.07  | 87.44       | 105.20   |
| 1   | 1     | 1216 | U    | C2-N1-C1' | 8.01   | 127.32      | 117.70   |
| 2   | 2     | 1275 | C    | N1-C2-O2  | 7.88   | 123.63      | 118.90   |
| 1   | 1     | 1270 | U    | N1-C2-O2  | 7.83   | 128.28      | 122.80   |
| 26  | R     | 22   | PRO  | N-CA-CB   | 7.49   | 112.29      | 103.30   |
| 1   | 1     | 1270 | U    | C2-N1-C1' | 7.48   | 126.68      | 117.70   |
| 1   | 1     | 1216 | U    | N1-C2-O2  | 7.48   | 128.03      | 122.80   |
| 2   | 2     | 24   | C    | N1-C2-O2  | 7.32   | 123.29      | 118.90   |
| 1   | 1     | 1216 | U    | N3-C2-O2  | -7.12  | 117.22      | 122.20   |
| 6   | 6     | 38   | C    | P-O3'-C3' | 7.06   | 128.18      | 119.70   |
| 2   | 2     | 776  | C    | N3-C2-O2  | -7.05  | 116.97      | 121.90   |
| 2   | 2     | 540  | C    | C2-N1-C1' | 6.94   | 126.43      | 118.80   |
| 1   | 1     | 1270 | U    | N3-C2-O2  | -6.94  | 117.34      | 122.20   |
| 1   | 1     | 1576 | C    | OP1-P-OP2 | 6.93   | 129.99      | 119.60   |
| 2   | 2     | 1275 | C    | C2-N1-C1' | 6.89   | 126.38      | 118.80   |
| 1   | 1     | 973  | U    | C2-N1-C1' | 6.86   | 125.93      | 117.70   |
| 2   | 2     | 1275 | C    | N3-C2-O2  | -6.76  | 117.17      | 121.90   |
| 1   | 1     | 1757 | U    | N1-C2-O2  | 6.72   | 127.50      | 122.80   |
| 18  | J     | 112  | LYS  | CB-CA-C   | -6.67  | 97.06       | 110.40   |
| 2   | 2     | 552  | C    | N1-C2-O2  | 6.67   | 122.90      | 118.90   |
| 2   | 2     | 552  | C    | C2-N1-C1' | 6.65   | 126.11      | 118.80   |
| 1   | 1     | 1109 | U    | C2-N1-C1' | 6.62   | 125.64      | 117.70   |
| 1   | 1     | 1602 | U    | C4-C5-C6  | 6.58   | 123.65      | 119.70   |
| 1   | 1     | 1602 | U    | C5-C6-N1  | -6.54  | 119.43      | 122.70   |
| 4   | 4     | 86   | U    | N1-C2-O2  | 6.47   | 127.33      | 122.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | J     | 112  | LYS  | N-CA-C      | 6.45  | 128.41      | 111.00   |
| 1   | 1     | 1757 | U    | N3-C2-O2    | -6.36 | 117.75      | 122.20   |
| 2   | 2     | 360  | U    | OP2-P-O3'   | 6.33  | 119.13      | 105.20   |
| 28  | T     | 4    | TYR  | N-CA-C      | 6.17  | 127.67      | 111.00   |
| 2   | 2     | 776  | C    | C6-N1-C1'   | -6.17 | 113.40      | 120.80   |
| 4   | 4     | 86   | U    | C2-N1-C1'   | 6.16  | 125.09      | 117.70   |
| 15  | G     | 115  | ARG  | C-N-CD      | -6.10 | 107.18      | 120.60   |
| 7   | 7     | 62   | A    | C2-N3-C4    | -6.09 | 107.56      | 110.60   |
| 1   | 1     | 1757 | U    | C6-N1-C1'   | -6.07 | 112.70      | 121.20   |
| 6   | 6     | 31   | U    | C2'-C3'-O3' | 6.04  | 123.37      | 113.70   |
| 1   | 1     | 1618 | U    | C2-N1-C1'   | 5.99  | 124.89      | 117.70   |
| 1   | 1     | 912  | C    | C2-N1-C1'   | 5.96  | 125.36      | 118.80   |
| 2   | 2     | 1404 | H2U  | P-O3'-C3'   | -5.94 | 112.58      | 119.70   |
| 2   | 2     | 24   | C    | N3-C2-O2    | -5.93 | 117.75      | 121.90   |
| 2   | 2     | 61   | C    | C2-N1-C1'   | 5.78  | 125.16      | 118.80   |
| 4   | 4     | 86   | U    | N3-C2-O2    | -5.78 | 118.16      | 122.20   |
| 2   | 2     | 24   | C    | C6-N1-C1'   | -5.77 | 113.87      | 120.80   |
| 1   | 1     | 170  | U    | OP1-P-O3'   | 5.76  | 117.87      | 105.20   |
| 5   | 5     | 112  | A    | N7-C8-N9    | 5.72  | 116.66      | 113.80   |
| 2   | 2     | 1441 | G    | O4'-C1'-N9  | 5.65  | 112.72      | 108.20   |
| 1   | 1     | 665  | C    | O4'-C1'-N1  | 5.61  | 112.69      | 108.20   |
| 2   | 2     | 782  | G    | OP1-P-O3'   | 5.61  | 117.54      | 105.20   |
| 2   | 2     | 1289 | G    | C4-N9-C1'   | 5.59  | 133.77      | 126.50   |
| 1   | 1     | 205  | A    | OP1-P-O3'   | 5.58  | 117.49      | 105.20   |
| 1   | 1     | 912  | C    | N3-C2-O2    | -5.51 | 118.04      | 121.90   |
| 1   | 1     | 1012 | C    | N1-C2-O2    | 5.49  | 122.20      | 118.90   |
| 2   | 2     | 540  | C    | C6-N1-C1'   | -5.47 | 114.24      | 120.80   |
| 1   | 1     | 912  | C    | N1-C2-O2    | 5.42  | 122.15      | 118.90   |
| 2   | 2     | 776  | C    | C6-N1-C2    | -5.42 | 118.13      | 120.30   |
| 1   | 1     | 1657 | U    | O4'-C1'-N1  | 5.40  | 112.52      | 108.20   |
| 1   | 1     | 1012 | C    | C2-N1-C1'   | 5.39  | 124.73      | 118.80   |
| 1   | 1     | 1618 | U    | N3-C2-O2    | -5.38 | 118.43      | 122.20   |
| 6   | 6     | 41   | G    | C2'-C3'-O3' | 5.38  | 122.30      | 113.70   |
| 6   | 6     | 39   | U    | O5'-P-OP1   | -5.37 | 100.87      | 105.70   |
| 1   | 1     | 995  | C    | C2-N1-C1'   | 5.35  | 124.69      | 118.80   |
| 1   | 1     | 301  | A    | O4'-C1'-N9  | 5.34  | 112.48      | 108.20   |
| 3   | 3     | 108  | A    | P-O3'-C3'   | 5.34  | 126.11      | 119.70   |
| 1   | 1     | 458  | A    | O4'-C1'-N9  | 5.26  | 112.41      | 108.20   |
| 2   | 2     | 540  | C    | N1-C2-O2    | 5.20  | 122.02      | 118.90   |
| 5   | 5     | 112  | A    | C8-N9-C4    | -5.20 | 103.72      | 105.80   |
| 1   | 1     | 824  | U    | C2-N1-C1'   | 5.19  | 123.93      | 117.70   |
| 1   | 1     | 1434 | U    | C2-N1-C1'   | 5.17  | 123.91      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2   | 2     | 1155 | C    | N3-C2-O2   | -5.17 | 118.28      | 121.90   |
| 1   | 1     | 229  | C    | P-O3'-C3'  | 5.16  | 125.89      | 119.70   |
| 2   | 2     | 360  | U    | P-O3'-C3'  | 5.16  | 125.89      | 119.70   |
| 1   | 1     | 1263 | A    | P-O3'-C3'  | 5.13  | 125.86      | 119.70   |
| 1   | 1     | 1596 | A    | O5'-P-OP1  | -5.12 | 101.09      | 105.70   |
| 2   | 2     | 1393 | U    | P-O3'-C3'  | 5.12  | 125.85      | 119.70   |
| 1   | 1     | 141  | U    | P-O3'-C3'  | 5.12  | 125.85      | 119.70   |
| 1   | 1     | 1388 | U    | P-O3'-C3'  | 5.12  | 125.85      | 119.70   |
| 1   | 1     | 1600 | A    | O4'-C1'-N9 | 5.12  | 112.30      | 108.20   |
| 1   | 1     | 1618 | U    | N1-C2-O2   | 5.12  | 126.38      | 122.80   |
| 1   | 1     | 136  | G    | OP1-P-O3'  | 5.12  | 116.46      | 105.20   |
| 1   | 1     | 1239 | U    | P-O3'-C3'  | 5.11  | 125.83      | 119.70   |
| 5   | 5     | 113  | A    | P-O3'-C3'  | 5.09  | 125.80      | 119.70   |
| 1   | 1     | 542  | C    | P-O3'-C3'  | 5.08  | 125.80      | 119.70   |
| 1   | 1     | 1493 | G    | O4'-C1'-N9 | 5.08  | 112.27      | 108.20   |
| 1   | 1     | 1216 | U    | C6-N1-C1'  | -5.06 | 114.12      | 121.20   |
| 1   | 1     | 1602 | U    | N1-C2-N3   | 5.05  | 117.93      | 114.90   |
| 2   | 2     | 755  | U    | P-O3'-C3'  | 5.04  | 125.75      | 119.70   |
| 7   | 7     | 140  | U    | C2-N1-C1'  | 5.03  | 123.74      | 117.70   |
| 1   | 1     | 205  | A    | P-O3'-C3'  | 5.02  | 125.73      | 119.70   |
| 2   | 2     | 552  | C    | C6-N1-C1'  | -5.01 | 114.78      | 120.80   |
| 1   | 1     | 1216 | U    | C5-C6-N1   | 5.01  | 125.20      | 122.70   |

There are no chirality outliers.

All (13) planarity outliers are listed below:

| Mol | Chain | Res    | Type | Group     |
|-----|-------|--------|------|-----------|
| 9   | A     | 60[B]  | ARG  | Mainchain |
| 10  | B     | 337    | GLY  | Peptide   |
| 10  | B     | 373    | GLY  | Peptide   |
| 13  | E     | 136    | PRO  | Peptide   |
| 15  | G     | 114    | ALA  | Peptide   |
| 16  | H     | 151    | GLU  | Peptide   |
| 19  | K     | 107    | HIS  | Peptide   |
| 19  | K     | 126    | ASN  | Peptide   |
| 19  | K     | 40     | TYR  | Peptide   |
| 26  | R     | 17     | PRO  | Peptide   |
| 27  | S     | 100[B] | ARG  | Mainchain |
| 28  | T     | 3      | HIS  | Peptide   |
| 40  | f     | 9      | ALA  | Peptide   |

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 33313 | 0        | 16798    | 1118    | 0            |
| 2   | 2     | 23926 | 0        | 12113    | 740     | 0            |
| 3   | 3     | 3893  | 0        | 1971     | 147     | 0            |
| 4   | 4     | 3177  | 0        | 1611     | 112     | 0            |
| 5   | 5     | 1708  | 0        | 867      | 59      | 0            |
| 6   | 6     | 1288  | 0        | 657      | 184     | 0            |
| 7   | 7     | 3280  | 0        | 1664     | 103     | 0            |
| 8   | 8     | 2531  | 0        | 1281     | 155     | 0            |
| 9   | A     | 1859  | 0        | 1901     | 128     | 0            |
| 10  | B     | 3020  | 0        | 3003     | 172     | 0            |
| 11  | C     | 2237  | 0        | 2231     | 118     | 0            |
| 12  | D     | 799   | 0        | 374      | 5       | 0            |
| 13  | E     | 1509  | 0        | 1595     | 122     | 0            |
| 14  | F     | 1002  | 0        | 994      | 55      | 0            |
| 15  | G     | 1772  | 0        | 1853     | 108     | 0            |
| 16  | H     | 1596  | 0        | 1683     | 143     | 0            |
| 17  | I     | 1061  | 0        | 1123     | 64      | 0            |
| 18  | J     | 924   | 0        | 934      | 60      | 0            |
| 19  | K     | 1061  | 0        | 939      | 196     | 0            |
| 20  | L     | 1096  | 0        | 1096     | 52      | 0            |
| 21  | M     | 1714  | 0        | 1793     | 95      | 0            |
| 22  | N     | 1714  | 0        | 1786     | 111     | 0            |
| 23  | O     | 1557  | 0        | 1351     | 84      | 0            |
| 24  | P     | 1494  | 0        | 1554     | 83      | 0            |
| 25  | Q     | 1162  | 0        | 1130     | 74      | 0            |
| 26  | R     | 1019  | 0        | 981      | 52      | 0            |
| 27  | S     | 1112  | 0        | 1051     | 57      | 0            |
| 28  | T     | 1221  | 0        | 1230     | 98      | 0            |
| 29  | U     | 541   | 0        | 295      | 10      | 0            |
| 30  | V     | 892   | 0        | 903      | 48      | 0            |
| 31  | W     | 896   | 0        | 915      | 36      | 0            |
| 32  | X     | 508   | 0        | 477      | 25      | 0            |
| 33  | Y     | 914   | 0        | 813      | 40      | 0            |
| 34  | Z     | 538   | 0        | 479      | 18      | 0            |
| 35  | a     | 982   | 0        | 1029     | 0       | 0            |
| 36  | b     | 503   | 0        | 500      | 0       | 0            |
| 37  | c     | 1732  | 0        | 1768     | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 38  | d     | 518    | 0        | 462      | 0       | 0            |
| 39  | e     | 824    | 0        | 839      | 0       | 0            |
| 40  | f     | 982    | 0        | 985      | 0       | 0            |
| 41  | g     | 983    | 0        | 1006     | 0       | 0            |
| 42  | h     | 856    | 0        | 873      | 0       | 0            |
| 43  | i     | 494    | 0        | 535      | 0       | 0            |
| 44  | j     | 639    | 0        | 641      | 0       | 0            |
| 45  | k     | 373    | 0        | 302      | 0       | 0            |
| 46  | l     | 457    | 0        | 484      | 0       | 0            |
| 47  | m     | 668    | 0        | 648      | 0       | 0            |
| 48  | n     | 659    | 0        | 672      | 0       | 0            |
| 49  | 1     | 51     | 0        | 0        | 0       | 0            |
| 49  | 2     | 25     | 0        | 0        | 0       | 0            |
| 49  | 3     | 3      | 0        | 0        | 0       | 0            |
| 49  | 4     | 2      | 0        | 0        | 0       | 0            |
| 49  | 5     | 4      | 0        | 0        | 0       | 0            |
| 49  | 7     | 9      | 0        | 0        | 0       | 0            |
| 49  | C     | 1      | 0        | 0        | 0       | 0            |
| 49  | K     | 1      | 0        | 0        | 0       | 0            |
| 49  | M     | 3      | 0        | 0        | 0       | 0            |
| 49  | V     | 1      | 0        | 0        | 0       | 0            |
| 49  | a     | 1      | 0        | 0        | 0       | 0            |
| 49  | f     | 2      | 0        | 0        | 0       | 0            |
| 49  | g     | 1      | 0        | 0        | 0       | 0            |
| 49  | h     | 1      | 0        | 0        | 0       | 0            |
| 49  | j     | 4      | 0        | 0        | 0       | 0            |
| 50  | 1     | 72     | 0        | 0        | 18      | 0            |
| 50  | 2     | 40     | 0        | 0        | 17      | 0            |
| 50  | 4     | 4      | 0        | 0        | 1       | 0            |
| 50  | 5     | 4      | 0        | 0        | 0       | 0            |
| 50  | 7     | 16     | 0        | 0        | 2       | 0            |
| 50  | 8     | 1      | 0        | 0        | 1       | 0            |
| 50  | A     | 2      | 0        | 0        | 1       | 0            |
| 50  | G     | 1      | 0        | 0        | 0       | 0            |
| 50  | M     | 2      | 0        | 0        | 0       | 0            |
| 50  | i     | 1      | 0        | 0        | 0       | 0            |
| 50  | j     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 117257 | 0        | 80190    | 3902    | 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 25.

All (3902) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:57:U:H2'     | 3:3:58:C:C5      | 1.26                     | 1.62              |
| 19:K:89:VAL:CG1  | 26:R:73:ALA:HB2  | 1.26                     | 1.56              |
| 19:K:89:VAL:HG12 | 26:R:73:ALA:CB   | 1.38                     | 1.50              |
| 24:P:17:HIS:CE1  | 24:P:18:HIS:HD1  | 1.29                     | 1.50              |
| 25:Q:23:TRP:CE3  | 25:Q:51:ILE:CD1  | 2.02                     | 1.42              |
| 24:P:17:HIS:CE1  | 24:P:18:HIS:ND1  | 1.85                     | 1.39              |
| 19:K:78:ARG:HH12 | 19:K:107:HIS:CE1 | 1.41                     | 1.38              |
| 16:H:200:ALA:HB1 | 19:K:185:VAL:CG1 | 1.51                     | 1.36              |
| 1:1:1392:G:C6    | 19:K:105:TRP:HH2 | 1.43                     | 1.36              |
| 1:1:1392:G:O6    | 19:K:105:TRP:CH2 | 1.78                     | 1.36              |
| 16:H:203:GLU:OE2 | 19:K:185:VAL:CG2 | 1.75                     | 1.34              |
| 19:K:95:LEU:HD11 | 19:K:106:ARG:CD  | 1.55                     | 1.34              |
| 16:H:49:LYS:NZ   | 19:K:37:THR:N    | 1.73                     | 1.34              |
| 3:3:57:U:C2'     | 3:3:58:C:C5      | 2.09                     | 1.33              |
| 19:K:89:VAL:CG1  | 26:R:73:ALA:CB   | 1.95                     | 1.31              |
| 22:N:121:LYS:HD2 | 22:N:122:PRO:CD  | 1.61                     | 1.30              |
| 1:1:1392:G:O6    | 19:K:105:TRP:HH2 | 1.02                     | 1.30              |
| 6:6:17:U:H5      | 19:K:43:PRO:CG   | 1.42                     | 1.29              |
| 19:K:78:ARG:NH1  | 19:K:107:HIS:HE1 | 1.31                     | 1.28              |
| 1:1:439:U:O5'    | 28:T:2:THR:N     | 1.68                     | 1.27              |
| 25:Q:23:TRP:CE3  | 25:Q:51:ILE:HD13 | 1.62                     | 1.27              |
| 4:4:95:U:OP2     | 25:Q:62:ARG:NH2  | 1.65                     | 1.26              |
| 3:3:106:U:O2     | 3:3:129:G:O6     | 1.53                     | 1.26              |
| 19:K:69:ARG:O    | 19:K:84:VAL:HG23 | 1.10                     | 1.26              |
| 10:B:282:GLN:NE2 | 10:B:336:SER:OG  | 1.68                     | 1.26              |
| 25:Q:23:TRP:HE3  | 25:Q:51:ILE:CD1  | 1.42                     | 1.25              |
| 1:1:238:A:N6     | 1:1:239:U:O4     | 1.71                     | 1.24              |
| 6:6:17:U:C5      | 19:K:43:PRO:HG2  | 1.71                     | 1.23              |
| 22:N:121:LYS:CD  | 22:N:122:PRO:HD2 | 1.68                     | 1.23              |
| 16:H:49:LYS:HZ2  | 19:K:37:THR:N    | 1.27                     | 1.22              |
| 18:J:106:ASN:OD1 | 18:J:107:PRO:HD2 | 1.38                     | 1.20              |
| 24:P:17:HIS:CE1  | 24:P:18:HIS:CE1  | 2.28                     | 1.20              |
| 1:1:1392:G:C6    | 19:K:105:TRP:CH2 | 2.30                     | 1.18              |
| 14:F:195:TRP:O   | 19:K:164:THR:OG1 | 1.59                     | 1.18              |
| 28:T:6:ARG:NH2   | 28:T:116:HIS:HB2 | 1.57                     | 1.17              |
| 10:B:369:SER:OG  | 10:B:378:GLN:OE1 | 1.62                     | 1.17              |
| 13:E:137:SER:O   | 13:E:140:LYS:HG2 | 1.44                     | 1.17              |
| 1:1:439:U:C5'    | 28:T:2:THR:N     | 2.08                     | 1.16              |
| 1:1:1674:U:O4    | 1:1:1728:G:N2    | 1.78                     | 1.15              |
| 8:8:48:G:N2      | 8:8:49:U:H1'     | 1.58                     | 1.15              |
| 19:K:89:VAL:HG12 | 26:R:73:ALA:HB1  | 1.29                     | 1.14              |
| 22:N:121:LYS:CD  | 22:N:122:PRO:CD  | 2.25                     | 1.13              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:8:48:G:N2      | 8:8:49:U:C1'      | 2.10                     | 1.13              |
| 6:6:17:U:C5      | 19:K:43:PRO:CG    | 2.30                     | 1.11              |
| 3:3:106:U:O2     | 3:3:129:G:C6      | 2.04                     | 1.11              |
| 19:K:78:ARG:NH1  | 19:K:107:HIS:CE1  | 2.08                     | 1.10              |
| 2:2:1151:U:H2'   | 2:2:1152:U:H5'    | 1.34                     | 1.09              |
| 1:1:439:U:O4     | 28:T:3:HIS:CE1    | 2.04                     | 1.09              |
| 2:2:690:C:O2     | 2:2:749:G:N2      | 1.85                     | 1.08              |
| 3:3:4:U:C4       | 33:Y:17:ARG:NH1   | 2.21                     | 1.08              |
| 6:6:10:C:H2'     | 6:6:13:C:H41      | 1.16                     | 1.08              |
| 8:8:2:C:C4       | 8:8:120:C:O2      | 2.07                     | 1.08              |
| 19:K:180:HIS:NE2 | 19:K:184:LYS:HE2  | 1.67                     | 1.08              |
| 8:8:40:U:O2'     | 8:8:44:A:N6       | 1.85                     | 1.08              |
| 19:K:69:ARG:O    | 19:K:84:VAL:CG2   | 2.00                     | 1.08              |
| 16:H:200:ALA:HB1 | 19:K:185:VAL:HG12 | 1.33                     | 1.08              |
| 2:2:1079:OMG:N2  | 2:2:1237:C:O2     | 1.88                     | 1.07              |
| 2:2:1318:OMC:H6  | 2:2:1318:OMC:H5'  | 1.19                     | 1.06              |
| 3:3:209:G:H2'    | 3:3:210:G:H5'     | 1.33                     | 1.06              |
| 6:6:34:C:H3'     | 6:6:35:U:H6       | 1.19                     | 1.06              |
| 16:H:200:ALA:CB  | 19:K:185:VAL:CG1  | 2.33                     | 1.05              |
| 19:K:95:LEU:CD1  | 19:K:106:ARG:HD3  | 1.86                     | 1.05              |
| 22:N:121:LYS:HD2 | 22:N:122:PRO:HD3  | 1.12                     | 1.04              |
| 1:1:1729:A:C2    | 1:1:1730:A:N7     | 2.25                     | 1.04              |
| 6:6:30:C:H5'     | 6:6:30:C:H6       | 1.19                     | 1.04              |
| 18:J:112:LYS:HG3 | 18:J:112:LYS:O    | 1.24                     | 1.04              |
| 16:H:148:TYR:CD1 | 19:K:59:MET:CB    | 2.40                     | 1.04              |
| 18:J:106:ASN:OD1 | 18:J:107:PRO:CD   | 2.05                     | 1.03              |
| 1:1:353:C:OP2    | 17:I:107:LYS:NZ   | 1.91                     | 1.03              |
| 6:6:28:A:C2      | 6:6:29:G:C6       | 2.47                     | 1.03              |
| 25:Q:23:TRP:CZ3  | 25:Q:51:ILE:HD11  | 1.93                     | 1.03              |
| 25:Q:23:TRP:HE3  | 25:Q:51:ILE:HD12  | 1.21                     | 1.03              |
| 25:Q:23:TRP:CZ3  | 25:Q:51:ILE:CD1   | 2.41                     | 1.03              |
| 6:6:41:G:H3'     | 19:K:180:HIS:CE1  | 1.93                     | 1.02              |
| 10:B:367:ASP:OD2 | 32:X:17:HIS:NE2   | 1.91                     | 1.02              |
| 2:2:1444:A:N7    | 6:6:6:G:N2        | 2.05                     | 1.02              |
| 19:K:180:HIS:HA  | 19:K:183:ARG:HG2  | 1.40                     | 1.02              |
| 3:3:106:U:C2     | 3:3:129:G:O6      | 2.12                     | 1.02              |
| 19:K:93:ARG:HD2  | 19:K:108:VAL:CG1  | 1.89                     | 1.02              |
| 1:1:48:OMU:HM22  | 1:1:49:C:C5'      | 1.90                     | 1.02              |
| 2:2:1079:OMG:N1  | 2:2:1237:C:N3     | 2.06                     | 1.02              |
| 2:2:591:A2M:HM'2 | 2:2:592:C:H5'     | 1.42                     | 1.02              |
| 2:2:569:G:O2'    | 2:2:571:OMG:OP2   | 1.78                     | 1.01              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:452:G:N2      | 2:2:482:G:N7      | 2.08                     | 1.01              |
| 18:J:106:ASN:CG   | 18:J:107:PRO:HD2  | 1.80                     | 1.01              |
| 2:2:1151:U:C2'    | 2:2:1152:U:H5'    | 1.89                     | 1.01              |
| 2:2:749:G:O2'     | 2:2:750:U:O5'     | 1.79                     | 1.01              |
| 6:6:22:G:O6       | 6:6:27:G:OP2      | 1.76                     | 1.01              |
| 8:8:37:C:N4       | 8:8:48:G:H1'      | 1.76                     | 1.00              |
| 1:1:48:OMU:HM22   | 1:1:49:C:H5'      | 1.00                     | 0.99              |
| 1:1:34:C:H2'      | 1:1:35:U:H5'      | 1.45                     | 0.99              |
| 16:H:203:GLU:OE2  | 19:K:185:VAL:HG21 | 0.81                     | 0.98              |
| 6:6:34:C:H3'      | 6:6:35:U:C6       | 1.98                     | 0.98              |
| 22:N:121:LYS:CE   | 22:N:122:PRO:HD2  | 1.92                     | 0.98              |
| 25:Q:8:ALA:HB1    | 25:Q:19:ARG:NH1   | 1.79                     | 0.98              |
| 7:7:55:U:H3       | 7:7:62:A:H2       | 1.10                     | 0.97              |
| 18:J:112:LYS:O    | 18:J:112:LYS:CG   | 2.10                     | 0.97              |
| 6:6:7:A:N1        | 6:6:59:C:N4       | 2.13                     | 0.97              |
| 24:P:101:ARG:HH21 | 24:P:101:ARG:HG2  | 1.27                     | 0.97              |
| 1:1:959:OMG:HM23  | 21:M:81:TYR:OH    | 1.62                     | 0.97              |
| 2:2:666:C:N4      | 2:2:1034:G:O6     | 1.96                     | 0.97              |
| 21:M:71:ARG:HG2   | 21:M:94:LEU:HB2   | 1.47                     | 0.96              |
| 1:1:439:U:P       | 28:T:2:THR:N      | 2.37                     | 0.96              |
| 8:8:3:G:H1        | 8:8:120:C:H42     | 1.04                     | 0.95              |
| 23:O:18:VAL:CG2   | 23:O:24:ARG:HH21  | 1.78                     | 0.95              |
| 1:1:1540:U:OP1    | 28:T:82:ARG:NH2   | 1.97                     | 0.95              |
| 2:2:1317:G:O6     | 2:2:1387:C:N4     | 2.00                     | 0.95              |
| 6:6:17:U:H4'      | 6:6:18:A:H5'      | 1.46                     | 0.95              |
| 2:2:973:C:N4      | 2:2:977:A:N7      | 2.15                     | 0.95              |
| 1:1:454:U:HO2'    | 1:1:455:G:H8      | 0.99                     | 0.95              |
| 10:B:19:ARG:HB2   | 10:B:237:ARG:HH21 | 1.31                     | 0.95              |
| 6:6:40:C:H3'      | 6:6:40:C:P        | 2.08                     | 0.94              |
| 2:2:1254:OMG:H5'' | 2:2:1255:G:OP2    | 1.65                     | 0.94              |
| 1:1:439:U:H5'     | 28:T:2:THR:N      | 1.78                     | 0.94              |
| 7:7:145:G:H4'     | 30:V:52:ARG:HH11  | 1.32                     | 0.93              |
| 2:2:667:OMU:C5'   | 2:2:667:OMU:H6    | 1.98                     | 0.93              |
| 19:K:68:GLY:HA2   | 19:K:85:ILE:O     | 1.69                     | 0.93              |
| 2:2:628:A2M:OP1   | 16:H:103:ARG:NH1  | 2.02                     | 0.93              |
| 25:Q:8:ALA:HB1    | 25:Q:19:ARG:HH12  | 1.30                     | 0.93              |
| 28:T:6:ARG:HH21   | 28:T:116:HIS:HB2  | 1.34                     | 0.93              |
| 3:3:42:U:H3       | 3:3:178:G:H1      | 1.17                     | 0.93              |
| 6:6:33:G:H5'      | 19:K:42:VAL:CG2   | 1.99                     | 0.93              |
| 8:8:2:C:N3        | 8:8:120:C:O2      | 2.00                     | 0.93              |
| 24:P:17:HIS:NE2   | 24:P:18:HIS:CE1   | 2.35                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:130:U:H3      | 1:1:136:G:H1      | 0.93                     | 0.92              |
| 1:1:678:A2M:N6    | 2:2:617:G:N3      | 2.16                     | 0.92              |
| 23:O:18:VAL:HG22  | 23:O:24:ARG:HH21  | 1.32                     | 0.92              |
| 1:1:1674:U:C4     | 1:1:1728:G:N2     | 2.38                     | 0.92              |
| 1:1:844:C:H5''    | 20:L:5:PHE:O      | 1.69                     | 0.92              |
| 1:1:48:OMU:CM2    | 1:1:49:C:H5'      | 1.96                     | 0.92              |
| 2:2:667:OMU:H5'   | 2:2:667:OMU:H6    | 1.52                     | 0.92              |
| 2:2:443:OMC:H5''  | 2:2:488:A:N6      | 1.84                     | 0.91              |
| 19:K:95:LEU:HD11  | 19:K:106:ARG:HD3  | 0.92                     | 0.91              |
| 19:K:180:HIS:HB2  | 19:K:183:ARG:HH11 | 1.35                     | 0.91              |
| 1:1:239:U:O2'     | 1:1:240:U:OP2     | 1.86                     | 0.91              |
| 6:6:10:C:H2'      | 6:6:13:C:N4       | 1.84                     | 0.91              |
| 6:6:28:A:N3       | 6:6:29:G:C5       | 2.38                     | 0.91              |
| 1:1:174:U:H3      | 1:1:283:G:H1      | 0.92                     | 0.91              |
| 8:8:2:C:N4        | 8:8:120:C:O2      | 2.03                     | 0.90              |
| 1:1:895:G:H1      | 1:1:900:C:H42     | 1.18                     | 0.90              |
| 8:8:74:U:H3       | 8:8:105:C:H42     | 1.18                     | 0.90              |
| 6:6:30:C:H5'      | 6:6:30:C:C6       | 2.07                     | 0.90              |
| 2:2:390:A:H1'     | 2:2:527:A2M:N6    | 1.85                     | 0.90              |
| 19:K:73:ILE:HG13  | 19:K:114:VAL:HG22 | 1.52                     | 0.90              |
| 2:2:103:G:N2      | 2:2:117:A:N7      | 2.19                     | 0.90              |
| 3:3:57:U:O2'      | 3:3:58:C:C6       | 2.23                     | 0.90              |
| 7:7:145:G:H4'     | 30:V:52:ARG:NH1   | 1.87                     | 0.90              |
| 16:H:200:ALA:HB1  | 19:K:185:VAL:HG13 | 1.52                     | 0.89              |
| 16:H:203:GLU:CD   | 19:K:185:VAL:HG21 | 1.92                     | 0.89              |
| 9:A:65:HIS:HB2    | 9:A:72:VAL:HG13   | 1.51                     | 0.89              |
| 2:2:1318:OMC:HM21 | 10:B:244:PRO:HD3  | 1.55                     | 0.89              |
| 1:1:439:U:O4      | 28:T:3:HIS:HE1    | 1.50                     | 0.89              |
| 22:N:121:LYS:CG   | 22:N:122:PRO:HD2  | 2.02                     | 0.88              |
| 19:K:180:HIS:O    | 19:K:183:ARG:HG2  | 1.72                     | 0.88              |
| 1:1:990:U:OP2     | 20:L:26:ARG:NH1   | 2.06                     | 0.88              |
| 1:1:1048:A:N6     | 1:1:1102:U:O4     | 2.06                     | 0.88              |
| 1:1:412:G:H22     | 1:1:415:A:H5''    | 1.38                     | 0.88              |
| 2:2:70:A:C2'      | 2:2:71:OMG:H5'    | 2.03                     | 0.88              |
| 4:4:133:C:N3      | 4:4:157:A:N6      | 2.20                     | 0.88              |
| 6:6:30:C:O2'      | 6:6:31:U:OP1      | 1.91                     | 0.88              |
| 2:2:1340:G:H5'    | 13:E:169:LYS:HE2  | 1.56                     | 0.88              |
| 6:6:38:C:OP1      | 19:K:176:ARG:NH2  | 2.07                     | 0.88              |
| 19:K:89:VAL:HG11  | 26:R:73:ALA:HB2   | 0.91                     | 0.88              |
| 6:6:54:A:C2'      | 6:6:55:U:H5'      | 2.04                     | 0.88              |
| 2:2:400:U:H5''    | 9:A:242:ARG:O     | 1.74                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:72:G:H5''     | 10:B:250:GLY:HA3  | 1.54                     | 0.87              |
| 2:2:443:OMC:C5'   | 2:2:488:A:H61     | 1.86                     | 0.87              |
| 6:6:41:G:H22      | 19:K:173:VAL:HG12 | 1.36                     | 0.87              |
| 16:H:138:VAL:HG22 | 19:K:44:LEU:O     | 1.74                     | 0.87              |
| 2:2:1318:OMC:HM21 | 10:B:244:PRO:CD   | 2.03                     | 0.87              |
| 2:2:70:A:H2'      | 2:2:71:OMG:H5'    | 1.54                     | 0.87              |
| 2:2:362:A:H8      | 4:4:90:G:H21      | 1.18                     | 0.87              |
| 8:8:48:G:H21      | 8:8:49:U:C1'      | 1.83                     | 0.87              |
| 19:K:180:HIS:CA   | 19:K:183:ARG:HG2  | 2.04                     | 0.87              |
| 1:1:36:OMU:H4'    | 20:L:32:ARG:HD2   | 1.56                     | 0.87              |
| 22:N:121:LYS:HE3  | 22:N:122:PRO:HD2  | 1.56                     | 0.87              |
| 2:2:1157:G:N7     | 27:S:87:LYS:NZ    | 2.22                     | 0.87              |
| 4:4:76:C:H5       | 4:4:119:A:H62     | 1.21                     | 0.87              |
| 13:E:8:CYS:SG     | 13:E:70:ASN:ND2   | 2.48                     | 0.87              |
| 1:1:1443:U:H1'    | 24:P:17:HIS:CE1   | 2.09                     | 0.87              |
| 7:7:70:C:N3       | 7:7:88:A:N6       | 2.23                     | 0.86              |
| 1:1:439:U:C6      | 28:T:2:THR:HA     | 2.10                     | 0.86              |
| 19:K:180:HIS:O    | 19:K:183:ARG:CG   | 2.23                     | 0.86              |
| 2:2:1005:G:O2'    | 15:G:119:PHE:CD2  | 2.28                     | 0.86              |
| 1:1:36:OMU:CM2    | 1:1:94:A:O2'      | 2.23                     | 0.86              |
| 1:1:1057:A:H61    | 1:1:1095:U:H3     | 1.21                     | 0.86              |
| 2:2:425:C:H5      | 9:A:173:GLY:H     | 1.22                     | 0.86              |
| 26:R:40:LYS:NZ    | 26:R:63:CYS:SG    | 2.48                     | 0.86              |
| 1:1:243:G:H1      | 1:1:259:G:H1      | 1.22                     | 0.86              |
| 25:Q:51:ILE:HD12  | 25:Q:51:ILE:H     | 1.38                     | 0.86              |
| 2:2:1398:OMC:HM22 | 2:2:1399:C:O4'    | 1.76                     | 0.86              |
| 6:6:17:U:H5       | 19:K:43:PRO:HG3   | 1.41                     | 0.86              |
| 28:T:6:ARG:HH22   | 28:T:116:HIS:HB2  | 1.40                     | 0.86              |
| 1:1:1543:C:O2     | 2:2:599:G:N2      | 2.09                     | 0.86              |
| 19:K:95:LEU:HD11  | 19:K:106:ARG:NE   | 1.90                     | 0.85              |
| 1:1:778:C:H42     | 1:1:797:A:H61     | 1.23                     | 0.85              |
| 19:K:95:LEU:CD1   | 19:K:106:ARG:CD   | 2.50                     | 0.85              |
| 23:O:152:LEU:HG   | 23:O:169:LEU:HD12 | 1.59                     | 0.85              |
| 1:1:35:U:C2'      | 1:1:36:OMU:H5''   | 2.06                     | 0.85              |
| 1:1:547:U:C5      | 1:1:1393:A:C6     | 2.65                     | 0.85              |
| 4:4:95:U:H5       | 25:Q:62:ARG:CZ    | 1.90                     | 0.84              |
| 2:2:535:U:O2'     | 2:2:536:C:H5'     | 1.75                     | 0.84              |
| 3:3:22:G:O6       | 3:3:209:G:N1      | 2.10                     | 0.84              |
| 2:2:749:G:H2'     | 2:2:750:U:C6      | 2.13                     | 0.84              |
| 3:3:57:U:O2'      | 3:3:58:C:C5       | 2.29                     | 0.84              |
| 25:Q:23:TRP:HZ3   | 25:Q:51:ILE:HD11  | 1.42                     | 0.84              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:4:95:U:C5      | 25:Q:62:ARG:CZ    | 2.60                     | 0.84              |
| 6:6:17:U:C6      | 19:K:43:PRO:HG2   | 2.12                     | 0.84              |
| 1:1:1778:G:H1    | 2:2:6:A:H61       | 1.26                     | 0.84              |
| 25:Q:19:ARG:HD2  | 25:Q:20:ALA:H     | 1.42                     | 0.84              |
| 22:N:99:ILE:HG22 | 22:N:121:LYS:O    | 1.78                     | 0.84              |
| 8:8:48:G:H21     | 8:8:49:U:H1'      | 1.41                     | 0.83              |
| 8:8:66:A:H3'     | 8:8:67:G:H21      | 1.43                     | 0.83              |
| 10:B:337:GLY:HA3 | 10:B:343:MET:HE1  | 1.60                     | 0.83              |
| 23:O:38:LEU:HD21 | 27:S:70:ARG:HE    | 1.43                     | 0.83              |
| 3:3:107:U:O4     | 3:3:128:C:C5      | 2.31                     | 0.83              |
| 5:5:125:A:H5'    | 5:5:125:A:C8      | 2.14                     | 0.83              |
| 19:K:180:HIS:CB  | 19:K:183:ARG:HH11 | 1.92                     | 0.83              |
| 4:4:43:U:H3      | 4:4:67:A:H61      | 1.27                     | 0.83              |
| 1:1:959:OMG:HN21 | 21:M:76:HIS:CG    | 1.96                     | 0.83              |
| 1:1:204:A:N6     | 1:1:228:U:O4      | 2.12                     | 0.83              |
| 10:B:49:PHE:CE1  | 10:B:342:VAL:CG2  | 2.62                     | 0.83              |
| 15:G:118:ASN:ND2 | 15:G:123:GLN:OE1  | 2.12                     | 0.83              |
| 2:2:1012:G:H21   | 15:G:149:VAL:HG23 | 1.40                     | 0.83              |
| 3:3:28:U:H3      | 3:3:203:A:H61     | 1.25                     | 0.83              |
| 13:E:24:LYS:NZ   | 13:E:37:ASP:OD1   | 2.11                     | 0.83              |
| 3:3:58:C:O2'     | 3:3:60:U:C5'      | 2.26                     | 0.82              |
| 8:8:3:G:H1       | 8:8:120:C:N4      | 1.76                     | 0.82              |
| 25:Q:43:LYS:O    | 25:Q:47:ASP:OD1   | 1.97                     | 0.82              |
| 2:2:602:A:N3     | 28:T:131:ARG:NH2  | 2.26                     | 0.82              |
| 1:1:831:C:OP1    | 24:P:192:ARG:NH2  | 2.12                     | 0.82              |
| 19:K:93:ARG:HD2  | 19:K:108:VAL:HG12 | 1.61                     | 0.82              |
| 2:2:1077:G:O2'   | 2:2:1078:OMU:H5'' | 1.79                     | 0.82              |
| 1:1:778:C:HO2'   | 1:1:779:A:H8      | 1.27                     | 0.82              |
| 1:1:186:G:H1     | 1:1:267:A:H61     | 1.27                     | 0.82              |
| 16:H:146:VAL:CG1 | 19:K:55:ALA:HB1   | 2.09                     | 0.82              |
| 1:1:1012:C:N4    | 2:2:1043:G:O2'    | 2.12                     | 0.82              |
| 13:E:59:TRP:CH2  | 19:K:64:TYR:CB    | 2.63                     | 0.82              |
| 1:1:35:U:H2'     | 1:1:36:OMU:H5''   | 1.61                     | 0.81              |
| 8:8:72:A:N6      | 8:8:107:U:O4      | 2.11                     | 0.81              |
| 10:B:10:ARG:NH2  | 10:B:268:THR:O    | 2.13                     | 0.81              |
| 3:3:95:C:N3      | 3:3:139:G:N2      | 2.26                     | 0.81              |
| 7:7:75:G:OP2     | 31:W:71:TYR:OH    | 1.97                     | 0.81              |
| 2:2:616:G:N2     | 2:2:621:G:O6      | 2.12                     | 0.81              |
| 8:8:2:C:N4       | 8:8:120:C:C2      | 2.46                     | 0.81              |
| 31:W:37:ARG:O    | 31:W:41:ASN:N     | 2.12                     | 0.81              |
| 6:6:26:G:N3      | 6:6:26:G:H5''     | 1.95                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:S:100[A]:ARG:O | 27:S:102:GLN:N    | 2.12                     | 0.81              |
| 1:1:1392:G:O2'    | 1:1:1393:A:OP2    | 1.96                     | 0.81              |
| 2:2:458:C:N3      | 2:2:479:C:N4      | 2.28                     | 0.81              |
| 1:1:1674:U:O4     | 1:1:1728:G:C2     | 2.34                     | 0.81              |
| 1:1:836:G:OP1     | 24:P:149:ARG:NH1  | 2.13                     | 0.81              |
| 2:2:71:OMG:HM22   | 2:2:72:G:O4'      | 1.81                     | 0.81              |
| 16:H:148:TYR:CG   | 19:K:59:MET:CB    | 2.63                     | 0.81              |
| 30:V:118:ARG:HD3  | 30:V:124:LYS:HE3  | 1.62                     | 0.81              |
| 1:1:370:G:N2      | 1:1:374:G:N7      | 2.29                     | 0.81              |
| 1:1:424:G:H21     | 1:1:427:A:H8      | 1.27                     | 0.81              |
| 3:3:209:G:C2'     | 3:3:210:G:H5'     | 2.09                     | 0.81              |
| 22:N:67:ALA:O     | 22:N:71:GLN:N     | 2.12                     | 0.81              |
| 26:R:71:LEU:HD12  | 26:R:99:VAL:HG11  | 1.63                     | 0.81              |
| 6:6:4:U:H4'       | 6:6:4:U:OP1       | 1.80                     | 0.81              |
| 16:H:200:ALA:CB   | 19:K:185:VAL:HG13 | 2.10                     | 0.81              |
| 3:3:129:G:H21     | 3:3:130:G:H1'     | 1.44                     | 0.81              |
| 19:K:89:VAL:HG11  | 26:R:73:ALA:CB    | 1.83                     | 0.81              |
| 2:2:1057:U:O2     | 2:2:1077:G:N2     | 2.14                     | 0.81              |
| 2:2:1131:A:C2     | 23:O:23:ARG:NH1   | 2.49                     | 0.81              |
| 1:1:329:G:OP2     | 21:M:68:ARG:NH2   | 2.13                     | 0.81              |
| 4:4:77:U:H4'      | 10:B:371:LYS:HE3  | 1.60                     | 0.81              |
| 1:1:659:G:O2'     | 7:7:7:OMU:HM21    | 1.81                     | 0.80              |
| 1:1:959:OMG:HN21  | 21:M:76:HIS:CD2   | 1.98                     | 0.80              |
| 4:4:128:U:H3      | 4:4:162:A:H61     | 1.28                     | 0.80              |
| 8:8:34:A:C6       | 8:8:43:G:N3       | 2.49                     | 0.80              |
| 1:1:423:U:O4      | 1:1:428:A:N6      | 2.12                     | 0.80              |
| 9:A:40:TYR:HA     | 9:A:91:GLY:HA3    | 1.63                     | 0.80              |
| 1:1:1540:U:O2     | 2:2:602:A:N6      | 2.14                     | 0.80              |
| 3:3:57:U:C2'      | 3:3:58:C:C6       | 2.63                     | 0.80              |
| 19:K:74:LEU:HD23  | 19:K:74:LEU:H     | 1.43                     | 0.80              |
| 14:F:51:ALA:HB2   | 14:F:74:VAL:HG21  | 1.63                     | 0.80              |
| 17:I:83:ALA:HB3   | 17:I:108:ASN:ND2  | 1.97                     | 0.80              |
| 16:H:148:TYR:HB3  | 19:K:59:MET:H     | 1.45                     | 0.80              |
| 23:O:23:ARG:HD3   | 23:O:23:ARG:O     | 1.81                     | 0.80              |
| 1:1:1253:U:H5'    | 16:H:74:GLN:HE22  | 1.47                     | 0.80              |
| 1:1:1278:G:H1     | 1:1:1351:C:H42    | 1.25                     | 0.80              |
| 3:3:39:U:O4       | 3:3:181:A:N6      | 2.12                     | 0.80              |
| 10:B:321:TYR:CD1  | 10:B:340:ARG:HG2  | 2.16                     | 0.80              |
| 3:3:195:A:OP2     | 21:M:49:ARG:NH1   | 83.69                    | 0.79              |
| 16:H:146:VAL:CG1  | 19:K:55:ALA:CB    | 2.60                     | 0.79              |
| 10:B:93:ARG:HG3   | 10:B:102:ILE:HG21 | 1.62                     | 0.79              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 2:2:654:U:O2'     | 2:2:655:OMG:H5'     | 1.82                     | 0.79              |
| 18:J:28:ALA:O     | 18:J:116:ILE:HG23   | 1.82                     | 0.79              |
| 1:1:779:A:N6      | 1:1:796:G:O6        | 2.14                     | 0.79              |
| 5:5:38:G:OP1      | 32:X:37:ARG:NH2     | 2.15                     | 0.79              |
| 18:J:116:ILE:H    | 18:J:116:ILE:HD12   | 1.46                     | 0.79              |
| 9:A:35:ALA:HA     | 15:G:121:ILE:HD11   | 1.64                     | 0.79              |
| 1:1:543:G:H5'     | 1:1:543:G:N3        | 1.98                     | 0.79              |
| 2:2:1318:OMC:H5'  | 2:2:1318:OMC:C6     | 2.15                     | 0.79              |
| 1:1:779:A:OP1     | 24:P:141:LYS:HB3    | 1.83                     | 0.79              |
| 22:N:76:MET:SD    | 22:N:147:GLN:NE2    | 2.55                     | 0.78              |
| 1:1:1247:U:O2     | 1:1:1379:A:N6       | 2.15                     | 0.78              |
| 2:2:655:OMG:CM2   | 2:2:657:U:H5''      | 2.14                     | 0.78              |
| 19:K:93:ARG:HD2   | 19:K:108:VAL:HG11   | 1.64                     | 0.78              |
| 2:2:734:A:OP2     | 2:2:736:C:N4        | 2.16                     | 0.78              |
| 2:2:1253:G:OP1    | 11:C:74:ARG:NH1     | 2.16                     | 0.78              |
| 1:1:713:A:H62     | 1:1:737:U:H3        | 1.31                     | 0.78              |
| 1:1:1529:OMC:CM2  | 11:C:94:MET:HG2     | 2.14                     | 0.78              |
| 1:1:109:A:OP1     | 17:I:101:ARG:NH1    | 2.17                     | 0.78              |
| 1:1:34:C:C2'      | 1:1:35:U:H5'        | 2.14                     | 0.78              |
| 13:E:107:GLN:NE2  | 13:E:125:VAL:O      | 2.16                     | 0.78              |
| 25:Q:15:LEU:HD13  | 25:Q:52:ARG:HB3     | 1.66                     | 0.78              |
| 2:2:729:G:N1      | 2:2:732:A:OP2       | 2.17                     | 0.78              |
| 3:3:106:U:C2      | 3:3:129:G:C6        | 2.70                     | 0.78              |
| 1:1:1659:G:H1'    | 2:2:414:G:H22       | 1.47                     | 0.78              |
| 1:1:244:C:H42     | 1:1:248:A:H61       | 1.28                     | 0.78              |
| 2:2:1255:G:H1     | 2:2:1259:A:H62      | 1.29                     | 0.78              |
| 9:A:9:ARG:NH2     | 9:A:16:TYR:OH       | 2.16                     | 0.78              |
| 26:R:14:ARG:HG3   | 26:R:61:LEU:HD11    | 1.66                     | 0.78              |
| 33:Y:76:ASN:HB3   | 33:Y:79:HIS:HD2     | 1.49                     | 0.78              |
| 10:B:234:VAL:HG11 | 10:B:254:VAL:HG23   | 1.66                     | 0.77              |
| 16:H:103:ARG:HH11 | 16:H:103:ARG:HG3    | 1.49                     | 0.77              |
| 1:1:845:OMU:H6    | 1:1:845:OMU:O5'     | 1.84                     | 0.77              |
| 2:2:1044:C:O2     | 2:2:1052:G:N2       | 2.13                     | 0.77              |
| 2:2:1280:G:O2'    | 2:2:1286:A:N6       | 2.16                     | 0.77              |
| 19:K:70:LEU:HA    | 19:K:84:VAL:HA      | 1.65                     | 0.77              |
| 2:2:654:U:C2'     | 2:2:655:OMG:H5'     | 2.15                     | 0.77              |
| 4:4:71:C:OP1      | 18:J:47:ARG:NH2     | 2.16                     | 0.77              |
| 8:8:37:C:H42      | 8:8:48:G:H1'        | 1.47                     | 0.77              |
| 11:C:34:ASP:OD1   | 24:P:22:THR:OG1     | 2.01                     | 0.77              |
| 1:1:1042:G:OP1    | 27:S:100[B]:ARG:NH1 | 2.18                     | 0.77              |
| 1:1:490:C:N3      | 1:1:645:G:N2        | 2.31                     | 0.77              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 2:2:443:OMC:H5'' | 2:2:488:A:H61       | 1.44                     | 0.77              |
| 6:6:22:G:H2'     | 6:6:22:G:N3         | 1.98                     | 0.77              |
| 27:S:48:VAL:HG21 | 27:S:94:GLU:HG3     | 1.66                     | 0.77              |
| 1:1:183:G:O6     | 1:1:270:C:N4        | 2.16                     | 0.77              |
| 2:2:1145:U:H3    | 2:2:1168:G:H1       | 1.28                     | 0.77              |
| 3:3:129:G:N2     | 3:3:130:G:N9        | 2.32                     | 0.77              |
| 6:6:7:A:C2       | 6:6:60:A:C2         | 2.72                     | 0.77              |
| 2:2:655:OMG:HM21 | 2:2:657:U:H5''      | 1.67                     | 0.77              |
| 8:8:71:C:H2'     | 8:8:72:A:H5''       | 1.65                     | 0.77              |
| 6:6:30:C:O2'     | 6:6:31:U:P          | 2.42                     | 0.77              |
| 7:7:29:C:OP1     | 17:I:36:GLN:NE2     | 2.19                     | 0.77              |
| 1:1:1732:A:O2'   | 30:V:36:ARG:NH2     | 2.18                     | 0.76              |
| 14:F:49:ARG:HH11 | 14:F:181:VAL:HG13   | 1.50                     | 0.76              |
| 1:1:35:U:O2'     | 1:1:36:OMU:H5''     | 1.84                     | 0.76              |
| 4:4:140:G:H21    | 4:4:150:A:H62       | 1.33                     | 0.76              |
| 10:B:337:GLY:HA3 | 10:B:343:MET:CE     | 2.15                     | 0.76              |
| 16:H:195:GLU:HA  | 16:H:198:LYS:HG2    | 1.67                     | 0.76              |
| 16:H:141:ARG:NH2 | 19:K:48:LEU:O       | 2.14                     | 0.76              |
| 25:Q:8:ALA:CB    | 25:Q:19:ARG:HH12    | 1.97                     | 0.76              |
| 1:1:233:U:O2     | 1:1:255:G:N2        | 2.16                     | 0.76              |
| 10:B:26:ARG:NH2  | 10:B:183:VAL:O      | 2.18                     | 0.76              |
| 4:4:62:C:O2      | 13:E:119:ARG:NH1    | 2.18                     | 0.76              |
| 15:G:298:ASN:OD1 | 15:G:301[B]:ARG:NH2 | 2.17                     | 0.76              |
| 3:3:4:U:O4       | 33:Y:17:ARG:NH1     | 2.18                     | 0.76              |
| 31:W:14:ARG:O    | 31:W:18:GLN:HB2     | 1.84                     | 0.76              |
| 1:1:970:U:OP1    | 50:1:1955:HOH:O     | 2.03                     | 0.76              |
| 6:6:19:C:H4'     | 6:6:19:C:OP1        | 1.84                     | 0.76              |
| 17:I:80:PHE:O    | 17:I:106:ARG:NH1    | 2.17                     | 0.76              |
| 1:1:1260:G:N2    | 1:1:1261:U:O4       | 2.19                     | 0.76              |
| 1:1:239:U:H1'    | 1:1:240:U:H5'       | 1.67                     | 0.76              |
| 2:2:1369:A:O2'   | 18:J:40:SER:OG      | 2.03                     | 0.76              |
| 13:E:103:SER:HB2 | 13:E:110:GLU:HB2    | 1.66                     | 0.76              |
| 8:8:66:A:OP2     | 8:8:67:G:N2         | 2.18                     | 0.76              |
| 9:A:130:SER:OG   | 9:A:174:ARG:NH1     | 2.18                     | 0.76              |
| 8:8:8:C:OP1      | 23:O:54:ARG:NE      | 2.19                     | 0.75              |
| 2:2:1333:C:H5'   | 13:E:167:LYS:HG2    | 1.67                     | 0.75              |
| 6:6:38:C:O2'     | 14:F:179:ARG:O      | 2.02                     | 0.75              |
| 28:T:41:LEU:HD21 | 28:T:99:GLU:HG2     | 1.68                     | 0.75              |
| 6:6:33:G:H5'     | 19:K:42:VAL:HG21    | 1.67                     | 0.75              |
| 19:K:95:LEU:CD1  | 19:K:106:ARG:HE     | 1.99                     | 0.75              |
| 6:6:30:C:H6      | 6:6:30:C:C5'        | 1.97                     | 0.75              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:8:48:G:N2       | 8:8:49:U:N1        | 2.34                     | 0.75              |
| 19:K:95:LEU:CD1   | 19:K:106:ARG:NE    | 2.49                     | 0.75              |
| 27:S:118:ALA:HA   | 27:S:122:GLY:HA3   | 1.68                     | 0.75              |
| 28:T:33:ALA:HB1   | 28:T:117:VAL:HG11  | 1.67                     | 0.75              |
| 2:2:54:U:OP2      | 50:2:1710:HOH:O    | 2.05                     | 0.75              |
| 5:5:46:G:O6       | 5:5:101:C:N4       | 2.19                     | 0.75              |
| 9:A:116:VAL:HG23  | 9:A:126:LEU:HB2    | 1.67                     | 0.75              |
| 1:1:995:C:H5      | 1:1:1467:G:H1      | 1.32                     | 0.75              |
| 8:8:48:G:C2       | 8:8:49:U:N1        | 2.55                     | 0.75              |
| 18:J:104:ILE:N    | 18:J:104:ILE:HD12  | 2.02                     | 0.75              |
| 8:8:34:A:C6       | 8:8:43:G:C2        | 2.75                     | 0.75              |
| 1:1:1205:G:O6     | 1:1:1212:C:N4      | 2.19                     | 0.75              |
| 1:1:1586:U:OP2    | 50:2:1710:HOH:O    | 2.05                     | 0.75              |
| 2:2:457:U:N3      | 2:2:480:G:O6       | 2.19                     | 0.75              |
| 27:S:100[B]:ARG:O | 27:S:102:GLN:N     | 2.18                     | 0.75              |
| 3:3:4:U:C5        | 33:Y:17:ARG:NH1    | 2.43                     | 0.75              |
| 16:H:108:ARG:HG2  | 16:H:108:ARG:HH11  | 1.49                     | 0.75              |
| 19:K:81:ARG:NH1   | 19:K:102:ALA:O     | 2.19                     | 0.75              |
| 1:1:1228:G:H1     | 1:1:1398:C:H5      | 1.32                     | 0.74              |
| 2:2:782:G:O2'     | 2:2:784:U:OP1      | 2.04                     | 0.74              |
| 19:K:180:HIS:HA   | 19:K:183:ARG:CG    | 2.16                     | 0.74              |
| 16:H:49:LYS:HZ1   | 19:K:37:THR:N      | 1.85                     | 0.74              |
| 4:4:76:C:OP2      | 10:B:227[A]:LYS:NZ | 2.20                     | 0.74              |
| 2:2:1338:C:H2'    | 13:E:170:ASP:HB2   | 1.69                     | 0.74              |
| 2:2:1318:OMC:C5'  | 2:2:1318:OMC:H6    | 1.99                     | 0.74              |
| 23:O:18:VAL:CG2   | 23:O:24:ARG:NH2    | 2.50                     | 0.74              |
| 2:2:1254:OMG:N7   | 2:2:1309:C:O2'     | 2.20                     | 0.74              |
| 5:5:125:A:H5'     | 5:5:125:A:H8       | 1.52                     | 0.74              |
| 8:8:28:C:O2       | 8:8:58:G:N2        | 2.20                     | 0.74              |
| 6:6:17:U:O2       | 6:6:30:C:O2'       | 2.03                     | 0.74              |
| 1:1:855:C:OP1     | 11:C:99:ARG:NH2    | 2.20                     | 0.74              |
| 18:J:86:SER:HA    | 18:J:96:TYR:HB3    | 1.70                     | 0.74              |
| 2:2:591:A2M:HM'2  | 2:2:592:C:C5'      | 2.16                     | 0.74              |
| 2:2:762:U:OP1     | 21:M:31:ARG:NH1    | 2.20                     | 0.74              |
| 3:3:78:C:O2'      | 3:3:79:U:OP1       | 2.04                     | 0.74              |
| 8:8:37:C:C4       | 8:8:48:G:H1'       | 2.22                     | 0.74              |
| 1:1:193:A:H2'     | 1:1:194:A:H8       | 1.53                     | 0.74              |
| 2:2:783:U:O2      | 2:2:810:G:N1       | 2.19                     | 0.74              |
| 9:A:65:HIS:HD2    | 9:A:68:LYS:H       | 1.34                     | 0.74              |
| 12:D:16:VAL:HA    | 12:D:133:LEU:HA    | 1.69                     | 0.74              |
| 1:1:511:A:N1      | 1:1:541:A:N6       | 2.35                     | 0.74              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 9:A:229:SER:O     | 9:A:234:LYS:NZ   | 2.20                     | 0.74              |
| 2:2:1319:U:O2     | 10:B:255:ALA:HB3 | 1.87                     | 0.74              |
| 19:K:180:HIS:C    | 19:K:183:ARG:HG2 | 2.08                     | 0.74              |
| 22:N:121:LYS:HG3  | 22:N:122:PRO:HD2 | 1.68                     | 0.74              |
| 1:1:260:C:O2'     | 1:1:261:C:OP1    | 2.06                     | 0.74              |
| 19:K:73:ILE:N     | 19:K:73:ILE:HD12 | 2.02                     | 0.74              |
| 2:2:1043:G:O6     | 2:2:1053:C:N4    | 2.18                     | 0.73              |
| 1:1:501:C:N4      | 1:1:553:A:N3     | 2.36                     | 0.73              |
| 1:1:934:A:OP1     | 50:1:1971:HOH:O  | 2.06                     | 0.73              |
| 2:2:639:G:O2'     | 2:2:1421:A:N6    | 2.19                     | 0.73              |
| 33:Y:28:ASN:HA    | 33:Y:41:ALA:HA   | 1.69                     | 0.73              |
| 1:1:163:U:H3      | 1:1:292:A:H61    | 1.33                     | 0.73              |
| 2:2:104:U:O2'     | 2:2:116:A:N7     | 2.20                     | 0.73              |
| 13:E:58:ARG:HD2   | 13:E:69:LEU:HD22 | 1.70                     | 0.73              |
| 16:H:108:ARG:HG3  | 16:H:109:TYR:CE2 | 2.24                     | 0.73              |
| 1:1:1615:C:N4     | 2:2:62:A:OP1     | 2.21                     | 0.73              |
| 3:3:58:C:O2'      | 3:3:60:U:O5'     | 2.06                     | 0.73              |
| 6:6:41:G:C2       | 19:K:176:ARG:HD2 | 2.24                     | 0.73              |
| 13:E:5:LYS:HD2    | 13:E:66:ILE:HG21 | 1.69                     | 0.73              |
| 1:1:1266:A:H4'    | 22:N:162:ARG:HD3 | 1.71                     | 0.73              |
| 1:1:1540:U:H2'    | 1:1:1541:A2M:H8  | 1.68                     | 0.73              |
| 1:1:781:A:H61     | 1:1:794:U:H3     | 1.34                     | 0.73              |
| 13:E:137:SER:O    | 13:E:140:LYS:CG  | 2.31                     | 0.73              |
| 15:G:146:LYS:HB3  | 21:M:28:TRP:HH2  | 1.53                     | 0.73              |
| 2:2:986:A:H61     | 2:2:1000:U:H3    | 1.35                     | 0.73              |
| 11:C:54:ASN:HB3   | 11:C:57:SER:HB3  | 1.70                     | 0.73              |
| 19:K:180:HIS:HE2  | 19:K:184:LYS:HE2 | 1.50                     | 0.73              |
| 2:2:459:A:O2'     | 2:2:1029:A:O2'   | 2.06                     | 0.73              |
| 2:2:1238:A:O2'    | 20:L:42:ARG:NH1  | 2.22                     | 0.73              |
| 2:2:71:OMG:HM22   | 2:2:72:G:C4'     | 2.19                     | 0.73              |
| 1:1:1392:G:O6     | 19:K:105:TRP:CZ3 | 2.42                     | 0.73              |
| 1:1:237:U:OP1     | 1:1:257:U:O2'    | 2.05                     | 0.73              |
| 1:1:411:U:O2      | 1:1:415:A:N6     | 2.19                     | 0.73              |
| 2:2:760:U:OP1     | 15:G:153:ARG:NE  | 2.17                     | 0.73              |
| 15:G:166:VAL:HG21 | 15:G:266:LYS:HD3 | 1.70                     | 0.73              |
| 6:6:11:G:O2'      | 16:H:190:GLN:NE2 | 2.21                     | 0.73              |
| 1:1:1369:G:H5'    | 16:H:78:LYS:HE3  | 1.71                     | 0.73              |
| 2:2:1100:G:H1     | 2:2:1110:C:H42   | 1.37                     | 0.73              |
| 2:2:1338:C:H4'    | 2:2:1343:G:H22   | 1.52                     | 0.73              |
| 7:7:7:OMU:H6      | 7:7:7:OMU:OP2    | 1.89                     | 0.73              |
| 19:K:180:HIS:NE2  | 19:K:184:LYS:CE  | 2.50                     | 0.73              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 24:P:17:HIS:NE2   | 24:P:18:HIS:ND1     | 2.35                     | 0.73              |
| 1:1:1041:U:OP1    | 27:S:100[B]:ARG:NH2 | 2.22                     | 0.72              |
| 8:8:2:C:N3        | 8:8:120:C:C2        | 2.55                     | 0.72              |
| 10:B:368:THR:H    | 10:B:378:GLN:NE2    | 1.87                     | 0.72              |
| 1:1:955:A2M:HM'1  | 9:A:14:SER:O        | 1.89                     | 0.72              |
| 8:8:54:U:O2'      | 8:8:56:A:N7         | 2.22                     | 0.72              |
| 2:2:422:U:OP1     | 9:A:54:ARG:NH2      | 2.22                     | 0.72              |
| 13:E:23:ARG:NH1   | 13:E:43:LEU:O       | 2.22                     | 0.72              |
| 1:1:172:G:H2'     | 1:1:173:G:H8        | 1.54                     | 0.72              |
| 2:2:523:C:N4      | 2:2:553:G:O6        | 2.16                     | 0.72              |
| 7:7:6:G:H2'       | 7:7:7:OMU:H6        | 1.70                     | 0.72              |
| 1:1:85:U:O2       | 1:1:98:A:N6         | 2.19                     | 0.72              |
| 2:2:1159:A:H8     | 2:2:1159:A:H5''     | 1.55                     | 0.72              |
| 22:N:184:LEU:HD22 | 22:N:189:LYS:HG3    | 1.71                     | 0.72              |
| 23:O:107:ARG:NH1  | 23:O:119:PHE:O      | 2.17                     | 0.72              |
| 1:1:90:G:OP2      | 1:1:92:C:N4         | 2.20                     | 0.72              |
| 2:2:1310:G:H5'    | 2:2:1311:A:H5''     | 1.70                     | 0.72              |
| 2:2:655:OMG:HM21  | 2:2:657:U:C5'       | 2.19                     | 0.72              |
| 3:3:112:C:O2      | 3:3:120:G:N2        | 2.15                     | 0.72              |
| 1:1:12:U:O4       | 7:7:156:A:N6        | 2.19                     | 0.72              |
| 2:2:1310:G:OP2    | 50:2:1735:HOH:O     | 2.07                     | 0.72              |
| 2:2:957:C:H1'     | 2:2:958:C:OP1       | 1.89                     | 0.72              |
| 16:H:148:TYR:HB3  | 19:K:59:MET:N       | 2.04                     | 0.72              |
| 7:7:145:G:C4'     | 30:V:52:ARG:NH1     | 2.51                     | 0.72              |
| 2:2:1153:OMU:OP1  | 27:S:57:TYR:OH      | 2.06                     | 0.72              |
| 1:1:19:G:H1       | 7:7:149:A:H61       | 1.37                     | 0.72              |
| 8:8:34:A:N1       | 8:8:43:G:N2         | 2.37                     | 0.72              |
| 8:8:42:C:O2'      | 8:8:44:A:N7         | 2.23                     | 0.72              |
| 6:6:46:C:N4       | 14:F:179:ARG:HE     | 1.88                     | 0.72              |
| 18:J:116:ILE:N    | 18:J:116:ILE:HD12   | 2.03                     | 0.72              |
| 1:1:1548:A:H61    | 1:1:1584:A:H4'      | 1.54                     | 0.72              |
| 14:F:51:ALA:HA    | 14:F:67:GLY:HA2     | 1.71                     | 0.72              |
| 21:M:71:ARG:CG    | 21:M:94:LEU:HB2     | 2.20                     | 0.72              |
| 2:2:1280:G:N2     | 2:2:1285:U:OP1      | 2.22                     | 0.71              |
| 11:C:222:ILE:HG21 | 11:C:225:LEU:HD23   | 1.71                     | 0.71              |
| 17:I:28:LYS:HB2   | 21:M:197:ARG:HD2    | 1.71                     | 0.71              |
| 23:O:53:VAL:HG21  | 23:O:168:VAL:HG21   | 1.72                     | 0.71              |
| 1:1:385:G:O2'     | 7:7:24:G:N3         | 2.22                     | 0.71              |
| 25:Q:123:LEU:HD21 | 25:Q:138:LEU:HD11   | 1.71                     | 0.71              |
| 1:1:24:A:N3       | 1:1:366:C:O2'       | 2.22                     | 0.71              |
| 1:1:36:OMU:HM22   | 1:1:37:A:H5'        | 1.73                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:129:G:N2      | 3:3:130:G:C4      | 2.58                     | 0.71              |
| 10:B:56:ILE:HD12  | 10:B:363:LEU:HD22 | 1.70                     | 0.71              |
| 16:H:108:ARG:NH1  | 16:H:108:ARG:HG2  | 2.02                     | 0.71              |
| 16:H:49:LYS:HZ3   | 19:K:37:THR:N     | 1.87                     | 0.71              |
| 3:3:91:G:N2       | 3:3:92:G:O2'      | 2.24                     | 0.71              |
| 18:J:81:ILE:HG22  | 18:J:82:ARG:HG3   | 1.72                     | 0.71              |
| 8:8:107:U:H3'     | 22:N:203:LYS:HE3  | 1.71                     | 0.71              |
| 1:1:1757:U:H4'    | 2:2:18:A:H4'      | 1.72                     | 0.71              |
| 10:B:49:PHE:CE1   | 10:B:342:VAL:HG23 | 2.25                     | 0.71              |
| 11:C:237:HIS:O    | 11:C:246:ARG:NH1  | 2.24                     | 0.71              |
| 1:1:439:U:OP2     | 28:T:2:THR:N      | 2.23                     | 0.71              |
| 1:1:1440:A:O2'    | 1:1:1442:G:N1     | 2.23                     | 0.71              |
| 2:2:1056:A:H61    | 2:2:1078:OMU:HN3  | 1.36                     | 0.71              |
| 2:2:459:A:HO2'    | 2:2:1029:A:HO2'   | 1.33                     | 0.71              |
| 23:O:60:ILE:HD11  | 23:O:101:THR:HG21 | 1.73                     | 0.71              |
| 33:Y:11:VAL:HG12  | 33:Y:82:PRO:HA    | 1.71                     | 0.71              |
| 1:1:439:U:O4'     | 28:T:2:THR:OG1    | 2.07                     | 0.71              |
| 2:2:421:A:N6      | 9:A:20:GLY:O      | 2.22                     | 0.71              |
| 10:B:310:LYS:HE3  | 10:B:368:THR:OG1  | 1.90                     | 0.71              |
| 15:G:153:ARG:NH1  | 15:G:322:GLN:O    | 2.23                     | 0.71              |
| 4:4:41:U:H3       | 4:4:69:G:H1       | 1.38                     | 0.71              |
| 16:H:55:ARG:HE    | 16:H:126:ILE:HD11 | 1.56                     | 0.71              |
| 18:J:74:LYS:HE3   | 18:J:76:LEU:HD13  | 1.72                     | 0.71              |
| 2:2:1090:A:OP1    | 50:2:1727:HOH:O   | 2.07                     | 0.71              |
| 4:4:25:G:O6       | 4:4:180:C:N4      | 2.20                     | 0.71              |
| 27:S:68:THR:HB    | 27:S:69:PRO:HD2   | 1.71                     | 0.71              |
| 2:2:1268:U:N3     | 2:2:1300:U:O2     | 2.24                     | 0.71              |
| 3:3:57:U:C2'      | 3:3:58:C:H5       | 1.71                     | 0.71              |
| 6:6:42:A:N6       | 19:K:169:TYR:OH   | 2.24                     | 0.71              |
| 1:1:326:A:O2'     | 21:M:93:LYS:O     | 2.08                     | 0.71              |
| 6:6:40:C:H3'      | 6:6:40:C:OP2      | 1.89                     | 0.70              |
| 10:B:216:GLN:NE2  | 10:B:288:TYR:O    | 2.23                     | 0.70              |
| 16:H:137:VAL:HG13 | 19:K:45:SER:O     | 1.91                     | 0.70              |
| 16:H:146:VAL:HG13 | 19:K:55:ALA:HB3   | 1.73                     | 0.70              |
| 23:O:65:VAL:HG22  | 23:O:74:VAL:HG22  | 1.74                     | 0.70              |
| 2:2:585:C:OP1     | 18:J:50:ARG:NH1   | 2.25                     | 0.70              |
| 6:6:13:C:O2'      | 6:6:14:A:H5'      | 1.91                     | 0.70              |
| 8:8:96:C:OP1      | 26:R:45:ARG:NH1   | 2.23                     | 0.70              |
| 23:O:64:ILE:HD12  | 23:O:109:THR:HG21 | 1.72                     | 0.70              |
| 1:1:253:G:OP1     | 31:W:13:ARG:NH2   | 2.24                     | 0.70              |
| 10:B:56:ILE:HG22  | 10:B:366:ILE:HG23 | 1.73                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:H:140:PRO:HD3  | 19:K:46:PRO:HB3   | 1.74                     | 0.70              |
| 1:1:546:G:N1      | 26:R:63:CYS:SG    | 2.64                     | 0.70              |
| 1:1:409:U:O2'     | 1:1:410:U:OP2     | 2.09                     | 0.70              |
| 1:1:1651:G:H21    | 2:2:414:G:H21     | 1.39                     | 0.70              |
| 1:1:892:C:O2'     | 25:Q:126:ARG:NH2  | 2.24                     | 0.70              |
| 2:2:1131:A:N6     | 23:O:27:LYS:O     | 2.24                     | 0.70              |
| 6:6:14:A:H4'      | 6:6:15:C:OP1      | 1.91                     | 0.70              |
| 13:E:18:VAL:HG22  | 13:E:27:VAL:HG22  | 1.73                     | 0.70              |
| 13:E:135:ASP:HB2  | 13:E:136:PRO:HD3  | 1.71                     | 0.70              |
| 1:1:385:G:O6      | 50:1:1954:HOH:O   | 2.08                     | 0.70              |
| 2:2:1079:OMG:H4'  | 2:2:1080:U:OP2    | 1.91                     | 0.70              |
| 6:6:34:C:C4       | 6:6:35:U:C4       | 2.79                     | 0.70              |
| 16:H:53:VAL:HB    | 16:H:122:ALA:HA   | 1.73                     | 0.70              |
| 28:T:19:VAL:HG13  | 28:T:94:LEU:HD12  | 1.72                     | 0.70              |
| 1:1:1235:A:OP2    | 50:1:1960:HOH:O   | 2.09                     | 0.70              |
| 2:2:1392:U:H3'    | 2:2:1393:U:H3'    | 1.74                     | 0.70              |
| 10:B:365:PHE:CE2  | 10:B:367:ASP:OD1  | 2.45                     | 0.70              |
| 16:H:200:ALA:HB1  | 19:K:185:VAL:HG11 | 1.64                     | 0.70              |
| 1:1:1615:C:OP1    | 28:T:127:ARG:NH1  | 2.25                     | 0.70              |
| 1:1:291:A:H2'     | 1:1:292:A:H8      | 1.56                     | 0.69              |
| 1:1:753:A:N1      | 1:1:832:G:O2'     | 2.22                     | 0.69              |
| 2:2:378:C:OP1     | 50:2:1716:HOH:O   | 2.09                     | 0.69              |
| 13:E:89:PHE:HB2   | 13:E:145:PHE:HB2  | 1.74                     | 0.69              |
| 16:H:28:ASP:OD2   | 16:H:55:ARG:NH1   | 2.25                     | 0.69              |
| 22:N:121:LYS:CG   | 22:N:122:PRO:CD   | 2.67                     | 0.69              |
| 1:1:1729:A:N3     | 1:1:1729:A:H3'    | 2.07                     | 0.69              |
| 2:2:1078:OMU:O2   | 2:2:1078:OMU:HM23 | 1.92                     | 0.69              |
| 10:B:290:ILE:HG13 | 10:B:329:VAL:HG22 | 1.72                     | 0.69              |
| 16:H:138:VAL:O    | 19:K:46:PRO:HA    | 1.92                     | 0.69              |
| 19:K:163:SER:O    | 19:K:168:ARG:NH1  | 2.26                     | 0.69              |
| 1:1:238:A:C6      | 1:1:239:U:O4      | 2.46                     | 0.69              |
| 1:1:435:G:N1      | 1:1:438:A:OP2     | 2.23                     | 0.69              |
| 2:2:978:C:O2'     | 2:2:979:C:O5'     | 2.10                     | 0.69              |
| 1:1:1480:G:O2'    | 1:1:1510:A:N1     | 2.24                     | 0.69              |
| 1:1:461:G:N2      | 1:1:462:A:N7      | 2.36                     | 0.69              |
| 2:2:990:C:O2'     | 2:2:996:G:N2      | 2.25                     | 0.69              |
| 8:8:48:G:H22      | 8:8:49:U:H1'      | 1.55                     | 0.69              |
| 4:4:52:A:O2'      | 13:E:176:ASP:OD1  | 2.07                     | 0.69              |
| 14:F:77:ARG:HH11  | 14:F:77:ARG:HG3   | 1.57                     | 0.69              |
| 15:G:175:ALA:HA   | 15:G:299:LEU:HD11 | 1.73                     | 0.69              |
| 18:J:56:LEU:HD23  | 18:J:123:GLU:HB2  | 1.74                     | 0.69              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 21:M:121:VAL:HG21 | 21:M:131:GLU:HG3    | 1.75                     | 0.69              |
| 28:T:45:GLN:NE2   | 28:T:99:GLU:OE2     | 2.24                     | 0.69              |
| 1:1:735:U:OP1     | 11:C:273:LYS:NZ     | 2.24                     | 0.69              |
| 10:B:240:VAL:HG23 | 10:B:241:ALA:H      | 1.58                     | 0.69              |
| 16:H:200:ALA:CA   | 19:K:185:VAL:HG11   | 2.23                     | 0.69              |
| 1:1:1269:G:O2'    | 1:1:1270:U:O2       | 2.09                     | 0.69              |
| 2:2:1231:A:H5'    | 22:N:84:VAL:HG21    | 88.75                    | 0.69              |
| 2:2:19:C:OP2      | 50:2:1712:HOH:O     | 2.09                     | 0.69              |
| 2:2:749:G:C2'     | 2:2:750:U:C6        | 2.76                     | 0.69              |
| 2:2:866:U:H2'     | 2:2:867:G:H8        | 1.58                     | 0.69              |
| 13:E:5:LYS:H      | 13:E:58:ARG:NH1     | 1.90                     | 0.69              |
| 23:O:18:VAL:HG21  | 23:O:24:ARG:NH2     | 2.07                     | 0.69              |
| 27:S:98:LYS:O     | 27:S:100[A]:ARG:NH1 | 2.26                     | 0.69              |
| 1:1:1599:G:H1'    | 2:2:26:C:H5''       | 1.75                     | 0.69              |
| 3:3:129:G:H21     | 3:3:130:G:C1'       | 2.05                     | 0.69              |
| 6:6:54:A:H2'      | 6:6:55:U:H5'        | 1.74                     | 0.69              |
| 18:J:115:GLY:HA2  | 18:J:134:HIS:HB3    | 1.74                     | 0.69              |
| 2:2:1275:C:O2'    | 22:N:154:ARG:NH2    | 2.26                     | 0.69              |
| 1:1:752:G:HO2'    | 1:1:810:C:HO2'      | 1.34                     | 0.69              |
| 2:2:1057:U:H3     | 2:2:1077:G:H1       | 1.38                     | 0.69              |
| 18:J:19:LEU:HB2   | 18:J:54:ALA:HB3     | 1.75                     | 0.69              |
| 1:1:1208:U:N3     | 1:1:1260:G:O6       | 2.23                     | 0.69              |
| 1:1:956:U:H2'     | 1:1:957:C:H5''      | 1.75                     | 0.69              |
| 2:2:1043:G:N1     | 2:2:1053:C:N3       | 2.38                     | 0.69              |
| 2:2:1079:OMG:OP1  | 2:2:1080:U:H1'      | 1.93                     | 0.69              |
| 2:2:360:U:OP2     | 32:X:48:LYS:NZ      | 2.19                     | 0.69              |
| 4:4:141:A:N7      | 4:4:146:C:N4        | 2.35                     | 0.69              |
| 1:1:1186:A:N3     | 2:2:1265:U:O2'      | 2.25                     | 0.68              |
| 9:A:89:PHE:H      | 9:A:100:ASN:HD22    | 1.41                     | 0.68              |
| 1:1:1763:A:H2'    | 30:V:128:ARG:NH2    | 2.08                     | 0.68              |
| 1:1:1778:G:H1     | 2:2:6:A:N6          | 1.92                     | 0.68              |
| 2:2:806:C:N3      | 2:2:807:A:N6        | 2.41                     | 0.68              |
| 8:8:117:A:N6      | 8:8:118:C:N4        | 2.41                     | 0.68              |
| 10:B:310:LYS:CE   | 10:B:368:THR:OG1    | 2.41                     | 0.68              |
| 19:K:93:ARG:CD    | 19:K:108:VAL:HG12   | 2.24                     | 0.68              |
| 1:1:238:A:C6      | 1:1:239:U:C4        | 2.82                     | 0.68              |
| 2:2:1254:OMG:H4'  | 2:2:1254:OMG:HM23   | 1.75                     | 0.68              |
| 2:2:390:A:H1'     | 2:2:527:A2M:H61     | 1.56                     | 0.68              |
| 4:4:95:U:P        | 25:Q:62:ARG:NH2     | 2.65                     | 0.68              |
| 13:E:117:GLU:OE2  | 13:E:119:ARG:NE     | 2.27                     | 0.68              |
| 25:Q:23:TRP:CE3   | 25:Q:51:ILE:HD12    | 2.03                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:884:G:H1     | 1:1:912:C:H5      | 1.41                     | 0.68              |
| 3:3:77:U:O4      | 3:3:140:A:N6      | 2.20                     | 0.68              |
| 8:8:13:A:N1      | 8:8:68:G:O2'      | 2.24                     | 0.68              |
| 16:H:181:GLU:OE1 | 16:H:185:ARG:NH1  | 2.25                     | 0.68              |
| 1:1:251:A:N1     | 31:W:8:SER:N      | 2.41                     | 0.68              |
| 1:1:417:G:O2'    | 1:1:442:A:N6      | 2.27                     | 0.68              |
| 1:1:498:G:H1     | 1:1:555:U:H3      | 1.39                     | 0.68              |
| 2:2:973:C:H3'    | 9:A:89:PHE:HZ     | 1.58                     | 0.68              |
| 1:1:776:U:H3'    | 1:1:777:G:H8      | 1.59                     | 0.68              |
| 5:5:125:A:C2'    | 5:5:126:G:H5'     | 2.23                     | 0.68              |
| 1:1:1248:C:N3    | 16:H:152:ARG:NH2  | 2.41                     | 0.68              |
| 21:M:138:MET:HG2 | 21:M:143:ARG:HH21 | 1.58                     | 0.68              |
| 1:1:1602:U:H5    | 2:2:18:A:N1       | 1.92                     | 0.68              |
| 2:2:1198:C:H3'   | 2:2:1199:G:H5''   | 1.76                     | 0.68              |
| 1:1:1273:U:OP1   | 13:E:62:SER:OG    | 2.10                     | 0.68              |
| 24:P:165:PRO:HB3 | 24:P:193:LYS:HB3  | 1.76                     | 0.68              |
| 28:T:6:ARG:HD3   | 28:T:116:HIS:CD2  | 2.29                     | 0.68              |
| 3:3:209:G:H2'    | 3:3:210:G:C5'     | 2.17                     | 0.68              |
| 6:6:13:C:H2'     | 6:6:14:A:H2'      | 1.74                     | 0.68              |
| 1:1:697:A:H1'    | 17:I:13:GLN:HE22  | 1.57                     | 0.68              |
| 19:K:67:ALA:HB3  | 19:K:123:VAL:HA   | 1.75                     | 0.68              |
| 6:6:41:G:H1      | 19:K:176:ARG:NH1  | 1.91                     | 0.68              |
| 1:1:1258:A:O2'   | 1:1:1259:C:O5'    | 2.12                     | 0.68              |
| 1:1:754:G:C6     | 20:L:114:HIS:HB3  | 2.29                     | 0.68              |
| 2:2:1174:G:N2    | 2:2:1177:A:OP2    | 2.27                     | 0.68              |
| 4:4:140:G:H2'    | 4:4:141:A:C8      | 2.29                     | 0.68              |
| 8:8:30:C:OP2     | 23:O:57:ASN:ND2   | 2.27                     | 0.68              |
| 22:N:152:LEU:O   | 22:N:156:LYS:N    | 2.22                     | 0.68              |
| 1:1:1062:A:OP1   | 22:N:39:ARG:NE    | 2.26                     | 0.68              |
| 1:1:1541:A2M:H2' | 1:1:1542:OMG:O4'  | 1.94                     | 0.68              |
| 1:1:1746:A:O2'   | 1:1:1771:A:N3     | 2.27                     | 0.68              |
| 1:1:380:C:OP2    | 11:C:196:ARG:NH2  | 2.18                     | 0.68              |
| 1:1:740:C:H2'    | 1:1:741:G:H5'     | 1.74                     | 0.68              |
| 2:2:1310:G:N7    | 50:2:1737:HOH:O   | 2.27                     | 0.68              |
| 8:8:44:A:C8      | 8:8:45:U:C5       | 2.82                     | 0.68              |
| 16:H:73:LEU:HD23 | 16:H:76:LEU:HD12  | 1.75                     | 0.68              |
| 1:1:679:A:H4'    | 1:1:680:C:OP2     | 1.93                     | 0.67              |
| 1:1:839:U:H2'    | 1:1:840:G:H8      | 1.60                     | 0.67              |
| 1:1:889:G:N2     | 3:3:118:U:OP1     | 2.27                     | 0.67              |
| 2:2:443:OMC:H5'  | 2:2:488:A:H61     | 1.57                     | 0.67              |
| 6:6:20:A:N1      | 6:6:27:G:N7       | 2.42                     | 0.67              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:1:1672:A:C2     | 1:1:1729:A:N6    | 2.62                     | 0.67              |
| 1:1:174:U:O2      | 1:1:283:G:N2     | 2.27                     | 0.67              |
| 1:1:242:A:H61     | 1:1:260:C:H42    | 1.41                     | 0.67              |
| 1:1:799:U:OP2     | 24:P:73:ARG:NH1  | 2.27                     | 0.67              |
| 2:2:98:G:OP1      | 2:2:115:G:N1     | 2.27                     | 0.67              |
| 2:2:1386:G:OP1    | 2:2:1421:A:N6    | 2.23                     | 0.67              |
| 1:1:1769:A:O2'    | 3:3:70:A:N1      | 2.24                     | 0.67              |
| 1:1:1594:G:O6     | 50:1:1970:HOH:O  | 2.10                     | 0.67              |
| 11:C:30:PRO:HB3   | 24:P:25:TYR:HE2  | 1.59                     | 0.67              |
| 15:G:323:LEU:HB2  | 15:G:328:ARG:HD2 | 1.75                     | 0.67              |
| 18:J:30:ASN:CB    | 18:J:114:SER:HB2 | 2.24                     | 0.67              |
| 28:T:64:ASN:O     | 28:T:67:ILE:HG23 | 1.95                     | 0.67              |
| 1:1:1061:G:OP1    | 22:N:39:ARG:NH1  | 2.21                     | 0.67              |
| 1:1:1062:A:H61    | 1:1:1090:U:H3    | 1.41                     | 0.67              |
| 1:1:77:U:H5''     | 21:M:186:PRO:HG3 | 1.75                     | 0.67              |
| 1:1:843:C:H5''    | 20:L:2:PRO:HG2   | 1.75                     | 0.67              |
| 1:1:376:A:O2'     | 11:C:49:GLN:NE2  | 2.28                     | 0.67              |
| 1:1:487:G:H22     | 1:1:648:A:H2     | 1.43                     | 0.67              |
| 2:2:1159:A:C8     | 2:2:1159:A:H5''  | 2.29                     | 0.67              |
| 1:1:1778:G:N2     | 2:2:6:A:N1       | 2.40                     | 0.67              |
| 19:K:71:VAL:O     | 19:K:82:VAL:HG23 | 1.93                     | 0.67              |
| 2:2:749:G:HO2'    | 2:2:750:U:H6     | 1.42                     | 0.67              |
| 8:8:48:G:H2'      | 8:8:48:G:N3      | 2.08                     | 0.67              |
| 9:A:246:ILE:C     | 9:A:246:ILE:HD12 | 2.15                     | 0.67              |
| 1:1:1529:OMC:HM22 | 11:C:94:MET:HG2  | 1.76                     | 0.67              |
| 23:O:185:ARG:O    | 23:O:185:ARG:NH2 | 2.28                     | 0.67              |
| 1:1:1144:G:H2'    | 1:1:1145:G:H8    | 1.59                     | 0.67              |
| 2:2:70:A:O2'      | 2:2:71:OMG:H5'   | 1.95                     | 0.67              |
| 3:3:129:G:N2      | 3:3:130:G:C1'    | 2.57                     | 0.67              |
| 5:5:34:G:H1       | 5:5:116:U:H3     | 1.42                     | 0.67              |
| 6:6:28:A:C2       | 6:6:29:G:N1      | 2.62                     | 0.67              |
| 8:8:13:A:O2'      | 8:8:15:A:OP2     | 2.12                     | 0.67              |
| 1:1:953:G:C2'     | 1:1:954:U:H5'    | 2.25                     | 0.67              |
| 2:2:387:U:OP1     | 50:2:1706:HOH:O  | 2.11                     | 0.67              |
| 1:1:1538:C:H5     | 2:2:603:A:H62    | 1.43                     | 0.67              |
| 3:3:129:G:N2      | 3:3:130:G:H1'    | 2.09                     | 0.67              |
| 8:8:95:A:O2'      | 26:R:122:ASN:ND2 | 2.28                     | 0.67              |
| 21:M:181:ALA:HB1  | 21:M:184:LEU:HB2 | 1.76                     | 0.67              |
| 1:1:1443:U:H1'    | 24:P:17:HIS:HE1  | 1.58                     | 0.67              |
| 1:1:490:C:H42     | 1:1:645:G:H1     | 1.41                     | 0.67              |
| 2:2:1178:G:O2'    | 23:O:35:GLN:OE1  | 2.13                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:F:80:ASP:OD1   | 14:F:81:SER:N     | 2.25                     | 0.67              |
| 2:2:769:A:O2'     | 15:G:134:PHE:O    | 2.06                     | 0.67              |
| 19:K:180:HIS:CB   | 19:K:183:ARG:NH1  | 2.58                     | 0.67              |
| 11:C:206:PRO:HB3  | 11:C:247:PHE:HD2  | 1.58                     | 0.67              |
| 16:H:44:GLN:CD    | 19:K:48:LEU:HD21  | 2.15                     | 0.67              |
| 22:N:45:GLU:O     | 22:N:141:LYS:NZ   | 2.26                     | 0.67              |
| 2:2:446:U:O2'     | 2:2:664:G:N2      | 2.28                     | 0.66              |
| 6:6:26:G:N3       | 6:6:26:G:H3'      | 2.09                     | 0.66              |
| 14:F:53:ILE:HA    | 14:F:65:VAL:HG12  | 1.77                     | 0.66              |
| 1:1:79:U:OP1      | 21:M:197:ARG:NH2  | 2.28                     | 0.66              |
| 2:2:749:G:H4'     | 2:2:749:G:OP2     | 1.94                     | 0.66              |
| 9:A:65:HIS:CD2    | 9:A:68:LYS:H      | 2.13                     | 0.66              |
| 10:B:86:ILE:HD13  | 10:B:164:ALA:HB2  | 1.77                     | 0.66              |
| 15:G:193:ARG:HH12 | 15:G:213:ALA:HA   | 1.59                     | 0.66              |
| 1:1:222:A:H2'     | 1:1:223:A:H8      | 1.60                     | 0.66              |
| 6:6:6:G:OP1       | 15:G:136:ARG:NH2  | 139.37                   | 0.66              |
| 7:7:127:C:O2      | 7:7:136:G:N2      | 2.26                     | 0.66              |
| 19:K:69:ARG:C     | 19:K:84:VAL:HG23  | 2.09                     | 0.66              |
| 2:2:390:A:C1'     | 2:2:527:A2M:N6    | 2.58                     | 0.66              |
| 5:5:33:G:H1       | 5:5:117:U:H3      | 1.41                     | 0.66              |
| 6:6:17:U:C2       | 6:6:30:C:O2'      | 2.49                     | 0.66              |
| 8:8:117:A:C6      | 8:8:118:C:N4      | 2.63                     | 0.66              |
| 13:E:135:ASP:O    | 13:E:140:LYS:HD2  | 1.96                     | 0.66              |
| 23:O:108:ARG:NE   | 23:O:260:PRO:O    | 2.25                     | 0.66              |
| 24:P:101:ARG:NH2  | 24:P:101:ARG:HG2  | 2.01                     | 0.66              |
| 25:Q:15:LEU:HD12  | 25:Q:22:VAL:HG12  | 1.75                     | 0.66              |
| 1:1:1621:U:OP1    | 50:1:1968:HOH:O   | 2.14                     | 0.66              |
| 1:1:1537:G:H21    | 2:2:604:A:H62     | 1.43                     | 0.66              |
| 6:6:42:A:N3       | 6:6:43:A:N7       | 2.44                     | 0.66              |
| 18:J:81:ILE:HD11  | 18:J:103:VAL:HG13 | 1.77                     | 0.66              |
| 1:1:819:C:O2      | 1:1:821:C:O2'     | 2.13                     | 0.66              |
| 2:2:1343:G:H2'    | 2:2:1344:A:H8     | 1.61                     | 0.66              |
| 2:2:749:G:O2'     | 2:2:750:U:O4'     | 2.13                     | 0.66              |
| 6:6:10:C:H42      | 6:6:33:G:H1       | 1.41                     | 0.66              |
| 1:1:19:G:N2       | 7:7:149:A:N1      | 2.32                     | 0.66              |
| 8:8:48:G:C2       | 8:8:49:U:C2       | 2.83                     | 0.66              |
| 10:B:176:VAL:HG22 | 10:B:340:ARG:HB3  | 1.76                     | 0.66              |
| 22:N:65:LEU:HD21  | 22:N:135:LEU:HD22 | 1.78                     | 0.66              |
| 23:O:31:HIS:CD2   | 23:O:34:ARG:HH21  | 2.14                     | 0.66              |
| 1:1:47:C:N4       | 21:M:188:TYR:CE1  | 2.64                     | 0.66              |
| 1:1:894:G:O6      | 1:1:901:C:N4      | 2.28                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:2:751:U:H2'    | 2:2:752:G:C8      | 2.31                     | 0.66              |
| 2:2:1151:U:O2'   | 27:S:88:ARG:O     | 2.11                     | 0.66              |
| 1:1:1285:A:H2    | 1:1:1350:U:H1'    | 1.61                     | 0.66              |
| 1:1:931:G:OP1    | 28:T:131:ARG:NH1  | 2.29                     | 0.66              |
| 1:1:1445:U:O4'   | 1:1:1466:G:O2'    | 2.13                     | 0.66              |
| 1:1:36:OMU:HM22  | 1:1:37:A:C5'      | 2.26                     | 0.66              |
| 1:1:429:G:H4'    | 28:T:18:LYS:HB2   | 1.77                     | 0.66              |
| 1:1:672:U:O4     | 50:1:1946:HOH:O   | 2.14                     | 0.66              |
| 2:2:619:A:H62    | 2:2:1306:C:H1'    | 1.61                     | 0.66              |
| 2:2:490:A:O4'    | 9:A:243:THR:HG21  | 1.96                     | 0.66              |
| 2:2:70:A:H2'     | 2:2:71:OMG:C5'    | 2.26                     | 0.66              |
| 10:B:57:VAL:HB   | 10:B:365:PHE:HB3  | 1.78                     | 0.66              |
| 5:5:37:G:H4'     | 10:B:373:GLY:HA3  | 1.77                     | 0.66              |
| 7:7:145:G:C4'    | 30:V:52:ARG:HH11  | 2.06                     | 0.66              |
| 2:2:439:U:H5''   | 2:2:440:G:H5'     | 1.77                     | 0.66              |
| 7:7:36:G:O2'     | 7:7:103:A:N1      | 2.24                     | 0.66              |
| 16:H:29:LEU:HD13 | 16:H:59:LEU:HD21  | 1.77                     | 0.66              |
| 19:K:180:HIS:CE1 | 19:K:181:TRP:CD1  | 2.84                     | 0.66              |
| 22:N:99:ILE:HD12 | 22:N:123:ASN:HD22 | 1.59                     | 0.66              |
| 4:4:168:A:O2'    | 4:4:169:A:OP2     | 2.12                     | 0.65              |
| 4:4:116:G:OP1    | 10:B:339:ARG:NH1  | 2.29                     | 0.65              |
| 2:2:1450:A:H2'   | 2:2:1451:G:C8     | 2.31                     | 0.65              |
| 2:2:392:C:OP1    | 9:A:200:ARG:NH2   | 2.30                     | 0.65              |
| 10:B:93:ARG:HG3  | 10:B:102:ILE:CG2  | 2.27                     | 0.65              |
| 1:1:1578:U:H5''  | 25:Q:5:LYS:HD3    | 1.76                     | 0.65              |
| 1:1:1608:C:N4    | 1:1:1620:G:OP2    | 2.28                     | 0.65              |
| 1:1:752:G:N7     | 20:L:108:LYS:NZ   | 2.37                     | 0.65              |
| 6:6:16:C:O2      | 6:6:30:C:H1'      | 1.95                     | 0.65              |
| 13:E:5:LYS:H     | 13:E:58:ARG:HH12  | 1.42                     | 0.65              |
| 19:K:180:HIS:HE1 | 19:K:181:TRP:CD1  | 2.15                     | 0.65              |
| 31:W:82:VAL:HG21 | 31:W:96:ILE:HD11  | 1.77                     | 0.65              |
| 1:1:931:G:H5'    | 28:T:132:ALA:HB2  | 1.77                     | 0.65              |
| 2:2:1248:C:H2'   | 2:2:1249:OMC:H4'  | 1.79                     | 0.65              |
| 1:1:959:OMG:HN1  | 21:M:76:HIS:HD2   | 1.44                     | 0.65              |
| 3:3:209:G:C5     | 3:3:210:G:H2'     | 2.32                     | 0.65              |
| 8:8:72:A:HO2'    | 8:8:73:G:H8       | 1.44                     | 0.65              |
| 10:B:311:THR:O   | 10:B:368:THR:HG21 | 1.97                     | 0.65              |
| 16:H:200:ALA:CB  | 19:K:185:VAL:HG11 | 2.23                     | 0.65              |
| 1:1:83:A:H61     | 1:1:98:A:H3'      | 1.61                     | 0.65              |
| 2:2:575:C:OP1    | 50:2:1725:HOH:O   | 2.15                     | 0.65              |
| 6:6:28:A:C4      | 6:6:29:G:C5       | 2.84                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:P:30:ILE:HG23  | 24:P:49:TYR:HE1    | 1.61                     | 0.65              |
| 2:2:1133:A:H2     | 27:S:49:ARG:HH21   | 1.45                     | 0.65              |
| 1:1:1738:A:OP2    | 50:1:1969:HOH:O    | 2.13                     | 0.65              |
| 1:1:511:A:N6      | 1:1:541:A:N7       | 2.45                     | 0.65              |
| 2:2:526:A:O2'     | 2:2:527:A2M:O5'    | 2.12                     | 0.65              |
| 2:2:591:A2M:CM'   | 2:2:592:C:H5'      | 2.21                     | 0.65              |
| 6:6:28:A:N3       | 6:6:29:G:C6        | 2.63                     | 0.65              |
| 19:K:180:HIS:CD2  | 19:K:184:LYS:HE2   | 2.32                     | 0.65              |
| 23:O:21:ARG:C     | 23:O:21:ARG:HD3    | 2.18                     | 0.65              |
| 27:S:40:VAL:HB    | 27:S:96:VAL:HG13   | 1.78                     | 0.65              |
| 2:2:779:U:O2'     | 15:G:328:ARG:NH1   | 2.29                     | 0.65              |
| 6:6:17:U:C5       | 19:K:43:PRO:CD     | 2.79                     | 0.65              |
| 1:1:373:G:N2      | 7:7:29:C:O2        | 2.23                     | 0.65              |
| 13:E:93:CYS:N     | 13:E:141:ASP:OD2   | 2.28                     | 0.65              |
| 17:I:59:LEU:HD22  | 17:I:80:PHE:HZ     | 1.61                     | 0.65              |
| 21:M:73:ARG:HH12  | 21:M:86:THR:HB     | 1.62                     | 0.65              |
| 7:7:6:G:H2'       | 7:7:7:OMU:C6       | 2.26                     | 0.65              |
| 10:B:48:VAL:HG21  | 10:B:79:LEU:HD13   | 1.78                     | 0.65              |
| 17:I:79:GLY:HA3   | 17:I:103:ASP:HB2   | 1.79                     | 0.65              |
| 1:1:831:C:N4      | 24:P:179:GLU:O     | 2.30                     | 0.64              |
| 7:7:52:A:OP2      | 50:7:313:HOH:O     | 2.14                     | 0.64              |
| 11:C:170:LEU:HD11 | 11:C:225:LEU:HD22  | 1.79                     | 0.64              |
| 11:C:189:ARG:HD2  | 11:C:193:GLY:HA3   | 1.79                     | 0.64              |
| 23:O:185:ARG:O    | 23:O:185:ARG:HD2   | 1.97                     | 0.64              |
| 8:8:85:G:C8       | 8:8:85:G:H5''      | 2.32                     | 0.64              |
| 10:B:366:ILE:HD12 | 10:B:366:ILE:N     | 2.13                     | 0.64              |
| 21:M:159:ARG:HB2  | 21:M:164:LEU:HB2   | 1.79                     | 0.64              |
| 1:1:1041:U:H5''   | 27:S:100[B]:ARG:CZ | 2.28                     | 0.64              |
| 1:1:1115:C:H4'    | 1:1:1116:A:H5'     | 1.79                     | 0.64              |
| 1:1:852:A:N6      | 17:I:18:ASN:OD1    | 2.30                     | 0.64              |
| 2:2:1436:A:O2'    | 2:2:1438:A:OP2     | 2.15                     | 0.64              |
| 11:C:43:MET:HB2   | 11:C:236:LEU:HD11  | 1.80                     | 0.64              |
| 11:C:45:LYS:O     | 11:C:48:ARG:HG2    | 1.98                     | 0.64              |
| 13:E:34:LEU:HD22  | 13:E:149:ASP:HA    | 1.80                     | 0.64              |
| 24:P:152:GLY:HA2  | 24:P:157:ARG:HH21  | 1.63                     | 0.64              |
| 2:2:1385:A:H5''   | 2:2:1386:G:H5'     | 1.79                     | 0.64              |
| 2:2:749:G:H2'     | 2:2:750:U:C5       | 2.32                     | 0.64              |
| 2:2:815:G:H4'     | 2:2:816:G:OP1      | 1.98                     | 0.64              |
| 8:8:2:C:C4        | 8:8:120:C:C2       | 2.85                     | 0.64              |
| 9:A:82:MET:HG3    | 9:A:86:GLN:OE1     | 1.97                     | 0.64              |
| 1:1:395:A:N1      | 11:C:83:THR:HG22   | 2.13                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:M:122:ASN:HD22 | 21:M:123:MET:H    | 1.45                     | 0.64              |
| 28:T:127:ARG:O    | 28:T:139:TYR:HB3  | 1.97                     | 0.64              |
| 1:1:1539:G:OP1    | 28:T:65:GLY:HA3   | 1.96                     | 0.64              |
| 1:1:962:C:OP1     | 9:A:14:SER:OG     | 2.15                     | 0.64              |
| 3:3:22:G:O6       | 3:3:209:G:C2      | 2.35                     | 0.64              |
| 4:4:139:U:H4'     | 13:E:150:LEU:HD21 | 1.79                     | 0.64              |
| 14:F:42:LEU:HD11  | 14:F:85:ILE:HG13  | 1.79                     | 0.64              |
| 21:M:73:ARG:NH1   | 21:M:86:THR:HB    | 2.12                     | 0.64              |
| 24:P:186:THR:HA   | 24:P:191:LYS:HB2  | 1.79                     | 0.64              |
| 1:1:1672:A:C6     | 1:1:1729:A:N6     | 2.66                     | 0.64              |
| 1:1:171:U:H3'     | 1:1:172:G:H8      | 1.61                     | 0.64              |
| 2:2:828:U:O2      | 2:2:956:C:N4      | 2.30                     | 0.64              |
| 3:3:88:G:O2'      | 3:3:89:C:O4'      | 2.15                     | 0.64              |
| 1:1:1555:G:H1     | 1:1:1576:C:H42    | 1.46                     | 0.64              |
| 2:2:1151:U:C2'    | 2:2:1152:U:C5'    | 2.71                     | 0.64              |
| 8:8:14:U:OP2      | 8:8:69:C:O2'      | 2.15                     | 0.64              |
| 1:1:179:G:O2'     | 1:1:180:A:O5'     | 2.15                     | 0.64              |
| 1:1:238:A:N6      | 1:1:239:U:C4      | 2.61                     | 0.64              |
| 2:2:1042:G:H1     | 2:2:1055:U:H3     | 1.46                     | 0.64              |
| 6:6:54:A:O2'      | 6:6:55:U:H5'      | 1.97                     | 0.64              |
| 7:7:139:A:O2'     | 7:7:140:U:OP1     | 2.15                     | 0.64              |
| 10:B:102:ILE:HD11 | 10:B:157:ALA:HB2  | 1.80                     | 0.64              |
| 13:E:95:TYR:CZ    | 13:E:100:ILE:HG12 | 2.33                     | 0.64              |
| 23:O:17:GLN:NE2   | 27:S:21:LYS:HA    | 2.13                     | 0.64              |
| 31:W:33:SER:HA    | 31:W:102:GLU:OE2  | 1.97                     | 0.64              |
| 1:1:1253:U:OP1    | 16:H:74:GLN:NE2   | 2.31                     | 0.64              |
| 1:1:1278:G:N2     | 1:1:1351:C:N3     | 2.35                     | 0.64              |
| 1:1:728:C:H1'     | 1:1:730:G:C6      | 2.33                     | 0.64              |
| 2:2:997:C:H2'     | 2:2:998:A:H8      | 1.61                     | 0.64              |
| 1:1:490:C:O2'     | 6:6:54:A:H2       | 1.81                     | 0.64              |
| 7:7:28:C:H5''     | 17:I:32:ASN:HB3   | 1.80                     | 0.64              |
| 13:E:43:LEU:HD21  | 13:E:72:THR:HG21  | 1.79                     | 0.64              |
| 22:N:100:ASN:ND2  | 22:N:118:ALA:O    | 2.30                     | 0.64              |
| 23:O:107:ARG:HG3  | 23:O:256:ILE:HG22 | 1.81                     | 0.64              |
| 3:3:137:A:O2'     | 3:3:138:A:O5'     | 2.16                     | 0.63              |
| 1:1:1750:G:HO2'   | 3:3:149:U:HO2'    | 1.43                     | 0.63              |
| 1:1:136:G:H4'     | 1:1:137:G:OP1     | 1.98                     | 0.63              |
| 1:1:171:U:O2'     | 1:1:172:G:OP1     | 2.15                     | 0.63              |
| 1:1:346:U:HO2'    | 2:2:468:A:H8      | 1.46                     | 0.63              |
| 1:1:560:G:H4'     | 1:1:561:G:OP2     | 1.98                     | 0.63              |
| 2:2:1184:C:O2'    | 2:2:1185:C:OP1    | 2.15                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:4:153:C:O2      | 13:E:155:ARG:NH2  | 2.31                     | 0.63              |
| 6:6:10:C:N4       | 6:6:33:G:H1       | 1.96                     | 0.63              |
| 8:8:2:C:H2'       | 8:8:3:G:C8        | 2.33                     | 0.63              |
| 2:2:459:A:OP2     | 2:2:477:G:N1      | 2.31                     | 0.63              |
| 4:4:157:A:O2'     | 4:4:158:A:OP1     | 2.11                     | 0.63              |
| 8:8:48:G:N2       | 8:8:49:U:C2       | 2.67                     | 0.63              |
| 9:A:112:ILE:HD11  | 9:A:133:TYR:CD1   | 2.33                     | 0.63              |
| 22:N:76:MET:O     | 22:N:80:ALA:N     | 2.30                     | 0.63              |
| 24:P:139:THR:HG23 | 24:P:141:LYS:HG2  | 1.80                     | 0.63              |
| 13:E:91:VAL:HG21  | 13:E:160:LEU:HD11 | 1.80                     | 0.63              |
| 19:K:180:HIS:HE2  | 19:K:184:LYS:CE   | 2.09                     | 0.63              |
| 25:Q:14:ILE:HD11  | 25:Q:38:ARG:HB2   | 1.81                     | 0.63              |
| 1:1:1394:U:H2'    | 1:1:1395:U:H5'    | 1.79                     | 0.63              |
| 2:2:806:C:H2'     | 2:2:807:A:C8      | 2.32                     | 0.63              |
| 2:2:972:A:OP1     | 15:G:123:GLN:NE2  | 2.31                     | 0.63              |
| 3:3:92:G:O2'      | 3:3:93:G:N7       | 2.30                     | 0.63              |
| 9:A:137:ILE:HD11  | 9:A:149:LYS:HB2   | 1.79                     | 0.63              |
| 2:2:803:A:H4'     | 15:G:313:VAL:HG21 | 1.81                     | 0.63              |
| 16:H:92:ARG:HG2   | 16:H:165:GLY:HA3  | 1.79                     | 0.63              |
| 2:2:351:C:OP1     | 25:Q:88:ARG:NH2   | 2.32                     | 0.63              |
| 33:Y:48:LYS:HB3   | 33:Y:69:GLY:H     | 1.64                     | 0.63              |
| 4:4:112:C:O2'     | 5:5:39:C:OP1      | 2.16                     | 0.63              |
| 8:8:4:A:O2'       | 8:8:5:G:H8        | 1.80                     | 0.63              |
| 15:G:263:ALA:HB2  | 15:G:303:VAL:HG21 | 1.80                     | 0.63              |
| 18:J:111:MET:HG2  | 18:J:134:HIS:CD2  | 2.34                     | 0.63              |
| 21:M:71:ARG:O     | 21:M:71:ARG:HD3   | 1.98                     | 0.63              |
| 28:T:6:ARG:NH2    | 28:T:116:HIS:CB   | 2.50                     | 0.63              |
| 1:1:1551:U:H2'    | 1:1:1552:A:C8     | 2.34                     | 0.63              |
| 2:2:1175:A:H1'    | 23:O:185:ARG:HH11 | 1.63                     | 0.63              |
| 2:2:871:U:O2      | 2:2:939:G:N2      | 2.31                     | 0.63              |
| 6:6:53:U:O2       | 14:F:80:ASP:HB2   | 1.98                     | 0.63              |
| 8:8:81:U:H2'      | 8:8:82:G:C8       | 2.34                     | 0.63              |
| 19:K:180:HIS:O    | 19:K:183:ARG:HG3  | 1.99                     | 0.63              |
| 1:1:1143:C:H2'    | 1:1:1144:G:C8     | 2.34                     | 0.63              |
| 8:8:34:A:N6       | 8:8:43:G:N3       | 2.45                     | 0.63              |
| 10:B:292:ARG:HG2  | 10:B:293:SER:H    | 1.64                     | 0.63              |
| 15:G:218:VAL:HB   | 15:G:284:ALA:HB3  | 1.80                     | 0.63              |
| 21:M:200:PHE:HB3  | 21:M:204:ARG:HH21 | 1.63                     | 0.63              |
| 2:2:1408:A:N7     | 9:A:215:ASN:ND2   | 2.46                     | 0.63              |
| 3:3:139:G:H2'     | 3:3:140:A:H8      | 1.64                     | 0.63              |
| 6:6:37:C:C5       | 14:F:185:LYS:HD3  | 2.33                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:7:33:U:O2'      | 7:7:34:U:OP2      | 2.16                     | 0.63              |
| 8:8:11:C:C5'      | 8:8:12:C:OP2      | 2.47                     | 0.63              |
| 13:E:88:ARG:HB2   | 13:E:186:ILE:HB   | 1.81                     | 0.63              |
| 1:1:995:C:H5      | 1:1:1467:G:N1     | 1.97                     | 0.62              |
| 1:1:1780:G:N2     | 3:3:14:A:O2'      | 2.32                     | 0.62              |
| 1:1:491:A:N1      | 1:1:644:G:N2      | 2.47                     | 0.62              |
| 1:1:568:U:C4      | 1:1:634:G:O6      | 2.51                     | 0.62              |
| 2:2:442:C:H2'     | 2:2:488:A:N6      | 2.14                     | 0.62              |
| 1:1:923:G:O2'     | 2:2:92:A:OP1      | 2.13                     | 0.62              |
| 7:7:168:G:H2'     | 7:7:169:A:C8      | 2.34                     | 0.62              |
| 5:5:36:U:O2'      | 10:B:372:ILE:CG2  | 2.47                     | 0.62              |
| 10:B:368:THR:H    | 10:B:378:GLN:HE22 | 1.47                     | 0.62              |
| 16:H:95:SER:OG    | 16:H:124:GLU:OE1  | 2.16                     | 0.62              |
| 24:P:117:ARG:NH1  | 24:P:127:CYS:SG   | 2.71                     | 0.62              |
| 26:R:103:GLY:O    | 26:R:107:GLN:NE2  | 2.32                     | 0.62              |
| 1:1:1122:U:O2'    | 1:1:1144:G:N2     | 2.32                     | 0.62              |
| 1:1:193:A:H2'     | 1:1:194:A:C8      | 2.34                     | 0.62              |
| 2:2:1270:G:N2     | 2:2:1297:U:O2     | 2.21                     | 0.62              |
| 2:2:755:U:HO2'    | 2:2:756:C:H6      | 1.45                     | 0.62              |
| 8:8:63:C:O2'      | 8:8:64:A:O5'      | 2.17                     | 0.62              |
| 6:6:41:G:N2       | 19:K:173:VAL:HG12 | 2.12                     | 0.62              |
| 1:1:1611:A:N1     | 1:1:1622:A:O2'    | 2.30                     | 0.62              |
| 3:3:82:G:N2       | 3:3:91:G:O6       | 2.16                     | 0.62              |
| 14:F:174:LYS:HA   | 14:F:177:TYR:HB3  | 1.81                     | 0.62              |
| 14:F:40:ILE:HB    | 14:F:85:ILE:HB    | 1.81                     | 0.62              |
| 8:8:85:G:H8       | 8:8:85:G:C5'      | 2.11                     | 0.62              |
| 10:B:321:TYR:HD1  | 10:B:340:ARG:CG   | 2.11                     | 0.62              |
| 15:G:224:VAL:HG13 | 15:G:284:ALA:HB2  | 1.80                     | 0.62              |
| 16:H:108:ARG:CG   | 16:H:108:ARG:HH11 | 2.12                     | 0.62              |
| 16:H:52:THR:HG23  | 16:H:121:VAL:HB   | 1.80                     | 0.62              |
| 23:O:41:LYS:NZ    | 27:S:32:THR:O     | 2.33                     | 0.62              |
| 1:1:1180:U:H1'    | 1:1:1181:U:H5'    | 1.82                     | 0.62              |
| 1:1:754:G:N2      | 1:1:768:C:OP2     | 2.33                     | 0.62              |
| 6:6:16:C:N3       | 6:6:17:U:C4       | 2.67                     | 0.62              |
| 6:6:42:A:O2'      | 6:6:43:A:O4'      | 2.16                     | 0.62              |
| 1:1:1063:G:N2     | 1:1:1089:C:O2     | 2.32                     | 0.62              |
| 1:1:1268:G:O6     | 1:1:1360:C:N4     | 2.30                     | 0.62              |
| 1:1:1727:U:H3'    | 1:1:1728:G:C8     | 2.34                     | 0.62              |
| 1:1:491:A:H61     | 1:1:644:G:H1      | 1.47                     | 0.62              |
| 1:1:953:G:H2'     | 1:1:954:U:H5'     | 1.80                     | 0.62              |
| 2:2:1011:U:O3'    | 15:G:148:ARG:NH1  | 2.32                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:606:G:O2'     | 2:2:608:C:OP2     | 2.16                     | 0.62              |
| 4:4:173:C:O2'     | 4:4:175:G:OP1     | 2.16                     | 0.62              |
| 9:A:111:CYS:SG    | 9:A:112:ILE:N     | 2.70                     | 0.62              |
| 10:B:292:ARG:HE   | 10:B:296:VAL:HG11 | 1.64                     | 0.62              |
| 13:E:26:THR:HA    | 13:E:35:THR:HG22  | 1.82                     | 0.62              |
| 1:1:1481:A:N6     | 1:1:1510:A:O2'    | 2.32                     | 0.62              |
| 1:1:251:A:N6      | 1:1:376:A:OP1     | 2.32                     | 0.62              |
| 1:1:154:A:H8      | 1:1:301:A:H62     | 1.46                     | 0.62              |
| 1:1:892:C:O3'     | 25:Q:126:ARG:NH1  | 2.31                     | 0.62              |
| 6:6:21:A:H1'      | 6:6:22:G:P        | 2.39                     | 0.62              |
| 16:H:103:ARG:HH11 | 16:H:103:ARG:CG   | 2.12                     | 0.62              |
| 1:1:561:G:O2'     | 1:1:1424:A:O3'    | 2.17                     | 0.62              |
| 1:1:988:G:N2      | 1:1:1012:C:OP1    | 2.33                     | 0.62              |
| 4:4:180:C:H1'     | 5:5:3:C:H1'       | 1.82                     | 0.62              |
| 9:A:28:LYS:O      | 9:A:74:GLU:OE2    | 2.17                     | 0.62              |
| 10:B:25:ILE:HG22  | 10:B:277:TYR:HE1  | 1.65                     | 0.62              |
| 6:6:51:A:C8       | 14:F:45:ARG:NH1   | 2.68                     | 0.62              |
| 2:2:1012:G:H22    | 15:G:153:ARG:HH12 | 1.48                     | 0.62              |
| 1:1:208:C:N3      | 1:1:209:C:N4      | 2.47                     | 0.62              |
| 1:1:398:G:N1      | 1:1:401:A:OP2     | 2.31                     | 0.62              |
| 1:1:543:G:H3'     | 1:1:543:G:N3      | 2.15                     | 0.62              |
| 1:1:847:OMU:H5'   | 17:I:2:PRO:O      | 2.00                     | 0.62              |
| 18:J:116:ILE:H    | 18:J:116:ILE:CD1  | 2.12                     | 0.62              |
| 1:1:1057:A:H3'    | 1:1:1058:U:C6     | 2.35                     | 0.62              |
| 2:2:526:A:H4'     | 2:2:527:A2M:OP1   | 2.00                     | 0.62              |
| 2:2:663:U:O2'     | 2:2:1404:H2U:H52  | 2.00                     | 0.62              |
| 2:2:834:G:O6      | 2:2:951:G:N2      | 2.31                     | 0.62              |
| 2:2:362:A:N6      | 4:4:90:G:O2'      | 2.31                     | 0.62              |
| 1:1:1163:G:O6     | 24:P:13:ARG:NH2   | 2.29                     | 0.61              |
| 1:1:458:A:C2      | 1:1:459:A:H1'     | 2.35                     | 0.61              |
| 9:A:105:GLY:HA3   | 9:A:160:SER:HB3   | 1.81                     | 0.61              |
| 20:L:75:LEU:HG    | 20:L:111:GLY:HA2  | 1.81                     | 0.61              |
| 23:O:23:ARG:HD3   | 23:O:23:ARG:C     | 2.20                     | 0.61              |
| 25:Q:147:ASN:O    | 25:Q:151:LYS:N    | 2.33                     | 0.61              |
| 2:2:1449:A:H3'    | 2:2:1450:A:C8     | 2.35                     | 0.61              |
| 13:E:150:LEU:HD23 | 13:E:151:GLU:HB2  | 1.82                     | 0.61              |
| 22:N:43:VAL:HG12  | 22:N:171:TRP:HE1  | 1.64                     | 0.61              |
| 1:1:1202:G:N2     | 1:1:1401:U:O2'    | 2.33                     | 0.61              |
| 1:1:905:G:H4'     | 25:Q:130:ASN:HD22 | 1.65                     | 0.61              |
| 2:2:1152:U:H2'    | 2:2:1153:OMU:H6   | 1.82                     | 0.61              |
| 3:3:39:U:H1'      | 3:3:139:G:H5"     | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:B:321:TYR:HD1  | 10:B:340:ARG:HG2  | 1.64                     | 0.61              |
| 19:K:108:VAL:O    | 19:K:108:VAL:HG12 | 1.99                     | 0.61              |
| 16:H:137:VAL:HA   | 19:K:45:SER:O     | 2.00                     | 0.61              |
| 16:H:146:VAL:HG12 | 19:K:55:ALA:HB1   | 1.81                     | 0.61              |
| 1:1:770:G:H22     | 1:1:806:A:H2      | 1.49                     | 0.61              |
| 1:1:801:G:N3      | 24:P:147:ARG:NH1  | 2.48                     | 0.61              |
| 1:1:831:C:OP1     | 24:P:184:ARG:NH2  | 2.33                     | 0.61              |
| 2:2:787:G:H1      | 2:2:807:A:H61     | 1.48                     | 0.61              |
| 6:6:41:G:H3'      | 19:K:180:HIS:NE2  | 2.14                     | 0.61              |
| 11:C:158:GLN:HA   | 11:C:215:GLY:HA3  | 1.82                     | 0.61              |
| 18:J:82:ARG:NH1   | 18:J:118:GLY:HA3  | 2.15                     | 0.61              |
| 18:J:64:VAL:HG21  | 18:J:71:LEU:HD13  | 1.82                     | 0.61              |
| 19:K:94:VAL:CG2   | 19:K:109:GLN:O    | 2.49                     | 0.61              |
| 1:1:317:U:O2'     | 1:1:319:G:N7      | 2.28                     | 0.61              |
| 1:1:839:U:H2'     | 1:1:840:G:C8      | 2.35                     | 0.61              |
| 8:8:40:U:C2'      | 8:8:44:A:H62      | 2.13                     | 0.61              |
| 8:8:34:A:N1       | 8:8:43:G:C2       | 2.69                     | 0.61              |
| 10:B:346:ARG:HH12 | 10:B:349:MET:HG2  | 1.64                     | 0.61              |
| 1:1:1245:G:N3     | 26:R:114:SER:OG   | 2.28                     | 0.61              |
| 1:1:1495:G:N2     | 1:1:1498:A:OP2    | 2.30                     | 0.61              |
| 1:1:367:A:H4'     | 1:1:368:G:OP2     | 2.01                     | 0.61              |
| 2:2:772:A:O2'     | 2:2:1016:C:OP1    | 2.15                     | 0.61              |
| 2:2:455:U:H3'     | 2:2:456:G:H8      | 1.63                     | 0.61              |
| 2:2:610:G:H1      | 2:2:642:G:H21     | 1.49                     | 0.61              |
| 2:2:729:G:H2'     | 2:2:730:A:H3'     | 1.83                     | 0.61              |
| 16:H:146:VAL:HG13 | 19:K:55:ALA:CB    | 2.28                     | 0.61              |
| 15:G:130:ASP:OD2  | 15:G:132:SER:OG   | 2.17                     | 0.61              |
| 20:L:72:THR:HB    | 20:L:110:LEU:HD23 | 1.81                     | 0.61              |
| 1:1:1440:A:O4'    | 34:Z:39:THR:OG1   | 2.17                     | 0.61              |
| 1:1:1242:U:O2'    | 1:1:1243:G:O4'    | 2.18                     | 0.61              |
| 1:1:381:G:N2      | 7:7:21:U:O2'      | 2.34                     | 0.61              |
| 2:2:590:U:H2'     | 2:2:591:A2M:C8    | 2.30                     | 0.61              |
| 2:2:747:A:N6      | 2:2:749:G:C6      | 2.68                     | 0.61              |
| 2:2:771:G:N2      | 2:2:969:U:H3      | 1.98                     | 0.61              |
| 1:1:1743:A:O2'    | 3:3:201:A:N1      | 2.31                     | 0.61              |
| 5:5:125:A:H2'     | 5:5:126:G:H5'     | 1.81                     | 0.61              |
| 11:C:139:ARG:HD2  | 11:C:245:GLY:HA3  | 1.81                     | 0.61              |
| 15:G:131:LEU:O    | 15:G:133:ARG:N    | 2.34                     | 0.61              |
| 16:H:147:CYS:HA   | 19:K:57:CYS:O     | 2.00                     | 0.61              |
| 32:X:37:ARG:HD3   | 32:X:39:LYS:HE2   | 1.81                     | 0.61              |
| 1:1:848:U:H6      | 1:1:848:U:C5'     | 2.13                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:527:A2M:HM'1  | 2:2:1399:C:H1'    | 1.83                     | 0.61              |
| 2:2:44:C:O2'      | 4:4:94:G:OP1      | 2.14                     | 0.61              |
| 8:8:2:C:N3        | 8:8:120:C:N3      | 2.49                     | 0.61              |
| 18:J:18:ALA:HB2   | 18:J:83:GLN:HE21  | 1.66                     | 0.61              |
| 33:Y:17:ARG:NH2   | 33:Y:18:TYR:OH    | 2.34                     | 0.61              |
| 1:1:1062:A:H5'    | 22:N:39:ARG:HG2   | 1.83                     | 0.61              |
| 2:2:1273:G:N1     | 2:2:1294:C:N3     | 2.49                     | 0.61              |
| 5:5:37:G:H4'      | 10:B:373:GLY:CA   | 2.31                     | 0.61              |
| 1:1:1530:U:H5''   | 11:C:75:ILE:HD11  | 1.83                     | 0.61              |
| 22:N:141:LYS:HB2  | 22:N:144:TYR:HD2  | 1.66                     | 0.61              |
| 31:W:28:MET:SD    | 31:W:72:ARG:HG3   | 2.41                     | 0.61              |
| 1:1:229:C:HO2'    | 1:1:230:A:H8      | 1.47                     | 0.60              |
| 1:1:1549:U:OP2    | 2:2:60:A:O2'      | 2.16                     | 0.60              |
| 2:2:685:G:N2      | 2:2:754:U:O2      | 2.22                     | 0.60              |
| 3:3:195:A:H8      | 3:3:195:A:H5''    | 1.66                     | 0.60              |
| 22:N:176:ILE:HG13 | 22:N:190:LEU:HD11 | 1.83                     | 0.60              |
| 28:T:120:ASP:OD1  | 28:T:145:HIS:HB2  | 2.01                     | 0.60              |
| 4:4:63:U:O4'      | 13:E:119:ARG:NH2  | 2.33                     | 0.60              |
| 29:U:29:ASP:HB3   | 29:U:118:GLN:HA   | 1.83                     | 0.60              |
| 1:1:1126:U:H2'    | 1:1:1127:U:H4'    | 1.83                     | 0.60              |
| 1:1:806:A:O2'     | 1:1:807:C:O5'     | 2.19                     | 0.60              |
| 6:6:16:C:H3'      | 6:6:16:C:H6       | 1.66                     | 0.60              |
| 9:A:89:PHE:H      | 9:A:100:ASN:ND2   | 1.97                     | 0.60              |
| 22:N:100:ASN:HD21 | 22:N:118:ALA:HB1  | 1.64                     | 0.60              |
| 22:N:86:HIS:HB2   | 22:N:139:ARG:HB2  | 1.83                     | 0.60              |
| 1:1:1122:U:H1'    | 1:1:1144:G:H22    | 1.65                     | 0.60              |
| 1:1:660:U:H5'     | 7:7:7:OMU:HM22    | 1.83                     | 0.60              |
| 2:2:97:A:O2'      | 2:2:366:C:O2      | 2.17                     | 0.60              |
| 2:2:451:U:H3      | 2:2:483:C:H42     | 1.49                     | 0.60              |
| 1:1:216:G:O2'     | 4:4:183:C:N3      | 2.34                     | 0.60              |
| 10:B:288:TYR:CZ   | 10:B:332:LYS:HG3  | 2.36                     | 0.60              |
| 13:E:89:PHE:O     | 13:E:145:PHE:N    | 2.32                     | 0.60              |
| 18:J:106:ASN:OD1  | 18:J:107:PRO:HD3  | 1.98                     | 0.60              |
| 25:Q:55:VAL:HG13  | 25:Q:56:LYS:H     | 1.65                     | 0.60              |
| 1:1:1061:G:H2'    | 1:1:1062:A:C8     | 2.36                     | 0.60              |
| 1:1:236:G:O2'     | 1:1:237:U:OP1     | 2.19                     | 0.60              |
| 1:1:849:U:O2'     | 1:1:850:G:O5'     | 2.19                     | 0.60              |
| 9:A:91:GLY:O      | 9:A:103:PRO:HD3   | 2.01                     | 0.60              |
| 3:3:8:A:OP2       | 33:Y:73:ARG:NH2   | 2.35                     | 0.60              |
| 1:1:388:A:H4'     | 1:1:407:A:N6      | 2.16                     | 0.60              |
| 1:1:669:C:O2'     | 1:1:670:C:O5'     | 2.18                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:2:1317:G:N1    | 2:2:1387:C:N3     | 2.50                     | 0.60              |
| 1:1:696:A:H5''   | 11:C:108:ARG:HA   | 1.84                     | 0.60              |
| 4:4:74:G:N2      | 4:4:123:C:O2      | 2.24                     | 0.60              |
| 2:2:1434:G:N2    | 4:4:170:G:N7      | 2.37                     | 0.60              |
| 8:8:12:C:O2      | 8:8:15:A:C2       | 2.55                     | 0.60              |
| 8:8:4:A:N6       | 8:8:119:U:O4      | 2.34                     | 0.60              |
| 1:1:1674:U:N3    | 1:1:1728:G:N2     | 2.50                     | 0.60              |
| 2:2:443:OMC:N4   | 2:2:487:U:H2'     | 2.16                     | 0.60              |
| 2:2:957:C:H1'    | 2:2:958:C:P       | 2.41                     | 0.60              |
| 2:2:996:G:H2'    | 2:2:997:C:C6      | 2.37                     | 0.60              |
| 16:H:45:LEU:HD11 | 16:H:120:LEU:HG   | 1.84                     | 0.60              |
| 17:I:83:ALA:CB   | 17:I:108:ASN:ND2  | 2.64                     | 0.60              |
| 1:1:1209:G:N2    | 1:1:1209:G:OP2    | 2.24                     | 0.60              |
| 4:4:181:C:H1'    | 5:5:2:A:C4        | 2.36                     | 0.60              |
| 13:E:169:LYS:HZ2 | 13:E:174:PHE:HE1  | 1.50                     | 0.60              |
| 1:1:1042:G:H1    | 1:1:1109:U:H5     | 1.50                     | 0.60              |
| 1:1:778:C:O2'    | 1:1:779:A:H8      | 1.83                     | 0.60              |
| 2:2:676:G:OP2    | 50:2:1702:HOH:O   | 2.16                     | 0.60              |
| 11:C:7:VAL:HG11  | 11:C:255:PHE:HE2  | 1.67                     | 0.60              |
| 1:1:1058:U:H1'   | 22:N:94:PHE:HE1   | 1.67                     | 0.60              |
| 28:T:13:LYS:HA   | 28:T:107:LEU:HD21 | 1.84                     | 0.60              |
| 10:B:376:ARG:NH2 | 32:X:11:PHE:HD1   | 1.99                     | 0.60              |
| 1:1:1433:U:O2'   | 1:1:1434:U:H5''   | 2.02                     | 0.59              |
| 1:1:1458:G:O6    | 50:1:1956:HOH:O   | 2.15                     | 0.59              |
| 3:3:32:A:N1      | 3:3:33:A:N6       | 2.49                     | 0.59              |
| 5:5:44:G:H1      | 5:5:103:U:H3      | 1.49                     | 0.59              |
| 8:8:85:G:C8      | 8:8:85:G:C5'      | 2.85                     | 0.59              |
| 33:Y:50:PRO:HD3  | 33:Y:68:VAL:HG22  | 1.84                     | 0.59              |
| 1:1:1238:C:H5'   | 1:1:1239:U:H5''   | 1.84                     | 0.59              |
| 2:2:1184:C:H2'   | 2:2:1185:C:O4'    | 2.02                     | 0.59              |
| 2:2:590:U:H2'    | 2:2:591:A2M:H8    | 1.84                     | 0.59              |
| 8:8:116:U:H2'    | 8:8:117:A:C8      | 2.37                     | 0.59              |
| 1:1:1145:G:C2    | 1:1:1146:A:H1'    | 2.37                     | 0.59              |
| 1:1:695:OMC:HM22 | 1:1:696:A:H5'     | 1.84                     | 0.59              |
| 1:1:73:U:H5''    | 17:I:63:VAL:HB    | 1.84                     | 0.59              |
| 1:1:895:G:O6     | 1:1:901:C:N4      | 2.34                     | 0.59              |
| 1:1:1651:G:H21   | 2:2:414:G:N2      | 2.00                     | 0.59              |
| 6:6:17:U:N3      | 6:6:30:C:O2'      | 2.35                     | 0.59              |
| 8:8:34:A:H4'     | 8:8:35:U:H5'      | 1.84                     | 0.59              |
| 24:P:36:LEU:O    | 24:P:40:THR:OG1   | 2.12                     | 0.59              |
| 28:T:109:PRO:HA  | 28:T:112:MET:HG2  | 1.83                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:T:124:ARG:NH1  | 28:T:142:SER:OG   | 2.35                     | 0.59              |
| 1:1:1122:U:O2     | 1:1:1144:G:N1     | 2.35                     | 0.59              |
| 1:1:1129:G:H1     | 1:1:1137:C:H42    | 1.51                     | 0.59              |
| 1:1:502:U:O2'     | 1:1:503:A:O4'     | 2.21                     | 0.59              |
| 1:1:895:G:H1      | 1:1:900:C:N4      | 1.97                     | 0.59              |
| 2:2:553:G:H4'     | 2:2:554:OMC:OP2   | 2.02                     | 0.59              |
| 5:5:12:C:O2'      | 5:5:14:A:N6       | 2.34                     | 0.59              |
| 13:E:20:VAL:HG21  | 13:E:46:ARG:HA    | 1.84                     | 0.59              |
| 21:M:119:TYR:OH   | 21:M:131:GLU:OE1  | 2.15                     | 0.59              |
| 22:N:121:LYS:CE   | 22:N:122:PRO:CD   | 2.70                     | 0.59              |
| 22:N:152:LEU:HD13 | 22:N:165:ILE:HG12 | 1.83                     | 0.59              |
| 26:R:13:GLY:HA2   | 26:R:61:LEU:HG    | 1.83                     | 0.59              |
| 28:T:36:ILE:O     | 28:T:36:ILE:HD12  | 2.02                     | 0.59              |
| 1:1:255:G:H1      | 31:W:59:THR:HG23  | 1.67                     | 0.59              |
| 2:2:527:A2M:HM'3  | 2:2:1398:OMC:CM2  | 2.33                     | 0.59              |
| 3:3:163:C:H41     | 25:Q:46:LYS:CB    | 2.16                     | 0.59              |
| 19:K:74:LEU:HD23  | 19:K:113:ASN:O    | 2.02                     | 0.59              |
| 19:K:94:VAL:HG22  | 19:K:109:GLN:O    | 2.03                     | 0.59              |
| 1:1:1271:G:N2     | 1:1:1359:C:O2     | 2.33                     | 0.59              |
| 1:1:930:U:O2      | 2:2:603:A:O2'     | 2.16                     | 0.59              |
| 2:2:603:A:H2'     | 2:2:604:A:C8      | 2.38                     | 0.59              |
| 2:2:743:C:H2'     | 2:2:744:G:H8      | 1.68                     | 0.59              |
| 6:6:27:G:H2'      | 6:6:28:A:H5'      | 1.83                     | 0.59              |
| 10:B:19:ARG:HB2   | 10:B:237:ARG:NH2  | 2.12                     | 0.59              |
| 10:B:56:ILE:HD11  | 10:B:288:TYR:HD2  | 1.67                     | 0.59              |
| 18:J:47:ARG:HE    | 18:J:50:ARG:HB2   | 1.68                     | 0.59              |
| 24:P:144:TYR:CE2  | 24:P:146:LEU:HD21 | 2.36                     | 0.59              |
| 1:1:1389:A:H3'    | 19:K:77:PRO:CG    | 2.32                     | 0.59              |
| 1:1:1727:U:C5     | 1:1:1728:G:C5     | 2.90                     | 0.59              |
| 3:3:45:C:H2'      | 3:3:46:A:C8       | 2.37                     | 0.59              |
| 4:4:45:G:H2'      | 4:4:46:G:C8       | 2.38                     | 0.59              |
| 8:8:14:U:O4'      | 8:8:110:G:N2      | 2.35                     | 0.59              |
| 9:A:45:VAL:O      | 9:A:85:GLY:N      | 2.36                     | 0.59              |
| 10:B:192:ASN:O    | 10:B:195:ALA:N    | 2.35                     | 0.59              |
| 1:1:1763:A:H2'    | 30:V:128:ARG:HH22 | 1.65                     | 0.59              |
| 1:1:779:A:P       | 24:P:142:ASN:H    | 2.26                     | 0.59              |
| 3:3:31:C:H4'      | 3:3:32:A:OP2      | 2.02                     | 0.59              |
| 8:8:44:A:N7       | 8:8:45:U:C5       | 2.71                     | 0.59              |
| 11:C:299:VAL:HG21 | 24:P:138:PRO:HG2  | 1.84                     | 0.59              |
| 20:L:112:ASN:HD22 | 20:L:113:GLY:N    | 2.00                     | 0.59              |
| 22:N:14:ASN:OD1   | 22:N:15:LYS:N     | 2.35                     | 0.59              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 2:2:1019:G:H4'   | 2:2:1021:C:C2       | 2.37                     | 0.59              |
| 1:1:429:G:H1'    | 28:T:97:ASN:HD21    | 1.68                     | 0.59              |
| 1:1:1189:C:H2'   | 1:1:1190:G:C8       | 2.38                     | 0.59              |
| 2:2:771:G:N7     | 9:A:67:TYR:OH       | 2.24                     | 0.59              |
| 4:4:136:G:H22    | 4:4:155:A:H1'       | 1.67                     | 0.59              |
| 4:4:181:C:H2'    | 4:4:182:A:H8        | 1.68                     | 0.59              |
| 6:6:22:G:N7      | 6:6:26:G:N2         | 2.50                     | 0.59              |
| 13:E:42:GLN:HG3  | 13:E:60:PHE:HB2     | 1.85                     | 0.59              |
| 28:T:6:ARG:HH21  | 28:T:116:HIS:CB     | 2.11                     | 0.59              |
| 1:1:1393:A:H3'   | 1:1:1393:A:OP1      | 2.02                     | 0.58              |
| 1:1:167:U:O2'    | 1:1:168:G:N7        | 2.30                     | 0.58              |
| 1:1:237:U:OP2    | 50:1:1928:HOH:O     | 2.17                     | 0.58              |
| 1:1:301:A:H2'    | 1:1:302:G:C8        | 2.38                     | 0.58              |
| 2:2:1078:OMU:CM2 | 2:2:1079:OMG:H5'    | 2.33                     | 0.58              |
| 2:2:655:OMG:O2'  | 2:2:657:U:H5''      | 2.03                     | 0.58              |
| 3:3:116:C:H5''   | 25:Q:99:LEU:HD12    | 1.85                     | 0.58              |
| 7:7:105:C:OP2    | 50:7:316:HOH:O      | 2.17                     | 0.58              |
| 1:1:1041:U:H4'   | 27:S:100[A]:ARG:HB2 | 1.85                     | 0.58              |
| 1:1:300:A:N3     | 1:1:301:A:H1'       | 2.18                     | 0.58              |
| 2:2:1095:A:O2'   | 2:2:1119:A:OP1      | 2.21                     | 0.58              |
| 2:2:387:U:O2     | 2:2:1415:G:N2       | 2.35                     | 0.58              |
| 2:2:387:U:OP2    | 50:2:1715:HOH:O     | 2.16                     | 0.58              |
| 9:A:45:VAL:HG22  | 9:A:61:VAL:HG22     | 1.85                     | 0.58              |
| 19:K:72:ARG:HD2  | 19:K:72:ARG:O       | 2.03                     | 0.58              |
| 22:N:53:VAL:C    | 22:N:163:GLN:HE22   | 2.05                     | 0.58              |
| 23:O:189:TYR:HA  | 23:O:194:SER:HA     | 1.85                     | 0.58              |
| 23:O:19:LYS:NZ   | 23:O:19:LYS:HB2     | 2.18                     | 0.58              |
| 1:1:1655:U:OP1   | 21:M:105:ARG:NE     | 2.32                     | 0.58              |
| 2:2:1189:G:N2    | 2:2:1239:G:O4'      | 2.37                     | 0.58              |
| 2:2:68:A:O2'     | 2:2:69:A:O5'        | 2.13                     | 0.58              |
| 6:6:13:C:N4      | 6:6:14:A:N6         | 2.50                     | 0.58              |
| 15:G:158:PRO:HB3 | 15:G:317:GLN:H      | 1.68                     | 0.58              |
| 22:N:130:ARG:NH2 | 22:N:131:ILE:O      | 2.31                     | 0.58              |
| 2:2:1051:G:N2    | 2:2:1072:C:O2       | 2.36                     | 0.58              |
| 2:2:1153:OMU:OP2 | 2:2:1155:C:N4       | 2.36                     | 0.58              |
| 2:2:1317:G:O6    | 2:2:1387:C:C4       | 2.55                     | 0.58              |
| 3:3:106:U:C5     | 3:3:128:C:N4        | 2.71                     | 0.58              |
| 11:C:257:GLN:O   | 11:C:261:ILE:N      | 2.31                     | 0.58              |
| 1:1:777:G:H21    | 24:P:144:TYR:HA     | 1.68                     | 0.58              |
| 25:Q:19:ARG:HD2  | 25:Q:20:ALA:N       | 2.17                     | 0.58              |
| 1:1:237:U:H3'    | 1:1:238:A:C8        | 2.38                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:705:C:H4'     | 11:C:34:ASP:OD2   | 2.03                     | 0.58              |
| 2:2:1332:G:H4'    | 4:4:157:A:H1'     | 1.85                     | 0.58              |
| 8:8:73:G:H2'      | 8:8:74:U:O4'      | 2.03                     | 0.58              |
| 23:O:44:PHE:CE1   | 27:S:33:ASN:HB3   | 2.38                     | 0.58              |
| 31:W:29:SER:HA    | 31:W:46:PRO:HA    | 1.84                     | 0.58              |
| 1:1:1491:U:H2'    | 1:1:1492:G:C8     | 2.37                     | 0.58              |
| 1:1:1493:G:O2'    | 1:1:1494:C:OP2    | 2.14                     | 0.58              |
| 1:1:157:U:H3      | 1:1:297:A:H61     | 1.51                     | 0.58              |
| 1:1:179:G:O2'     | 1:1:180:A:O4'     | 2.22                     | 0.58              |
| 2:2:1056:A:N6     | 2:2:1078:OMU:HN3  | 2.00                     | 0.58              |
| 2:2:1316:G:H2'    | 2:2:1317:G:O4'    | 2.03                     | 0.58              |
| 8:8:54:U:H1'      | 8:8:56:A:H62      | 1.68                     | 0.58              |
| 20:L:70:LYS:HD3   | 20:L:108:LYS:HD2  | 1.84                     | 0.58              |
| 1:1:204:A:H2'     | 1:1:205:A:H5'     | 1.86                     | 0.58              |
| 1:1:547:U:C4      | 1:1:1393:A:N6     | 2.71                     | 0.58              |
| 2:2:527:A2M:H4'   | 2:2:528:U:OP1     | 2.04                     | 0.58              |
| 3:3:8:A:P         | 33:Y:73:ARG:HH21  | 2.25                     | 0.58              |
| 9:A:65:HIS:HB2    | 9:A:72:VAL:CG1    | 2.31                     | 0.58              |
| 2:2:1386:G:C2     | 10:B:255:ALA:HB1  | 2.39                     | 0.58              |
| 13:E:16:VAL:HG11  | 13:E:80:ILE:HG23  | 1.86                     | 0.58              |
| 2:2:802:U:O3'     | 15:G:310:ARG:NH2  | 2.37                     | 0.58              |
| 1:1:422:U:O2'     | 1:1:423:U:H5''    | 2.03                     | 0.58              |
| 1:1:836:G:OP2     | 24:P:63:SER:OG    | 2.21                     | 0.58              |
| 2:2:1443:G:O6     | 15:G:133:ARG:NH1  | 147.47                   | 0.58              |
| 5:5:46:G:N1       | 5:5:101:C:N3      | 2.39                     | 0.58              |
| 6:6:16:C:C4       | 6:6:17:U:C5       | 2.91                     | 0.58              |
| 10:B:315:MET:O    | 10:B:370:SER:HB2  | 2.04                     | 0.58              |
| 18:J:98:GLU:HG3   | 32:X:24:PHE:H     | 1.69                     | 0.58              |
| 22:N:170:TYR:O    | 22:N:178:ARG:NE   | 2.33                     | 0.58              |
| 23:O:61:ILE:HG23  | 23:O:79:TYR:CE1   | 2.39                     | 0.58              |
| 25:Q:102:LEU:HD22 | 25:Q:138:LEU:HD22 | 1.85                     | 0.58              |
| 4:4:95:U:C5       | 25:Q:62:ARG:NE    | 2.71                     | 0.58              |
| 1:1:242:A:N6      | 1:1:260:C:H42     | 2.01                     | 0.58              |
| 10:B:379:THR:O    | 10:B:381:LYS:N    | 2.37                     | 0.58              |
| 13:E:16:VAL:HG11  | 13:E:80:ILE:HG12  | 1.86                     | 0.58              |
| 15:G:141:VAL:HG12 | 15:G:145:ARG:HH12 | 1.69                     | 0.58              |
| 15:G:141:VAL:HG12 | 15:G:145:ARG:NH1  | 2.19                     | 0.58              |
| 27:S:116:LEU:O    | 27:S:120:LYS:N    | 2.32                     | 0.58              |
| 30:V:68:TYR:CE1   | 30:V:88:ILE:HD12  | 2.39                     | 0.58              |
| 1:1:488:G:N2      | 1:1:648:A:N3      | 2.51                     | 0.58              |
| 1:1:676:G:H2'     | 2:2:618:A:N7      | 2.19                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:872:U:H4'     | 1:1:963:G:H5'     | 1.85                     | 0.58              |
| 2:2:654:U:H2'     | 2:2:655:OMG:H5'   | 1.86                     | 0.58              |
| 8:8:93:U:HO2'     | 8:8:94:G:H8       | 1.50                     | 0.58              |
| 21:M:23:GLN:HA    | 21:M:26:ARG:HG2   | 1.84                     | 0.58              |
| 26:R:8:HIS:HD2    | 26:R:66:VAL:HG21  | 1.68                     | 0.58              |
| 27:S:103:GLU:HA   | 27:S:106:LYS:HB2  | 1.84                     | 0.58              |
| 1:1:1189:C:H2'    | 1:1:1190:G:H8     | 1.68                     | 0.57              |
| 1:1:1523:G:OP2    | 20:L:9:ARG:NH1    | 2.31                     | 0.57              |
| 1:1:933:A:OP1     | 2:2:30:A:N6       | 2.32                     | 0.57              |
| 2:2:47:A:H5'      | 25:Q:88:ARG:HG2   | 1.86                     | 0.57              |
| 2:2:716:C:H2'     | 2:2:717:G:O4'     | 2.04                     | 0.57              |
| 15:G:215:LEU:HD21 | 15:G:288:VAL:HA   | 1.86                     | 0.57              |
| 22:N:53:VAL:HG22  | 22:N:134:ILE:HG12 | 1.85                     | 0.57              |
| 27:S:56:TYR:OH    | 27:S:79:PRO:HD2   | 2.04                     | 0.57              |
| 28:T:31:GLU:HG2   | 28:T:60:PHE:HA    | 1.83                     | 0.57              |
| 1:1:1445:U:O2     | 34:Z:26:ARG:CZ    | 2.52                     | 0.57              |
| 1:1:270:C:H2'     | 1:1:271:A:H4'     | 1.86                     | 0.57              |
| 1:1:61:A:N3       | 1:1:76:U:O2'      | 2.29                     | 0.57              |
| 2:2:12:G:H5''     | 2:2:13:A:H5'      | 1.85                     | 0.57              |
| 8:8:37:C:H42      | 8:8:48:G:C1'      | 2.17                     | 0.57              |
| 12:D:105:GLY:HA3  | 12:D:130:TYR:HA   | 1.85                     | 0.57              |
| 30:V:106:TYR:O    | 30:V:108:VAL:N    | 2.35                     | 0.57              |
| 1:1:673:C:H42     | 1:1:677:A:H8      | 1.50                     | 0.57              |
| 2:2:1146:A:O2'    | 2:2:1167:A:N1     | 2.35                     | 0.57              |
| 2:2:442:C:H2'     | 2:2:488:A:H61     | 1.70                     | 0.57              |
| 4:4:123:C:H2'     | 4:4:124:A:C8      | 2.40                     | 0.57              |
| 14:F:57:LEU:HB2   | 14:F:61:GLY:HA3   | 1.86                     | 0.57              |
| 2:2:1012:G:N2     | 15:G:153:ARG:HH12 | 2.02                     | 0.57              |
| 19:K:68:GLY:CA    | 19:K:85:ILE:O     | 2.49                     | 0.57              |
| 21:M:184:LEU:HD13 | 21:M:188:TYR:CE1  | 2.39                     | 0.57              |
| 1:1:893:G:P       | 25:Q:126:ARG:HH12 | 2.27                     | 0.57              |
| 2:2:512:U:H2'     | 2:2:513:C:C6      | 2.39                     | 0.57              |
| 9:A:117:GLU:HB2   | 9:A:122:ASP:OD1   | 2.05                     | 0.57              |
| 9:A:198:LYS:O     | 50:A:302:HOH:O    | 2.17                     | 0.57              |
| 11:C:105:LYS:HE2  | 17:I:18:ASN:HD21  | 1.68                     | 0.57              |
| 14:F:50:ARG:NH1   | 14:F:180:SER:OG   | 2.37                     | 0.57              |
| 15:G:173:ASN:OD1  | 15:G:174:GLU:N    | 2.37                     | 0.57              |
| 15:G:271:LEU:HD23 | 15:G:283:VAL:HG23 | 1.87                     | 0.57              |
| 21:M:40:ARG:HH12  | 21:M:41:ARG:CZ    | 2.18                     | 0.57              |
| 26:R:40:LYS:HE3   | 26:R:60:VAL:HG11  | 1.85                     | 0.57              |
| 1:1:547:U:H5      | 1:1:1393:A:C6     | 2.20                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:209:C:N4      | 1:1:223:A:H61     | 2.02                     | 0.57              |
| 1:1:966:A:OP2     | 50:1:1972:HOH:O   | 2.17                     | 0.57              |
| 8:8:17:U:O2'      | 8:8:18:U:O5'      | 2.15                     | 0.57              |
| 10:B:49:PHE:CE1   | 10:B:342:VAL:HG22 | 2.38                     | 0.57              |
| 25:Q:142:ILE:HA   | 25:Q:145:ILE:HG12 | 1.87                     | 0.57              |
| 2:2:557:G:OP1     | 50:2:1723:HOH:O   | 2.17                     | 0.57              |
| 3:3:115:G:OP2     | 25:Q:124:TYR:OH   | 2.21                     | 0.57              |
| 22:N:112:GLN:OE1  | 22:N:113:THR:OG1  | 2.17                     | 0.57              |
| 22:N:88:ARG:NH2   | 22:N:89:THR:O     | 2.37                     | 0.57              |
| 1:1:243:G:N2      | 1:1:260:C:O2      | 2.37                     | 0.57              |
| 1:1:659:G:O2'     | 7:7:7:OMU:CM2     | 2.51                     | 0.57              |
| 1:1:817:C:H2'     | 1:1:818:C:O4'     | 2.05                     | 0.57              |
| 7:7:55:U:N3       | 7:7:62:A:H2       | 1.91                     | 0.57              |
| 7:7:7:OMU:CM2     | 7:7:7:OMU:H4'     | 2.35                     | 0.57              |
| 10:B:226:THR:O    | 10:B:341:ARG:NH2  | 2.37                     | 0.57              |
| 19:K:179:ALA:O    | 19:K:182:ALA:HB3  | 2.05                     | 0.57              |
| 20:L:16:PHE:CZ    | 20:L:21:ARG:HG2   | 2.40                     | 0.57              |
| 1:1:490:C:O2'     | 6:6:54:A:C2       | 2.54                     | 0.57              |
| 2:2:1317:G:O6     | 2:2:1387:C:N3     | 2.38                     | 0.57              |
| 3:3:106:U:N3      | 3:3:129:G:O6      | 2.37                     | 0.57              |
| 3:3:30:A:O4'      | 3:3:31:C:C5       | 2.58                     | 0.57              |
| 8:8:43:G:H8       | 8:8:43:G:OP2      | 1.88                     | 0.57              |
| 4:4:52:A:N9       | 13:E:174:PHE:HB2  | 2.20                     | 0.57              |
| 18:J:59:MET:HE2   | 18:J:77:ASN:HB3   | 1.87                     | 0.57              |
| 19:K:164:THR:HG22 | 19:K:167:GLU:OE1  | 2.04                     | 0.57              |
| 7:7:152:C:O2      | 21:M:112:ASN:ND2  | 2.38                     | 0.57              |
| 26:R:46:MET:O     | 26:R:50:LYS:N     | 2.38                     | 0.57              |
| 31:W:71:TYR:CE1   | 31:W:74:LYS:HG2   | 2.39                     | 0.57              |
| 32:X:4:ILE:HD11   | 32:X:20:ARG:HH21  | 1.68                     | 0.57              |
| 1:1:1183:G:N2     | 1:1:1189:C:O2     | 2.34                     | 0.57              |
| 1:1:47:C:OP1      | 17:I:15:LYS:NZ    | 2.29                     | 0.57              |
| 1:1:498:G:H2'     | 1:1:499:C:C6      | 2.39                     | 0.57              |
| 1:1:543:G:OP2     | 1:1:544:A:N1      | 2.38                     | 0.57              |
| 2:2:1312:U:H3'    | 2:2:1313:G:H5''   | 1.86                     | 0.57              |
| 3:3:58:C:HO2'     | 3:3:60:U:C5'      | 2.10                     | 0.57              |
| 4:4:140:G:N1      | 4:4:149:U:OP1     | 2.35                     | 0.57              |
| 16:H:74:GLN:O     | 16:H:78:LYS:NZ    | 2.38                     | 0.57              |
| 23:O:187:PRO:HD2  | 23:O:199:LYS:NZ   | 2.20                     | 0.57              |
| 1:1:205:A:H62     | 1:1:224:C:P       | 2.28                     | 0.57              |
| 2:2:535:U:C2'     | 2:2:536:C:H5'     | 2.34                     | 0.57              |
| 2:2:991:C:N4      | 2:2:996:G:O2'     | 2.37                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:3:47:C:N3       | 3:3:173:U:H5     | 2.03                     | 0.57              |
| 1:1:836:G:O4'     | 24:P:98:ARG:NH2  | 2.37                     | 0.57              |
| 1:1:945:U:H4'     | 1:1:946:G:O4'    | 2.05                     | 0.56              |
| 2:2:1151:U:O2'    | 2:2:1152:U:C5'   | 2.53                     | 0.56              |
| 2:2:1152:U:H2'    | 2:2:1153:OMU:C6  | 2.35                     | 0.56              |
| 2:2:379:U:O2'     | 50:2:1705:HOH:O  | 2.17                     | 0.56              |
| 6:6:48:C:H3'      | 6:6:49:C:H6      | 1.70                     | 0.56              |
| 8:8:3:G:H2'       | 8:8:4:A:O4'      | 2.05                     | 0.56              |
| 11:C:191:GLY:H    | 11:C:194:LYS:NZ  | 2.03                     | 0.56              |
| 23:O:187:PRO:HD2  | 23:O:199:LYS:HZ3 | 1.69                     | 0.56              |
| 24:P:17:HIS:NE2   | 24:P:18:HIS:HE1  | 1.95                     | 0.56              |
| 26:R:17:PRO:HB3   | 26:R:24:PRO:HD2  | 1.87                     | 0.56              |
| 29:U:94:THR:O     | 29:U:98:LEU:N    | 2.24                     | 0.56              |
| 1:1:1529:OMC:H5'  | 1:1:1529:OMC:H6  | 1.70                     | 0.56              |
| 1:1:694:U:H2'     | 1:1:695:OMC:C6   | 2.40                     | 0.56              |
| 6:6:59:C:H6       | 6:6:59:C:H5''    | 1.70                     | 0.56              |
| 10:B:371:LYS:HD2  | 10:B:371:LYS:N   | 2.19                     | 0.56              |
| 11:C:206:PRO:HB3  | 11:C:247:PHE:CD2 | 2.40                     | 0.56              |
| 17:I:27:VAL:HG12  | 21:M:198:ILE:HB  | 1.87                     | 0.56              |
| 23:O:94:ASN:HD22  | 23:O:95:TYR:N    | 2.02                     | 0.56              |
| 27:S:52:MET:HG2   | 27:S:95:HIS:CE1  | 2.40                     | 0.56              |
| 1:1:893:G:OP1     | 25:Q:126:ARG:NH1 | 2.38                     | 0.56              |
| 2:2:723:G:O2'     | 2:2:734:A:N6     | 2.38                     | 0.56              |
| 4:4:115:A:HO2'    | 5:5:111:G:H22    | 1.47                     | 0.56              |
| 7:7:142:C:H4'     | 30:V:96:THR:HG21 | 1.88                     | 0.56              |
| 7:7:79:A:H2'      | 7:7:80:A:H5''    | 1.86                     | 0.56              |
| 10:B:376:ARG:NH2  | 32:X:11:PHE:CD1  | 2.73                     | 0.56              |
| 15:G:273:ASP:OD1  | 15:G:274:ALA:N   | 2.38                     | 0.56              |
| 27:S:100[B]:ARG:C | 27:S:102:GLN:H   | 2.08                     | 0.56              |
| 1:1:159:U:C5      | 1:1:160:C:N3     | 2.73                     | 0.56              |
| 1:1:265:U:H2'     | 1:1:266:G:H8     | 1.70                     | 0.56              |
| 1:1:278:U:N3      | 1:1:279:G:N7     | 2.53                     | 0.56              |
| 2:2:1078:OMU:HM22 | 2:2:1079:OMG:H5' | 1.85                     | 0.56              |
| 1:1:873:G:H1'     | 9:A:15:VAL:HG13  | 1.88                     | 0.56              |
| 9:A:15:VAL:HG12   | 9:A:194:ASN:HD22 | 1.71                     | 0.56              |
| 19:K:75:ARG:NH1   | 19:K:112:LYS:O   | 2.37                     | 0.56              |
| 28:T:122:ALA:HB3  | 28:T:143:PRO:HG2 | 1.86                     | 0.56              |
| 32:X:8:PHE:HB3    | 32:X:40:CYS:SG   | 2.45                     | 0.56              |
| 1:1:1477:U:H2'    | 1:1:1478:A:O4'   | 2.05                     | 0.56              |
| 1:1:1656:A:H2'    | 1:1:1657:U:H5''  | 1.88                     | 0.56              |
| 1:1:1677:A:H61    | 1:1:1725:A:N6    | 2.03                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:763:U:H2'     | 1:1:764:G:C8       | 2.41                     | 0.56              |
| 2:2:100:U:H2'     | 2:2:101:G:H8       | 1.70                     | 0.56              |
| 2:2:690:C:H2'     | 2:2:691:A:C4       | 2.40                     | 0.56              |
| 3:3:139:G:H2'     | 3:3:140:A:C8       | 2.39                     | 0.56              |
| 3:3:173:U:H2'     | 3:3:174:U:O4'      | 2.06                     | 0.56              |
| 5:5:104:G:H8      | 5:5:104:G:OP1      | 1.88                     | 0.56              |
| 7:7:88:A:O2'      | 7:7:89:U:OP1       | 2.18                     | 0.56              |
| 1:1:874:C:H5'     | 9:A:19:HIS:CE1     | 2.40                     | 0.56              |
| 16:H:61:ILE:HD11  | 16:H:157:LEU:HD13  | 1.86                     | 0.56              |
| 16:H:124:GLU:HG3  | 16:H:172:VAL:HG21  | 1.86                     | 0.56              |
| 16:H:201:ARG:HG3  | 19:K:178:ARG:HD3   | 1.86                     | 0.56              |
| 19:K:92:ASN:O     | 19:K:111:LEU:HG    | 2.05                     | 0.56              |
| 23:O:40:ASP:OD1   | 23:O:43:LYS:NZ     | 2.36                     | 0.56              |
| 25:Q:105:LEU:HD12 | 25:Q:138:LEU:HD23  | 1.88                     | 0.56              |
| 1:1:1540:U:H4'    | 28:T:66[A]:LYS:HE2 | 1.88                     | 0.56              |
| 1:1:786:A:H61     | 1:1:791:C:H42      | 1.52                     | 0.56              |
| 2:2:3:C:H2'       | 2:2:4:C:C6         | 2.40                     | 0.56              |
| 8:8:27:A:H2'      | 8:8:28:C:C6        | 2.41                     | 0.56              |
| 15:G:137:TRP:HB2  | 15:G:142:THR:HG23  | 1.88                     | 0.56              |
| 19:K:89:VAL:HG12  | 26:R:73:ALA:HB3    | 1.67                     | 0.56              |
| 22:N:150:GLU:OE1  | 22:N:153:ARG:NH1   | 2.39                     | 0.56              |
| 1:1:1727:U:H3'    | 1:1:1728:G:H8      | 1.70                     | 0.56              |
| 1:1:556:U:H2'     | 1:1:557:U:O4'      | 2.04                     | 0.56              |
| 1:1:763:U:H2'     | 1:1:764:G:H8       | 1.69                     | 0.56              |
| 1:1:930:U:H3'     | 1:1:931:G:H5''     | 1.88                     | 0.56              |
| 1:1:927:A2M:H5''  | 2:2:73:U:H5''      | 1.87                     | 0.56              |
| 11:C:109:ARG:HA   | 21:M:204:ARG:HH12  | 1.70                     | 0.56              |
| 14:F:39:ALA:HB1   | 14:F:84:VAL:CG2    | 2.34                     | 0.56              |
| 16:H:144:ARG:CZ   | 16:H:154:TYR:HB3   | 2.36                     | 0.56              |
| 20:L:101:LEU:HB3  | 20:L:106:TYR:O     | 2.05                     | 0.56              |
| 1:1:1149:G:N1     | 1:1:1155:A:OP2     | 2.39                     | 0.56              |
| 1:1:1410:U:H2'    | 1:1:1411:G:C8      | 2.40                     | 0.56              |
| 1:1:9:G:H21       | 1:1:1669:G:H1      | 1.52                     | 0.56              |
| 1:1:36:OMU:HM21   | 1:1:94:A:O2'       | 2.02                     | 0.56              |
| 2:2:18:A:OP1      | 50:2:1712:HOH:O    | 2.17                     | 0.56              |
| 2:2:718:C:H2'     | 2:2:719:A:O4'      | 2.06                     | 0.56              |
| 23:O:17:GLN:HE22  | 27:S:22:HIS:H      | 1.54                     | 0.56              |
| 23:O:39:GLN:HE21  | 23:O:43:LYS:HZ2    | 1.54                     | 0.56              |
| 1:1:453:G:O2'     | 28:T:119:VAL:O     | 2.22                     | 0.56              |
| 2:2:653:C:H2'     | 2:2:654:U:C6       | 2.40                     | 0.56              |
| 2:2:667:OMU:H3'   | 2:2:668:C:H5''     | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:979:C:H5''    | 9:A:69:PHE:CE1    | 2.40                     | 0.56              |
| 3:3:168:U:O2      | 3:3:168:U:H3'     | 2.06                     | 0.56              |
| 3:3:58:C:C2'      | 3:3:60:U:H5''     | 2.36                     | 0.56              |
| 11:C:157:ILE:HG12 | 11:C:160:TYR:HE2  | 1.70                     | 0.56              |
| 11:C:194:LYS:HB2  | 11:C:199:ARG:HD2  | 1.87                     | 0.56              |
| 19:K:74:LEU:HD21  | 19:K:113:ASN:HA   | 1.87                     | 0.56              |
| 22:N:31:ILE:HG13  | 22:N:69:ARG:HD3   | 1.87                     | 0.56              |
| 33:Y:42:LEU:HA    | 33:Y:74:VAL:HA    | 1.86                     | 0.56              |
| 1:1:456:A:H2'     | 1:1:457:C:O4'     | 2.05                     | 0.56              |
| 1:1:776:U:O2      | 24:P:51:ARG:NH2   | 2.37                     | 0.56              |
| 2:2:1077:G:C2'    | 2:2:1078:OMU:H5'' | 2.36                     | 0.56              |
| 9:A:126:LEU:HD13  | 9:A:150:LEU:HD21  | 1.88                     | 0.56              |
| 20:L:136:LYS:O    | 20:L:136:LYS:HD3  | 2.06                     | 0.56              |
| 1:1:1044:G:N3     | 2:2:1065:A:H2'    | 2.21                     | 0.56              |
| 1:1:1631:G:O2'    | 1:1:1633:U:OP1    | 2.23                     | 0.56              |
| 1:1:299:U:H4'     | 1:1:300:A:N7      | 2.21                     | 0.56              |
| 1:1:370:G:O2'     | 1:1:372:A:N7      | 2.39                     | 0.56              |
| 1:1:533:G:O2'     | 1:1:534:G:H5'     | 2.06                     | 0.56              |
| 2:2:1177:A:H4'    | 23:O:151:ILE:HG21 | 1.88                     | 0.56              |
| 2:2:827:A:O2'     | 2:2:828:U:O5'     | 2.23                     | 0.56              |
| 7:7:37:U:OP1      | 7:7:38:U:O2'      | 2.18                     | 0.56              |
| 8:8:50:G:C4       | 8:8:51:A:H2       | 2.24                     | 0.56              |
| 6:6:41:G:N1       | 19:K:176:ARG:NH1  | 2.52                     | 0.56              |
| 26:R:14:ARG:CZ    | 26:R:17:PRO:HG3   | 2.36                     | 0.56              |
| 2:2:1035:G:H5'    | 9:A:233:GLN:HB2   | 1.88                     | 0.55              |
| 2:2:957:C:C1'     | 2:2:958:C:P       | 2.94                     | 0.55              |
| 3:3:207:G:H2'     | 3:3:208:G:C8      | 2.41                     | 0.55              |
| 4:4:115:A:OP1     | 50:4:303:HOH:O    | 2.18                     | 0.55              |
| 6:6:28:A:C4       | 6:6:29:G:N7       | 2.75                     | 0.55              |
| 19:K:180:HIS:ND1  | 19:K:181:TRP:N    | 2.54                     | 0.55              |
| 22:N:150:GLU:O    | 22:N:154:ARG:N    | 2.37                     | 0.55              |
| 30:V:95:LYS:HE3   | 30:V:113:VAL:O    | 2.05                     | 0.55              |
| 4:4:77:U:O2'      | 10:B:55:HIS:HD2   | 1.89                     | 0.55              |
| 15:G:304:ASN:HB2  | 15:G:308:LEU:HB2  | 1.87                     | 0.55              |
| 22:N:38:ARG:HG2   | 22:N:41:ALA:HB2   | 1.87                     | 0.55              |
| 1:1:458:A:H2      | 1:1:459:A:H1'     | 1.70                     | 0.55              |
| 3:3:39:U:O2'      | 3:3:139:G:O3'     | 2.22                     | 0.55              |
| 4:4:179:C:O2'     | 5:5:3:C:O2'       | 2.21                     | 0.55              |
| 1:1:543:G:N7      | 19:K:105:TRP:CD1  | 2.74                     | 0.55              |
| 20:L:134:ILE:HD12 | 20:L:141:VAL:HG22 | 1.87                     | 0.55              |
| 21:M:31:ARG:HD3   | 21:M:124:ASP:OD2  | 2.06                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:30:C:H5''    | 21:M:71:ARG:HH22  | 1.71                     | 0.55              |
| 28:T:3:HIS:HB2   | 28:T:4:TYR:HD2    | 1.71                     | 0.55              |
| 2:2:635:A:H5'    | 28:T:80:LYS:HE2   | 1.89                     | 0.55              |
| 30:V:90:ASP:OD1  | 30:V:93:ALA:HB2   | 2.06                     | 0.55              |
| 1:1:240:U:H2'    | 1:1:241:G:C8      | 2.40                     | 0.55              |
| 2:2:395:A:N6     | 2:2:433:G:O2'     | 2.35                     | 0.55              |
| 6:6:33:G:H2'     | 6:6:34:C:O4'      | 2.06                     | 0.55              |
| 7:7:71:A:OP2     | 31:W:48:ARG:NH1   | 2.39                     | 0.55              |
| 7:7:76:C:O2'     | 7:7:77:A:O4'      | 2.23                     | 0.55              |
| 8:8:34:A:C2      | 8:8:43:G:N2       | 2.74                     | 0.55              |
| 9:A:140:ASN:O    | 9:A:144:GLY:N     | 2.34                     | 0.55              |
| 23:O:55:ILE:HG23 | 23:O:60:ILE:HG22  | 1.88                     | 0.55              |
| 26:R:14:ARG:NH2  | 26:R:17:PRO:HG3   | 2.21                     | 0.55              |
| 1:1:729:A:N1     | 7:7:27:U:O2'      | 2.36                     | 0.55              |
| 2:2:1132:A:H4'   | 23:O:31:HIS:CE1   | 2.42                     | 0.55              |
| 8:8:7:A:N6       | 8:8:117:A:N1      | 2.55                     | 0.55              |
| 11:C:235:LEU:O   | 11:C:236:LEU:HB2  | 2.05                     | 0.55              |
| 14:F:176:GLY:HA2 | 14:F:179:ARG:HH11 | 1.72                     | 0.55              |
| 15:G:238:ILE:N   | 15:G:263:ALA:O    | 2.33                     | 0.55              |
| 4:4:162:A:OP1    | 16:H:92:ARG:NH2   | 2.38                     | 0.55              |
| 27:S:115:TYR:O   | 27:S:119:LYS:N    | 2.39                     | 0.55              |
| 1:1:1355:C:H2'   | 1:1:1356:G:H8     | 1.71                     | 0.55              |
| 1:1:893:G:H2'    | 1:1:894:G:H5'     | 1.88                     | 0.55              |
| 2:2:467:G:N2     | 2:2:470:A:OP2     | 2.24                     | 0.55              |
| 3:3:104:U:H4'    | 33:Y:37:PRO:HB2   | 1.88                     | 0.55              |
| 8:8:48:G:C2      | 8:8:49:U:C6       | 2.94                     | 0.55              |
| 9:A:43:GLY:O     | 9:A:88:VAL:N      | 2.40                     | 0.55              |
| 15:G:255:CYS:O   | 15:G:259:LYS:N    | 2.40                     | 0.55              |
| 1:1:987:A:OP1    | 20:L:32:ARG:NH2   | 2.40                     | 0.55              |
| 24:P:17:HIS:CG   | 24:P:18:HIS:HD1   | 2.23                     | 0.55              |
| 1:1:326:A:H2'    | 1:1:327:G:C8      | 2.41                     | 0.55              |
| 1:1:35:U:H2'     | 1:1:36:OMU:C5'    | 2.33                     | 0.55              |
| 9:A:90:CYS:HB2   | 9:A:101:VAL:HB    | 1.89                     | 0.55              |
| 1:1:712:G:H2'    | 1:1:713:A:O4'     | 2.06                     | 0.55              |
| 2:2:1340:G:H5'   | 13:E:169:LYS:CE   | 2.32                     | 0.55              |
| 2:2:1403:G:N2    | 2:2:1406:A:OP2    | 2.35                     | 0.55              |
| 2:2:668:C:H6     | 2:2:668:C:C5'     | 2.20                     | 0.55              |
| 3:3:36:C:N3      | 3:3:185:C:N4      | 2.55                     | 0.55              |
| 4:4:115:A:O2'    | 5:5:111:G:N2      | 2.31                     | 0.55              |
| 5:5:45:C:H2'     | 5:5:46:G:C8       | 2.42                     | 0.55              |
| 6:6:31:U:H6      | 6:6:31:U:H3'      | 1.72                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:8:40:U:C2'      | 8:8:44:A:N6       | 2.68                     | 0.55              |
| 9:A:135:ILE:HD13  | 9:A:149:LYS:NZ    | 2.22                     | 0.55              |
| 11:C:207:MET:HB3  | 11:C:226:ASP:HB3  | 1.89                     | 0.55              |
| 16:H:186:HIS:NE2  | 16:H:190:GLN:OE1  | 2.40                     | 0.55              |
| 18:J:56:LEU:O     | 18:J:124:SER:OG   | 2.24                     | 0.55              |
| 23:O:244:SER:O    | 23:O:248:MET:N    | 2.38                     | 0.55              |
| 1:1:353:C:OP2     | 17:I:107:LYS:CE   | 2.54                     | 0.55              |
| 1:1:505:U:H2'     | 1:1:506:G:C8      | 2.42                     | 0.55              |
| 1:1:814:C:H2'     | 1:1:815:G:C8      | 2.42                     | 0.55              |
| 1:1:893:G:O6      | 1:1:902:C:N4      | 2.27                     | 0.55              |
| 2:2:1254:OMG:C4'  | 2:2:1254:OMG:HM23 | 2.36                     | 0.55              |
| 2:2:403:G:N1      | 2:2:424:U:OP2     | 2.31                     | 0.55              |
| 1:1:678:A2M:C6    | 2:2:617:G:H21     | 2.14                     | 0.55              |
| 5:5:42:G:N7       | 5:5:106:G:O2'     | 2.37                     | 0.55              |
| 10:B:321:TYR:CD1  | 10:B:340:ARG:CG   | 2.87                     | 0.55              |
| 27:S:117:ALA:O    | 27:S:122:GLY:N    | 2.39                     | 0.55              |
| 28:T:16:LYS:O     | 28:T:101:ASN:ND2  | 2.40                     | 0.55              |
| 1:1:1656:A:N6     | 2:2:412:A:N1      | 2.54                     | 0.55              |
| 6:6:16:C:C4       | 6:6:17:U:C4       | 2.95                     | 0.55              |
| 11:C:207:MET:HB3  | 11:C:246:ARG:HH21 | 1.72                     | 0.55              |
| 16:H:40:VAL:O     | 16:H:44:GLN:HG2   | 2.06                     | 0.55              |
| 17:I:128:LEU:HD21 | 17:I:130:LEU:HB2  | 1.88                     | 0.55              |
| 29:U:92:TYR:O     | 29:U:96:LYS:N     | 2.38                     | 0.55              |
| 32:X:4:ILE:HD11   | 32:X:20:ARG:HE    | 1.71                     | 0.55              |
| 33:Y:77:HIS:HA    | 33:Y:80:PHE:CD2   | 2.41                     | 0.55              |
| 2:2:534:OMG:H3'   | 2:2:535:U:H5      | 1.72                     | 0.54              |
| 6:6:16:C:H3'      | 6:6:16:C:C6       | 2.42                     | 0.54              |
| 2:2:423:A:O2'     | 9:A:125:THR:O     | 2.15                     | 0.54              |
| 2:2:393:A:O3'     | 9:A:197:PRO:HB3   | 2.07                     | 0.54              |
| 22:N:75:TYR:OH    | 22:N:154:ARG:NE   | 2.40                     | 0.54              |
| 27:S:48:VAL:HG11  | 27:S:94:GLU:OE2   | 2.07                     | 0.54              |
| 31:W:79:ILE:HD12  | 31:W:96:ILE:HD13  | 1.89                     | 0.54              |
| 1:1:1114:A:H2     | 1:1:1148:A:C4     | 2.26                     | 0.54              |
| 1:1:312:C:N4      | 1:1:313:U:O4      | 2.40                     | 0.54              |
| 1:1:956:U:C2'     | 1:1:957:C:H5''    | 2.37                     | 0.54              |
| 2:2:776:C:O2'     | 2:2:777:A:O5'     | 2.24                     | 0.54              |
| 13:E:88:ARG:NH1   | 13:E:186:ILE:HG22 | 2.22                     | 0.54              |
| 28:T:112:MET:HA   | 28:T:151:SER:O    | 2.07                     | 0.54              |
| 34:Z:21:LYS:NZ    | 34:Z:23:GLY:O     | 2.28                     | 0.54              |
| 1:1:442:A:H1'     | 1:1:444:C:C4      | 2.42                     | 0.54              |
| 1:1:848:U:H5''    | 1:1:848:U:H6      | 1.71                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:1254:OMG:C4'  | 2:2:1254:OMG:CM2  | 2.86                     | 0.54              |
| 1:1:1595:G:N2     | 2:2:37:C:O2       | 2.19                     | 0.54              |
| 3:3:28:U:H3       | 3:3:203:A:N6      | 2.00                     | 0.54              |
| 1:1:147:G:O6      | 15:G:220:GLY:HA3  | 2.07                     | 0.54              |
| 1:1:120:G:N7      | 15:G:226:ARG:NH1  | 2.55                     | 0.54              |
| 19:K:78:ARG:HB2   | 19:K:81:ARG:HE    | 1.72                     | 0.54              |
| 24:P:45:ASN:HA    | 24:P:48:VAL:HG12  | 1.90                     | 0.54              |
| 2:2:1128:G:H21    | 27:S:49:ARG:HH22  | 1.55                     | 0.54              |
| 1:1:1525:A:O2'    | 1:1:1526:OMG:OP2  | 2.22                     | 0.54              |
| 1:1:178:G:O6      | 1:1:274:A:O2'     | 2.24                     | 0.54              |
| 1:1:769:U:O2      | 24:P:66:ARG:NH1   | 2.36                     | 0.54              |
| 10:B:240:VAL:HG23 | 10:B:241:ALA:N    | 2.22                     | 0.54              |
| 1:1:147:G:H4'     | 21:M:55:THR:HG21  | 1.90                     | 0.54              |
| 22:N:55:ARG:NH1   | 22:N:162:ARG:HH11 | 2.06                     | 0.54              |
| 24:P:17:HIS:HE1   | 24:P:18:HIS:CE1   | 2.16                     | 0.54              |
| 1:1:517:U:H3      | 1:1:534:G:H1      | 1.55                     | 0.54              |
| 2:2:390:A:N9      | 2:2:527:A2M:N6    | 2.56                     | 0.54              |
| 2:2:699:U:N3      | 2:2:707:A:O5'     | 2.39                     | 0.54              |
| 6:6:33:G:C5'      | 19:K:42:VAL:CG2   | 2.80                     | 0.54              |
| 7:7:154:A:O2'     | 21:M:57:GLN:NE2   | 2.40                     | 0.54              |
| 22:N:76:MET:HE3   | 22:N:80:ALA:HB3   | 1.90                     | 0.54              |
| 27:S:115:TYR:HA   | 27:S:118:ALA:HB3  | 1.88                     | 0.54              |
| 30:V:70:LEU:HD13  | 30:V:88:ILE:HD11  | 1.90                     | 0.54              |
| 1:1:1751:G:N2     | 1:1:1752:G:N7     | 2.55                     | 0.54              |
| 1:1:771:U:H2'     | 1:1:772:G:C8      | 2.43                     | 0.54              |
| 2:2:1437:A:O2'    | 2:2:1438:A:OP1    | 2.18                     | 0.54              |
| 2:2:473:C:H2'     | 2:2:474:A:O4'     | 2.07                     | 0.54              |
| 2:2:729:G:N3      | 2:2:731:A:H8      | 2.05                     | 0.54              |
| 5:5:18:G:H1'      | 28:T:69:ARG:HE    | 1.73                     | 0.54              |
| 6:6:21:A:C1'      | 6:6:22:G:P        | 2.95                     | 0.54              |
| 9:A:73:LYS:NZ     | 9:A:73:LYS:HB2    | 2.23                     | 0.54              |
| 18:J:106:ASN:CG   | 18:J:107:PRO:CD   | 2.64                     | 0.54              |
| 20:L:54:GLY:C     | 24:P:181:LYS:HD2  | 2.27                     | 0.54              |
| 27:S:75:ILE:HG22  | 27:S:88:ARG:HD3   | 1.88                     | 0.54              |
| 1:1:180:A:N6      | 1:1:271:A:H62     | 2.06                     | 0.54              |
| 2:2:1318:OMC:HM21 | 10:B:244:PRO:CG   | 2.37                     | 0.54              |
| 19:K:89:VAL:O     | 19:K:89:VAL:HG23  | 2.07                     | 0.54              |
| 25:Q:10:LEU:HD11  | 25:Q:41:VAL:HG21  | 1.90                     | 0.54              |
| 1:1:1158:U:H2'    | 1:1:1159:A:H4'    | 1.90                     | 0.54              |
| 1:1:195:G:N2      | 1:1:237:U:O4      | 2.41                     | 0.54              |
| 1:1:373:G:H2'     | 1:1:374:G:O4'     | 2.07                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:107:U:O4      | 3:3:128:C:C6      | 2.61                     | 0.54              |
| 6:6:43:A:H2'      | 6:6:44:G:O4'      | 2.07                     | 0.54              |
| 7:7:168:G:H2'     | 7:7:169:A:H8      | 1.70                     | 0.54              |
| 8:8:19:G:O6       | 8:8:64:A:N6       | 2.40                     | 0.54              |
| 14:F:38:ILE:HG21  | 14:F:177:TYR:HE2  | 1.72                     | 0.54              |
| 19:K:73:ILE:HD12  | 19:K:73:ILE:H     | 1.70                     | 0.54              |
| 1:1:172:G:H2'     | 1:1:173:G:C8      | 2.39                     | 0.54              |
| 1:1:422:U:HO2'    | 1:1:423:U:H6      | 1.56                     | 0.54              |
| 2:2:1110:C:H3'    | 2:2:1111:U:H5''   | 1.90                     | 0.54              |
| 2:2:768:G:H1'     | 30:V:34:GLN:HE22  | 1.73                     | 0.54              |
| 4:4:45:G:H2'      | 4:4:46:G:H8       | 1.73                     | 0.54              |
| 4:4:64:C:O2'      | 4:4:65:C:OP1      | 2.22                     | 0.54              |
| 5:5:111:G:N2      | 5:5:115:U:OP1     | 2.40                     | 0.54              |
| 11:C:127:LEU:HD23 | 11:C:238:LEU:HD11 | 1.90                     | 0.54              |
| 11:C:59:MET:SD    | 11:C:99:ARG:HD3   | 2.48                     | 0.54              |
| 11:C:94:MET:N     | 11:C:94:MET:SD    | 2.81                     | 0.54              |
| 14:F:55:LYS:NZ    | 14:F:99:ALA:O     | 2.29                     | 0.54              |
| 22:N:121:LYS:HG3  | 22:N:122:PRO:CD   | 2.34                     | 0.54              |
| 29:U:111:ALA:HA   | 29:U:117:TYR:HA   | 1.90                     | 0.54              |
| 30:V:69:PRO:HA    | 30:V:87:PHE:HA    | 1.88                     | 0.54              |
| 2:2:551:G:N2      | 2:2:551:G:OP2     | 2.39                     | 0.54              |
| 2:2:715:G:H2'     | 2:2:716:C:C6      | 2.43                     | 0.54              |
| 6:6:37:C:C2       | 19:K:172:ARG:HD2  | 2.43                     | 0.54              |
| 7:7:76:C:O2'      | 7:7:77:A:N3       | 2.41                     | 0.54              |
| 7:7:7:OMU:CM2     | 7:7:7:OMU:C4'     | 2.86                     | 0.54              |
| 10:B:50:LYS:HA    | 10:B:79:LEU:HD23  | 1.90                     | 0.54              |
| 21:M:121:VAL:HG21 | 21:M:131:GLU:CG   | 2.38                     | 0.54              |
| 1:1:1257:U:O2'    | 1:1:1258:A:O5'    | 2.24                     | 0.53              |
| 1:1:218:A:H2'     | 1:1:219:U:C6      | 2.43                     | 0.53              |
| 1:1:237:U:H3'     | 1:1:238:A:H8      | 1.72                     | 0.53              |
| 2:2:396:G:O2'     | 2:2:435:U:OP1     | 2.18                     | 0.53              |
| 2:2:451:U:H3      | 2:2:483:C:N4      | 2.06                     | 0.53              |
| 2:2:981:A:O2'     | 2:2:982:C:OP1     | 2.22                     | 0.53              |
| 10:B:302:THR:CG2  | 10:B:310:LYS:HG2  | 2.39                     | 0.53              |
| 15:G:166:VAL:HG12 | 15:G:264:ILE:HG22 | 1.90                     | 0.53              |
| 16:H:92:ARG:HB3   | 16:H:166:TRP:HB2  | 1.89                     | 0.53              |
| 19:K:78:ARG:H     | 19:K:78:ARG:HD2   | 1.73                     | 0.53              |
| 20:L:111:GLY:N    | 20:L:130:ALA:HB2  | 2.23                     | 0.53              |
| 24:P:101:ARG:HH21 | 24:P:101:ARG:CG   | 2.11                     | 0.53              |
| 1:1:777:G:H22     | 24:P:144:TYR:HD1  | 1.56                     | 0.53              |
| 1:1:1628:OMG:H5'' | 30:V:74:LYS:HD3   | 1.89                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:V:78:LYS:HB3   | 30:V:84:THR:OG1  | 2.09                     | 0.53              |
| 1:1:138:C:O2'     | 1:1:139:C:O5'    | 2.22                     | 0.53              |
| 1:1:208:C:O2'     | 1:1:226:C:N3     | 2.38                     | 0.53              |
| 1:1:439:U:H5      | 28:T:3:HIS:HD1   | 1.54                     | 0.53              |
| 1:1:461:G:O2'     | 1:1:462:A:O4'    | 2.15                     | 0.53              |
| 1:1:464:A:N1      | 2:2:608:C:O2'    | 2.34                     | 0.53              |
| 4:4:95:U:H5       | 25:Q:62:ARG:NH1  | 2.07                     | 0.53              |
| 10:B:108:HIS:CE1  | 10:B:109:HIS:HD2 | 2.25                     | 0.53              |
| 1:1:1669:G:H21    | 30:V:38:PRO:HD2  | 1.74                     | 0.53              |
| 32:X:6:CYS:SG     | 32:X:7:GLU:N     | 2.81                     | 0.53              |
| 1:1:219:U:H2'     | 1:1:220:A:C8     | 2.44                     | 0.53              |
| 1:1:807:C:H2'     | 1:1:808:A:O4'    | 2.08                     | 0.53              |
| 1:1:855:C:O2'     | 1:1:856:OMG:H5'  | 2.08                     | 0.53              |
| 1:1:951:G:H1'     | 1:1:1741:A:N6    | 2.24                     | 0.53              |
| 2:2:973:C:H3'     | 9:A:89:PHE:CZ    | 2.43                     | 0.53              |
| 11:C:269:SER:OG   | 11:C:272:LYS:O   | 2.27                     | 0.53              |
| 13:E:22:GLY:O     | 13:E:23:ARG:HG3  | 2.08                     | 0.53              |
| 19:K:180:HIS:HB2  | 19:K:183:ARG:HD2 | 1.90                     | 0.53              |
| 25:Q:118:HIS:CD2  | 25:Q:122:ASP:HB3 | 2.43                     | 0.53              |
| 1:1:1263:A:H1'    | 1:1:1264:A:OP2   | 2.08                     | 0.53              |
| 1:1:155:A:H4'     | 1:1:156:A:O5'    | 2.08                     | 0.53              |
| 1:1:23:U:H1'      | 1:1:25:C:H41     | 1.74                     | 0.53              |
| 1:1:279:G:H2'     | 1:1:280:A:H4'    | 1.90                     | 0.53              |
| 1:1:53:G:C2'      | 1:1:54:G:H5'     | 2.38                     | 0.53              |
| 4:4:128:U:H3      | 4:4:162:A:N6     | 2.02                     | 0.53              |
| 4:4:140:G:H21     | 4:4:150:A:N6     | 2.05                     | 0.53              |
| 4:4:95:U:P        | 25:Q:62:ARG:HH21 | 2.29                     | 0.53              |
| 2:2:1275:C:H5     | 2:2:1292:G:H1    | 1.55                     | 0.53              |
| 4:4:39:A:N1       | 4:4:71:C:O2'     | 2.35                     | 0.53              |
| 8:8:72:A:O2'      | 8:8:73:G:H8      | 1.92                     | 0.53              |
| 14:F:40:ILE:HD13  | 14:F:50:ARG:HG2  | 1.90                     | 0.53              |
| 20:L:112:ASN:HD22 | 20:L:113:GLY:H   | 1.56                     | 0.53              |
| 22:N:133:GLN:NE2  | 22:N:134:ILE:O   | 2.41                     | 0.53              |
| 22:N:191:GLU:O    | 22:N:197:CYS:HB2 | 2.09                     | 0.53              |
| 1:1:133:C:OP1     | 1:1:134:A:N6     | 2.41                     | 0.53              |
| 1:1:209:C:H42     | 1:1:223:A:H61    | 1.57                     | 0.53              |
| 8:8:85:G:H8       | 8:8:85:G:H5''    | 1.72                     | 0.53              |
| 17:I:81:SER:HB3   | 17:I:84:GLU:OE1  | 2.09                     | 0.53              |
| 1:1:754:G:C5      | 20:L:114:HIS:HB3 | 2.44                     | 0.53              |
| 22:N:36:ILE:HB    | 22:N:87:MET:HB3  | 1.90                     | 0.53              |
| 1:1:454:U:OP1     | 28:T:62:ARG:NH2  | 2.42                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:36:OMU:HM22   | 1:1:37:A:C4'      | 2.39                     | 0.53              |
| 1:1:465:A:H2'     | 1:1:466:U:O4'     | 2.09                     | 0.53              |
| 1:1:558:U:O2'     | 1:1:559:G:OP2     | 2.26                     | 0.53              |
| 4:4:179:C:HO2'    | 5:5:3:C:HO2'      | 1.56                     | 0.53              |
| 10:B:95:THR:OG1   | 10:B:96:PRO:HD2   | 2.08                     | 0.53              |
| 14:F:30:ARG:NH2   | 14:F:33:CYS:SG    | 2.82                     | 0.53              |
| 1:1:252:G:H5''    | 31:W:9:ARG:HD2    | 1.91                     | 0.53              |
| 1:1:1091:A:H3'    | 1:1:1092:U:H5''   | 1.90                     | 0.53              |
| 2:2:541:A:N3      | 2:2:1368:C:O2'    | 2.36                     | 0.53              |
| 2:2:598:A:OP1     | 28:T:82:ARG:HB3   | 2.09                     | 0.53              |
| 2:2:729:G:C2      | 2:2:731:A:H3'     | 2.43                     | 0.53              |
| 6:6:33:G:C8       | 19:K:42:VAL:HG11  | 2.43                     | 0.53              |
| 8:8:101:G:O6      | 26:R:54:LYS:NZ    | 2.37                     | 0.53              |
| 8:8:9:G:OP2       | 23:O:28:THR:OG1   | 2.21                     | 0.53              |
| 11:C:226:ASP:OD1  | 11:C:227:LEU:N    | 2.41                     | 0.53              |
| 18:J:20:PRO:HA    | 18:J:53:SER:HA    | 1.91                     | 0.53              |
| 22:N:190:LEU:HD22 | 22:N:199:LEU:HG   | 1.91                     | 0.53              |
| 2:2:1131:A:N6     | 23:O:28:THR:O     | 2.42                     | 0.53              |
| 23:O:94:ASN:HD22  | 23:O:95:TYR:H     | 1.57                     | 0.53              |
| 1:1:1442:G:O2'    | 1:1:1443:U:OP1    | 2.24                     | 0.53              |
| 1:1:491:A:HO2'    | 14:F:83:TYR:HH    | 1.56                     | 0.53              |
| 2:2:452:G:O2'     | 2:2:454:A:OP2     | 2.18                     | 0.53              |
| 2:2:728:U:H1'     | 2:2:729:G:C2      | 2.44                     | 0.53              |
| 2:2:768:G:H1'     | 30:V:34:GLN:NE2   | 2.23                     | 0.53              |
| 10:B:294:VAL:HG13 | 10:B:300:GLN:NE2  | 2.23                     | 0.53              |
| 11:C:246:ARG:O    | 11:C:248:VAL:HG13 | 2.08                     | 0.53              |
| 14:F:34:ALA:HB1   | 14:F:35:PRO:HD2   | 1.91                     | 0.53              |
| 26:R:16:SER:OG    | 26:R:57:HIS:O     | 2.23                     | 0.53              |
| 33:Y:76:ASN:OD1   | 33:Y:77:HIS:N     | 2.42                     | 0.53              |
| 1:1:650:G:O2'     | 1:1:651:G:N2      | 2.41                     | 0.53              |
| 2:2:1285:U:H1'    | 2:2:1288:C:H5     | 1.73                     | 0.53              |
| 2:2:1394:U:H5''   | 2:2:1416:G:H22    | 1.73                     | 0.53              |
| 8:8:59:C:H2'      | 8:8:60:A:C8       | 2.44                     | 0.53              |
| 2:2:1386:G:N3     | 10:B:255:ALA:HB1  | 2.24                     | 0.53              |
| 28:T:60:PHE:HE2   | 28:T:82:ARG:HD2   | 1.73                     | 0.53              |
| 1:1:1587:G:N7     | 50:2:1710:HOH:O   | 2.34                     | 0.52              |
| 1:1:160:C:H2'     | 1:1:161:A:C8      | 2.45                     | 0.52              |
| 1:1:564:U:O5'     | 1:1:564:U:H6      | 1.91                     | 0.52              |
| 1:1:708:A:N6      | 24:P:92:ASP:OD2   | 2.42                     | 0.52              |
| 2:2:387:U:H1'     | 2:2:1415:G:H21    | 1.73                     | 0.52              |
| 3:3:57:U:H2'      | 3:3:58:C:H5       | 0.77                     | 0.52              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 13:E:7:LEU:HD21   | 13:E:55:THR:HG23    | 1.91                     | 0.52              |
| 28:T:64:ASN:OD1   | 28:T:65:GLY:N       | 2.35                     | 0.52              |
| 1:1:1273:U:H3     | 1:1:1356:G:H22      | 1.57                     | 0.52              |
| 1:1:158:A:H2'     | 1:1:159:U:C2        | 2.45                     | 0.52              |
| 1:1:1754:U:N3     | 1:1:1757:U:OP2      | 2.29                     | 0.52              |
| 1:1:770:G:O2'     | 1:1:771:U:OP2       | 2.21                     | 0.52              |
| 2:2:1229:A:H2'    | 2:2:1230:OMG:O4'    | 2.08                     | 0.52              |
| 7:7:167:C:H2'     | 7:7:168:G:C8        | 2.44                     | 0.52              |
| 8:8:17:U:O2'      | 8:8:18:U:O4'        | 2.26                     | 0.52              |
| 9:A:92:GLN:NE2    | 9:A:106:GLN:OE1     | 2.42                     | 0.52              |
| 13:E:123:GLN:HE22 | 13:E:159:VAL:HB     | 1.74                     | 0.52              |
| 1:1:959:OMG:HN1   | 21:M:76:HIS:CD2     | 2.25                     | 0.52              |
| 28:T:119:VAL:HG22 | 28:T:146:VAL:HG22   | 1.90                     | 0.52              |
| 28:T:22:LEU:O     | 28:T:22:LEU:HD13    | 2.09                     | 0.52              |
| 33:Y:9:LYS:HZ2    | 33:Y:9:LYS:HB2      | 1.74                     | 0.52              |
| 1:1:47:C:N4       | 21:M:188:TYR:CD1    | 2.77                     | 0.52              |
| 1:1:857:A:N3      | 2:2:1251:C:O2'      | 2.39                     | 0.52              |
| 3:3:58:C:O2'      | 3:3:60:U:C4'        | 2.57                     | 0.52              |
| 3:3:58:C:H6       | 3:3:58:C:O5'        | 1.92                     | 0.52              |
| 8:8:117:A:N6      | 8:8:118:C:H42       | 2.07                     | 0.52              |
| 8:8:39:G:O2'      | 8:8:40:U:H5''       | 2.09                     | 0.52              |
| 10:B:386:TRP:HD1  | 10:B:387:PHE:CD1    | 2.28                     | 0.52              |
| 1:1:1041:U:H5''   | 27:S:100[B]:ARG:NH2 | 2.24                     | 0.52              |
| 1:1:1626:G:H2'    | 1:1:1627:A:O4'      | 2.09                     | 0.52              |
| 1:1:657:G:C2'     | 1:1:658:G:H5'       | 2.39                     | 0.52              |
| 1:1:669:C:HO2'    | 1:1:670:C:C5'       | 2.22                     | 0.52              |
| 1:1:669:C:H2'     | 1:1:670:C:C6        | 2.44                     | 0.52              |
| 1:1:784:U:H3      | 1:1:786:A:H62       | 1.56                     | 0.52              |
| 2:2:499:G:H1      | 2:2:510:U:H3        | 1.58                     | 0.52              |
| 4:4:101:G:H2'     | 4:4:102:G:O4'       | 2.09                     | 0.52              |
| 4:4:51:U:H2'      | 13:E:98:PHE:CZ      | 2.44                     | 0.52              |
| 5:5:23:A:H2'      | 5:5:24:A:O4'        | 2.10                     | 0.52              |
| 7:7:146:U:H5''    | 30:V:51:ASN:HB2     | 1.91                     | 0.52              |
| 8:8:19:G:N1       | 8:8:64:A:N1         | 2.57                     | 0.52              |
| 8:8:47:U:OP1      | 23:O:158:ARG:N      | 2.40                     | 0.52              |
| 10:B:379:THR:HG23 | 10:B:382:GLU:HG2    | 1.92                     | 0.52              |
| 7:7:168:G:H5''    | 15:G:172:ARG:NH2    | 2.23                     | 0.52              |
| 20:L:98:VAL:HG22  | 20:L:120:ILE:HD11   | 1.91                     | 0.52              |
| 1:1:150:G:OP2     | 21:M:147:ARG:NH2    | 2.42                     | 0.52              |
| 23:O:19:LYS:NZ    | 23:O:19:LYS:CB      | 2.73                     | 0.52              |
| 23:O:53:VAL:HG23  | 23:O:62:ALA:HB2     | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:439:U:C4      | 28:T:3:HIS:CE1    | 2.93                     | 0.52              |
| 1:1:198:C:C4      | 1:1:199:A:H1'     | 2.44                     | 0.52              |
| 1:1:931:G:O2'     | 1:1:932:C:H3'     | 2.09                     | 0.52              |
| 2:2:1036:G:H2'    | 2:2:1037:A:C8     | 2.45                     | 0.52              |
| 2:2:1318:OMC:C5'  | 2:2:1318:OMC:C6   | 2.85                     | 0.52              |
| 2:2:701:U:H3'     | 2:2:702:A:C8      | 2.43                     | 0.52              |
| 2:2:749:G:C2'     | 2:2:750:U:O5'     | 2.58                     | 0.52              |
| 4:4:139:U:H2'     | 4:4:140:G:O4'     | 2.09                     | 0.52              |
| 6:6:10:C:N3       | 6:6:33:G:N2       | 2.53                     | 0.52              |
| 8:8:117:A:C6      | 8:8:118:C:C4      | 2.97                     | 0.52              |
| 10:B:58:ARG:NH2   | 10:B:74:GLU:OE2   | 2.42                     | 0.52              |
| 11:C:30:PRO:HG2   | 11:C:121:PHE:HE1  | 1.74                     | 0.52              |
| 13:E:8:CYS:HB3    | 13:E:73:LYS:HE3   | 1.92                     | 0.52              |
| 19:K:71:VAL:HG23  | 19:K:116:PRO:HA   | 1.91                     | 0.52              |
| 22:N:169:LYS:HE3  | 22:N:177:LEU:HD13 | 1.91                     | 0.52              |
| 30:V:138:THR:O    | 30:V:142:ILE:N    | 2.36                     | 0.52              |
| 1:1:816:G:H22     | 1:1:823:G:N2      | 2.06                     | 0.52              |
| 1:1:1528:U:N3     | 2:2:648:A:OP1     | 2.40                     | 0.52              |
| 2:2:677:C:H2'     | 2:2:678:U:O4'     | 2.10                     | 0.52              |
| 2:2:5:A:H2'       | 2:2:6:A:C8        | 2.45                     | 0.52              |
| 2:2:1430:A:O2'    | 5:5:18:G:N7       | 2.43                     | 0.52              |
| 7:7:75:G:O6       | 7:7:76:C:N4       | 2.42                     | 0.52              |
| 9:A:73:LYS:NZ     | 9:A:73:LYS:CB     | 2.73                     | 0.52              |
| 14:F:49:ARG:HH11  | 14:F:181:VAL:CG1  | 2.21                     | 0.52              |
| 15:G:163:PHE:O    | 15:G:240:ASN:ND2  | 2.43                     | 0.52              |
| 1:1:1539:G:N7     | 28:T:27:LYS:HB2   | 2.25                     | 0.52              |
| 1:1:1683:G:O3'    | 1:1:1718:G:N2     | 2.40                     | 0.52              |
| 1:1:1729:A:C3'    | 1:1:1729:A:N3     | 2.73                     | 0.52              |
| 1:1:273:A:O2'     | 1:1:275:A:N7      | 2.43                     | 0.52              |
| 1:1:910:G:O2'     | 1:1:912:C:O2      | 2.26                     | 0.52              |
| 2:2:1252:A:H2'    | 2:2:1253:G:O4'    | 2.10                     | 0.52              |
| 2:2:1433:U:H2'    | 2:2:1434:G:C8     | 2.44                     | 0.52              |
| 2:2:706:U:OP1     | 2:2:706:U:H4'     | 2.08                     | 0.52              |
| 3:3:108:A:H1'     | 3:3:109:C:OP2     | 2.09                     | 0.52              |
| 8:8:44:A:N7       | 8:8:45:U:C4       | 2.78                     | 0.52              |
| 10:B:168:LEU:HD12 | 10:B:180:LYS:O    | 2.10                     | 0.52              |
| 13:E:23:ARG:HH21  | 13:E:24:LYS:HZ1   | 1.58                     | 0.52              |
| 17:I:84:GLU:HA    | 17:I:118:VAL:HG22 | 1.92                     | 0.52              |
| 18:J:66:LYS:HA    | 18:J:72:ARG:HH12  | 1.74                     | 0.52              |
| 21:M:173:GLY:HA3  | 21:M:184:LEU:CD1  | 2.40                     | 0.52              |
| 26:R:92:MET:SD    | 26:R:112:LEU:HD21 | 2.49                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:S:63:ILE:HB    | 27:S:75:ILE:HG12  | 1.91                     | 0.52              |
| 2:2:1334:G:H1     | 2:2:1345:C:H42    | 1.56                     | 0.52              |
| 2:2:29:C:O2'      | 2:2:30:A:H8       | 1.92                     | 0.52              |
| 6:6:20:A:OP2      | 6:6:20:A:H3'      | 2.09                     | 0.52              |
| 6:6:24:C:O2'      | 6:6:25:U:O5'      | 2.24                     | 0.52              |
| 1:1:1475:G:OP2    | 11:C:204:ARG:NH2  | 2.43                     | 0.52              |
| 13:E:59:TRP:CZ2   | 19:K:64:TYR:CB    | 2.93                     | 0.52              |
| 20:L:70:LYS:HE2   | 20:L:125:TYR:CD2  | 2.44                     | 0.52              |
| 15:G:143:MET:HE2  | 21:M:29:GLU:HA    | 1.90                     | 0.52              |
| 1:1:454:U:P       | 28:T:62:ARG:HH22  | 2.32                     | 0.52              |
| 1:1:499:C:H42     | 1:1:554:A:H61     | 1.56                     | 0.52              |
| 1:1:843:C:H2'     | 1:1:844:C:C6      | 2.44                     | 0.52              |
| 1:1:975:G:N3      | 2:2:660:G:O2'     | 2.38                     | 0.52              |
| 2:2:1290:A:H5'    | 2:2:1291:C:H5     | 1.75                     | 0.52              |
| 2:2:685:G:H1      | 2:2:754:U:H3      | 1.57                     | 0.52              |
| 3:3:179:U:H2'     | 3:3:180:G:O4'     | 2.10                     | 0.52              |
| 6:6:35:U:O2       | 6:6:35:U:H2'      | 2.08                     | 0.52              |
| 10:B:368:THR:N    | 10:B:378:GLN:HE22 | 2.06                     | 0.52              |
| 11:C:100:MET:CE   | 11:C:103:PRO:HA   | 2.40                     | 0.52              |
| 11:C:39:VAL:HG13  | 11:C:114:ILE:HD13 | 1.90                     | 0.52              |
| 22:N:123:ASN:OD1  | 22:N:124:GLY:N    | 2.43                     | 0.52              |
| 1:1:1602:U:C5     | 2:2:18:A:N1       | 2.74                     | 0.52              |
| 1:1:652:A:H1'     | 1:1:653:A:C8      | 2.45                     | 0.52              |
| 2:2:1153:OMU:HM23 | 2:2:1153:OMU:O2   | 2.10                     | 0.52              |
| 2:2:1254:OMG:HM21 | 2:2:1256:A:H2'    | 1.91                     | 0.52              |
| 5:5:42:G:OP2      | 5:5:104:G:N2      | 2.43                     | 0.52              |
| 9:A:60[B]:ARG:NH1 | 9:A:73:LYS:HD2    | 2.25                     | 0.52              |
| 10:B:122:TRP:O    | 10:B:127:GLN:NE2  | 2.41                     | 0.52              |
| 10:B:173:ASN:HD22 | 10:B:174[A]:HIS:N | 2.07                     | 0.52              |
| 18:J:27:CYS:SG    | 18:J:36:LEU:HG    | 2.50                     | 0.52              |
| 22:N:98:ARG:NH1   | 22:N:122:PRO:HG3  | 2.25                     | 0.52              |
| 23:O:83:LEU:N     | 23:O:84:PRO:HD2   | 2.25                     | 0.52              |
| 29:U:40:SER:O     | 29:U:44:LEU:N     | 2.39                     | 0.52              |
| 2:2:811:U:O2'     | 2:2:812:C:O5'     | 2.23                     | 0.51              |
| 2:2:996:G:O2'     | 2:2:997:C:OP1     | 2.26                     | 0.51              |
| 16:H:219:PHE:HE1  | 19:K:163:SER:HB3  | 1.76                     | 0.51              |
| 19:K:164:THR:HG23 | 19:K:166:PHE:H    | 1.75                     | 0.51              |
| 21:M:62:PHE:O     | 21:M:131:GLU:HA   | 2.09                     | 0.51              |
| 1:1:1274:G:OP1    | 13:E:1:MET:N      | 2.31                     | 0.51              |
| 1:1:1276:U:H2'    | 1:1:1277:G:C8     | 2.45                     | 0.51              |
| 1:1:497:A:O2'     | 1:1:498:G:H8      | 1.93                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:2:1151:U:O2'    | 2:2:1152:U:H5''  | 2.10                     | 0.51              |
| 2:2:708:G:N7      | 2:2:740:A:O2'    | 2.35                     | 0.51              |
| 6:6:34:C:O2       | 6:6:34:C:H2'     | 2.10                     | 0.51              |
| 7:7:161:C:H2'     | 7:7:161:C:O2     | 2.11                     | 0.51              |
| 11:C:59:MET:SD    | 11:C:91:PHE:HB2  | 2.50                     | 0.51              |
| 16:H:103:ARG:NH1  | 16:H:103:ARG:CG  | 2.72                     | 0.51              |
| 21:M:26:ARG:HA    | 21:M:29:GLU:OE1  | 2.10                     | 0.51              |
| 28:T:3:HIS:CD2    | 28:T:4:TYR:HB2   | 2.46                     | 0.51              |
| 1:1:1015:G:H4'    | 20:L:30:SER:HB3  | 1.91                     | 0.51              |
| 1:1:244:C:H42     | 1:1:248:A:N6     | 2.04                     | 0.51              |
| 1:1:994:U:H5      | 1:1:1523:G:OP1   | 1.93                     | 0.51              |
| 2:2:1037:A:H2'    | 2:2:1038:G:C8    | 2.45                     | 0.51              |
| 2:2:424:U:H2'     | 9:A:152:SER:HB3  | 1.92                     | 0.51              |
| 2:2:830:U:H5''    | 2:2:955:A:N6     | 2.24                     | 0.51              |
| 6:6:56:A:O2'      | 15:G:136:ARG:NH1 | 142.91                   | 0.51              |
| 1:1:1185:U:H5     | 22:N:102:MET:HE2 | 1.75                     | 0.51              |
| 22:N:79:ARG:HH12  | 22:N:150:GLU:HB3 | 1.74                     | 0.51              |
| 23:O:172:ALA:HB1  | 23:O:177:MET:HG3 | 1.92                     | 0.51              |
| 25:Q:32:ILE:HD11  | 25:Q:49:PHE:HB3  | 1.92                     | 0.51              |
| 33:Y:10:VAL:HA    | 33:Y:24:VAL:HA   | 1.91                     | 0.51              |
| 1:1:1263:A:H4'    | 1:1:1264:A:O5'   | 2.11                     | 0.51              |
| 1:1:687:C:H2'     | 1:1:688:A:C8     | 2.46                     | 0.51              |
| 2:2:1120:A:N6     | 2:2:1128:G:O6    | 2.43                     | 0.51              |
| 2:2:534:OMG:H3'   | 2:2:535:U:C5     | 2.45                     | 0.51              |
| 2:2:760:U:OP2     | 2:2:1013:U:N3    | 2.41                     | 0.51              |
| 2:2:363:C:O2'     | 4:4:108:G:H1'    | 2.09                     | 0.51              |
| 10:B:371:LYS:N    | 10:B:371:LYS:CD  | 2.74                     | 0.51              |
| 13:E:172:ARG:HH11 | 13:E:173:LYS:HZ1 | 1.58                     | 0.51              |
| 15:G:185:GLU:HG3  | 15:G:190:ARG:HB2 | 1.91                     | 0.51              |
| 17:I:29:VAL:HG12  | 17:I:31:LEU:HG   | 1.93                     | 0.51              |
| 24:P:65:SER:HA    | 24:P:99:MET:HG3  | 1.92                     | 0.51              |
| 33:Y:83:THR:OG1   | 33:Y:84:ARG:N    | 2.32                     | 0.51              |
| 1:1:801:G:H1      | 1:1:1028:A:H2    | 1.58                     | 0.51              |
| 1:1:1158:U:C4     | 1:1:1159:A:H1'   | 2.45                     | 0.51              |
| 1:1:1682:U:O2'    | 1:1:1683:G:N7    | 2.42                     | 0.51              |
| 1:1:222:A:H2'     | 1:1:223:A:C8     | 2.43                     | 0.51              |
| 1:1:240:U:H2'     | 1:1:241:G:H8     | 1.74                     | 0.51              |
| 2:2:1131:A:N3     | 23:O:23:ARG:NH1  | 2.57                     | 0.51              |
| 4:4:168:A:HO2'    | 4:4:169:A:P      | 2.32                     | 0.51              |
| 6:6:14:A:C4'      | 6:6:15:C:OP1     | 2.58                     | 0.51              |
| 6:6:22:G:C5       | 6:6:26:G:N2      | 2.78                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:6:8:A:H2'       | 6:6:9:U:C6       | 2.45                     | 0.51              |
| 6:6:46:C:H42      | 14:F:179:ARG:HE  | 1.56                     | 0.51              |
| 15:G:185:GLU:OE2  | 15:G:193:ARG:NH2 | 2.44                     | 0.51              |
| 16:H:79:ARG:HH21  | 16:H:84:PRO:HG3  | 1.75                     | 0.51              |
| 18:J:25:VAL:O     | 18:J:36:LEU:N    | 2.44                     | 0.51              |
| 1:1:304:G:N2      | 21:M:50:MET:O    | 2.43                     | 0.51              |
| 1:1:1116:A:N3     | 1:1:1118:A:N6    | 2.58                     | 0.51              |
| 1:1:1259:C:H2'    | 1:1:1260:G:H4'   | 1.93                     | 0.51              |
| 1:1:1221:G:H1     | 1:1:1405:U:H3    | 1.58                     | 0.51              |
| 1:1:1674:U:H3     | 1:1:1728:G:N2    | 2.08                     | 0.51              |
| 1:1:696:A:H2'     | 1:1:697:A:C8     | 2.45                     | 0.51              |
| 2:2:1090:A:H2'    | 2:2:1091:G:H8    | 1.75                     | 0.51              |
| 2:2:1441:G:O2'    | 2:2:1443:G:N2    | 2.44                     | 0.51              |
| 2:2:449:U:H2'     | 2:2:450:C:C6     | 2.46                     | 0.51              |
| 2:2:701:U:H3'     | 2:2:702:A:H8     | 1.75                     | 0.51              |
| 6:6:27:G:N3       | 6:6:27:G:C5'     | 2.73                     | 0.51              |
| 8:8:42:C:O2'      | 8:8:43:G:H5''    | 2.11                     | 0.51              |
| 10:B:204:LEU:O    | 10:B:205:GLU:HG2 | 2.10                     | 0.51              |
| 10:B:47:MET:HE1   | 10:B:182:HIS:O   | 2.10                     | 0.51              |
| 19:K:155:GLU:HG2  | 19:K:158:LYS:HE2 | 1.92                     | 0.51              |
| 21:M:120:TRP:HZ2  | 21:M:123:MET:HG2 | 1.75                     | 0.51              |
| 22:N:30:LYS:HB3   | 22:N:66:GLU:OE1  | 2.10                     | 0.51              |
| 23:O:101:THR:HA   | 23:O:104:LEU:HB3 | 1.91                     | 0.51              |
| 23:O:22:ARG:NE    | 23:O:28:THR:OG1  | 2.44                     | 0.51              |
| 1:1:708:A:OP2     | 24:P:111:ARG:NH1 | 2.43                     | 0.51              |
| 26:R:5:HIS:ND1    | 26:R:6:LEU:HB2   | 2.26                     | 0.51              |
| 33:Y:22:LYS:NZ    | 33:Y:127:TRP:O   | 2.40                     | 0.51              |
| 1:1:157:U:H2'     | 1:1:158:A:H4'    | 1.92                     | 0.51              |
| 1:1:238:A:OP2     | 50:1:1929:HOH:O  | 2.18                     | 0.51              |
| 1:1:670:C:H2'     | 1:1:671:G:C8     | 2.46                     | 0.51              |
| 1:1:739:U:H2'     | 1:1:740:C:C6     | 2.46                     | 0.51              |
| 2:2:1151:U:O2'    | 2:2:1152:U:H5'   | 2.10                     | 0.51              |
| 6:6:42:A:H1'      | 6:6:43:A:N7      | 2.25                     | 0.51              |
| 7:7:135:U:H2'     | 7:7:136:G:O4'    | 2.10                     | 0.51              |
| 10:B:338:PRO:HD2  | 10:B:341:ARG:HD2 | 1.93                     | 0.51              |
| 14:F:188:ASP:HB2  | 14:F:193:TRP:CZ2 | 2.46                     | 0.51              |
| 15:G:247:LEU:HD12 | 21:M:45:PRO:HG2  | 1.92                     | 0.51              |
| 24:P:112:PHE:CZ   | 24:P:127:CYS:HB2 | 2.46                     | 0.51              |
| 30:V:65:VAL:HG23  | 30:V:66:ILE:H    | 1.74                     | 0.51              |
| 1:1:1659:G:H1'    | 2:2:414:G:N2     | 2.20                     | 0.51              |
| 1:1:452:C:H2'     | 1:1:453:G:C8     | 2.45                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:913:C:OP2     | 50:1:1952:HOH:O    | 2.19                     | 0.51              |
| 2:2:1254:OMG:C5   | 2:2:1309:C:O2'     | 2.62                     | 0.51              |
| 2:2:535:U:HO2'    | 2:2:536:C:H5'      | 1.73                     | 0.51              |
| 2:2:745:G:H2'     | 2:2:746:A:C8       | 2.46                     | 0.51              |
| 11:C:139:ARG:HH11 | 11:C:240:PRO:HD2   | 1.76                     | 0.51              |
| 13:E:19:ASP:OD1   | 13:E:26:THR:N      | 2.44                     | 0.51              |
| 14:F:173:GLU:O    | 14:F:177:TYR:N     | 2.39                     | 0.51              |
| 21:M:108:LYS:HE3  | 21:M:161:GLN:NE2   | 2.26                     | 0.51              |
| 1:1:1613:G:OP2    | 28:T:127:ARG:NH2   | 2.44                     | 0.51              |
| 30:V:83:ASN:H     | 30:V:128:ARG:NH1   | 2.09                     | 0.51              |
| 1:1:559:G:HO2'    | 1:1:560:G:H8       | 1.54                     | 0.51              |
| 1:1:669:C:O2      | 1:1:684:G:N2       | 2.31                     | 0.51              |
| 1:1:84:G:H4'      | 1:1:85:U:H5'       | 1.93                     | 0.51              |
| 2:2:780:G:O6      | 2:2:812:C:N4       | 2.44                     | 0.51              |
| 10:B:365:PHE:HE2  | 10:B:367:ASP:OD1   | 1.91                     | 0.51              |
| 14:F:23:SER:O     | 14:F:25:GLU:N      | 2.35                     | 0.51              |
| 14:F:76:ILE:H     | 14:F:76:ILE:HD12   | 1.75                     | 0.51              |
| 2:2:1445:G:N2     | 16:H:119:SER:O     | 2.39                     | 0.51              |
| 16:H:208:MET:SD   | 19:K:181:TRP:CD2   | 3.04                     | 0.51              |
| 20:L:75:LEU:HD21  | 20:L:109:LEU:HD11  | 1.93                     | 0.51              |
| 22:N:191:GLU:HG2  | 22:N:192:GLN:H     | 1.75                     | 0.51              |
| 23:O:76:MET:HE2   | 23:O:108:ARG:HB2   | 1.93                     | 0.51              |
| 23:O:41:LYS:N     | 27:S:69:PRO:O      | 2.40                     | 0.51              |
| 1:1:547:U:C4      | 1:1:1393:A:C6      | 2.99                     | 0.51              |
| 1:1:178:G:N7      | 1:1:274:A:O2'      | 2.42                     | 0.51              |
| 2:2:833:U:H3      | 2:2:952:G:N2       | 2.09                     | 0.51              |
| 5:5:101:C:H1'     | 5:5:102:U:H5'      | 1.92                     | 0.51              |
| 5:5:24:A:H5''     | 10:B:123:LYS:HG3   | 1.91                     | 0.51              |
| 6:6:22:G:N3       | 6:6:22:G:C2'       | 2.73                     | 0.51              |
| 22:N:44:ASP:HA    | 22:N:171:TRP:HZ2   | 1.76                     | 0.51              |
| 22:N:47:PRO:HD2   | 22:N:141:LYS:HA    | 1.92                     | 0.51              |
| 1:1:434:U:O2'     | 31:W:84[A]:ARG:NH1 | 2.44                     | 0.51              |
| 1:1:1452:U:H2'    | 1:1:1453:C:C6      | 2.46                     | 0.50              |
| 1:1:159:U:C5      | 1:1:160:C:C4       | 2.99                     | 0.50              |
| 1:1:567:G:H2'     | 1:1:568:U:C6       | 2.45                     | 0.50              |
| 1:1:781:A:HO2'    | 1:1:782:C:C5'      | 2.24                     | 0.50              |
| 2:2:1024:C:O2     | 2:2:1025:U:H5      | 1.94                     | 0.50              |
| 2:2:533:C:C5      | 2:2:544:U:C6       | 2.99                     | 0.50              |
| 5:5:6:C:O3'       | 28:T:74:LYS:NZ     | 2.39                     | 0.50              |
| 6:6:10:C:O2'      | 6:6:12:C:OP2       | 2.28                     | 0.50              |
| 8:8:27:A:N6       | 8:8:55:U:O4        | 2.44                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:1375:G:H5'   | 16:H:101:THR:HG23 | 1.93                     | 0.50              |
| 18:J:67:GLY:O    | 18:J:72:ARG:NH2   | 2.44                     | 0.50              |
| 1:1:752:G:C4     | 20:L:110:LEU:HD11 | 2.46                     | 0.50              |
| 21:M:168:GLY:HA2 | 21:M:171:HIS:CD2  | 2.46                     | 0.50              |
| 22:N:150:GLU:O   | 22:N:154:ARG:HG2  | 2.11                     | 0.50              |
| 26:R:8:HIS:CD2   | 26:R:66:VAL:HG21  | 2.46                     | 0.50              |
| 1:1:1729:A:N3    | 1:1:1729:A:C2'    | 2.74                     | 0.50              |
| 1:1:478:C:H2'    | 1:1:479:A:C8      | 2.45                     | 0.50              |
| 1:1:788:A:H2'    | 1:1:789:U:O4'     | 2.11                     | 0.50              |
| 2:2:1239:G:O6    | 20:L:42:ARG:NH2   | 2.40                     | 0.50              |
| 2:2:622:G:H2'    | 2:2:623:A:C8      | 2.46                     | 0.50              |
| 2:2:777:A:H62    | 2:2:812:C:H6      | 1.59                     | 0.50              |
| 6:6:22:G:C6      | 6:6:26:G:N2       | 2.80                     | 0.50              |
| 2:2:1383:U:H1'   | 10:B:256:CYS:SG   | 2.50                     | 0.50              |
| 16:H:58:GLN:HA   | 16:H:156:VAL:HG13 | 1.93                     | 0.50              |
| 19:K:88:ILE:HD12 | 19:K:88:ILE:N     | 2.26                     | 0.50              |
| 20:L:4:ARG:H     | 20:L:4:ARG:HD3    | 1.77                     | 0.50              |
| 25:Q:147:ASN:OD1 | 25:Q:148:GLU:N    | 2.40                     | 0.50              |
| 1:1:1236:A:OP2   | 50:1:1960:HOH:O   | 2.19                     | 0.50              |
| 1:1:409:U:HO2'   | 1:1:410:U:P       | 2.32                     | 0.50              |
| 1:1:700:A:H4'    | 24:P:172:TYR:CE1  | 2.46                     | 0.50              |
| 1:1:847:OMU:H2'  | 1:1:848:U:H5''    | 1.92                     | 0.50              |
| 4:4:33:G:H21     | 4:4:171:A:H2      | 1.58                     | 0.50              |
| 6:6:26:G:N3      | 6:6:26:G:C3'      | 2.73                     | 0.50              |
| 6:6:56:A:C2      | 6:6:58:U:OP2      | 2.64                     | 0.50              |
| 9:A:133:TYR:HE1  | 9:A:135:ILE:HD11  | 1.74                     | 0.50              |
| 13:E:91:VAL:HG22 | 13:E:180:VAL:HA   | 1.91                     | 0.50              |
| 2:2:971:A:N7     | 15:G:118:ASN:HB2  | 2.27                     | 0.50              |
| 1:1:1512:C:OP2   | 11:C:194:LYS:NZ   | 2.32                     | 0.50              |
| 1:1:1773:U:H2'   | 1:1:1774:G:C8     | 2.46                     | 0.50              |
| 1:1:780:C:H2'    | 1:1:781:A:C8      | 2.46                     | 0.50              |
| 2:2:1255:G:H1    | 2:2:1259:A:N6     | 2.04                     | 0.50              |
| 1:1:1590:G:N2    | 2:2:56:U:O4       | 2.37                     | 0.50              |
| 8:8:110:G:H1'    | 8:8:111:U:H5'     | 1.93                     | 0.50              |
| 13:E:111:VAL:HB  | 13:E:121:ARG:HB2  | 1.93                     | 0.50              |
| 15:G:128:ALA:HB1 | 30:V:31:THR:HG21  | 1.93                     | 0.50              |
| 16:H:107:PRO:O   | 16:H:113:GLY:HA3  | 2.11                     | 0.50              |
| 21:M:193:ARG:O   | 21:M:197:ARG:HG3  | 2.12                     | 0.50              |
| 25:Q:99:LEU:HD11 | 25:Q:103:ARG:CZ   | 2.42                     | 0.50              |
| 2:2:14:C:OP2     | 30:V:95:LYS:HD3   | 2.11                     | 0.50              |
| 31:W:28:MET:HB3  | 31:W:98:PRO:HG2   | 1.93                     | 0.50              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 34:Z:113:ARG:O    | 34:Z:117:ILE:HG13   | 2.11                     | 0.50              |
| 1:1:1483:G:O2'    | 1:1:1508:G:O6       | 2.30                     | 0.50              |
| 1:1:1547:G:H4'    | 4:4:106:G:H22       | 1.76                     | 0.50              |
| 1:1:1548:A:N6     | 1:1:1584:A:HO2'     | 2.09                     | 0.50              |
| 1:1:930:U:H3'     | 1:1:931:G:C5'       | 2.40                     | 0.50              |
| 2:2:1012:G:O2'    | 2:2:1013:U:OP2      | 2.25                     | 0.50              |
| 4:4:33:G:H5''     | 10:B:98:GLY:HA3     | 1.94                     | 0.50              |
| 4:4:77:U:C2       | 10:B:75:PRO:HB3     | 2.46                     | 0.50              |
| 10:B:173:ASN:HD22 | 10:B:174[B]:HIS:N   | 2.07                     | 0.50              |
| 10:B:365:PHE:C    | 10:B:366:ILE:HD12   | 2.31                     | 0.50              |
| 11:C:127:LEU:HD22 | 11:C:250:TRP:HZ2    | 1.76                     | 0.50              |
| 13:E:126:PRO:HD3  | 13:E:156:GLU:CD     | 2.32                     | 0.50              |
| 15:G:227:ALA:HB1  | 15:G:233:ALA:HB2    | 1.93                     | 0.50              |
| 2:2:800:G:O5'     | 15:G:301[A]:ARG:NH1 | 2.44                     | 0.50              |
| 16:H:79:ARG:HA    | 16:H:88:PRO:HD2     | 1.94                     | 0.50              |
| 2:2:603:A:H5'     | 28:T:137:THR:OG1    | 2.11                     | 0.50              |
| 1:1:1729:A:C6     | 1:1:1730:A:N6       | 2.80                     | 0.50              |
| 1:1:282:C:H2'     | 1:1:283:G:C8        | 2.47                     | 0.50              |
| 1:1:520:G:N2      | 1:1:531:C:N3        | 2.44                     | 0.50              |
| 2:2:1446:A:H3'    | 16:H:129:ASN:ND2    | 2.26                     | 0.50              |
| 2:2:468:A:HO2'    | 2:2:469:G:P         | 2.35                     | 0.50              |
| 2:2:509:C:H2'     | 2:2:510:U:C6        | 2.46                     | 0.50              |
| 2:2:638:C:O2'     | 10:B:271:ARG:NH1    | 2.43                     | 0.50              |
| 2:2:958:C:O2      | 2:2:958:C:H2'       | 2.10                     | 0.50              |
| 1:1:491:A:O4'     | 6:6:54:A:C2         | 2.65                     | 0.50              |
| 9:A:192:LYS:HB3   | 9:A:193:ARG:NH2     | 2.27                     | 0.50              |
| 9:A:62:GLU:OE1    | 9:A:71:ARG:NH2      | 2.45                     | 0.50              |
| 10:B:28:ARG:H     | 10:B:279:HIS:CE1    | 2.30                     | 0.50              |
| 15:G:306:ARG:O    | 15:G:310:ARG:HD3    | 2.12                     | 0.50              |
| 10:B:96:PRO:HD3   | 16:H:175:LEU:CD1    | 2.41                     | 0.50              |
| 16:H:30:LYS:HB2   | 16:H:55:ARG:NH2     | 2.26                     | 0.50              |
| 19:K:110:ASN:OD1  | 19:K:111:LEU:N      | 2.44                     | 0.50              |
| 6:6:14:A:OP2      | 19:K:42:VAL:HB      | 2.11                     | 0.50              |
| 1:1:1135:U:H3'    | 1:1:1136:G:C8       | 2.47                     | 0.50              |
| 1:1:1166:C:H2'    | 1:1:1167:C:C6       | 2.46                     | 0.50              |
| 1:1:173:G:C4      | 1:1:174:U:H1'       | 2.47                     | 0.50              |
| 1:1:229:C:O2'     | 1:1:230:A:H8        | 1.95                     | 0.50              |
| 1:1:452:C:H2'     | 1:1:453:G:H8        | 1.76                     | 0.50              |
| 1:1:664:C:C2'     | 1:1:665:C:H5'       | 2.42                     | 0.50              |
| 1:1:681:A2M:H2'   | 1:1:682:C:C6        | 2.47                     | 0.50              |
| 2:2:1089:G:H1     | 2:2:1137:U:H3       | 1.60                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:1443:G:H4'    | 2:2:1444:A:O5'    | 2.10                     | 0.50              |
| 2:2:628:A2M:OP1   | 16:H:103:ARG:CZ   | 2.58                     | 0.50              |
| 3:3:93:G:H2'      | 3:3:94:G:O4'      | 2.11                     | 0.50              |
| 8:8:11:C:H5''     | 8:8:12:C:OP2      | 2.10                     | 0.50              |
| 9:A:116:VAL:HG21  | 9:A:148:LEU:HD11  | 1.94                     | 0.50              |
| 2:2:1005:G:O3'    | 15:G:117:LYS:O    | 2.16                     | 0.50              |
| 2:2:1005:G:O2'    | 15:G:119:PHE:CE2  | 2.57                     | 0.50              |
| 1:1:1539:G:O6     | 28:T:25:HIS:ND1   | 2.45                     | 0.50              |
| 31:W:52:GLU:HA    | 31:W:66:LYS:HA    | 1.94                     | 0.50              |
| 1:1:129:C:H2'     | 1:1:130:U:O4'     | 2.12                     | 0.50              |
| 1:1:1489:U:H1'    | 1:1:1491:U:OP1    | 2.12                     | 0.50              |
| 1:1:1631:G:N2     | 1:1:1759:U:O2'    | 2.45                     | 0.50              |
| 1:1:232:G:O2'     | 1:1:233:U:OP1     | 2.26                     | 0.50              |
| 2:2:776:C:H2'     | 2:2:776:C:O2      | 2.12                     | 0.50              |
| 3:3:108:A:H5''    | 3:3:109:C:H5      | 1.77                     | 0.50              |
| 3:3:55:U:O2'      | 3:3:57:U:OP2      | 2.18                     | 0.50              |
| 10:B:153:PHE:O    | 10:B:157:ALA:HB3  | 2.12                     | 0.50              |
| 7:7:20:C:OP1      | 11:C:194:LYS:HD2  | 2.11                     | 0.50              |
| 13:E:23:ARG:HB3   | 13:E:46:ARG:HH22  | 1.77                     | 0.50              |
| 19:K:93:ARG:CG    | 19:K:108:VAL:HG12 | 2.42                     | 0.50              |
| 19:K:74:LEU:HD12  | 19:K:75:ARG:HG3   | 1.93                     | 0.50              |
| 1:1:765:C:OP2     | 20:L:136:LYS:HE2  | 2.12                     | 0.50              |
| 21:M:122:ASN:HD22 | 21:M:123:MET:N    | 2.09                     | 0.50              |
| 28:T:60:PHE:O     | 28:T:64:ASN:HB3   | 2.11                     | 0.50              |
| 1:1:1161:A:N6     | 24:P:13:ARG:HD2   | 2.27                     | 0.50              |
| 1:1:1278:G:H1     | 1:1:1351:C:N4     | 2.01                     | 0.50              |
| 1:1:242:A:H61     | 1:1:260:C:N4      | 2.10                     | 0.50              |
| 1:1:568:U:O4      | 1:1:634:G:O6      | 2.30                     | 0.50              |
| 1:1:672:U:OP1     | 20:L:21:ARG:NH2   | 2.45                     | 0.50              |
| 2:2:772:A:C8      | 15:G:134:PHE:HZ   | 2.29                     | 0.50              |
| 6:6:34:C:C3'      | 6:6:35:U:C6       | 2.85                     | 0.50              |
| 6:6:40:C:H5''     | 6:6:41:G:C8       | 2.46                     | 0.50              |
| 7:7:124:A:H2'     | 7:7:125:A:C8      | 2.46                     | 0.50              |
| 13:E:149:ASP:O    | 13:E:153:VAL:HG22 | 2.12                     | 0.50              |
| 16:H:94:PRO:HA    | 16:H:97:VAL:HB    | 1.93                     | 0.50              |
| 28:T:41:LEU:HD13  | 28:T:150:MET:HE2  | 1.94                     | 0.50              |
| 1:1:1032:G:N2     | 1:1:1164:C:OP1    | 2.44                     | 0.49              |
| 1:1:368:G:H22     | 7:7:34:U:H3       | 1.59                     | 0.49              |
| 1:1:872:U:C4'     | 1:1:963:G:H5'     | 2.42                     | 0.49              |
| 2:2:700:G:H2'     | 2:2:701:U:H5''    | 1.94                     | 0.49              |
| 2:2:69:A:C2'      | 2:2:70:A:H5'      | 2.42                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:5:28:G:O6       | 5:5:122:C:N4      | 2.43                     | 0.49              |
| 7:7:145:G:H2'     | 7:7:146:U:C6      | 2.47                     | 0.49              |
| 17:I:59:LEU:HD22  | 17:I:80:PHE:CZ    | 2.46                     | 0.49              |
| 28:T:60:PHE:CE2   | 28:T:82:ARG:HD2   | 2.46                     | 0.49              |
| 1:1:215:U:H3'     | 1:1:217:A:H2      | 1.77                     | 0.49              |
| 1:1:306:G:OP2     | 21:M:44:ARG:NH1   | 2.41                     | 0.49              |
| 1:1:453:G:OP1     | 28:T:62:ARG:HD3   | 2.12                     | 0.49              |
| 2:2:1277:A:C5     | 2:2:1278:G:H1'    | 2.47                     | 0.49              |
| 2:2:459:A:N6      | 2:2:479:C:N3      | 2.60                     | 0.49              |
| 2:2:71:OMG:O5'    | 2:2:71:OMG:H8     | 1.96                     | 0.49              |
| 6:6:42:A:H1'      | 6:6:43:A:C5       | 2.47                     | 0.49              |
| 2:2:1387:C:P      | 10:B:249:ARG:HH21 | 2.36                     | 0.49              |
| 17:I:52:PHE:CD1   | 17:I:53:PRO:HA    | 2.47                     | 0.49              |
| 23:O:103:LEU:HA   | 23:O:106:ALA:HB3  | 1.94                     | 0.49              |
| 24:P:93:VAL:HB    | 24:P:112:PHE:CD1  | 2.48                     | 0.49              |
| 1:1:235:A:H2'     | 1:1:235:A:N3      | 2.27                     | 0.49              |
| 1:1:291:A:H2'     | 1:1:292:A:C8      | 2.43                     | 0.49              |
| 1:1:53:G:O2'      | 21:M:161:GLN:NE2  | 2.44                     | 0.49              |
| 1:1:740:C:C2'     | 1:1:741:G:H5'     | 2.40                     | 0.49              |
| 1:1:776:U:H3'     | 1:1:777:G:C8      | 2.42                     | 0.49              |
| 1:1:751:G:O2'     | 1:1:811:G:H5"     | 2.11                     | 0.49              |
| 1:1:88:G:OP2      | 50:1:1926:HOH:O   | 2.20                     | 0.49              |
| 2:2:620:C:OP1     | 2:2:1262:G:O2'    | 2.30                     | 0.49              |
| 3:3:128:C:O2      | 3:3:128:C:H3'     | 2.12                     | 0.49              |
| 3:3:51:G:H5'      | 3:3:153:G:O2'     | 2.13                     | 0.49              |
| 4:4:35:G:H5"      | 16:H:90:HIS:O     | 2.12                     | 0.49              |
| 7:7:76:C:O2'      | 7:7:77:A:O5'      | 2.29                     | 0.49              |
| 8:8:48:G:N1       | 8:8:49:U:C2       | 2.79                     | 0.49              |
| 10:B:92:TYR:HD2   | 10:B:99:LEU:HD13  | 1.76                     | 0.49              |
| 11:C:192:ARG:O    | 11:C:196:ARG:HD3  | 2.11                     | 0.49              |
| 13:E:104:VAL:HG22 | 13:E:109:ILE:HG13 | 1.93                     | 0.49              |
| 13:E:108:ASN:HD21 | 13:E:122:ARG:HB3  | 1.77                     | 0.49              |
| 13:E:161:HIS:CD2  | 13:E:180:VAL:HG12 | 2.48                     | 0.49              |
| 13:E:182:THR:HG22 | 13:E:184:THR:OG1  | 2.12                     | 0.49              |
| 13:E:40:HIS:CE1   | 13:E:41:LEU:HB3   | 2.46                     | 0.49              |
| 17:I:33:GLN:HE21  | 21:M:202:ARG:HE   | 1.59                     | 0.49              |
| 22:N:193:ARG:HH11 | 22:N:198:LYS:HE3  | 1.77                     | 0.49              |
| 23:O:18:VAL:HG22  | 23:O:24:ARG:NH2   | 2.15                     | 0.49              |
| 28:T:36:ILE:HG22  | 28:T:39:MET:SD    | 2.52                     | 0.49              |
| 1:1:1102:U:O2'    | 1:1:1103:U:O5'    | 2.29                     | 0.49              |
| 1:1:1554:C:H2'    | 1:1:1555:G:C8     | 2.46                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:273:A:H2'     | 1:1:274:A:H4'     | 1.94                     | 0.49              |
| 1:1:308:A:H2'     | 1:1:309:G:O4'     | 2.13                     | 0.49              |
| 1:1:543:G:C5'     | 1:1:543:G:N3      | 2.73                     | 0.49              |
| 2:2:1113:A:O2'    | 2:2:1114:C:O4'    | 2.21                     | 0.49              |
| 2:2:1398:OMC:HM22 | 2:2:1399:C:C4'    | 2.41                     | 0.49              |
| 7:7:12:A:O2'      | 28:T:121:GLN:O    | 2.30                     | 0.49              |
| 9:A:30:ARG:O      | 9:A:163:ARG:NH2   | 2.40                     | 0.49              |
| 10:B:248:HIS:CE1  | 10:B:249:ARG:HD3  | 2.46                     | 0.49              |
| 11:C:10:TYR:CE2   | 11:C:147:PRO:HB2  | 2.47                     | 0.49              |
| 11:C:207:MET:HB3  | 11:C:246:ARG:NH2  | 2.27                     | 0.49              |
| 16:H:30:LYS:HE3   | 16:H:55:ARG:NH2   | 2.27                     | 0.49              |
| 19:K:134:ASP:O    | 19:K:138:SER:N    | 2.45                     | 0.49              |
| 24:P:89:VAL:HG22  | 24:P:91:GLY:H     | 1.78                     | 0.49              |
| 1:1:1144:G:H2'    | 1:1:1145:G:C8     | 2.46                     | 0.49              |
| 1:1:1662:U:H4'    | 1:1:1663:U:O5'    | 2.11                     | 0.49              |
| 1:1:212:U:H3      | 1:1:221:C:H42     | 1.59                     | 0.49              |
| 1:1:300:A:C2      | 1:1:301:A:H1'     | 2.47                     | 0.49              |
| 1:1:519:G:H21     | 1:1:531:C:N4      | 2.10                     | 0.49              |
| 1:1:819:C:H2'     | 1:1:820:U:H4'     | 1.95                     | 0.49              |
| 2:2:527:A2M:HM'3  | 2:2:1398:OMC:HM23 | 1.95                     | 0.49              |
| 2:2:1440:U:O2'    | 2:2:1441:G:H5''   | 2.12                     | 0.49              |
| 2:2:373:U:H3      | 2:2:572:A2M:C2    | 2.26                     | 0.49              |
| 2:2:782:G:C4      | 2:2:783:U:C5      | 3.00                     | 0.49              |
| 2:2:988:U:H2'     | 2:2:989:G:C8      | 2.48                     | 0.49              |
| 6:6:7:A:C2        | 6:6:60:A:N1       | 2.81                     | 0.49              |
| 7:7:41:A:H61      | 7:7:102:G:C2'     | 2.25                     | 0.49              |
| 2:2:410:C:O2'     | 9:A:12:ASN:OD1    | 2.19                     | 0.49              |
| 19:K:78:ARG:HH12  | 19:K:107:HIS:HE1  | 0.65                     | 0.49              |
| 22:N:96:VAL:HA    | 22:N:125:VAL:HG22 | 1.94                     | 0.49              |
| 1:1:779:A:OP1     | 24:P:142:ASN:N    | 2.46                     | 0.49              |
| 25:Q:21:ARG:NH2   | 25:Q:52:ARG:HH11  | 2.09                     | 0.49              |
| 25:Q:32:ILE:HD12  | 25:Q:50:ILE:HD11  | 1.93                     | 0.49              |
| 31:W:50:ASP:C     | 31:W:66:LYS:HE2   | 2.33                     | 0.49              |
| 1:1:777:G:N2      | 24:P:144:TYR:HA   | 2.28                     | 0.49              |
| 6:6:16:C:H2'      | 6:6:17:U:O4'      | 2.13                     | 0.49              |
| 6:6:8:A:N6        | 6:6:34:C:N4       | 2.60                     | 0.49              |
| 3:3:24:C:H5''     | 9:A:70:ARG:HG2    | 1.95                     | 0.49              |
| 1:1:1530:U:H5''   | 11:C:75:ILE:CD1   | 2.43                     | 0.49              |
| 16:H:93:ALA:H     | 16:H:166:TRP:HB2  | 1.78                     | 0.49              |
| 31:W:77:ILE:HD11  | 31:W:101:VAL:HG21 | 1.93                     | 0.49              |
| 31:W:80:ASP:O     | 31:W:80:ASP:OD1   | 2.30                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:1165:A:H2'   | 1:1:1166:C:C6     | 2.46                     | 0.49              |
| 1:1:1576:C:H2'   | 1:1:1577:G:C8     | 2.47                     | 0.49              |
| 2:2:1021:C:H2'   | 2:2:1022:A:O4'    | 2.13                     | 0.49              |
| 2:2:969:U:O2'    | 2:2:970:A:O4'     | 2.30                     | 0.49              |
| 3:3:36:C:H2'     | 3:3:37:A:C8       | 2.47                     | 0.49              |
| 5:5:113:A:H1'    | 5:5:114:A:OP2     | 2.12                     | 0.49              |
| 5:5:32:G:H2'     | 5:5:33:G:H8       | 1.77                     | 0.49              |
| 8:8:109:A:N6     | 8:8:110:G:O6      | 2.46                     | 0.49              |
| 9:A:113:VAL:HG12 | 9:A:166:ILE:HD13  | 1.93                     | 0.49              |
| 9:A:192:LYS:HD3  | 9:A:193:ARG:HH22  | 1.77                     | 0.49              |
| 13:E:108:ASN:OD1 | 13:E:109:ILE:N    | 2.44                     | 0.49              |
| 14:F:25:GLU:O    | 14:F:26:TYR:HB3   | 2.13                     | 0.49              |
| 2:2:768:G:H8     | 30:V:34:GLN:HE22  | 1.59                     | 0.49              |
| 1:1:1368:G:O6    | 2:2:612:C:O2'     | 2.29                     | 0.49              |
| 1:1:649:U:O2'    | 1:1:650:G:O4'     | 2.30                     | 0.49              |
| 2:2:455:U:H3'    | 2:2:456:G:C8      | 2.46                     | 0.49              |
| 2:2:522:G:N2     | 2:2:562:G:O2'     | 2.44                     | 0.49              |
| 4:4:140:G:N2     | 4:4:150:A:H62     | 2.06                     | 0.49              |
| 6:6:37:C:C6      | 14:F:185:LYS:HD3  | 2.48                     | 0.49              |
| 6:6:41:G:H1      | 19:K:176:ARG:HH11 | 1.56                     | 0.49              |
| 8:8:76:A:N1      | 8:8:102:A:H5'     | 2.27                     | 0.49              |
| 8:8:27:A:OP2     | 8:8:27:A:H8       | 1.96                     | 0.49              |
| 10:B:300:GLN:HB3 | 10:B:312:ILE:HG12 | 1.93                     | 0.49              |
| 1:1:1357:G:H2'   | 1:1:1358:C:C6     | 2.48                     | 0.49              |
| 1:1:1752:G:H2'   | 1:1:1754:U:OP2    | 2.13                     | 0.49              |
| 2:2:1044:C:H2'   | 2:2:1045:U:C2     | 2.48                     | 0.49              |
| 2:2:1140:U:H2'   | 2:2:1141:U:C6     | 2.48                     | 0.49              |
| 2:2:601:G:H4'    | 28:T:139:TYR:CE1  | 2.48                     | 0.49              |
| 6:6:18:A:H1'     | 6:6:29:G:H22      | 1.78                     | 0.49              |
| 9:A:79:PRO:HD2   | 9:A:82:MET:CE     | 2.42                     | 0.49              |
| 10:B:301:ALA:HB2 | 10:B:312:ILE:HD13 | 1.94                     | 0.49              |
| 16:H:123:TYR:CG  | 16:H:127:PRO:HG2  | 2.48                     | 0.49              |
| 16:H:200:ALA:HA  | 19:K:185:VAL:HG11 | 1.93                     | 0.49              |
| 1:1:70:C:H1'     | 17:I:66:PRO:O     | 2.13                     | 0.49              |
| 18:J:81:ILE:HG23 | 18:J:120:VAL:HG22 | 1.94                     | 0.49              |
| 1:1:1677:A:O5'   | 1:1:1677:A:H8     | 1.95                     | 0.49              |
| 1:1:300:A:C2'    | 1:1:301:A:H4'     | 2.43                     | 0.49              |
| 1:1:353:C:P      | 17:I:107:LYS:HE3  | 2.53                     | 0.49              |
| 1:1:1651:G:O2'   | 2:2:414:G:O2'     | 2.30                     | 0.49              |
| 2:2:94:A:H2'     | 2:2:95:A:O4'      | 2.13                     | 0.49              |
| 3:3:194:A:H8     | 3:3:196:A:HO2'    | 1.59                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:5:132:C:H4'     | 5:5:133:A:O5'    | 2.13                     | 0.49              |
| 8:8:29:A:OP2      | 23:O:56:THR:OG1  | 2.31                     | 0.49              |
| 9:A:237:LEU:HB3   | 9:A:240:ALA:HB2  | 1.95                     | 0.49              |
| 13:E:137:SER:HA   | 13:E:140:LYS:HD3 | 1.95                     | 0.49              |
| 2:2:1012:G:N2     | 15:G:153:ARG:NH1 | 2.61                     | 0.49              |
| 15:G:166:VAL:HG21 | 15:G:266:LYS:CD  | 2.40                     | 0.49              |
| 16:H:188:GLU:HA   | 16:H:191:ALA:HB2 | 1.94                     | 0.49              |
| 17:I:16:HIS:HD2   | 17:I:23:GLN:HG3  | 1.78                     | 0.49              |
| 26:R:14:ARG:HG2   | 26:R:26:VAL:HG22 | 1.94                     | 0.49              |
| 1:1:1629:U:O4     | 30:V:119:PRO:HG3 | 2.13                     | 0.49              |
| 34:Z:18:PHE:O     | 34:Z:28:SER:HA   | 2.13                     | 0.49              |
| 1:1:1505:G:H2'    | 1:1:1507:U:C6    | 2.48                     | 0.48              |
| 2:2:1277:A:OP1    | 22:N:154:ARG:NH1 | 2.46                     | 0.48              |
| 2:2:393:A:H2'     | 2:2:394:U:O4'    | 2.14                     | 0.48              |
| 2:2:483:C:O2'     | 2:2:484:G:O4'    | 2.25                     | 0.48              |
| 2:2:749:G:H2'     | 2:2:750:U:H6     | 1.74                     | 0.48              |
| 5:5:102:U:H2'     | 5:5:103:U:C6     | 2.47                     | 0.48              |
| 5:5:36:U:H2'      | 5:5:37:G:O4'     | 2.12                     | 0.48              |
| 6:6:5:C:N4        | 6:6:6:G:C6       | 2.81                     | 0.48              |
| 9:A:60[B]:ARG:HD2 | 9:A:73:LYS:HD2   | 1.95                     | 0.48              |
| 25:Q:98:ARG:NH2   | 25:Q:132:PHE:O   | 2.46                     | 0.48              |
| 26:R:29:PHE:CZ    | 26:R:43:PHE:HA   | 2.47                     | 0.48              |
| 2:2:1164:U:O2'    | 27:S:90:CYS:O    | 2.30                     | 0.48              |
| 10:B:376:ARG:HD3  | 32:X:37:ARG:HH12 | 1.78                     | 0.48              |
| 34:Z:53:VAL:HG12  | 34:Z:54:LYS:H    | 1.77                     | 0.48              |
| 1:1:1169:A:N3     | 1:1:1461:G:O2'   | 2.46                     | 0.48              |
| 1:1:1472:G:N2     | 1:1:1518:C:O2    | 2.31                     | 0.48              |
| 1:1:1674:U:H3     | 1:1:1728:G:H21   | 1.62                     | 0.48              |
| 1:1:215:U:H3'     | 1:1:217:A:C2     | 2.47                     | 0.48              |
| 1:1:494:A:H2'     | 1:1:495:C:C6     | 2.48                     | 0.48              |
| 1:1:959:OMG:H2'   | 1:1:959:OMG:N3   | 2.28                     | 0.48              |
| 2:2:1446:A:H1'    | 4:4:174:A:O2'    | 2.12                     | 0.48              |
| 3:3:57:U:O2'      | 3:3:58:C:P       | 2.71                     | 0.48              |
| 6:6:10:C:C2'      | 6:6:13:C:H41     | 2.07                     | 0.48              |
| 7:7:12:A:H2'      | 7:7:13:U:C6      | 2.48                     | 0.48              |
| 1:1:956:U:C4'     | 9:A:14:SER:HB2   | 2.44                     | 0.48              |
| 2:2:427:C:H5"     | 9:A:193:ARG:NH1  | 2.28                     | 0.48              |
| 10:B:248:HIS:ND1  | 10:B:249:ARG:HD3 | 2.28                     | 0.48              |
| 15:G:253:ASN:ND2  | 15:G:253:ASN:O   | 2.41                     | 0.48              |
| 17:I:61:PRO:HD2   | 17:I:77:GLY:O    | 2.12                     | 0.48              |
| 1:1:113:C:P       | 21:M:147:ARG:HE  | 2.36                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 21:M:7:LEU:HB3   | 21:M:46:GLU:HG2   | 1.94                     | 0.48              |
| 22:N:60:ILE:HG23 | 22:N:160:PRO:HD2  | 1.94                     | 0.48              |
| 23:O:31:HIS:HD2  | 23:O:34:ARG:HH21  | 1.57                     | 0.48              |
| 26:R:32:PHE:HE2  | 26:R:128:VAL:HG21 | 1.77                     | 0.48              |
| 1:1:1414:A:H8    | 1:1:1414:A:OP2    | 1.96                     | 0.48              |
| 1:1:708:A:O2'    | 1:1:710:G:O2'     | 2.31                     | 0.48              |
| 1:1:848:U:O2     | 17:I:11:VAL:HG11  | 2.12                     | 0.48              |
| 1:1:35:U:O3'     | 1:1:986:U:H4'     | 2.13                     | 0.48              |
| 2:2:100:U:H2'    | 2:2:101:G:C8      | 2.47                     | 0.48              |
| 2:2:572:A2M:O2'  | 2:2:573:U:H5'     | 2.12                     | 0.48              |
| 5:5:125:A:C6     | 5:5:126:G:N1      | 2.82                     | 0.48              |
| 6:6:5:C:H2'      | 6:6:6:G:H5'       | 1.94                     | 0.48              |
| 10:B:288:TYR:OH  | 10:B:332:LYS:HG3  | 2.13                     | 0.48              |
| 13:E:126:PRO:HD3 | 13:E:156:GLU:OE2  | 2.13                     | 0.48              |
| 13:E:24:LYS:HZ3  | 13:E:38:LEU:H     | 1.60                     | 0.48              |
| 19:K:73:ILE:HA   | 19:K:113:ASN:O    | 2.13                     | 0.48              |
| 23:O:105:LEU:O   | 23:O:109:THR:HG23 | 2.13                     | 0.48              |
| 26:R:12:VAL:HG23 | 26:R:28:LYS:HB3   | 1.94                     | 0.48              |
| 1:1:765:C:H2'    | 1:1:766:A:H8      | 1.79                     | 0.48              |
| 8:8:12:C:O2      | 8:8:15:A:H2       | 1.96                     | 0.48              |
| 14:F:38:ILE:HG21 | 14:F:177:TYR:CE2  | 2.49                     | 0.48              |
| 16:H:27:ILE:HD11 | 16:H:139:ILE:HG13 | 1.94                     | 0.48              |
| 22:N:34:PHE:HD1  | 22:N:89:THR:HB    | 1.77                     | 0.48              |
| 1:1:1548:A:N6    | 1:1:1584:A:H4'    | 2.27                     | 0.48              |
| 1:1:22:C:H2'     | 1:1:23:U:H5'      | 1.94                     | 0.48              |
| 1:1:787:A:N7     | 1:1:788:A:H8      | 2.11                     | 0.48              |
| 1:1:892:C:H2'    | 1:1:893:G:C8      | 2.49                     | 0.48              |
| 2:2:1317:G:C6    | 2:2:1387:C:N3     | 2.81                     | 0.48              |
| 2:2:541:A:C8     | 18:J:39:ILE:HD12  | 2.49                     | 0.48              |
| 2:2:776:C:O2'    | 2:2:777:A:O4'     | 2.27                     | 0.48              |
| 2:2:962:C:N4     | 2:2:963:G:O6      | 2.46                     | 0.48              |
| 3:3:182:G:OP2    | 3:3:182:G:H8      | 1.97                     | 0.48              |
| 3:3:201:A:H2'    | 3:3:202:A:C8      | 2.48                     | 0.48              |
| 3:3:97:U:O2'     | 3:3:98:G:H8       | 1.97                     | 0.48              |
| 4:4:43:U:H2'     | 4:4:44:G:C8       | 2.49                     | 0.48              |
| 6:6:8:A:H61      | 6:6:34:C:N4       | 2.12                     | 0.48              |
| 6:6:3:A:H2'      | 6:6:4:U:H5''      | 1.95                     | 0.48              |
| 7:7:164:U:H5''   | 7:7:165:G:OP1     | 2.13                     | 0.48              |
| 9:A:19:HIS:CD2   | 9:A:192:LYS:O     | 2.66                     | 0.48              |
| 13:E:145:PHE:HD2 | 13:E:157:ALA:HB2  | 1.78                     | 0.48              |
| 1:1:1092:U:OP1   | 1:1:1092:U:H4'    | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:114:G:H2'     | 1:1:115:U:O4'     | 2.13                     | 0.48              |
| 2:2:342:U:O2      | 2:2:343:U:N3      | 2.46                     | 0.48              |
| 2:2:966:C:H5''    | 2:2:967:U:OP2     | 2.12                     | 0.48              |
| 3:3:155:U:H2'     | 3:3:156:C:O4'     | 2.13                     | 0.48              |
| 5:5:46:G:H2'      | 5:5:47:G:C8       | 2.49                     | 0.48              |
| 7:7:119:G:C2'     | 7:7:120:G:H5'     | 2.43                     | 0.48              |
| 9:A:108:THR:CG2   | 21:M:146:PRO:HG2  | 86.11                    | 0.48              |
| 9:A:60[B]:ARG:HD2 | 9:A:73:LYS:CD     | 2.44                     | 0.48              |
| 13:E:93:CYS:SG    | 13:E:94:ALA:N     | 2.86                     | 0.48              |
| 2:2:971:A:C5      | 15:G:118:ASN:HB2  | 2.48                     | 0.48              |
| 19:K:180:HIS:HA   | 19:K:183:ARG:CD   | 2.42                     | 0.48              |
| 22:N:98:ARG:HB3   | 22:N:120:GLY:HA3  | 1.95                     | 0.48              |
| 22:N:57:LEU:HA    | 22:N:130:ARG:HA   | 1.96                     | 0.48              |
| 27:S:80:VAL:HG21  | 27:S:85:LEU:HD23  | 1.96                     | 0.48              |
| 2:2:1159:A:H3'    | 2:2:1160:OMC:H6   | 1.78                     | 0.48              |
| 2:2:822:G:C6      | 2:2:823:A:C6      | 3.02                     | 0.48              |
| 3:3:182:G:C4'     | 16:H:36:ARG:HH12  | 126.38                   | 0.48              |
| 1:1:447:G:H1'     | 7:7:15:G:N2       | 2.29                     | 0.48              |
| 1:1:454:U:H3      | 7:7:9:G:H1        | 1.61                     | 0.48              |
| 9:A:173:GLY:O     | 9:A:176:GLU:HG2   | 2.13                     | 0.48              |
| 10:B:25:ILE:HG22  | 10:B:277:TYR:CE1  | 2.46                     | 0.48              |
| 17:I:123:THR:O    | 17:I:126:SER:OG   | 2.23                     | 0.48              |
| 18:J:78:ALA:N     | 18:J:105:VAL:HG22 | 2.29                     | 0.48              |
| 23:O:19:LYS:CB    | 23:O:19:LYS:HZ3   | 2.26                     | 0.48              |
| 26:R:115:ARG:HG3  | 26:R:116:HIS:ND1  | 2.29                     | 0.48              |
| 31:W:40:TYR:CG    | 31:W:116:LEU:HD21 | 2.48                     | 0.48              |
| 1:1:1042:G:N1     | 1:1:1109:U:H5     | 2.12                     | 0.48              |
| 1:1:1150:A:OP1    | 27:S:116:LEU:HD21 | 2.14                     | 0.48              |
| 1:1:766:A:N6      | 1:1:767:U:O2      | 2.47                     | 0.48              |
| 2:2:1029:A:H2'    | 2:2:1030:G:C8     | 2.49                     | 0.48              |
| 3:3:82:G:H2'      | 3:3:83:G:N7       | 2.29                     | 0.48              |
| 9:A:65:HIS:HD2    | 9:A:68:LYS:N      | 2.08                     | 0.48              |
| 9:A:79:PRO:HD2    | 9:A:82:MET:HE2    | 1.96                     | 0.48              |
| 5:5:13:C:C4       | 10:B:340:ARG:O    | 2.67                     | 0.48              |
| 19:K:73:ILE:HG21  | 19:K:109:GLN:NE2  | 2.29                     | 0.48              |
| 1:1:1185:U:H4'    | 22:N:8:CYS:HB3    | 1.95                     | 0.48              |
| 32:X:54:PRO:HA    | 32:X:59:TYR:CD2   | 2.48                     | 0.48              |
| 1:1:1446:A:C8     | 34:Z:24:GLY:HA3   | 2.49                     | 0.48              |
| 1:1:244:C:N4      | 1:1:248:A:H61     | 2.05                     | 0.48              |
| 1:1:287:C:H2'     | 1:1:288:A:O4'     | 2.14                     | 0.48              |
| 1:1:33:A:C8       | 1:1:46:A:N6       | 2.81                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:947:A:N1     | 2:2:393:A:O2'     | 2.39                     | 0.48              |
| 1:1:967:G:O4'    | 9:A:205:ASN:ND2   | 2.47                     | 0.48              |
| 2:2:1012:G:C6    | 15:G:324:SER:HA   | 2.49                     | 0.48              |
| 2:2:512:U:H2'    | 2:2:513:C:H6      | 1.79                     | 0.48              |
| 2:2:967:U:H4'    | 2:2:968:G:C8      | 2.49                     | 0.48              |
| 3:3:78:C:HO2'    | 3:3:79:U:P        | 2.33                     | 0.48              |
| 6:6:26:G:H3'     | 6:6:27:G:H4'      | 1.96                     | 0.48              |
| 6:6:52:G:H8      | 6:6:52:G:OP2      | 1.96                     | 0.48              |
| 1:1:248:A:H2'    | 11:C:221:ASN:OD1  | 2.14                     | 0.48              |
| 11:C:297:ARG:HA  | 11:C:300:LEU:HG   | 1.95                     | 0.48              |
| 16:H:28:ASP:OD1  | 16:H:29:LEU:N     | 2.47                     | 0.48              |
| 21:M:71:ARG:HG2  | 21:M:94:LEU:CB    | 2.33                     | 0.48              |
| 1:1:1050:G:H4'   | 8:8:104:C:O2'     | 2.13                     | 0.48              |
| 1:1:1262:G:C2    | 1:1:1263:A:H2'    | 2.48                     | 0.48              |
| 2:2:1442:C:H42   | 6:6:3:A:H61       | 1.61                     | 0.48              |
| 2:2:528:U:O2     | 2:2:556:U:H4'     | 2.13                     | 0.48              |
| 2:2:667:OMU:C4'  | 2:2:667:OMU:H6    | 2.44                     | 0.48              |
| 2:2:984:G:H2'    | 2:2:985:G:C8      | 2.49                     | 0.48              |
| 3:3:45:C:H2'     | 3:3:46:A:H8       | 1.78                     | 0.48              |
| 6:6:21:A:H1'     | 6:6:22:G:OP1      | 2.14                     | 0.48              |
| 6:6:49:C:H5'     | 14:F:45:ARG:HH12  | 1.79                     | 0.48              |
| 6:6:5:C:C2'      | 6:6:6:G:H5'       | 2.43                     | 0.48              |
| 11:C:257:GLN:HB3 | 11:C:261:ILE:HG23 | 1.96                     | 0.48              |
| 4:4:52:A:H1'     | 13:E:174:PHE:HD2  | 1.79                     | 0.48              |
| 7:7:164:U:O4     | 15:G:133:ARG:HA   | 2.13                     | 0.48              |
| 15:G:193:ARG:NH1 | 15:G:214:PRO:HD3  | 2.28                     | 0.48              |
| 15:G:199:GLU:O   | 15:G:203:LYS:HD3  | 2.14                     | 0.48              |
| 16:H:192:LYS:HA  | 16:H:195:GLU:OE1  | 2.14                     | 0.48              |
| 19:K:81:ARG:CZ   | 19:K:102:ALA:O    | 2.62                     | 0.48              |
| 22:N:49:CYS:SG   | 22:N:172:GLY:HA2  | 2.53                     | 0.48              |
| 24:P:136:ILE:O   | 24:P:136:ILE:HG13 | 2.14                     | 0.48              |
| 27:S:75:ILE:HA   | 27:S:87:LYS:O     | 2.14                     | 0.48              |
| 1:1:1751:G:H5'   | 3:3:150:G:H5"     | 1.96                     | 0.47              |
| 1:1:35:U:C2'     | 1:1:36:OMU:C5'    | 2.86                     | 0.47              |
| 1:1:454:U:O2'    | 1:1:455:G:O5'     | 2.32                     | 0.47              |
| 2:2:1090:A:H2'   | 2:2:1091:G:C8     | 2.48                     | 0.47              |
| 2:2:467:G:HO2'   | 2:2:468:A:H2      | 1.60                     | 0.47              |
| 2:2:540:C:O2'    | 2:2:541:A:O5'     | 2.32                     | 0.47              |
| 2:2:544:U:O2'    | 2:2:545:A:H5'     | 2.14                     | 0.47              |
| 2:2:739:C:H2'    | 2:2:740:A:H5'     | 1.96                     | 0.47              |
| 3:3:195:A:C8     | 3:3:195:A:H5"     | 2.47                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:5:32:G:H2'     | 5:5:33:G:C8       | 2.48                     | 0.47              |
| 6:6:13:C:C4      | 6:6:14:A:N6       | 2.81                     | 0.47              |
| 10:B:310:LYS:NZ  | 10:B:368:THR:OG1  | 2.47                     | 0.47              |
| 13:E:16:VAL:HG21 | 13:E:80:ILE:HG23  | 1.96                     | 0.47              |
| 20:L:50:PRO:HG3  | 24:P:162:SER:O    | 2.14                     | 0.47              |
| 21:M:173:GLY:HA3 | 21:M:184:LEU:HD12 | 1.97                     | 0.47              |
| 21:M:71:ARG:HD3  | 21:M:71:ARG:C     | 2.34                     | 0.47              |
| 1:1:1123:G:O2'   | 1:1:1124:C:H5''   | 2.14                     | 0.47              |
| 2:2:789:G:H2'    | 2:2:790:U:H5'     | 1.96                     | 0.47              |
| 10:B:310:LYS:HE2 | 10:B:368:THR:CG2  | 2.43                     | 0.47              |
| 11:C:207:MET:CB  | 11:C:226:ASP:HB3  | 2.45                     | 0.47              |
| 15:G:146:LYS:HB3 | 21:M:28:TRP:CH2   | 2.42                     | 0.47              |
| 15:G:262:TYR:CZ  | 15:G:307:PHE:HB3  | 2.49                     | 0.47              |
| 19:K:94:VAL:HG23 | 19:K:109:GLN:O    | 2.14                     | 0.47              |
| 28:T:124:ARG:HA  | 28:T:143:PRO:HD2  | 1.97                     | 0.47              |
| 1:1:171:U:H3     | 1:1:287:C:H1'     | 1.79                     | 0.47              |
| 1:1:429:G:H5''   | 28:T:18:LYS:HD3   | 1.96                     | 0.47              |
| 1:1:555:U:H2'    | 1:1:556:U:C6      | 2.49                     | 0.47              |
| 7:7:119:G:H2'    | 7:7:120:G:H5'     | 1.95                     | 0.47              |
| 7:7:75:G:C6      | 7:7:76:C:C4       | 3.02                     | 0.47              |
| 9:A:116:VAL:HG12 | 9:A:164:ALA:HB1   | 1.96                     | 0.47              |
| 9:A:242:ARG:NH2  | 9:A:246:ILE:HA    | 2.29                     | 0.47              |
| 3:3:25:A:H4'     | 9:A:71:ARG:HH11   | 1.77                     | 0.47              |
| 10:B:165:HIS:HB2 | 10:B:181:ALA:HB1  | 1.97                     | 0.47              |
| 11:C:290:ILE:HA  | 11:C:293:SER:HB2  | 1.95                     | 0.47              |
| 22:N:59:GLN:NE2  | 22:N:128:ARG:HG3  | 2.28                     | 0.47              |
| 24:P:101:ARG:NH2 | 24:P:101:ARG:CG   | 2.72                     | 0.47              |
| 26:R:76:TYR:O    | 26:R:96:PHE:N     | 2.47                     | 0.47              |
| 30:V:68:TYR:HE1  | 30:V:88:ILE:HD12  | 1.79                     | 0.47              |
| 1:1:1268:G:H2'   | 1:1:1269:G:C8     | 2.48                     | 0.47              |
| 1:1:245:C:H4'    | 1:1:247:A:N7      | 2.30                     | 0.47              |
| 1:1:489:C:H2'    | 1:1:490:C:O4'     | 2.15                     | 0.47              |
| 1:1:636:U:H2'    | 1:1:637:C:C2      | 2.49                     | 0.47              |
| 1:1:801:G:N2     | 1:1:1027:U:O3'    | 2.48                     | 0.47              |
| 2:2:1158:U:OP2   | 24:P:165:PRO:HD2  | 2.14                     | 0.47              |
| 2:2:1077:G:O2'   | 2:2:1186:A2M:H2   | 2.13                     | 0.47              |
| 2:2:646:G:O2'    | 2:2:647:A:OP1     | 2.23                     | 0.47              |
| 5:5:17:C:N3      | 28:T:69:ARG:NH2   | 2.61                     | 0.47              |
| 6:6:20:A:H4'     | 6:6:21:A:OP1      | 2.13                     | 0.47              |
| 7:7:43:A:O2'     | 7:7:44:A:H8       | 1.97                     | 0.47              |
| 10:B:43:LEU:O    | 10:B:213:VAL:HG13 | 2.14                     | 0.47              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 10:B:319:VAL:O   | 10:B:339:ARG:HD2    | 2.14                     | 0.47              |
| 14:F:189:ALA:O   | 14:F:192:ARG:HB2    | 2.15                     | 0.47              |
| 14:F:87:THR:HG22 | 14:F:89:THR:H       | 1.79                     | 0.47              |
| 16:H:79:ARG:NH2  | 16:H:84:PRO:HG3     | 2.30                     | 0.47              |
| 24:P:182:ARG:HA  | 24:P:188:ARG:CB     | 2.44                     | 0.47              |
| 28:T:93:SER:HA   | 28:T:96:LYS:HG2     | 1.96                     | 0.47              |
| 1:1:169:G:H4'    | 1:1:170:U:H5'       | 1.96                     | 0.47              |
| 1:1:748:A:H2'    | 1:1:749:A:C8        | 2.49                     | 0.47              |
| 1:1:814:C:H2'    | 1:1:815:G:H8        | 1.79                     | 0.47              |
| 2:2:1233:G:H1'   | 2:2:1234:U:C6       | 2.50                     | 0.47              |
| 3:3:129:G:N3     | 3:3:129:G:H2'       | 2.28                     | 0.47              |
| 6:6:20:A:C2      | 6:6:27:G:N7         | 2.82                     | 0.47              |
| 7:7:121:G:O2'    | 7:7:122:A:O5'       | 2.30                     | 0.47              |
| 11:C:191:GLY:H   | 11:C:194:LYS:HZ2    | 1.60                     | 0.47              |
| 18:J:28:ALA:HB3  | 18:J:81:ILE:HD12    | 1.97                     | 0.47              |
| 16:H:219:PHE:CE1 | 19:K:163:SER:HB3    | 2.50                     | 0.47              |
| 19:K:78:ARG:N    | 19:K:78:ARG:HD2     | 2.30                     | 0.47              |
| 20:L:102:GLN:NE2 | 20:L:144:GLN:OE1    | 2.23                     | 0.47              |
| 23:O:147:PRO:HG2 | 23:O:178:ALA:HB2    | 1.97                     | 0.47              |
| 1:1:832:G:OP1    | 24:P:170[B]:LYS:HE3 | 2.14                     | 0.47              |
| 33:Y:113:ARG:O   | 33:Y:117:GLN:HG3    | 2.14                     | 0.47              |
| 16:H:77:ARG:HG2  | 33:Y:16:GLY:O       | 133.90                   | 0.47              |
| 1:1:1726:C:H2'   | 1:1:1727:U:O4'      | 2.14                     | 0.47              |
| 2:2:443:OMC:C5'  | 2:2:488:A:N6        | 2.54                     | 0.47              |
| 1:1:346:U:O2'    | 2:2:468:A:H8        | 1.97                     | 0.47              |
| 8:8:77:G:C8      | 26:R:52:LYS:HG3     | 2.49                     | 0.47              |
| 10:B:167:GLN:HB3 | 10:B:170:LYS:HB2    | 1.96                     | 0.47              |
| 13:E:62:SER:HB3  | 13:E:65:PRO:HD2     | 1.95                     | 0.47              |
| 18:J:104:ILE:N   | 18:J:104:ILE:CD1    | 2.73                     | 0.47              |
| 19:K:73:ILE:N    | 19:K:73:ILE:CD1     | 2.73                     | 0.47              |
| 22:N:48:VAL:HA   | 22:N:178:ARG:NH1    | 2.29                     | 0.47              |
| 27:S:109:GLU:HA  | 27:S:112:PHE:HB3    | 1.95                     | 0.47              |
| 1:1:1061:G:H2'   | 1:1:1062:A:H8       | 1.77                     | 0.47              |
| 1:1:1388:U:H4'   | 1:1:1389:A:O5'      | 2.15                     | 0.47              |
| 1:1:543:G:C3'    | 1:1:543:G:N3        | 2.78                     | 0.47              |
| 1:1:788:A:H3'    | 1:1:788:A:N3        | 2.29                     | 0.47              |
| 1:1:872:U:H2'    | 1:1:873:G:C8        | 2.50                     | 0.47              |
| 2:2:1088:C:O2'   | 2:2:1173:C:O2       | 2.31                     | 0.47              |
| 1:1:1595:G:N1    | 2:2:37:C:N3         | 2.40                     | 0.47              |
| 3:3:195:A:N1     | 9:A:175:ILE:HD12    | 2.29                     | 0.47              |
| 10:B:209:ARG:HG3 | 10:B:211:ASP:OD1    | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:B:386:TRP:HD1  | 10:B:387:PHE:CE1  | 2.33                     | 0.47              |
| 11:C:100:MET:HE1  | 11:C:104:THR:H    | 1.80                     | 0.47              |
| 11:C:151:LEU:HD21 | 11:C:173:ILE:HD13 | 1.96                     | 0.47              |
| 14:F:71:TYR:HD2   | 14:F:178:LEU:HD12 | 1.80                     | 0.47              |
| 16:H:72:TYR:OH    | 16:H:91:HIS:O     | 2.32                     | 0.47              |
| 19:K:94:VAL:HG23  | 19:K:96:VAL:HG23  | 1.97                     | 0.47              |
| 1:1:113:C:OP1     | 21:M:147:ARG:NE   | 2.47                     | 0.47              |
| 22:N:50:ILE:HG13  | 22:N:138:MET:HB2  | 1.96                     | 0.47              |
| 22:N:81:ASN:OD1   | 22:N:82:LYS:N     | 2.47                     | 0.47              |
| 24:P:66:ARG:O     | 24:P:70:VAL:HG22  | 2.15                     | 0.47              |
| 1:1:250:A:H4'     | 1:1:251:A:C2      | 2.50                     | 0.47              |
| 2:2:1336:C:OP2    | 2:2:1338:C:N4     | 2.48                     | 0.47              |
| 2:2:1441:G:O2'    | 2:2:1442:C:H2'    | 2.14                     | 0.47              |
| 2:2:1442:C:H42    | 6:6:3:A:N6        | 2.13                     | 0.47              |
| 2:2:442:C:O2'     | 2:2:516:A:N3      | 2.39                     | 0.47              |
| 8:8:50:G:O2'      | 8:8:51:A:H5'      | 2.14                     | 0.47              |
| 11:C:170:LEU:HD13 | 11:C:179:VAL:HG21 | 1.96                     | 0.47              |
| 11:C:78:ILE:HB    | 11:C:85:THR:O     | 2.15                     | 0.47              |
| 13:E:58:ARG:HD3   | 13:E:58:ARG:H     | 1.78                     | 0.47              |
| 14:F:77:ARG:HH11  | 14:F:77:ARG:CG    | 2.21                     | 0.47              |
| 20:L:62:HIS:CD2   | 20:L:64:LYS:HE3   | 2.50                     | 0.47              |
| 1:1:959:OMG:N2    | 21:M:76:HIS:CG    | 2.75                     | 0.47              |
| 26:R:32:PHE:CE2   | 26:R:105:VAL:HG21 | 2.50                     | 0.47              |
| 28:T:42:ARG:HG3   | 28:T:110:ASN:HD22 | 1.80                     | 0.47              |
| 28:T:31:GLU:OE2   | 28:T:63:TYR:HB2   | 2.14                     | 0.47              |
| 1:1:1145:G:N3     | 1:1:1146:A:H1'    | 2.30                     | 0.47              |
| 1:1:1176:C:H2'    | 1:1:1177:U:O4'    | 2.14                     | 0.47              |
| 1:1:1440:A:HO2'   | 1:1:1442:G:N2     | 2.12                     | 0.47              |
| 1:1:1729:A:C2     | 1:1:1730:A:C5     | 3.01                     | 0.47              |
| 1:1:569:G:P       | 1:1:569:G:H8      | 2.37                     | 0.47              |
| 2:2:992:U:N3      | 2:2:995:U:O4      | 2.48                     | 0.47              |
| 3:3:66:C:H2'      | 3:3:173:U:H3      | 1.78                     | 0.47              |
| 13:E:17:THR:HA    | 13:E:51:ASN:ND2   | 2.30                     | 0.47              |
| 18:J:78:ALA:CA    | 18:J:105:VAL:HG22 | 2.45                     | 0.47              |
| 22:N:46:PHE:HB3   | 22:N:140:THR:O    | 2.15                     | 0.47              |
| 25:Q:19:ARG:O     | 25:Q:20:ALA:HB3   | 2.15                     | 0.47              |
| 33:Y:45:GLY:O     | 33:Y:70:VAL:HA    | 2.15                     | 0.47              |
| 1:1:1111:C:H2'    | 1:1:1112:A:C8     | 2.50                     | 0.47              |
| 1:1:1228:G:OP1    | 8:8:86:U:O2'      | 2.24                     | 0.47              |
| 1:1:334:G:OP2     | 50:1:1937:HOH:O   | 2.20                     | 0.47              |
| 1:1:33:A:O2'      | 1:1:860:G:N3      | 2.48                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:453:G:H21     | 28:T:118:GLN:HE22  | 1.62                     | 0.47              |
| 1:1:453:G:H21     | 28:T:118:GLN:NE2   | 2.12                     | 0.47              |
| 1:1:781:A:N6      | 1:1:794:U:H3       | 2.09                     | 0.47              |
| 2:2:1036:G:H2'    | 2:2:1037:A:H8      | 1.79                     | 0.47              |
| 1:1:344:A:C2      | 2:2:1223:C:H1'     | 2.49                     | 0.47              |
| 2:2:1267:G:N2     | 2:2:1301:U:O2      | 2.26                     | 0.47              |
| 2:2:1387:C:OP1    | 10:B:249:ARG:NH2   | 2.47                     | 0.47              |
| 2:2:1423:C:OP1    | 28:T:66[B]:LYS:HE2 | 2.15                     | 0.47              |
| 3:3:38:A:N6       | 3:3:182:G:H1       | 2.12                     | 0.47              |
| 4:4:140:G:O6      | 4:4:147:U:O2'      | 2.31                     | 0.47              |
| 4:4:62:C:H2'      | 13:E:119:ARG:NH1   | 2.29                     | 0.47              |
| 16:H:25:ILE:HG12  | 19:K:47:LEU:HD21   | 1.97                     | 0.47              |
| 23:O:159:THR:HG22 | 23:O:166:PHE:HZ    | 1.80                     | 0.47              |
| 23:O:106:ALA:HB2  | 23:O:172:ALA:HA    | 1.97                     | 0.47              |
| 33:Y:84:ARG:NH1   | 33:Y:85:TYR:HE1    | 2.13                     | 0.47              |
| 1:1:245:C:O2      | 11:C:221:ASN:ND2   | 2.48                     | 0.47              |
| 1:1:42:U:H2'      | 1:1:43:A:O4'       | 2.15                     | 0.47              |
| 1:1:557:U:H6      | 1:1:557:U:O5'      | 1.98                     | 0.47              |
| 1:1:922:U:H5'     | 2:2:388:A:H3'      | 1.97                     | 0.47              |
| 2:2:125:C:H2'     | 2:2:126:U:C6       | 2.50                     | 0.47              |
| 2:2:1437:A:N6     | 2:2:1440:U:O2'     | 2.39                     | 0.47              |
| 2:2:460:A:H2      | 2:2:676:G:H1'      | 1.80                     | 0.47              |
| 2:2:787:G:H22     | 2:2:807:A:N6       | 2.12                     | 0.47              |
| 4:4:105:A:H5''    | 4:4:106:G:H5''     | 1.96                     | 0.47              |
| 6:6:41:G:N1       | 19:K:176:ARG:HD2   | 2.30                     | 0.47              |
| 8:8:44:A:C5       | 8:8:45:U:C4        | 3.03                     | 0.47              |
| 8:8:48:G:OP1      | 8:8:48:G:H4'       | 2.15                     | 0.47              |
| 2:2:419:G:OP1     | 9:A:18:VAL:HG12    | 2.15                     | 0.47              |
| 7:7:21:U:OP2      | 11:C:195:MET:HG2   | 2.15                     | 0.47              |
| 16:H:96:ASP:O     | 16:H:100:ARG:N     | 2.47                     | 0.47              |
| 17:I:18:ASN:HD22  | 17:I:19:PRO:N      | 2.13                     | 0.47              |
| 24:P:69:VAL:O     | 24:P:73:ARG:HG2    | 2.15                     | 0.47              |
| 25:Q:120:TYR:O    | 25:Q:124:TYR:N     | 2.48                     | 0.47              |
| 2:2:1151:U:H4'    | 27:S:88:ARG:HB2    | 1.96                     | 0.47              |
| 1:1:1669:G:H21    | 30:V:38:PRO:CD     | 2.27                     | 0.47              |
| 1:1:1472:G:H5''   | 11:C:191:GLY:O     | 2.14                     | 0.46              |
| 1:1:500:C:H2'     | 1:1:501:C:H5'      | 1.96                     | 0.46              |
| 2:2:1109:U:H2'    | 2:2:1110:C:C6      | 2.50                     | 0.46              |
| 2:2:755:U:O2'     | 2:2:756:C:H6       | 1.97                     | 0.46              |
| 2:2:865:G:H2'     | 2:2:866:U:O4'      | 2.15                     | 0.46              |
| 3:3:8:A:H5''      | 33:Y:15:ALA:O      | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:4:52:A:H1'      | 13:E:174:PHE:CD2  | 2.50                     | 0.46              |
| 8:8:103:A:H2'     | 8:8:104:C:C6      | 2.50                     | 0.46              |
| 8:8:26:A:C2'      | 8:8:27:A:H5'      | 2.44                     | 0.46              |
| 9:A:101:VAL:O     | 9:A:101:VAL:HG12  | 2.16                     | 0.46              |
| 10:B:159:VAL:HG13 | 10:B:187:GLN:HE22 | 1.78                     | 0.46              |
| 14:F:162:ILE:HD12 | 14:F:162:ILE:H    | 1.80                     | 0.46              |
| 19:K:180:HIS:CE1  | 19:K:184:LYS:HE2  | 2.46                     | 0.46              |
| 21:M:96:LYS:HE3   | 21:M:101:VAL:HG22 | 1.96                     | 0.46              |
| 1:1:519:G:H21     | 1:1:531:C:H41     | 1.63                     | 0.46              |
| 1:1:660:U:H2'     | 1:1:661:G:C8      | 2.50                     | 0.46              |
| 1:1:906:U:H2'     | 1:1:907:G:O4'     | 2.15                     | 0.46              |
| 2:2:431:C:C5'     | 9:A:219:ILE:HD11  | 2.45                     | 0.46              |
| 4:4:181:C:H2'     | 4:4:182:A:C8      | 2.50                     | 0.46              |
| 5:5:18:G:H3'      | 5:5:19:A:H8       | 1.80                     | 0.46              |
| 11:C:151:LEU:HD21 | 11:C:173:ILE:HG21 | 1.97                     | 0.46              |
| 13:E:125:VAL:HA   | 13:E:156:GLU:OE1  | 2.15                     | 0.46              |
| 15:G:316:ARG:HG3  | 15:G:316:ARG:O    | 2.16                     | 0.46              |
| 15:G:155:LYS:HE3  | 15:G:318:TRP:HB3  | 1.97                     | 0.46              |
| 23:O:60:ILE:CD1   | 23:O:101:THR:HG21 | 2.43                     | 0.46              |
| 23:O:69:ILE:H     | 23:O:69:ILE:HD12  | 1.80                     | 0.46              |
| 28:T:72:GLN:OE1   | 28:T:83:TRP:NE1   | 2.44                     | 0.46              |
| 1:1:157:U:H2'     | 1:1:158:A:C4'     | 2.46                     | 0.46              |
| 1:1:1732:A:H2'    | 1:1:1733:G:O4'    | 2.15                     | 0.46              |
| 1:1:243:G:N2      | 1:1:259:G:H22     | 2.13                     | 0.46              |
| 1:1:392:A:N1      | 1:1:405:A:H5''    | 2.29                     | 0.46              |
| 1:1:815:G:H1      | 1:1:825:G:H1      | 1.62                     | 0.46              |
| 2:2:619:A:N6      | 2:2:1306:C:H1'    | 2.28                     | 0.46              |
| 2:2:1345:C:H5''   | 2:2:1346:G:OP2    | 2.15                     | 0.46              |
| 2:2:428:A:C2'     | 2:2:429:A:H5'     | 2.44                     | 0.46              |
| 9:A:108:THR:HG23  | 21:M:146:PRO:HG2  | 86.07                    | 0.46              |
| 4:4:114:A:O3'     | 10:B:372:ILE:O    | 2.34                     | 0.46              |
| 15:G:231:LYS:HG2  | 15:G:258:ASN:HB3  | 1.98                     | 0.46              |
| 15:G:218:VAL:N    | 15:G:284:ALA:O    | 2.49                     | 0.46              |
| 13:E:41:LEU:HD13  | 16:H:150:SER:HB3  | 1.97                     | 0.46              |
| 32:X:13:VAL:HG22  | 32:X:36:SER:OG    | 2.15                     | 0.46              |
| 1:1:162:U:H2'     | 1:1:163:U:O4'     | 2.15                     | 0.46              |
| 1:1:312:C:C2'     | 1:1:313:U:H5'     | 2.45                     | 0.46              |
| 1:1:66:A:N6       | 1:1:352:G:O2'     | 2.48                     | 0.46              |
| 2:2:479:C:O2'     | 2:2:674:U:O3'     | 2.33                     | 0.46              |
| 2:2:534:OMG:H2'   | 2:2:534:OMG:N3    | 2.30                     | 0.46              |
| 2:2:591:A2M:H5''  | 2:2:591:A2M:H8    | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:956:C:O2'     | 2:2:957:C:O4'     | 2.30                     | 0.46              |
| 4:4:94:G:N2       | 4:4:103:C:O2      | 2.46                     | 0.46              |
| 4:4:43:U:H3       | 4:4:67:A:N6       | 2.05                     | 0.46              |
| 7:7:108:A:H2'     | 7:7:109:A:O4'     | 2.16                     | 0.46              |
| 10:B:367:ASP:HA   | 10:B:378:GLN:HE22 | 1.80                     | 0.46              |
| 1:1:692:A:H5''    | 11:C:101:PHE:CG   | 2.50                     | 0.46              |
| 11:C:211:PRO:HG3  | 11:C:253:SER:HB2  | 1.97                     | 0.46              |
| 11:C:24:PRO:HB2   | 11:C:26:VAL:HG12  | 1.97                     | 0.46              |
| 16:H:121:VAL:HG11 | 16:H:123:TYR:CZ   | 2.51                     | 0.46              |
| 17:I:79:GLY:HA2   | 17:I:101:ARG:C    | 2.36                     | 0.46              |
| 17:I:33:GLN:HE21  | 21:M:202:ARG:NE   | 2.13                     | 0.46              |
| 19:K:108:VAL:HG23 | 26:R:71:LEU:HD21  | 1.96                     | 0.46              |
| 1:1:1118:A:H2'    | 1:1:1119:C:O4'    | 2.16                     | 0.46              |
| 1:1:1390:G:H5''   | 1:1:1391:U:H3'    | 1.97                     | 0.46              |
| 1:1:13:G:H5''     | 30:V:43:LYS:O     | 2.15                     | 0.46              |
| 1:1:223:A:H2      | 1:1:224:C:C2      | 2.32                     | 0.46              |
| 1:1:52:C:H2'      | 1:1:53:G:O4'      | 2.16                     | 0.46              |
| 1:1:834:U:H5''    | 1:1:835:G:H5''    | 1.97                     | 0.46              |
| 2:2:1070:A:H2'    | 2:2:1071:A:C8     | 2.51                     | 0.46              |
| 2:2:1080:U:O2     | 2:2:1080:U:H2'    | 2.15                     | 0.46              |
| 2:2:495:G:H22     | 2:2:514:U:H1'     | 1.79                     | 0.46              |
| 2:2:526:A:O2'     | 2:2:527:A2M:P     | 2.74                     | 0.46              |
| 3:3:56:U:H3'      | 3:3:57:U:H6       | 1.80                     | 0.46              |
| 3:3:95:C:H42      | 3:3:139:G:H1      | 1.62                     | 0.46              |
| 8:8:61:C:H2'      | 8:8:62:U:C6       | 2.50                     | 0.46              |
| 9:A:150:LEU:HD11  | 9:A:156:LYS:HD2   | 1.97                     | 0.46              |
| 10:B:352:GLN:HA   | 10:B:357:LEU:HD23 | 1.95                     | 0.46              |
| 1:1:734:U:OP2     | 11:C:120:ARG:NH2  | 2.47                     | 0.46              |
| 14:F:54:LEU:HD11  | 14:F:66:SER:HB3   | 1.97                     | 0.46              |
| 19:K:74:LEU:CD2   | 19:K:74:LEU:H     | 2.21                     | 0.46              |
| 24:P:128:LEU:HD12 | 24:P:132:GLN:HG2  | 1.98                     | 0.46              |
| 26:R:6:LEU:HG     | 26:R:32:PHE:HB3   | 1.96                     | 0.46              |
| 2:2:635:A:H5''    | 28:T:66[B]:LYS:HA | 1.98                     | 0.46              |
| 1:1:1253:U:H5'    | 16:H:74:GLN:NE2   | 2.23                     | 0.46              |
| 1:1:1549:U:O2'    | 1:1:1550:C:O5'    | 2.33                     | 0.46              |
| 1:1:1556:G:N3     | 1:1:1618:U:H5     | 2.14                     | 0.46              |
| 1:1:181:G:H2'     | 1:1:182:U:O4'     | 2.15                     | 0.46              |
| 1:1:836:G:O6      | 24:P:97:VAL:HG22  | 2.15                     | 0.46              |
| 2:2:540:C:O2'     | 2:2:542:A:OP2     | 2.30                     | 0.46              |
| 1:1:685:A:H5''    | 2:2:607:A:C5'     | 2.45                     | 0.46              |
| 2:2:705:A:H2'     | 2:2:706:U:H5''    | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:4:94:G:H2'      | 4:4:95:U:O4'      | 2.15                     | 0.46              |
| 2:2:68:A:H2'      | 5:5:113:A:N6      | 2.30                     | 0.46              |
| 7:7:155:U:H2'     | 7:7:156:A:C8      | 2.50                     | 0.46              |
| 9:A:127:ALA:HB2   | 9:A:134:CYS:SG    | 2.56                     | 0.46              |
| 10:B:310:LYS:HE3  | 10:B:368:THR:HG1  | 1.79                     | 0.46              |
| 11:C:194:LYS:HA   | 11:C:199:ARG:HA   | 1.97                     | 0.46              |
| 15:G:124:ASP:OD1  | 15:G:125:VAL:N    | 2.47                     | 0.46              |
| 17:I:90:LEU:HD21  | 17:I:125:MET:SD   | 2.55                     | 0.46              |
| 19:K:150:THR:H    | 19:K:153:ARG:CZ   | 2.28                     | 0.46              |
| 1:1:133:C:H1'     | 1:1:172:G:H1'     | 1.97                     | 0.46              |
| 1:1:180:A:H2'     | 1:1:181:G:H8      | 1.80                     | 0.46              |
| 2:2:1044:C:N3     | 2:2:1052:G:N1     | 2.46                     | 0.46              |
| 2:2:1254:OMG:CM2  | 2:2:1254:OMG:H4'  | 2.45                     | 0.46              |
| 2:2:1433:U:H2'    | 2:2:1434:G:H8     | 1.80                     | 0.46              |
| 1:1:463:C:H2'     | 2:2:630:G:N2      | 2.31                     | 0.46              |
| 5:5:125:A:C5'     | 5:5:125:A:H8      | 2.26                     | 0.46              |
| 6:6:13:C:O2'      | 6:6:14:A:C5'      | 2.63                     | 0.46              |
| 11:C:206:PRO:O    | 11:C:225:LEU:HA   | 2.16                     | 0.46              |
| 2:2:1005:G:C2'    | 15:G:119:PHE:CD2  | 2.98                     | 0.46              |
| 17:I:65:CYS:O     | 17:I:71:ASN:HA    | 2.16                     | 0.46              |
| 22:N:95:HIS:O     | 22:N:125:VAL:HG13 | 2.15                     | 0.46              |
| 23:O:56:THR:HG23  | 23:O:59:ASP:H     | 1.80                     | 0.46              |
| 27:S:75:ILE:HG22  | 27:S:88:ARG:CD    | 2.46                     | 0.46              |
| 10:B:386:TRP:CZ2  | 32:X:57:ARG:HD3   | 2.51                     | 0.46              |
| 1:1:1004:G:H1'    | 1:1:1172:G:H5'    | 1.97                     | 0.46              |
| 1:1:1228:G:H2'    | 1:1:1229:G:O4'    | 2.16                     | 0.46              |
| 1:1:159:U:H2'     | 1:1:160:C:O4'     | 2.15                     | 0.46              |
| 1:1:208:C:H1'     | 1:1:226:C:H42     | 1.81                     | 0.46              |
| 1:1:296:U:O2'     | 1:1:297:A:O4'     | 2.25                     | 0.46              |
| 1:1:849:U:O2'     | 1:1:850:G:O4'     | 2.33                     | 0.46              |
| 1:1:901:C:O2'     | 1:1:902:C:O5'     | 2.34                     | 0.46              |
| 2:2:424:U:OP1     | 9:A:128:ARG:N     | 2.35                     | 0.46              |
| 6:6:16:C:C6       | 6:6:16:C:C3'      | 2.97                     | 0.46              |
| 11:C:157:ILE:HA   | 11:C:160:TYR:CD2  | 2.51                     | 0.46              |
| 11:C:197:ASN:HD21 | 31:W:8:SER:HB2    | 1.79                     | 0.46              |
| 8:8:57:A:O2'      | 12:D:151:GLY:HA3  | 2.16                     | 0.46              |
| 14:F:39:ALA:HB1   | 14:F:84:VAL:HG21  | 1.97                     | 0.46              |
| 14:F:46:PHE:HB3   | 14:F:49:ARG:HG3   | 1.98                     | 0.46              |
| 1:1:492:G:H4'     | 14:F:80:ASP:OD2   | 2.15                     | 0.46              |
| 15:G:163:PHE:HE2  | 15:G:249:LEU:HD12 | 1.80                     | 0.46              |
| 19:K:180:HIS:CA   | 19:K:183:ARG:NH1  | 2.79                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:L:60:HIS:CE1   | 20:L:63:ARG:HA    | 2.50                     | 0.46              |
| 23:O:149:LYS:HA   | 23:O:178:ALA:HB3  | 1.96                     | 0.46              |
| 23:O:184:ASN:HA   | 23:O:189:TYR:CE1  | 2.50                     | 0.46              |
| 1:1:1375:G:O2'    | 1:1:1380:A:N1     | 2.38                     | 0.46              |
| 1:1:1443:U:H2'    | 1:1:1444:G:O4'    | 2.15                     | 0.46              |
| 1:1:1445:U:O2     | 34:Z:26:ARG:NH2   | 2.49                     | 0.46              |
| 1:1:177:A:N1      | 1:1:280:A:H2      | 2.14                     | 0.46              |
| 2:2:1097:U:H2'    | 2:2:1098:G:C8     | 2.51                     | 0.46              |
| 2:2:1165:C:H2'    | 2:2:1166:G:O4'    | 2.15                     | 0.46              |
| 5:5:36:U:O2'      | 10:B:372:ILE:HG21 | 2.15                     | 0.46              |
| 6:6:19:C:O2       | 6:6:19:C:H2'      | 2.15                     | 0.46              |
| 7:7:62:A:H5''     | 7:7:63:G:O4'      | 2.16                     | 0.46              |
| 8:8:106:C:H2'     | 8:8:107:U:C6      | 2.51                     | 0.46              |
| 9:A:43:GLY:N      | 9:A:88:VAL:O      | 2.48                     | 0.46              |
| 15:G:157:PRO:HA   | 15:G:318:TRP:CZ3  | 2.51                     | 0.46              |
| 20:L:109:LEU:HD12 | 20:L:126:VAL:HG23 | 1.98                     | 0.46              |
| 22:N:9:TYR:CE2    | 22:N:97:LEU:HD11  | 2.51                     | 0.46              |
| 26:R:32:PHE:CE2   | 26:R:128:VAL:HG21 | 2.50                     | 0.46              |
| 27:S:18:LYS:HG3   | 27:S:19:PHE:H     | 1.80                     | 0.46              |
| 34:Z:21:LYS:NZ    | 34:Z:24:GLY:HA2   | 2.31                     | 0.46              |
| 1:1:1388:U:H1'    | 1:1:1389:A:OP2    | 2.15                     | 0.46              |
| 1:1:1494:C:O2'    | 1:1:1495:G:OP2    | 2.26                     | 0.46              |
| 1:1:1529:OMC:H5'  | 1:1:1529:OMC:C6   | 2.51                     | 0.46              |
| 1:1:1673:G:N3     | 1:1:1673:G:H2'    | 2.31                     | 0.46              |
| 1:1:1755:U:OP2    | 25:Q:38:ARG:HG2   | 2.16                     | 0.46              |
| 1:1:191:U:H4'     | 1:1:192:C:O5'     | 2.16                     | 0.46              |
| 1:1:907:G:OP1     | 25:Q:92:LYS:HG2   | 2.16                     | 0.46              |
| 1:1:960:A:H2'     | 1:1:961:G:H8      | 1.81                     | 0.46              |
| 2:2:1196:U:H2'    | 2:2:1197:G:C8     | 2.51                     | 0.46              |
| 2:2:1340:G:H3'    | 2:2:1341:A:C8     | 2.51                     | 0.46              |
| 2:2:591:A2M:C2'   | 2:2:592:C:H5'     | 2.46                     | 0.46              |
| 2:2:782:G:H4'     | 2:2:783:U:OP1     | 2.16                     | 0.46              |
| 3:3:102:C:H2'     | 3:3:103:U:C6      | 2.51                     | 0.46              |
| 3:3:113:U:OP2     | 25:Q:121:ARG:NE   | 2.38                     | 0.46              |
| 6:6:55:U:OP1      | 14:F:47:ARG:NH2   | 2.49                     | 0.46              |
| 7:7:163:G:O2'     | 7:7:165:G:OP2     | 2.22                     | 0.46              |
| 8:8:39:G:H21      | 8:8:46:U:H3       | 1.64                     | 0.46              |
| 14:F:24:PRO:HG3   | 14:F:59:HIS:NE2   | 2.31                     | 0.46              |
| 14:F:49:ARG:NH1   | 14:F:179:ARG:O    | 2.49                     | 0.46              |
| 25:Q:4:LEU:HD23   | 25:Q:24:LEU:HD23  | 1.98                     | 0.46              |
| 31:W:77:ILE:HG23  | 31:W:98:PRO:HG3   | 1.96                     | 0.46              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 33:Y:70:VAL:HG11  | 33:Y:112:VAL:HG23   | 1.98                     | 0.46              |
| 1:1:1241:A:O2'    | 19:K:75:ARG:NH1     | 2.49                     | 0.45              |
| 1:1:1448:C:H2'    | 1:1:1449:C:C6       | 2.51                     | 0.45              |
| 1:1:1630:U:H1'    | 30:V:114:ASN:HB3    | 1.98                     | 0.45              |
| 1:1:32:A:OP1      | 1:1:32:A:H4'        | 2.14                     | 0.45              |
| 1:1:816:G:H22     | 1:1:823:G:H21       | 1.64                     | 0.45              |
| 1:1:925:U:OP1     | 10:B:246:LYS:HG3    | 2.16                     | 0.45              |
| 2:2:768:G:O2'     | 2:2:769:A:O5'       | 2.20                     | 0.45              |
| 6:6:17:U:H1'      | 6:6:18:A:N3         | 2.31                     | 0.45              |
| 6:6:3:A:N3        | 6:6:4:U:H5''        | 2.31                     | 0.45              |
| 7:7:106:G:H4'     | 7:7:149:A:H5'       | 1.98                     | 0.45              |
| 7:7:37:U:H5       | 7:7:105:C:N3        | 2.14                     | 0.45              |
| 13:E:135:ASP:N    | 13:E:136:PRO:CD     | 2.78                     | 0.45              |
| 6:6:15:C:C5       | 16:H:187:HIS:CE1    | 3.05                     | 0.45              |
| 6:6:41:G:C3'      | 19:K:180:HIS:CE1    | 2.82                     | 0.45              |
| 16:H:140:PRO:CD   | 19:K:46:PRO:HB3     | 2.45                     | 0.45              |
| 20:L:70:LYS:HE2   | 20:L:125:TYR:CE2    | 2.51                     | 0.45              |
| 21:M:30:PHE:HB3   | 21:M:129:TRP:CE2    | 2.51                     | 0.45              |
| 23:O:109:THR:O    | 23:O:113:LEU:N      | 2.46                     | 0.45              |
| 23:O:17:GLN:HE22  | 27:S:21:LYS:HA      | 1.80                     | 0.45              |
| 1:1:934:A:O4'     | 28:T:133[A]:HIS:HA  | 2.16                     | 0.45              |
| 1:1:23:U:H4'      | 1:1:24:A:N7         | 2.31                     | 0.45              |
| 1:1:245:C:H2'     | 11:C:163:THR:HG21   | 1.98                     | 0.45              |
| 1:1:816:G:H1'     | 1:1:825:G:H22       | 1.81                     | 0.45              |
| 2:2:1147:A:OP2    | 2:2:1168:G:N2       | 2.49                     | 0.45              |
| 2:2:607:A:H61     | 2:2:623:A:H61       | 1.63                     | 0.45              |
| 2:2:867:G:N2      | 2:2:943:U:O2        | 2.49                     | 0.45              |
| 3:3:209:G:C3'     | 3:3:210:G:H5'       | 2.46                     | 0.45              |
| 3:3:95:C:H5''     | 3:3:96:U:OP2        | 2.15                     | 0.45              |
| 6:6:7:A:N1        | 6:6:60:A:C6         | 2.85                     | 0.45              |
| 8:8:112:G:C5      | 8:8:113:C:C4        | 3.04                     | 0.45              |
| 8:8:32:A:C6       | 8:8:50:G:C6         | 3.04                     | 0.45              |
| 10:B:102:ILE:HG13 | 10:B:153:PHE:CE1    | 2.50                     | 0.45              |
| 11:C:136:VAL:HG11 | 11:C:247:PHE:HB2    | 1.98                     | 0.45              |
| 11:C:121:PHE:CE1  | 11:C:278[A]:PRO:HG3 | 2.50                     | 0.45              |
| 13:E:89:PHE:CE2   | 13:E:153:VAL:HG23   | 2.51                     | 0.45              |
| 23:O:38:LEU:CD2   | 27:S:70:ARG:HE      | 2.20                     | 0.45              |
| 1:1:1126:U:O2     | 1:1:1127:U:O2'      | 2.26                     | 0.45              |
| 1:1:1535:U:H2'    | 1:1:1536:G:C8       | 2.52                     | 0.45              |
| 1:1:1604:C:H2'    | 1:1:1605:G:C8       | 2.51                     | 0.45              |
| 1:1:1653:U:N3     | 1:1:1656:A:OP2      | 2.45                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:912:C:OP1     | 2:2:379:U:O2'     | 2.20                     | 0.45              |
| 1:1:869:C:C2      | 1:1:971:C:H5'     | 2.51                     | 0.45              |
| 2:2:1276:A:H2     | 2:2:1291:C:H41    | 1.64                     | 0.45              |
| 2:2:578:U:H2'     | 2:2:579:C:O4'     | 2.16                     | 0.45              |
| 2:2:776:C:H1'     | 2:2:777:A:C5      | 2.52                     | 0.45              |
| 5:5:42:G:N7       | 5:5:104:G:N1      | 2.64                     | 0.45              |
| 10:B:28:ARG:H     | 10:B:279:HIS:HE1  | 1.64                     | 0.45              |
| 4:4:74:G:N2       | 10:B:334:SER:OG   | 2.40                     | 0.45              |
| 11:C:153:VAL:O    | 11:C:252:LYS:N    | 2.45                     | 0.45              |
| 12:D:24:CYS:HA    | 12:D:68:ALA:HA    | 1.98                     | 0.45              |
| 16:H:126:ILE:H    | 16:H:176:GLU:CD   | 2.19                     | 0.45              |
| 2:2:1370:C:OP1    | 18:J:61:MET:HE1   | 2.16                     | 0.45              |
| 1:1:1115:C:H1'    | 1:1:1147:A:N6     | 2.32                     | 0.45              |
| 1:1:1391:U:H4'    | 1:1:1392:G:H5'    | 1.98                     | 0.45              |
| 1:1:657:G:O2'     | 1:1:1493:G:OP2    | 2.27                     | 0.45              |
| 1:1:37:A:H2'      | 1:1:40:C:N4       | 2.31                     | 0.45              |
| 1:1:53:G:H2'      | 1:1:54:G:H5'      | 1.99                     | 0.45              |
| 1:1:551:A:H2'     | 1:1:552:G:C8      | 2.51                     | 0.45              |
| 1:1:647:G:C2'     | 1:1:648:A:H5'     | 2.46                     | 0.45              |
| 2:2:1114:C:H2'    | 2:2:1115:G:O4'    | 2.17                     | 0.45              |
| 2:2:1337:G:H5''   | 2:2:1339:A:OP2    | 2.16                     | 0.45              |
| 2:2:583:OMC:O2    | 2:2:583:OMC:HM23  | 2.16                     | 0.45              |
| 3:3:141:U:O2'     | 3:3:142:U:OP1     | 2.31                     | 0.45              |
| 1:1:876:U:H5''    | 3:3:199:A:C6      | 2.50                     | 0.45              |
| 6:6:28:A:N3       | 6:6:29:G:C4       | 2.82                     | 0.45              |
| 8:8:27:A:H2'      | 8:8:28:C:H6       | 1.78                     | 0.45              |
| 10:B:251:LEU:H    | 10:B:251:LEU:HD23 | 1.81                     | 0.45              |
| 16:H:25:ILE:HD11  | 16:H:137:VAL:HG21 | 1.98                     | 0.45              |
| 6:6:15:C:H1'      | 16:H:184:SER:HB2  | 1.99                     | 0.45              |
| 18:J:125:ALA:HB1  | 18:J:132:SER:HB3  | 1.98                     | 0.45              |
| 16:H:221:TYR:CD2  | 19:K:175:ARG:HD2  | 2.52                     | 0.45              |
| 21:M:174:LEU:HD22 | 21:M:185:ARG:NH1  | 2.32                     | 0.45              |
| 26:R:81:ALA:HA    | 26:R:91:ARG:HA    | 1.97                     | 0.45              |
| 26:R:77:LEU:HA    | 26:R:95:GLU:HA    | 1.98                     | 0.45              |
| 1:1:1266:A:H4'    | 22:N:162:ARG:HH21 | 1.82                     | 0.45              |
| 1:1:1467:G:O2'    | 1:1:1468:C:OP2    | 2.28                     | 0.45              |
| 1:1:171:U:C3'     | 1:1:172:G:H8      | 2.29                     | 0.45              |
| 1:1:307:U:H2'     | 1:1:308:A:H8      | 1.80                     | 0.45              |
| 1:1:50:A:H2'      | 1:1:51:G:H5'      | 1.97                     | 0.45              |
| 1:1:490:C:N4      | 1:1:645:G:H1      | 2.13                     | 0.45              |
| 2:2:1279:C:H42    | 2:2:1288:C:N4     | 2.14                     | 0.45              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 2:2:1340:G:OP2    | 2:2:1341:A:N6       | 2.48                     | 0.45              |
| 2:2:763:C:H2'     | 2:2:764:G:C8        | 2.52                     | 0.45              |
| 2:2:768:G:O6      | 2:2:770:A:N6        | 2.47                     | 0.45              |
| 3:3:141:U:H2'     | 3:3:142:U:C6        | 2.51                     | 0.45              |
| 8:8:11:C:H5'      | 8:8:12:C:OP2        | 2.14                     | 0.45              |
| 9:A:148:LEU:H     | 9:A:148:LEU:HD23    | 1.81                     | 0.45              |
| 9:A:219:ILE:HD12  | 9:A:219:ILE:H       | 1.82                     | 0.45              |
| 10:B:282:GLN:HB3  | 10:B:285:LYS:CE     | 2.46                     | 0.45              |
| 10:B:81:ALA:HB3   | 10:B:327:ASP:O      | 2.16                     | 0.45              |
| 13:E:33:THR:O     | 13:E:148:ASN:ND2    | 2.50                     | 0.45              |
| 22:N:129:VAL:HG13 | 22:N:133:GLN:HB3    | 1.98                     | 0.45              |
| 22:N:57:LEU:HD23  | 22:N:57:LEU:O       | 2.16                     | 0.45              |
| 22:N:73:ASN:O     | 22:N:76:MET:HG2     | 2.16                     | 0.45              |
| 1:1:779:A:OP2     | 24:P:141:LYS:CE     | 2.65                     | 0.45              |
| 1:1:893:G:P       | 25:Q:126:ARG:NH1    | 2.89                     | 0.45              |
| 28:T:61:LYS:HG2   | 28:T:78:GLN:NE2     | 2.32                     | 0.45              |
| 1:1:150:G:P       | 21:M:147:ARG:HH22   | 2.40                     | 0.45              |
| 1:1:161:A:H2'     | 1:1:162:U:C6        | 2.52                     | 0.45              |
| 1:1:171:U:H3'     | 1:1:172:G:C8        | 2.44                     | 0.45              |
| 1:1:205:A:H3'     | 1:1:205:A:N3        | 2.32                     | 0.45              |
| 1:1:422:U:O2'     | 1:1:423:U:H6        | 1.99                     | 0.45              |
| 1:1:472:U:H2'     | 1:1:473:A:C8        | 2.51                     | 0.45              |
| 1:1:766:A:H5''    | 1:1:767:U:H5        | 1.82                     | 0.45              |
| 2:2:1333:C:H2'    | 2:2:1334:G:H8       | 1.82                     | 0.45              |
| 2:2:361:U:O2      | 4:4:110:C:O2'       | 2.24                     | 0.45              |
| 2:2:414:G:OP2     | 2:2:414:G:H8        | 1.99                     | 0.45              |
| 2:2:778:A:H2'     | 2:2:779:U:H5''      | 1.99                     | 0.45              |
| 6:6:48:C:H3'      | 6:6:49:C:C6         | 2.50                     | 0.45              |
| 7:7:141:C:C2'     | 7:7:142:C:H5'       | 2.46                     | 0.45              |
| 4:4:166:C:H5''    | 10:B:279:HIS:O      | 2.16                     | 0.45              |
| 11:C:121:PHE:CD1  | 11:C:278[B]:PRO:HG2 | 2.51                     | 0.45              |
| 13:E:114:PHE:O    | 13:E:115:LEU:HG     | 2.16                     | 0.45              |
| 13:E:132:SER:OG   | 13:E:133:GLN:N      | 2.49                     | 0.45              |
| 14:F:77:ARG:NH1   | 14:F:77:ARG:CG      | 2.78                     | 0.45              |
| 15:G:146:LYS:HA   | 15:G:149:VAL:HG12   | 1.97                     | 0.45              |
| 16:H:41:VAL:HG11  | 16:H:120:LEU:HD21   | 1.99                     | 0.45              |
| 16:H:31:ASP:HA    | 16:H:60:ASN:ND2     | 2.31                     | 0.45              |
| 17:I:108:ASN:HB3  | 17:I:114:MET:HE2    | 1.99                     | 0.45              |
| 1:1:75:A:OP2      | 17:I:78:ARG:NH2     | 2.48                     | 0.45              |
| 18:J:138:ILE:O    | 18:J:138:ILE:HG23   | 2.15                     | 0.45              |
| 25:Q:126:ARG:HD3  | 25:Q:126:ARG:HA     | 1.62                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:S:9:SER:O      | 27:S:55:LYS:HD3   | 2.16                     | 0.45              |
| 1:1:1158:U:C5     | 1:1:1159:A:H1'    | 2.52                     | 0.45              |
| 1:1:1198:C:O2'    | 1:1:1210:A:N3     | 2.44                     | 0.45              |
| 1:1:1727:U:C5     | 1:1:1728:G:C6     | 3.05                     | 0.45              |
| 1:1:477:C:H4'     | 1:1:478:C:OP1     | 2.16                     | 0.45              |
| 1:1:758:C:N4      | 1:1:759:A:N1      | 2.63                     | 0.45              |
| 4:4:140:G:H2'     | 4:4:141:A:H8      | 1.78                     | 0.45              |
| 6:6:49:C:C6       | 6:6:49:C:OP2      | 2.70                     | 0.45              |
| 9:A:189:PHE:HA    | 9:A:192:LYS:HB2   | 1.99                     | 0.45              |
| 9:A:54:ARG:HD2    | 9:A:58:LEU:HD11   | 1.98                     | 0.45              |
| 10:B:376:ARG:HD2  | 32:X:11:PHE:CD1   | 2.52                     | 0.45              |
| 11:C:113:LYS:CG   | 21:M:203:LYS:HB3  | 2.47                     | 0.45              |
| 13:E:146:ASP:OD1  | 13:E:147:GLY:N    | 2.45                     | 0.45              |
| 13:E:17:THR:HG21  | 13:E:50:LYS:HE3   | 1.99                     | 0.45              |
| 13:E:34:LEU:HD11  | 13:E:79:MET:HA    | 1.98                     | 0.45              |
| 6:6:41:G:N2       | 19:K:176:ARG:HH11 | 2.14                     | 0.45              |
| 13:E:59:TRP:HB3   | 19:K:61:LYS:CA    | 2.35                     | 0.45              |
| 22:N:36:ILE:HG21  | 22:N:73:ASN:OD1   | 2.17                     | 0.45              |
| 25:Q:133:ARG:H    | 25:Q:137:ASN:ND2  | 2.15                     | 0.45              |
| 28:T:116:HIS:HB3  | 28:T:149:PHE:CE2  | 2.51                     | 0.45              |
| 34:Z:53:VAL:HG12  | 34:Z:54:LYS:N     | 2.32                     | 0.45              |
| 1:1:25:C:O2'      | 1:1:365:A:N3      | 2.47                     | 0.45              |
| 1:1:558:U:O2'     | 1:1:559:G:H8      | 2.00                     | 0.45              |
| 1:1:756:U:H2'     | 1:1:757:G:C8      | 2.52                     | 0.45              |
| 1:1:740:C:O2'     | 1:1:839:U:H5''    | 2.17                     | 0.45              |
| 2:2:1295:G:OP2    | 22:N:7:ARG:NH1    | 2.50                     | 0.45              |
| 2:2:71:OMG:O2'    | 2:2:72:G:H5'      | 2.17                     | 0.45              |
| 4:4:123:C:H2'     | 4:4:124:A:H8      | 1.82                     | 0.45              |
| 4:4:169:A:H2'     | 4:4:169:A:N3      | 2.32                     | 0.45              |
| 6:6:1:U:H6        | 6:6:1:U:H5''      | 1.82                     | 0.45              |
| 6:6:22:G:O6       | 6:6:26:G:N2       | 2.50                     | 0.45              |
| 9:A:116:VAL:HG12  | 9:A:164:ALA:CB    | 2.47                     | 0.45              |
| 10:B:48:VAL:HG12  | 10:B:81:ALA:HB2   | 1.99                     | 0.45              |
| 11:C:139:ARG:NH1  | 11:C:240:PRO:HG2  | 2.32                     | 0.45              |
| 14:F:36:GLY:HA2   | 14:F:53:ILE:O     | 2.16                     | 0.45              |
| 15:G:172:ARG:HG2  | 15:G:265:VAL:HG13 | 1.98                     | 0.45              |
| 21:M:146:PRO:HA   | 21:M:149:ASN:ND2  | 2.31                     | 0.45              |
| 22:N:152:LEU:HD23 | 22:N:156:LYS:HB2  | 1.99                     | 0.45              |
| 23:O:98:ALA:HB1   | 23:O:168:VAL:HG13 | 1.99                     | 0.45              |
| 1:1:439:U:C5      | 28:T:2:THR:HA     | 2.51                     | 0.45              |
| 32:X:50:PRO:HB2   | 32:X:58:THR:OG1   | 2.17                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 32:X:54:PRO:HA   | 32:X:59:TYR:CE2   | 2.51                     | 0.45              |
| 33:Y:43:LEU:HD23 | 33:Y:73:ARG:O     | 2.17                     | 0.45              |
| 34:Z:6:ASP:O     | 34:Z:10:ILE:HG12  | 2.17                     | 0.45              |
| 1:1:1090:U:H2'   | 1:1:1091:A:C8     | 2.51                     | 0.45              |
| 1:1:1369:G:OP2   | 16:H:77:ARG:NH2   | 2.49                     | 0.45              |
| 1:1:779:A:OP1    | 24:P:141:LYS:CB   | 2.62                     | 0.45              |
| 1:1:782:C:H2'    | 1:1:783:G:C8      | 2.52                     | 0.45              |
| 2:2:402:U:H3     | 2:2:426:G:H1      | 1.63                     | 0.45              |
| 4:4:136:G:N2     | 4:4:155:A:HI'     | 2.32                     | 0.45              |
| 4:4:77:U:H5''    | 10:B:371:LYS:HG3  | 1.99                     | 0.45              |
| 10:B:310:LYS:HZ1 | 10:B:378:GLN:HE21 | 1.65                     | 0.45              |
| 13:E:95:TYR:CE1  | 13:E:100:ILE:HG12 | 2.52                     | 0.45              |
| 13:E:23:ARG:NH2  | 13:E:24:LYS:HZ1   | 2.13                     | 0.45              |
| 13:E:23:ARG:O    | 13:E:24:LYS:HE2   | 2.17                     | 0.45              |
| 15:G:163:PHE:HA  | 15:G:264:ILE:HG21 | 1.98                     | 0.45              |
| 15:G:153:ARG:NH2 | 15:G:324:SER:OG   | 2.48                     | 0.45              |
| 18:J:81:ILE:HD13 | 18:J:116:ILE:HG21 | 1.98                     | 0.45              |
| 31:W:37:ARG:HG3  | 31:W:38:ALA:N     | 2.32                     | 0.45              |
| 31:W:68:THR:N    | 31:W:78:LEU:O     | 2.44                     | 0.45              |
| 1:1:1238:C:H5'   | 1:1:1239:U:C5'    | 2.47                     | 0.45              |
| 1:1:694:U:C5     | 1:1:694:U:OP2     | 2.70                     | 0.45              |
| 1:1:721:U:H2'    | 1:1:728:C:N3      | 2.31                     | 0.45              |
| 2:2:1100:G:H22   | 2:2:1110:C:N4     | 2.15                     | 0.45              |
| 2:2:760:U:HO2'   | 2:2:761:A:H8      | 1.65                     | 0.45              |
| 6:6:32:U:O2      | 6:6:32:U:H2'      | 2.17                     | 0.45              |
| 1:1:381:G:O2'    | 7:7:21:U:O4       | 2.27                     | 0.45              |
| 13:E:112:ARG:HD3 | 13:E:113:ASN:N    | 2.32                     | 0.45              |
| 17:I:69:ARG:HG3  | 20:L:69:TRP:CE2   | 2.52                     | 0.45              |
| 23:O:21:ARG:C    | 23:O:21:ARG:CD    | 2.86                     | 0.45              |
| 1:1:398:G:N2     | 1:1:401:A:OP2     | 2.50                     | 0.44              |
| 2:2:535:U:H2'    | 2:2:536:C:C5'     | 2.47                     | 0.44              |
| 2:2:540:C:N4     | 2:2:543:U:OP1     | 2.34                     | 0.44              |
| 2:2:649:G:OP1    | 50:2:1734:HOH:O   | 2.21                     | 0.44              |
| 2:2:684:C:H2'    | 2:2:685:G:O4'     | 2.17                     | 0.44              |
| 2:2:830:U:O2'    | 2:2:831:U:O4'     | 2.29                     | 0.44              |
| 4:4:113:G:H5''   | 4:4:114:A:OP1     | 2.17                     | 0.44              |
| 2:2:588:G:H5''   | 4:4:117:C:O2'     | 2.17                     | 0.44              |
| 6:6:22:G:C6      | 6:6:27:G:OP2      | 2.63                     | 0.44              |
| 10:B:301:ALA:HB3 | 10:B:310:LYS:HG3  | 1.98                     | 0.44              |
| 11:C:32:ARG:HG3  | 11:C:121:PHE:CZ   | 2.53                     | 0.44              |
| 14:F:53:ILE:HG12 | 14:F:63:LEU:HD13  | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:H:148:TYR:HB3  | 19:K:59:MET:CB    | 2.48                     | 0.44              |
| 17:I:59:LEU:HD12  | 17:I:124:TYR:CD1  | 2.51                     | 0.44              |
| 19:K:95:LEU:CG    | 19:K:106:ARG:HE   | 2.29                     | 0.44              |
| 1:1:752:G:N1      | 20:L:72:THR:HG21  | 2.32                     | 0.44              |
| 25:Q:55:VAL:HG13  | 25:Q:56:LYS:N     | 2.32                     | 0.44              |
| 26:R:39:ALA:O     | 26:R:43:PHE:N     | 2.50                     | 0.44              |
| 28:T:67:ILE:HD11  | 28:T:80:LYS:HB3   | 1.98                     | 0.44              |
| 34:Z:21:LYS:HZ3   | 34:Z:24:GLY:HA2   | 1.82                     | 0.44              |
| 1:1:1442:G:O2'    | 1:1:1443:U:H5''   | 2.17                     | 0.44              |
| 1:1:508:A:OP2     | 1:1:508:A:H8      | 2.00                     | 0.44              |
| 1:1:552:G:O5'     | 1:1:552:G:H8      | 2.00                     | 0.44              |
| 1:1:657:G:H2'     | 1:1:658:G:H5'     | 1.99                     | 0.44              |
| 2:2:120:A:H2'     | 2:2:121:U:C6      | 2.52                     | 0.44              |
| 2:2:352:A:H2'     | 2:2:353:G:C8      | 2.52                     | 0.44              |
| 2:2:357:U:C2'     | 2:2:358:G:H5'     | 2.47                     | 0.44              |
| 2:2:755:U:O2'     | 2:2:756:C:H5''    | 2.17                     | 0.44              |
| 2:2:787:G:H22     | 2:2:807:A:H61     | 1.66                     | 0.44              |
| 2:2:941:C:H2'     | 2:2:942:G:O4'     | 2.18                     | 0.44              |
| 4:4:98:A:H2'      | 4:4:99:A:O4'      | 2.17                     | 0.44              |
| 7:7:54:G:H2'      | 7:7:55:U:C6       | 2.53                     | 0.44              |
| 11:C:100:MET:HE2  | 11:C:103:PRO:HA   | 1.99                     | 0.44              |
| 15:G:332:ARG:NH1  | 15:G:333:LYS:HE2  | 2.32                     | 0.44              |
| 17:I:18:ASN:HD22  | 17:I:18:ASN:C     | 2.20                     | 0.44              |
| 19:K:72:ARG:C     | 19:K:72:ARG:CD    | 2.85                     | 0.44              |
| 22:N:156:LYS:HA   | 22:N:159:PHE:CD2  | 2.52                     | 0.44              |
| 1:1:1477:U:C5'    | 34:Z:17:ARG:HG3   | 2.47                     | 0.44              |
| 1:1:1279:A:H2'    | 1:1:1280:U:O4'    | 2.16                     | 0.44              |
| 1:1:715:G:H2'     | 1:1:716:A:O4'     | 2.17                     | 0.44              |
| 1:1:103:G:O2'     | 1:1:736:C:O2      | 2.30                     | 0.44              |
| 1:1:755:A:H4'     | 1:1:770:G:H5'     | 2.00                     | 0.44              |
| 1:1:783:G:H2'     | 1:1:784:U:O4'     | 2.18                     | 0.44              |
| 2:2:705:A:N3      | 2:2:705:A:H2'     | 2.32                     | 0.44              |
| 2:2:747:A:H2'     | 2:2:749:G:H5'     | 1.98                     | 0.44              |
| 3:3:58:C:H2'      | 3:3:60:U:O4'      | 2.17                     | 0.44              |
| 3:3:7:U:H1'       | 33:Y:76:ASN:HB2   | 1.99                     | 0.44              |
| 8:8:29:A:O2'      | 8:8:57:A:N1       | 2.36                     | 0.44              |
| 5:5:37:G:H5'      | 10:B:370:SER:OG   | 2.17                     | 0.44              |
| 10:B:46:PHE:HE2   | 10:B:81:ALA:HB1   | 1.82                     | 0.44              |
| 4:4:31:G:HO2'     | 10:B:92:TYR:HH    | 1.61                     | 0.44              |
| 13:E:111:VAL:HG12 | 13:E:114:PHE:HB2  | 1.97                     | 0.44              |
| 4:4:137:G:N2      | 13:E:155:ARG:HH22 | 2.16                     | 0.44              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 15:G:131:LEU:C    | 15:G:133:ARG:H      | 2.20                     | 0.44              |
| 19:K:95:LEU:HG    | 19:K:106:ARG:HE     | 1.82                     | 0.44              |
| 1:1:115:U:H4'     | 21:M:4:PHE:CD2      | 2.52                     | 0.44              |
| 23:O:103:LEU:H    | 23:O:103:LEU:HD23   | 1.82                     | 0.44              |
| 24:P:35:PHE:HD2   | 24:P:36:LEU:HD12    | 1.82                     | 0.44              |
| 30:V:84:THR:HA    | 30:V:127:ILE:O      | 2.17                     | 0.44              |
| 1:1:129:C:H1'     | 1:1:137:G:N2        | 2.33                     | 0.44              |
| 1:1:140:U:H5'     | 1:1:141:U:P         | 2.58                     | 0.44              |
| 1:1:1529:OMC:HM22 | 11:C:94:MET:CG      | 2.45                     | 0.44              |
| 1:1:1535:U:H2'    | 1:1:1536:G:H8       | 1.82                     | 0.44              |
| 1:1:1771:A:H2'    | 1:1:1772:U:O4'      | 2.17                     | 0.44              |
| 1:1:275:A:H8      | 1:1:275:A:P         | 2.41                     | 0.44              |
| 1:1:427:A:H3'     | 1:1:428:A:C8        | 2.53                     | 0.44              |
| 1:1:547:U:H1'     | 1:1:548:G:C2        | 2.52                     | 0.44              |
| 1:1:681:A2M:H1'   | 1:1:681:A2M:HM'3    | 1.82                     | 0.44              |
| 1:1:786:A:N6      | 1:1:791:C:H42       | 2.16                     | 0.44              |
| 2:2:650:A:N6      | 2:2:1311:A:H62      | 2.16                     | 0.44              |
| 2:2:477:G:C2      | 2:2:478:A:C6        | 3.05                     | 0.44              |
| 5:5:42:G:H2'      | 5:5:42:G:N3         | 2.33                     | 0.44              |
| 6:6:26:G:N3       | 6:6:26:G:C5'        | 2.73                     | 0.44              |
| 6:6:42:A:O2'      | 6:6:43:A:O5'        | 2.35                     | 0.44              |
| 6:6:7:A:N1        | 6:6:60:A:N1         | 2.66                     | 0.44              |
| 7:7:43:A:HO2'     | 7:7:44:A:C5'        | 2.31                     | 0.44              |
| 8:8:104:C:H2'     | 8:8:105:C:O4'       | 2.18                     | 0.44              |
| 8:8:22:U:H2'      | 8:8:23:G:C8         | 2.53                     | 0.44              |
| 13:E:112:ARG:HA   | 13:E:119:ARG:O      | 2.17                     | 0.44              |
| 17:I:13:GLN:HB3   | 17:I:17:TRP:HE1     | 1.82                     | 0.44              |
| 22:N:98:ARG:HH12  | 22:N:122:PRO:HG3    | 1.82                     | 0.44              |
| 23:O:30:TYR:HA    | 23:O:33:ARG:HB3     | 2.00                     | 0.44              |
| 27:S:67:VAL:O     | 27:S:67:VAL:HG13    | 2.17                     | 0.44              |
| 28:T:133[B]:HIS:O | 28:T:133[B]:HIS:CD2 | 2.71                     | 0.44              |
| 33:Y:89:MET:HA    | 33:Y:119:ARG:HH22   | 1.83                     | 0.44              |
| 33:Y:11:VAL:HG21  | 33:Y:80:PHE:CD1     | 2.52                     | 0.44              |
| 33:Y:90:SER:O     | 33:Y:95:GLY:N       | 2.45                     | 0.44              |
| 1:1:1045:G:O2'    | 1:1:1104:A:N6       | 2.50                     | 0.44              |
| 1:1:1248:C:H4'    | 1:1:1249:A:H5'      | 1.99                     | 0.44              |
| 1:1:176:C:O2'     | 1:1:177:A:H8        | 2.01                     | 0.44              |
| 1:1:263:A:H2'     | 1:1:264:U:O4'       | 2.17                     | 0.44              |
| 1:1:50:A:C2'      | 1:1:51:G:H5'        | 2.47                     | 0.44              |
| 1:1:658:G:HO2'    | 1:1:659:G:P         | 2.40                     | 0.44              |
| 1:1:786:A:H61     | 1:1:791:C:N4        | 2.15                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:2:1184:C:H3'    | 2:2:1185:C:C6    | 2.52                     | 0.44              |
| 2:2:1332:G:H2'    | 2:2:1333:C:C6    | 2.52                     | 0.44              |
| 2:2:1404:H2U:H51  | 2:2:1405:G:C4    | 2.52                     | 0.44              |
| 2:2:812:C:H4'     | 2:2:813:U:C5     | 2.53                     | 0.44              |
| 3:3:58:C:O2'      | 3:3:60:U:H5''    | 2.10                     | 0.44              |
| 4:4:138:C:H41     | 4:4:148:C:H1'    | 1.82                     | 0.44              |
| 6:6:40:C:P        | 6:6:40:C:C3'     | 2.94                     | 0.44              |
| 7:7:20:C:N4       | 7:7:21:U:C4      | 2.86                     | 0.44              |
| 2:2:661:U:OP1     | 9:A:2:GLY:HA2    | 2.18                     | 0.44              |
| 1:1:707:C:H5'     | 11:C:117:HIS:CE1 | 2.53                     | 0.44              |
| 11:C:178:ASP:CG   | 11:C:206:PRO:HD3 | 2.38                     | 0.44              |
| 13:E:92:ARG:HG2   | 13:E:93:CYS:H    | 1.82                     | 0.44              |
| 15:G:154:LEU:HD22 | 21:M:24:ARG:HH22 | 1.83                     | 0.44              |
| 22:N:46:PHE:CE1   | 22:N:141:LYS:HE2 | 2.53                     | 0.44              |
| 23:O:23:ARG:CD    | 23:O:23:ARG:C    | 2.85                     | 0.44              |
| 1:1:798:U:H5'     | 24:P:77:PHE:HD2  | 1.82                     | 0.44              |
| 2:2:1133:A:N6     | 27:S:47:ALA:O    | 2.50                     | 0.44              |
| 1:1:1629:U:OP1    | 30:V:126:TYR:OH  | 2.35                     | 0.44              |
| 31:W:71:TYR:CD1   | 31:W:74:LYS:HG2  | 2.53                     | 0.44              |
| 1:1:1442:G:N2     | 1:1:1448:C:O4'   | 2.51                     | 0.44              |
| 1:1:1485:A:N3     | 7:7:18:G:O2'     | 2.46                     | 0.44              |
| 1:1:1648:A:H2'    | 1:1:1649:A:O4'   | 2.17                     | 0.44              |
| 1:1:18:A:C6       | 1:1:19:G:C6      | 3.05                     | 0.44              |
| 1:1:333:A:O2'     | 1:1:334:G:O5'    | 2.29                     | 0.44              |
| 1:1:370:G:O5'     | 1:1:371:U:H5'    | 2.17                     | 0.44              |
| 1:1:786:A:O2'     | 1:1:787:A:OP1    | 2.28                     | 0.44              |
| 2:2:1103:C:H3'    | 2:2:1104:A:H2'   | 2.00                     | 0.44              |
| 2:2:1159:A:OP1    | 24:P:196:ARG:NH2 | 2.50                     | 0.44              |
| 2:2:1381:C:OP1    | 2:2:1382:G:H5''  | 2.18                     | 0.44              |
| 2:2:773:G:H2'     | 2:2:774:A:O4'    | 2.17                     | 0.44              |
| 2:2:834:G:H22     | 2:2:951:G:H1'    | 1.83                     | 0.44              |
| 3:3:38:A:N6       | 3:3:182:G:N1     | 2.66                     | 0.44              |
| 3:3:32:A:C6       | 3:3:33:A:C6      | 3.05                     | 0.44              |
| 8:8:36:C:C2       | 8:8:48:G:O2'     | 2.65                     | 0.44              |
| 9:A:181:LYS:HG3   | 9:A:184:ASN:H    | 1.82                     | 0.44              |
| 4:4:180:C:OP2     | 10:B:132:ARG:NH2 | 2.51                     | 0.44              |
| 2:2:1128:G:N2     | 27:S:49:ARG:HH22 | 2.15                     | 0.44              |
| 1:1:89:C:O2'      | 1:1:319:G:OP1    | 2.34                     | 0.44              |
| 1:1:347:U:H2'     | 1:1:348:G:O4'    | 2.18                     | 0.44              |
| 1:1:670:C:H2'     | 1:1:671:G:H8     | 1.83                     | 0.44              |
| 2:2:1451:G:H2'    | 2:2:1452:A:O4'   | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:666:C:OP2     | 2:2:666:C:C6      | 2.70                     | 0.44              |
| 3:3:108:A:H4'     | 3:3:109:C:O5'     | 2.17                     | 0.44              |
| 3:3:194:A:O2'     | 3:3:196:A:H5'     | 2.17                     | 0.44              |
| 4:4:158:A:H3'     | 4:4:159:G:H8      | 1.83                     | 0.44              |
| 9:A:116:VAL:CG2   | 9:A:126:LEU:HB2   | 2.42                     | 0.44              |
| 10:B:8:HIS:HB3    | 18:J:48:LEU:HG    | 2.00                     | 0.44              |
| 16:H:33:VAL:HG13  | 16:H:36:ARG:HB2   | 2.00                     | 0.44              |
| 17:I:61:PRO:O     | 17:I:76:LEU:HA    | 2.17                     | 0.44              |
| 17:I:94:TYR:OH    | 17:I:130:LEU:HD11 | 2.18                     | 0.44              |
| 18:J:77:ASN:OD1   | 18:J:107:PRO:HA   | 2.18                     | 0.44              |
| 1:1:1043:C:C2'    | 1:1:1044:G:H5'    | 2.48                     | 0.44              |
| 1:1:1049:A:H4'    | 8:8:103:A:C2      | 2.53                     | 0.44              |
| 1:1:1186:A:H2'    | 1:1:1187:A:C8     | 2.53                     | 0.44              |
| 1:1:1434:U:H1'    | 1:1:1435:G:N7     | 2.33                     | 0.44              |
| 1:1:854:C:C2'     | 1:1:855:C:H5'     | 2.48                     | 0.44              |
| 2:2:1254:OMG:C3'  | 2:2:1255:G:H5''   | 2.48                     | 0.44              |
| 2:2:808:C:H3'     | 2:2:809:C:C5      | 2.53                     | 0.44              |
| 2:2:809:C:C4      | 2:2:810:G:O6      | 2.71                     | 0.44              |
| 4:4:141:A:H3'     | 4:4:142:A:C8      | 2.53                     | 0.44              |
| 7:7:74:U:OP2      | 31:W:73:LEU:HD23  | 2.17                     | 0.44              |
| 8:8:107:U:H5''    | 22:N:202:PRO:HG2  | 1.99                     | 0.44              |
| 9:A:79:PRO:HD3    | 9:A:165:MET:SD    | 2.58                     | 0.44              |
| 17:I:60:ARG:NH1   | 17:I:76:LEU:O     | 2.50                     | 0.44              |
| 18:J:81:ILE:HD11  | 18:J:103:VAL:CG1  | 2.48                     | 0.44              |
| 18:J:83:GLN:HG2   | 18:J:85:LYS:H     | 1.81                     | 0.44              |
| 21:M:7:LEU:O      | 21:M:11:TRP:HD1   | 2.01                     | 0.44              |
| 24:P:61:PRO:HB3   | 24:P:92:ASP:OD1   | 2.18                     | 0.44              |
| 26:R:111:ASP:OD1  | 26:R:115:ARG:NE   | 2.42                     | 0.44              |
| 1:1:1394:U:C6     | 1:1:1394:U:O5'    | 2.71                     | 0.44              |
| 1:1:462:A:H62     | 7:7:3:C:H42       | 1.64                     | 0.44              |
| 1:1:56:G:H4'      | 21:M:155:VAL:HG12 | 1.99                     | 0.44              |
| 1:1:656:G:H2'     | 1:1:657:G:O4'     | 2.18                     | 0.44              |
| 1:1:659:G:H2'     | 1:1:660:U:C6      | 2.53                     | 0.44              |
| 2:2:426:G:H2'     | 2:2:427:C:C6      | 2.52                     | 0.44              |
| 1:1:1537:G:N2     | 2:2:604:A:H62     | 2.12                     | 0.44              |
| 2:2:827:A:O2'     | 2:2:828:U:O4'     | 2.33                     | 0.44              |
| 6:6:13:C:O2'      | 6:6:14:A:P        | 2.75                     | 0.44              |
| 6:6:32:U:O4       | 16:H:221:TYR:CE1  | 2.71                     | 0.44              |
| 6:6:39:U:C6       | 6:6:39:U:OP2      | 2.71                     | 0.44              |
| 8:8:20:A:H2'      | 8:8:21:G:H8       | 1.83                     | 0.44              |
| 10:B:312:ILE:HG13 | 10:B:328:TYR:CZ   | 2.52                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:I:59:LEU:HD23  | 17:I:60:ARG:N     | 2.33                     | 0.44              |
| 1:1:1392:G:N1     | 19:K:105:TRP:CH2  | 2.82                     | 0.44              |
| 16:H:146:VAL:HG11 | 19:K:55:ALA:CB    | 2.47                     | 0.44              |
| 21:M:155:VAL:O    | 21:M:162:ARG:NH2  | 2.41                     | 0.44              |
| 21:M:189:ARG:HA   | 21:M:192:TRP:HB3  | 1.99                     | 0.44              |
| 23:O:39:GLN:HE21  | 23:O:43:LYS:NZ    | 2.16                     | 0.44              |
| 24:P:64:LEU:HD22  | 24:P:120:ILE:HD11 | 2.00                     | 0.44              |
| 1:1:1208:U:H3'    | 1:1:1209:G:N2     | 2.33                     | 0.43              |
| 1:1:1257:U:HO2'   | 1:1:1258:A:P      | 2.40                     | 0.43              |
| 1:1:1443:U:H1'    | 24:P:17:HIS:ND1   | 2.30                     | 0.43              |
| 1:1:213:G:H22     | 1:1:220:A:H2      | 1.66                     | 0.43              |
| 1:1:319:G:H5''    | 1:1:320:G:OP1     | 2.18                     | 0.43              |
| 1:1:460:A:H2'     | 1:1:461:G:O4'     | 2.18                     | 0.43              |
| 1:1:492:G:C2      | 1:1:644:G:N2      | 2.86                     | 0.43              |
| 2:2:631:G:H1      | 2:2:1433:U:H3     | 1.66                     | 0.43              |
| 6:6:16:C:H3'      | 6:6:17:U:H5''     | 2.00                     | 0.43              |
| 13:E:109:ILE:O    | 13:E:122:ARG:HA   | 2.18                     | 0.43              |
| 13:E:112:ARG:CZ   | 13:E:118:LYS:HD2  | 2.48                     | 0.43              |
| 13:E:15:GLY:HA2   | 13:E:30:LYS:NZ    | 2.32                     | 0.43              |
| 23:O:41:LYS:HA    | 23:O:41:LYS:HE2   | 2.00                     | 0.43              |
| 26:R:9:TYR:CE1    | 26:R:65:VAL:HG12  | 2.53                     | 0.43              |
| 1:1:1371:U:O2'    | 1:1:1372:G:P      | 2.76                     | 0.43              |
| 1:1:1667:A:N3     | 15:G:139:THR:HG22 | 2.33                     | 0.43              |
| 1:1:180:A:H2'     | 1:1:181:G:C8      | 2.54                     | 0.43              |
| 1:1:300:A:O3'     | 1:1:301:A:H4'     | 2.18                     | 0.43              |
| 2:2:404:A:H4'     | 2:2:405:U:H5''    | 2.00                     | 0.43              |
| 2:2:483:C:H2'     | 2:2:484:G:C8      | 2.53                     | 0.43              |
| 2:2:525:A:H1'     | 2:2:529:G:C8      | 2.53                     | 0.43              |
| 2:2:554:OMC:HM22  | 2:2:555:A:OP1     | 2.18                     | 0.43              |
| 4:4:137:G:O2'     | 13:E:158:ALA:HB1  | 2.18                     | 0.43              |
| 7:7:7:OMU:HM23    | 7:7:7:OMU:H4'     | 2.00                     | 0.43              |
| 16:H:111:LYS:O    | 16:H:115:LYS:HG3  | 2.19                     | 0.43              |
| 16:H:96:ASP:HA    | 16:H:99:VAL:HB    | 2.00                     | 0.43              |
| 19:K:149:ARG:C    | 19:K:151:ALA:H    | 2.21                     | 0.43              |
| 1:1:1754:U:H5''   | 25:Q:38:ARG:HD2   | 2.00                     | 0.43              |
| 5:5:17:C:O2'      | 28:T:69:ARG:O     | 2.23                     | 0.43              |
| 1:1:1029:G:H8     | 1:1:1029:G:OP2    | 2.01                     | 0.43              |
| 1:1:1054:A:H2'    | 1:1:1055:U:H5'    | 2.00                     | 0.43              |
| 1:1:1435:G:C2     | 1:1:1436:G:C6     | 3.06                     | 0.43              |
| 1:1:1735:G:C2     | 1:1:1736:G:H1'    | 2.52                     | 0.43              |
| 1:1:67:C:H2'      | 1:1:68:A:O4'      | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:829:U:O2'    | 1:1:830:G:OP2     | 2.29                     | 0.43              |
| 1:1:984:A:C6     | 11:C:99:ARG:HD2   | 2.53                     | 0.43              |
| 2:2:1088:C:H2'   | 2:2:1089:G:C8     | 2.54                     | 0.43              |
| 2:2:1248:C:H5''  | 2:2:1395:A:H4'    | 2.00                     | 0.43              |
| 2:2:1290:A:H5'   | 2:2:1291:C:C5     | 2.53                     | 0.43              |
| 2:2:44:C:H2'     | 2:2:45:A:C8       | 2.54                     | 0.43              |
| 2:2:533:C:C5     | 2:2:544:U:C5      | 3.06                     | 0.43              |
| 2:2:812:C:H6     | 2:2:812:C:H2'     | 1.62                     | 0.43              |
| 2:2:812:C:H4'    | 2:2:813:U:C6      | 2.54                     | 0.43              |
| 1:1:1640:C:H4'   | 3:3:202:A:H1'     | 2.00                     | 0.43              |
| 5:5:102:U:H2'    | 5:5:103:U:O4'     | 2.19                     | 0.43              |
| 8:8:108:G:C6     | 8:8:109:A:C6      | 3.06                     | 0.43              |
| 8:8:85:G:OP2     | 50:8:201:HOH:O    | 2.21                     | 0.43              |
| 10:B:371:LYS:HD2 | 10:B:371:LYS:HA   | 1.80                     | 0.43              |
| 16:H:53:VAL:HG21 | 16:H:98:PHE:HE2   | 1.83                     | 0.43              |
| 18:J:94:VAL:O    | 32:X:20:ARG:N     | 2.51                     | 0.43              |
| 19:K:45:SER:HA   | 19:K:46:PRO:HD3   | 1.10                     | 0.43              |
| 26:R:29:PHE:CE1  | 26:R:43:PHE:HA    | 2.53                     | 0.43              |
| 30:V:109:LYS:H   | 30:V:133:HIS:CD2  | 2.35                     | 0.43              |
| 30:V:99:LYS:HE3  | 30:V:110:ALA:O    | 2.19                     | 0.43              |
| 32:X:8:PHE:CD1   | 32:X:44:TYR:HD1   | 2.36                     | 0.43              |
| 33:Y:68:VAL:H    | 33:Y:113:ARG:HH12 | 1.66                     | 0.43              |
| 1:1:1238:C:H5    | 19:K:50:CYS:HG    | 1.60                     | 0.43              |
| 1:1:1413:U:H4'   | 1:1:1414:A:H5'    | 2.00                     | 0.43              |
| 1:1:145:U:H5''   | 1:1:147:G:H5'     | 1.99                     | 0.43              |
| 1:1:1470:U:C2    | 1:1:1522:U:H1'    | 2.53                     | 0.43              |
| 1:1:270:C:C4     | 1:1:271:A:H1'     | 2.53                     | 0.43              |
| 1:1:487:G:H1     | 1:1:648:A:H2      | 1.62                     | 0.43              |
| 2:2:1088:C:H5''  | 2:2:1179:C:O2'    | 2.18                     | 0.43              |
| 2:2:1161:G:H2'   | 2:2:1162:A:O4'    | 2.18                     | 0.43              |
| 2:2:1275:C:H5    | 2:2:1292:G:N1     | 2.14                     | 0.43              |
| 2:2:1310:G:H5'   | 2:2:1311:A:C5'    | 2.45                     | 0.43              |
| 2:2:1347:C:C2'   | 2:2:1348:U:H5'    | 2.48                     | 0.43              |
| 2:2:581:G:N2     | 2:2:585:C:O2'     | 2.51                     | 0.43              |
| 5:5:122:C:H5'    | 5:5:123:U:OP2     | 2.18                     | 0.43              |
| 6:6:12:C:H3'     | 6:6:12:C:OP1      | 2.17                     | 0.43              |
| 7:7:39:G:H1'     | 7:7:104:A:N1      | 2.34                     | 0.43              |
| 7:7:95:A:H2'     | 7:7:96:A:O4'      | 2.19                     | 0.43              |
| 15:G:253:ASN:ND2 | 15:G:256:ARG:HE   | 2.16                     | 0.43              |
| 16:H:93:ALA:HA   | 16:H:166:TRP:CD1  | 2.54                     | 0.43              |
| 16:H:208:MET:SD  | 19:K:181:TRP:CE3  | 3.11                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:N:60:ILE:HG12 | 22:N:160:PRO:HG2  | 2.00                     | 0.43              |
| 23:O:33:ARG:O    | 23:O:37:VAL:HG22  | 2.17                     | 0.43              |
| 25:Q:136:ARG:O   | 25:Q:139:VAL:HG22 | 2.18                     | 0.43              |
| 1:1:1136:G:H2'   | 1:1:1137:C:H6     | 1.83                     | 0.43              |
| 1:1:1285:A:H2'   | 1:1:1285:A:N3     | 2.34                     | 0.43              |
| 1:1:1674:U:H2'   | 1:1:1675:G:C8     | 2.54                     | 0.43              |
| 1:1:171:U:O2'    | 1:1:172:G:H5'     | 2.18                     | 0.43              |
| 1:1:1772:U:H2'   | 1:1:1773:U:C6     | 2.53                     | 0.43              |
| 2:2:1190:A:O3'   | 24:P:189:SER:HB3  | 2.19                     | 0.43              |
| 2:2:1393:U:H1'   | 2:2:1394:U:OP2    | 2.18                     | 0.43              |
| 2:2:634:U:H1'    | 2:2:1431:G:N2     | 2.33                     | 0.43              |
| 2:2:946:C:H2'    | 2:2:947:U:C6      | 2.52                     | 0.43              |
| 3:3:119:U:HO2'   | 3:3:120:G:H8      | 1.62                     | 0.43              |
| 8:8:11:C:C5      | 8:8:12:C:N3       | 2.87                     | 0.43              |
| 13:E:24:LYS:NZ   | 13:E:38:LEU:H     | 2.17                     | 0.43              |
| 23:O:163:ALA:HB3 | 23:O:166:PHE:CD2  | 2.53                     | 0.43              |
| 1:1:1166:C:H5''  | 24:P:159:PHE:CG   | 2.54                     | 0.43              |
| 1:1:100:G:H2'    | 1:1:101:A:O4'     | 2.19                     | 0.43              |
| 1:1:1659:G:H2'   | 1:1:1660:U:C6     | 2.53                     | 0.43              |
| 1:1:240:U:O2'    | 1:1:241:G:O4'     | 2.34                     | 0.43              |
| 1:1:36:OMU:O5'   | 1:1:36:OMU:H6     | 2.19                     | 0.43              |
| 1:1:487:G:N2     | 1:1:648:A:H2      | 2.13                     | 0.43              |
| 2:2:1167:A:H2'   | 2:2:1168:G:H8     | 1.84                     | 0.43              |
| 2:2:650:A:N6     | 2:2:1311:A:N7     | 2.66                     | 0.43              |
| 2:2:668:C:N3     | 2:2:1036:G:N2     | 2.52                     | 0.43              |
| 2:2:71:OMG:H2'   | 2:2:72:G:O5'      | 2.19                     | 0.43              |
| 3:3:129:G:C2     | 3:3:130:G:C8      | 3.06                     | 0.43              |
| 3:3:197:G:H4'    | 3:3:198:C:O4'     | 2.17                     | 0.43              |
| 6:6:33:G:N7      | 19:K:42:VAL:HG11  | 2.33                     | 0.43              |
| 6:6:3:A:H2'      | 6:6:3:A:N3        | 2.33                     | 0.43              |
| 1:1:448:A:C2     | 7:7:16:A:H1'      | 2.54                     | 0.43              |
| 8:8:42:C:O2'     | 8:8:43:G:C5'      | 2.66                     | 0.43              |
| 8:8:61:C:H2'     | 8:8:62:U:H6       | 1.83                     | 0.43              |
| 9:A:21:HIS:HD2   | 9:A:22:LYS:NZ     | 2.16                     | 0.43              |
| 10:B:226:THR:HB  | 10:B:278:HIS:H    | 1.82                     | 0.43              |
| 16:H:27:ILE:HG22 | 16:H:53:VAL:HA    | 2.00                     | 0.43              |
| 16:H:30:LYS:HE3  | 16:H:30:LYS:HB3   | 3.23                     | 0.43              |
| 18:J:47:ARG:HH11 | 18:J:50:ARG:HD3   | 1.83                     | 0.43              |
| 1:1:752:G:H1     | 20:L:72:THR:HG21  | 1.83                     | 0.43              |
| 25:Q:14:ILE:HG21 | 25:Q:42:ARG:HG2   | 2.01                     | 0.43              |
| 26:R:93:VAL:HG13 | 26:R:94:LYS:H     | 1.84                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:934:A:O4'     | 28:T:133[B]:HIS:HA | 2.18                     | 0.43              |
| 30:V:102:MET:O    | 30:V:106:TYR:N     | 2.51                     | 0.43              |
| 30:V:129:LEU:HD12 | 30:V:135:ALA:HA    | 2.01                     | 0.43              |
| 33:Y:67:GLN:HB3   | 33:Y:113:ARG:HH22  | 1.83                     | 0.43              |
| 33:Y:68:VAL:O     | 33:Y:113:ARG:NH1   | 2.51                     | 0.43              |
| 1:1:1149:G:H2'    | 1:1:1149:G:N3      | 2.33                     | 0.43              |
| 1:1:1445:U:O2'    | 1:1:1446:A:H3'     | 2.18                     | 0.43              |
| 1:1:1681:G:O5'    | 1:1:1681:G:H8      | 2.02                     | 0.43              |
| 1:1:36:OMU:CM2    | 1:1:37:A:H5'       | 2.46                     | 0.43              |
| 1:1:504:C:C2      | 1:1:505:U:H1'      | 2.54                     | 0.43              |
| 2:2:1088:C:OP1    | 2:2:1179:C:O2'     | 2.35                     | 0.43              |
| 2:2:1171:U:H2'    | 2:2:1172:G:C8      | 2.54                     | 0.43              |
| 2:2:526:A:H2'     | 2:2:527:A2M:O3'    | 2.19                     | 0.43              |
| 2:2:592:C:H2'     | 2:2:593:U:O4'      | 2.19                     | 0.43              |
| 2:2:801:C:H2'     | 2:2:802:U:O4'      | 2.19                     | 0.43              |
| 3:3:58:C:O5'      | 3:3:58:C:C6        | 2.71                     | 0.43              |
| 5:5:41:U:H4'      | 5:5:42:G:O5'       | 2.19                     | 0.43              |
| 6:6:33:G:C5'      | 19:K:42:VAL:HG22   | 2.48                     | 0.43              |
| 2:2:1442:C:N4     | 6:6:3:A:H61        | 2.16                     | 0.43              |
| 7:7:37:U:C5       | 7:7:105:C:N3       | 2.87                     | 0.43              |
| 1:1:911:G:C5      | 9:A:181:LYS:HB2    | 2.54                     | 0.43              |
| 9:A:246:ILE:C     | 9:A:246:ILE:CD1    | 2.85                     | 0.43              |
| 10:B:226:THR:O    | 10:B:277:TYR:HA    | 2.19                     | 0.43              |
| 10:B:77:THR:OG1   | 10:B:333:GLY:O     | 2.32                     | 0.43              |
| 13:E:36:LYS:HZ3   | 13:E:38:LEU:HD21   | 1.84                     | 0.43              |
| 19:K:180:HIS:HE1  | 19:K:181:TRP:NE1   | 2.15                     | 0.43              |
| 22:N:92:HIS:HB3   | 22:N:94:PHE:CZ     | 2.53                     | 0.43              |
| 33:Y:77:HIS:HA    | 33:Y:80:PHE:HD2    | 1.84                     | 0.43              |
| 1:1:121:A:O2'     | 1:1:144:G:N2       | 2.51                     | 0.43              |
| 1:1:1521:G:C4     | 11:C:100:MET:SD    | 3.11                     | 0.43              |
| 1:1:307:U:H2'     | 1:1:308:A:C8       | 2.53                     | 0.43              |
| 1:1:330:U:H2'     | 1:1:331:C:O4'      | 2.18                     | 0.43              |
| 1:1:838:G:OP1     | 24:P:154:GLU:N     | 2.38                     | 0.43              |
| 1:1:927:A2M:H4'   | 2:2:73:U:O3'       | 2.19                     | 0.43              |
| 2:2:1023:U:C4     | 2:2:1024:C:H1'     | 2.54                     | 0.43              |
| 2:2:1159:A:H2'    | 2:2:1160:OMC:O4'   | 2.19                     | 0.43              |
| 2:2:1307:U:OP2    | 50:2:1736:HOH:O    | 2.21                     | 0.43              |
| 2:2:413:A:H2'     | 2:2:414:G:C8       | 2.54                     | 0.43              |
| 2:2:432:U:H2'     | 2:2:433:G:O4'      | 2.18                     | 0.43              |
| 2:2:729:G:C4      | 2:2:731:A:H5''     | 2.54                     | 0.43              |
| 8:8:48:G:C2'      | 8:8:48:G:N3        | 2.80                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:103:PRO:O     | 9:A:107:ILE:HG13  | 2.19                     | 0.43              |
| 9:A:147:ARG:HG2   | 9:A:157:SER:HB3   | 1.99                     | 0.43              |
| 4:4:141:A:O3'     | 13:E:70:ASN:HB2   | 2.19                     | 0.43              |
| 16:H:27:ILE:O     | 16:H:54:VAL:HG22  | 2.19                     | 0.43              |
| 1:1:80:C:OP1      | 21:M:199:VAL:HG11 | 2.18                     | 0.43              |
| 28:T:107:LEU:HD23 | 28:T:112:MET:HE1  | 2.01                     | 0.43              |
| 34:Z:19:LEU:CD2   | 34:Z:21:LYS:HB2   | 2.48                     | 0.43              |
| 1:1:1205:G:O2'    | 1:1:1206:A:H5'    | 2.19                     | 0.43              |
| 1:1:271:A:H2'     | 1:1:272:U:C6      | 2.53                     | 0.43              |
| 1:1:815:G:N2      | 1:1:825:G:N2      | 2.67                     | 0.43              |
| 1:1:887:A:C2      | 1:1:909:A:H1'     | 2.54                     | 0.43              |
| 2:2:1441:G:N2     | 2:2:1443:G:O2'    | 2.41                     | 0.43              |
| 2:2:526:A:HO2'    | 2:2:527:A2M:P     | 2.37                     | 0.43              |
| 2:2:780:G:O5'     | 15:G:328:ARG:NH2  | 2.49                     | 0.43              |
| 6:6:37:C:H3'      | 6:6:37:C:O2       | 2.18                     | 0.43              |
| 10:B:210:VAL:HG21 | 10:B:329:VAL:HG21 | 2.00                     | 0.43              |
| 13:E:148:ASN:OD1  | 13:E:149:ASP:N    | 2.51                     | 0.43              |
| 16:H:95:SER:OG    | 16:H:124:GLU:HB2  | 2.19                     | 0.43              |
| 17:I:64:ASN:OD1   | 17:I:74:ARG:NH2   | 2.52                     | 0.43              |
| 20:L:74:ASN:HA    | 20:L:110:LEU:O    | 2.19                     | 0.43              |
| 1:1:695:OMC:OP1   | 20:L:3:THR:HG22   | 2.18                     | 0.43              |
| 22:N:99:ILE:HB    | 22:N:123:ASN:ND2  | 2.34                     | 0.43              |
| 1:1:835:G:O2'     | 24:P:65:SER:OG    | 2.27                     | 0.43              |
| 29:U:57:LEU:H     | 29:U:61:LYS:HA    | 1.83                     | 0.43              |
| 1:1:1136:G:H2'    | 1:1:1137:C:C6     | 2.54                     | 0.43              |
| 1:1:23:U:H4'      | 1:1:24:A:C8       | 2.54                     | 0.43              |
| 1:1:424:G:N2      | 1:1:427:A:H8      | 2.06                     | 0.43              |
| 1:1:506:G:N2      | 1:1:549:C:O2      | 2.52                     | 0.43              |
| 1:1:709:A:H5''    | 1:1:837:A:H61     | 1.84                     | 0.43              |
| 2:2:535:U:C2'     | 2:2:536:C:C5'     | 2.97                     | 0.43              |
| 8:8:20:A:H2'      | 8:8:21:G:O4'      | 2.19                     | 0.43              |
| 10:B:282:GLN:HB3  | 10:B:285:LYS:HE2  | 2.01                     | 0.43              |
| 11:C:167:MET:SD   | 11:C:222:ILE:HD12 | 2.59                     | 0.43              |
| 11:C:30:PRO:HB3   | 24:P:25:TYR:CE2   | 2.48                     | 0.43              |
| 19:K:73:ILE:CG1   | 19:K:114:VAL:HG22 | 2.36                     | 0.43              |
| 13:E:59:TRP:HH2   | 19:K:64:TYR:CB    | 2.23                     | 0.43              |
| 1:1:1389:A:OP1    | 19:K:77:PRO:HG3   | 2.18                     | 0.43              |
| 1:1:306:G:O6      | 21:M:15:SER:HB3   | 2.19                     | 0.43              |
| 22:N:72:ALA:HA    | 22:N:151:ALA:HB1  | 2.01                     | 0.43              |
| 22:N:156:LYS:HG3  | 22:N:163:GLN:HB3  | 2.01                     | 0.43              |
| 23:O:51:LEU:N     | 23:O:151:ILE:O    | 2.52                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:8:116:U:O2'     | 23:O:74:VAL:O     | 2.35                     | 0.43              |
| 25:Q:18:GLY:O     | 25:Q:21:ARG:HB2   | 2.19                     | 0.43              |
| 28:T:36:ILE:HG23  | 28:T:47:LEU:HD23  | 2.01                     | 0.43              |
| 28:T:61:LYS:CG    | 28:T:78:GLN:HE22  | 2.32                     | 0.43              |
| 1:1:1108:G:H3'    | 1:1:1109:U:O2     | 2.19                     | 0.42              |
| 1:1:1119:C:H2'    | 1:1:1120:C:C6     | 2.54                     | 0.42              |
| 1:1:130:U:H3'     | 1:1:131:U:H5'     | 2.00                     | 0.42              |
| 1:1:1354:C:H2'    | 1:1:1355:C:C6     | 2.54                     | 0.42              |
| 1:1:403:C:O2'     | 11:C:79:SER:O     | 2.37                     | 0.42              |
| 1:1:59:A:H2'      | 1:1:60:A:O4'      | 2.18                     | 0.42              |
| 2:2:1277:A:OP1    | 22:N:75:TYR:OH    | 2.15                     | 0.42              |
| 2:2:29:C:HO2'     | 2:2:30:A:P        | 2.42                     | 0.42              |
| 3:3:112:C:N3      | 3:3:120:G:N1      | 2.53                     | 0.42              |
| 3:3:151:C:H2'     | 3:3:152:A:O4'     | 2.18                     | 0.42              |
| 8:8:43:G:C8       | 8:8:43:G:OP2      | 2.70                     | 0.42              |
| 8:8:37:C:N3       | 8:8:48:G:O4'      | 2.52                     | 0.42              |
| 8:8:6:U:O2'       | 8:8:7:A:H8        | 2.02                     | 0.42              |
| 10:B:321:TYR:HD1  | 10:B:340:ARG:HG3  | 1.81                     | 0.42              |
| 4:4:137:G:H21     | 13:E:155:ARG:HH22 | 1.67                     | 0.42              |
| 13:E:88:ARG:HH11  | 13:E:186:ILE:HG22 | 1.82                     | 0.42              |
| 1:1:1668:G:C2     | 15:G:136:ARG:HD3  | 2.53                     | 0.42              |
| 17:I:79:GLY:HA2   | 17:I:101:ARG:O    | 2.19                     | 0.42              |
| 26:R:6:LEU:O      | 26:R:102:THR:HG23 | 2.18                     | 0.42              |
| 27:S:100[B]:ARG:C | 27:S:102:GLN:N    | 2.68                     | 0.42              |
| 1:1:1112:A:O2'    | 27:S:105:PHE:HE1  | 2.02                     | 0.42              |
| 27:S:14:LEU:HD11  | 27:S:58:HIS:CD2   | 2.54                     | 0.42              |
| 7:7:147:G:C5'     | 30:V:51:ASN:HD21  | 2.32                     | 0.42              |
| 30:V:79:ILE:HG12  | 30:V:85:LEU:HD23  | 2.01                     | 0.42              |
| 1:1:1048:A:H2'    | 1:1:1049:A:O4'    | 2.20                     | 0.42              |
| 1:1:1394:U:H6     | 1:1:1394:U:O5'    | 2.01                     | 0.42              |
| 1:1:1450:C:H2'    | 1:1:1451:U:H5'    | 2.01                     | 0.42              |
| 1:1:1727:U:C4     | 1:1:1728:G:C4     | 3.07                     | 0.42              |
| 1:1:48:OMU:H2'    | 1:1:48:OMU:O2     | 2.18                     | 0.42              |
| 1:1:752:G:H4'     | 1:1:810:C:O3'     | 2.19                     | 0.42              |
| 1:1:851:G:H2'     | 1:1:852:A:C8      | 2.54                     | 0.42              |
| 1:1:939:C:H2'     | 1:1:940:U:O4'     | 2.19                     | 0.42              |
| 2:2:498:A:H2'     | 2:2:499:G:C8      | 2.54                     | 0.42              |
| 2:2:775:C:N4      | 2:2:814:A:OP2     | 2.52                     | 0.42              |
| 3:3:3:G:H2'       | 3:3:4:U:C6        | 2.53                     | 0.42              |
| 8:8:34:A:N1       | 8:8:48:G:C6       | 2.88                     | 0.42              |
| 10:B:165:HIS:HA   | 10:B:182:HIS:O    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:B:337:GLY:HA3  | 10:B:343:MET:HE3  | 1.99                     | 0.42              |
| 18:J:13:PHE:CD2   | 18:J:123:GLU:HG3  | 2.54                     | 0.42              |
| 19:K:51:ALA:O     | 19:K:52:GLN:HG3   | 2.19                     | 0.42              |
| 21:M:73:ARG:HG2   | 21:M:75:VAL:HG13  | 2.01                     | 0.42              |
| 2:2:1276:A:H4'    | 22:N:154:ARG:HH12 | 1.83                     | 0.42              |
| 22:N:47:PRO:HA    | 22:N:171:TRP:CZ3  | 2.54                     | 0.42              |
| 22:N:58:GLU:O     | 22:N:129:VAL:HB   | 2.19                     | 0.42              |
| 2:2:635:A:H5''    | 28:T:66[A]:LYS:HA | 2.01                     | 0.42              |
| 29:U:85:TYR:HH    | 29:U:90:PHE:HZ    | 1.63                     | 0.42              |
| 1:1:1531:U:H2'    | 1:1:1532:G:C8     | 2.53                     | 0.42              |
| 1:1:1541:A2M:OP2  | 50:1:1966:HOH:O   | 2.21                     | 0.42              |
| 1:1:827:G:H2'     | 1:1:828:U:O4'     | 2.19                     | 0.42              |
| 2:2:71:OMG:H2'    | 2:2:72:G:O4'      | 2.20                     | 0.42              |
| 6:6:33:G:H5'      | 19:K:42:VAL:HG22  | 1.94                     | 0.42              |
| 8:8:46:U:O2'      | 8:8:47:U:H5'      | 2.19                     | 0.42              |
| 10:B:26:ARG:HD3   | 10:B:184:GLN:OE1  | 2.19                     | 0.42              |
| 10:B:320:GLY:O    | 10:B:340:ARG:NE   | 2.48                     | 0.42              |
| 10:B:56:ILE:CG2   | 10:B:366:ILE:HG23 | 2.47                     | 0.42              |
| 15:G:117:LYS:HE2  | 15:G:117:LYS:HA   | 2.00                     | 0.42              |
| 1:1:6:C:H5''      | 15:G:278:LYS:HB3  | 2.01                     | 0.42              |
| 16:H:148:TYR:CB   | 19:K:59:MET:H     | 2.25                     | 0.42              |
| 20:L:120:ILE:HG13 | 20:L:120:ILE:O    | 2.19                     | 0.42              |
| 26:R:12:VAL:HG12  | 26:R:62:SER:O     | 2.20                     | 0.42              |
| 1:1:1183:G:OP1    | 22:N:17:TYR:OH    | 2.35                     | 0.42              |
| 1:1:22:C:C2'      | 1:1:23:U:H5'      | 2.50                     | 0.42              |
| 1:1:260:C:HO2'    | 1:1:261:C:P       | 2.39                     | 0.42              |
| 1:1:493:A:C2'     | 1:1:494:A:H5'     | 2.49                     | 0.42              |
| 1:1:497:A:O2'     | 1:1:498:G:P       | 2.78                     | 0.42              |
| 1:1:899:A:H3'     | 1:1:900:C:C6      | 2.54                     | 0.42              |
| 1:1:923:G:N2      | 1:1:940:U:H1'     | 2.33                     | 0.42              |
| 2:2:1078:OMU:O4'  | 2:2:1186:A2M:H2   | 2.19                     | 0.42              |
| 2:2:1230:OMG:HM23 | 2:2:1230:OMG:H1'  | 1.84                     | 0.42              |
| 2:2:805:G:H2'     | 2:2:806:C:C6      | 2.55                     | 0.42              |
| 6:6:26:G:C3'      | 6:6:27:G:H4'      | 2.49                     | 0.42              |
| 7:7:20:C:H2'      | 7:7:21:U:H5'      | 2.00                     | 0.42              |
| 9:A:101:VAL:HG22  | 9:A:165:MET:HG2   | 2.01                     | 0.42              |
| 1:1:874:C:H5'     | 9:A:19:HIS:ND1    | 2.34                     | 0.42              |
| 10:B:204:LEU:O    | 10:B:206:LYS:HD2  | 2.19                     | 0.42              |
| 15:G:324:SER:HB2  | 15:G:327:SER:H    | 1.83                     | 0.42              |
| 19:K:78:ARG:O     | 19:K:78:ARG:HG2   | 2.19                     | 0.42              |
| 28:T:127:ARG:O    | 28:T:127:ARG:HG3  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:W:74:LYS:HB2  | 31:W:76:VAL:HG22  | 2.00                     | 0.42              |
| 32:X:43:LEU:O    | 32:X:43:LEU:HD23  | 2.20                     | 0.42              |
| 33:Y:20:GLY:HA3  | 33:Y:134:PHE:CE1  | 2.54                     | 0.42              |
| 33:Y:43:LEU:HD13 | 33:Y:80:PHE:HE1   | 1.84                     | 0.42              |
| 1:1:1093:U:H2'   | 1:1:1094:C:C6     | 2.54                     | 0.42              |
| 1:1:1004:G:O2'   | 1:1:1172:G:H4'    | 2.20                     | 0.42              |
| 1:1:1450:C:C2'   | 1:1:1451:U:H5'    | 2.49                     | 0.42              |
| 1:1:1729:A:N1    | 1:1:1730:A:N6     | 2.66                     | 0.42              |
| 1:1:205:A:H4'    | 1:1:206:A:OP1     | 2.19                     | 0.42              |
| 1:1:243:G:H22    | 1:1:259:G:N2      | 2.18                     | 0.42              |
| 1:1:30:C:H2'     | 1:1:31:G:O4'      | 2.19                     | 0.42              |
| 1:1:405:A:O2'    | 11:C:85:THR:HG23  | 2.19                     | 0.42              |
| 1:1:73:U:H5'     | 17:I:64:ASN:O     | 2.20                     | 0.42              |
| 1:1:840:G:H2'    | 1:1:841:U:O4'     | 2.20                     | 0.42              |
| 2:2:1161:G:H4'   | 2:2:1188:C:H4'    | 2.01                     | 0.42              |
| 2:2:1198:C:H3'   | 2:2:1199:G:C5'    | 2.47                     | 0.42              |
| 2:2:628:A2M:H1'  | 2:2:628:A2M:HM'3  | 1.84                     | 0.42              |
| 2:2:639:G:OP1    | 10:B:253:LYS:HD3  | 2.20                     | 0.42              |
| 2:2:754:U:H2'    | 2:2:755:U:C6      | 2.54                     | 0.42              |
| 2:2:770:A:H61    | 9:A:68:LYS:HE3    | 1.84                     | 0.42              |
| 6:6:31:U:C6      | 6:6:31:U:H3'      | 2.53                     | 0.42              |
| 7:7:44:A:H2'     | 7:7:45:C:C6       | 2.54                     | 0.42              |
| 9:A:65:HIS:CB    | 9:A:72:VAL:HG13   | 2.35                     | 0.42              |
| 11:C:100:MET:HE1 | 11:C:103:PRO:HA   | 2.02                     | 0.42              |
| 16:H:161:CYS:HA  | 16:H:164:VAL:HG22 | 2.01                     | 0.42              |
| 25:Q:140:GLU:O   | 25:Q:144:LYS:HG2  | 2.19                     | 0.42              |
| 2:2:1060:G:O6    | 27:S:3:HIS:NE2    | 2.53                     | 0.42              |
| 1:1:1126:U:N3    | 1:1:1127:U:H1'    | 2.35                     | 0.42              |
| 1:1:1161:A:H2'   | 1:1:1162:G:C8     | 2.55                     | 0.42              |
| 1:1:1161:A:H2'   | 1:1:1162:G:H8     | 1.84                     | 0.42              |
| 1:1:1440:A:C6    | 1:1:1448:C:H4'    | 2.54                     | 0.42              |
| 1:1:231:U:H4'    | 1:1:232:G:H5'     | 2.00                     | 0.42              |
| 1:1:673:C:N4     | 1:1:677:A:H8      | 2.17                     | 0.42              |
| 2:2:1140:U:O2'   | 2:2:1172:G:O2'    | 2.20                     | 0.42              |
| 2:2:1413:U:H2'   | 2:2:1414:U:C6     | 2.54                     | 0.42              |
| 2:2:429:A:O2'    | 9:A:236:GLY:N     | 2.45                     | 0.42              |
| 2:2:747:A:C6     | 2:2:749:G:C6      | 3.08                     | 0.42              |
| 2:2:996:G:H2'    | 2:2:997:C:C5      | 2.55                     | 0.42              |
| 2:2:9:G:H2'      | 2:2:10:C:C6       | 2.54                     | 0.42              |
| 7:7:136:G:H2'    | 7:7:137:U:C6      | 2.54                     | 0.42              |
| 8:8:12:C:H1'     | 8:8:15:A:N1       | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:8:31:C:O2'      | 8:8:52:A:N6       | 2.53                     | 0.42              |
| 9:A:54:ARG:HG2    | 9:A:56:ALA:H      | 1.84                     | 0.42              |
| 13:E:161:HIS:HD2  | 13:E:179:TYR:HB2  | 1.84                     | 0.42              |
| 13:E:24:LYS:HE2   | 13:E:24:LYS:HA    | 2.01                     | 0.42              |
| 16:H:148:TYR:HE2  | 16:H:150:SER:HG   | 1.67                     | 0.42              |
| 16:H:49:LYS:NZ    | 19:K:37:THR:HG23  | 2.35                     | 0.42              |
| 18:J:78:ALA:HA    | 18:J:105:VAL:HG22 | 2.01                     | 0.42              |
| 19:K:155:GLU:O    | 19:K:159:ALA:N    | 2.53                     | 0.42              |
| 21:M:159:ARG:NH1  | 21:M:165:THR:HG22 | 2.35                     | 0.42              |
| 25:Q:90:PRO:O     | 25:Q:94:LEU:HD23  | 2.19                     | 0.42              |
| 1:1:1536:G:H2'    | 1:1:1537:G:O4'    | 2.20                     | 0.42              |
| 1:1:672:U:H2'     | 1:1:673:C:C6      | 2.55                     | 0.42              |
| 1:1:673:C:H2'     | 1:1:674:U:O4'     | 2.19                     | 0.42              |
| 1:1:846:G:O2'     | 1:1:847:OMU:H5''  | 2.20                     | 0.42              |
| 1:1:94:A:C5       | 1:1:95:G:H1'      | 2.55                     | 0.42              |
| 2:2:102:C:H2'     | 2:2:103:G:O4'     | 2.20                     | 0.42              |
| 2:2:1254:OMG:H3'  | 2:2:1255:G:H5''   | 2.00                     | 0.42              |
| 2:2:412:A:H2'     | 2:2:413:A:C8      | 2.54                     | 0.42              |
| 2:2:113:A:H4'     | 2:2:567:A:H5''    | 2.01                     | 0.42              |
| 2:2:813:U:O4      | 2:2:1009:C:O2'    | 2.26                     | 0.42              |
| 2:2:942:G:C6      | 2:2:943:U:C2      | 3.08                     | 0.42              |
| 7:7:141:C:H2'     | 7:7:142:C:H5'     | 2.01                     | 0.42              |
| 9:A:59:ALA:CB     | 9:A:82:MET:HE3    | 2.49                     | 0.42              |
| 10:B:257:ILE:HD12 | 10:B:271:ARG:NH2  | 2.34                     | 0.42              |
| 10:B:265:VAL:HG21 | 10:B:271:ARG:HH21 | 1.84                     | 0.42              |
| 3:3:182:G:H4'     | 16:H:36:ARG:HH12  | 126.55                   | 0.42              |
| 1:1:1369:G:C5     | 16:H:78:LYS:HD3   | 2.55                     | 0.42              |
| 21:M:174:LEU:O    | 21:M:175:ARG:HB3  | 2.19                     | 0.42              |
| 1:1:959:OMG:N2    | 21:M:76:HIS:CD2   | 2.78                     | 0.42              |
| 24:P:51:ARG:CZ    | 24:P:147:ARG:HD2  | 2.50                     | 0.42              |
| 28:T:8:PRO:HD3    | 28:T:16:LYS:NZ    | 2.34                     | 0.42              |
| 32:X:47:LYS:HA    | 32:X:47:LYS:HD2   | 1.83                     | 0.42              |
| 1:1:144:G:OP1     | 21:M:40:ARG:NH2   | 2.52                     | 0.42              |
| 1:1:1729:A:N3     | 1:1:1729:A:H2'    | 2.34                     | 0.42              |
| 1:1:293:C:H2'     | 1:1:294:U:C5      | 2.54                     | 0.42              |
| 1:1:516:G:H2'     | 1:1:517:U:C6      | 2.55                     | 0.42              |
| 1:1:770:G:O2'     | 1:1:771:U:H5'     | 2.19                     | 0.42              |
| 1:1:819:C:H6      | 1:1:819:C:O5'     | 2.02                     | 0.42              |
| 2:2:554:OMC:O3'   | 2:2:554:OMC:HM22  | 2.20                     | 0.42              |
| 1:1:930:U:N3      | 2:2:603:A:N3      | 2.67                     | 0.42              |
| 3:3:116:C:H2'     | 3:3:117:G:H5'     | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:5:105:A:N3      | 5:5:105:A:H3'     | 2.35                     | 0.42              |
| 6:6:46:C:H2'      | 6:6:47:G:C8       | 2.54                     | 0.42              |
| 7:7:118:U:H2'     | 7:7:119:G:C8      | 2.54                     | 0.42              |
| 8:8:78:U:H2'      | 8:8:79:A:H8       | 1.85                     | 0.42              |
| 2:2:431:C:H5''    | 9:A:219:ILE:HD11  | 2.02                     | 0.42              |
| 10:B:390:LEU:HD12 | 10:B:392:LYS:H    | 1.84                     | 0.42              |
| 15:G:296:LEU:O    | 15:G:299:LEU:N    | 2.53                     | 0.42              |
| 15:G:157:PRO:HA   | 15:G:318:TRP:CE3  | 2.55                     | 0.42              |
| 16:H:93:ALA:O     | 16:H:95:SER:N     | 2.53                     | 0.42              |
| 17:I:83:ALA:CB    | 17:I:108:ASN:HD22 | 2.30                     | 0.42              |
| 17:I:129:VAL:HG23 | 17:I:130:LEU:N    | 2.35                     | 0.42              |
| 29:U:32:ILE:O     | 29:U:36:ASP:N     | 2.53                     | 0.42              |
| 1:1:1357:G:C5     | 1:1:1358:C:C4     | 3.08                     | 0.42              |
| 1:1:1374:C:H2'    | 1:1:1375:G:O4'    | 2.19                     | 0.42              |
| 1:1:1423:A:H4'    | 1:1:1424:A:OP1    | 2.18                     | 0.42              |
| 1:1:247:A:OP2     | 11:C:221:ASN:HB2  | 2.20                     | 0.42              |
| 1:1:333:A:H2'     | 1:1:334:G:C8      | 2.55                     | 0.42              |
| 1:1:386:C:C2      | 7:7:24:G:H4'      | 2.55                     | 0.42              |
| 1:1:720:A:H2'     | 1:1:721:U:O4'     | 2.19                     | 0.42              |
| 2:2:1195:U:H2'    | 2:2:1196:U:C6     | 2.54                     | 0.42              |
| 2:2:1369:A:H2'    | 2:2:1370:C:H6     | 1.85                     | 0.42              |
| 2:2:447:G:H1'     | 9:A:222:PRO:HG2   | 2.01                     | 0.42              |
| 3:3:69:A:H2'      | 3:3:70:A:C8       | 2.54                     | 0.42              |
| 8:8:23:G:H4'      | 8:8:24:A:N7       | 2.35                     | 0.42              |
| 10:B:84:MET:HE2   | 10:B:164:ALA:CB   | 2.50                     | 0.42              |
| 4:4:137:G:H21     | 13:E:155:ARG:NH2  | 2.18                     | 0.42              |
| 6:6:37:C:H5       | 14:F:185:LYS:HZ3  | 1.68                     | 0.42              |
| 15:G:186:THR:C    | 15:G:188:LYS:H    | 2.23                     | 0.42              |
| 15:G:239:ALA:HB1  | 15:G:268:MET:HB3  | 2.01                     | 0.42              |
| 22:N:49:CYS:SG    | 22:N:139:ARG:HG2  | 2.60                     | 0.42              |
| 22:N:4:ARG:HA     | 22:N:5:PRO:HD3    | 1.90                     | 0.42              |
| 2:2:57:G:OP1      | 25:Q:21:ARG:HG3   | 2.19                     | 0.42              |
| 30:V:116:LEU:HD21 | 30:V:124:LYS:HD2  | 2.01                     | 0.42              |
| 1:1:1271:G:H1     | 1:1:1358:C:N4     | 2.18                     | 0.42              |
| 1:1:1448:C:H2'    | 1:1:1449:C:H6     | 1.84                     | 0.42              |
| 1:1:1555:G:H2'    | 1:1:1556:G:O4'    | 2.20                     | 0.42              |
| 1:1:1677:A:H2'    | 1:1:1678:G:O4'    | 2.20                     | 0.42              |
| 1:1:249:G:H1'     | 1:1:251:A:OP1     | 2.20                     | 0.42              |
| 1:1:302:G:HO2'    | 1:1:303:C:H6      | 1.65                     | 0.42              |
| 1:1:503:A:H8      | 1:1:504:C:C5      | 2.38                     | 0.42              |
| 1:1:844:C:H2'     | 1:1:845:OMU:C6    | 2.50                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:2:1079:OMG:O6   | 2:2:1237:C:N4    | 2.24                     | 0.42              |
| 1:1:990:U:O2'     | 2:2:648:A:N1     | 2.43                     | 0.42              |
| 2:2:967:U:H4'     | 2:2:968:G:H8     | 1.84                     | 0.42              |
| 4:4:120:U:H2'     | 4:4:120:U:H6     | 1.65                     | 0.42              |
| 7:7:102:G:OP2     | 7:7:104:A:O2'    | 2.35                     | 0.42              |
| 8:8:15:A:H5''     | 8:8:112:G:O5'    | 2.20                     | 0.42              |
| 8:8:47:U:H1'      | 8:8:48:G:H8      | 1.85                     | 0.42              |
| 9:A:193:ARG:HD3   | 9:A:195:CYS:SG   | 2.60                     | 0.42              |
| 11:C:151:LEU:O    | 11:C:250:TRP:HB2 | 2.20                     | 0.42              |
| 11:C:12:ALA:HB1   | 11:C:160:TYR:OH  | 2.20                     | 0.42              |
| 11:C:168:ALA:HA   | 11:C:171:LYS:HE2 | 2.01                     | 0.42              |
| 11:C:153:VAL:HG23 | 11:C:251:THR:HA  | 2.01                     | 0.42              |
| 13:E:92:ARG:HG2   | 13:E:93:CYS:N    | 2.35                     | 0.42              |
| 1:1:1001:G:OP2    | 50:1:1956:HOH:O  | 2.22                     | 0.41              |
| 1:1:1091:A:C2     | 1:1:1092:U:H1'   | 2.55                     | 0.41              |
| 1:1:1092:U:H2'    | 1:1:1093:U:O4'   | 2.20                     | 0.41              |
| 1:1:1371:U:O2'    | 1:1:1372:G:OP1   | 2.38                     | 0.41              |
| 1:1:1581:G:OP2    | 25:Q:53:LYS:NZ   | 2.52                     | 0.41              |
| 1:1:207:C:H2'     | 1:1:208:C:C6     | 2.55                     | 0.41              |
| 1:1:217:A:H2'     | 1:1:218:A:N9     | 2.34                     | 0.41              |
| 1:1:188:A:H1'     | 1:1:244:C:O2'    | 2.20                     | 0.41              |
| 1:1:370:G:H4'     | 1:1:371:U:C6     | 2.55                     | 0.41              |
| 1:1:498:G:N2      | 1:1:556:U:H3     | 2.18                     | 0.41              |
| 1:1:488:G:H1      | 1:1:647:G:H1     | 1.67                     | 0.41              |
| 2:2:1175:A:H2'    | 2:2:1176:A:O4'   | 2.20                     | 0.41              |
| 2:2:1199:G:N3     | 2:2:1199:G:H3'   | 2.35                     | 0.41              |
| 2:2:1270:G:OP2    | 2:2:1270:G:H8    | 2.02                     | 0.41              |
| 2:2:548:G:H2'     | 2:2:549:A:O4'    | 2.20                     | 0.41              |
| 2:2:723:G:H1'     | 2:2:734:A:C5     | 2.55                     | 0.41              |
| 2:2:749:G:O2'     | 2:2:750:U:C6     | 2.69                     | 0.41              |
| 3:3:147:A:N3      | 3:3:147:A:H2'    | 2.35                     | 0.41              |
| 8:8:109:A:C2'     | 8:8:110:G:H5'    | 2.50                     | 0.41              |
| 8:8:44:A:C5       | 8:8:45:U:C5      | 3.07                     | 0.41              |
| 8:8:3:G:N1        | 8:8:4:A:N3       | 2.68                     | 0.41              |
| 9:A:90:CYS:CB     | 9:A:101:VAL:HB   | 2.49                     | 0.41              |
| 9:A:73:LYS:HZ3    | 9:A:73:LYS:HB2   | 1.83                     | 0.41              |
| 10:B:101:THR:HG22 | 10:B:103:GLY:H   | 1.85                     | 0.41              |
| 11:C:106:ILE:HD12 | 17:I:29:VAL:HG21 | 2.02                     | 0.41              |
| 13:E:18:VAL:HG13  | 13:E:25:VAL:HG13 | 2.02                     | 0.41              |
| 17:I:61:PRO:HB3   | 17:I:80:PHE:CE2  | 2.55                     | 0.41              |
| 18:J:39:ILE:HG12  | 18:J:62:CYS:HA   | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:H:138:VAL:CG2  | 19:K:44:LEU:O     | 2.57                     | 0.41              |
| 20:L:75:LEU:HD12  | 20:L:133:LYS:HD2  | 2.02                     | 0.41              |
| 1:1:234:G:H4'     | 31:W:58:GLY:HA2   | 2.01                     | 0.41              |
| 31:W:79:ILE:O     | 31:W:82:VAL:HG12  | 2.20                     | 0.41              |
| 11:C:138:SER:HB2  | 34:Z:16:SER:HB2   | 2.01                     | 0.41              |
| 1:1:1586:U:H2'    | 1:1:1587:G:H5'    | 2.01                     | 0.41              |
| 1:1:1729:A:N3     | 1:1:1730:A:N7     | 2.65                     | 0.41              |
| 1:1:547:U:C5      | 1:1:1393:A:N6     | 2.86                     | 0.41              |
| 1:1:664:C:N4      | 1:1:665:C:N4      | 2.68                     | 0.41              |
| 1:1:955:A2M:H1'   | 1:1:955:A2M:HM'3  | 1.83                     | 0.41              |
| 2:2:1004:G:H2'    | 2:2:1005:G:O4'    | 2.19                     | 0.41              |
| 2:2:1175:A:OP1    | 2:2:1175:A:H8     | 2.03                     | 0.41              |
| 2:2:533:C:N4      | 2:2:544:U:C4      | 2.88                     | 0.41              |
| 2:2:657:U:H2'     | 2:2:658:G:O4'     | 2.19                     | 0.41              |
| 2:2:695:G:N7      | 2:2:697:G:H5"     | 2.34                     | 0.41              |
| 3:3:207:G:H2'     | 3:3:208:G:H8      | 1.83                     | 0.41              |
| 3:3:37:A:H2'      | 3:3:38:A:H8       | 1.85                     | 0.41              |
| 7:7:167:C:H5"     | 15:G:266:LYS:HG3  | 2.01                     | 0.41              |
| 8:8:66:A:O2'      | 8:8:67:G:OP1      | 2.25                     | 0.41              |
| 10:B:265:VAL:HG11 | 10:B:271:ARG:HH21 | 1.85                     | 0.41              |
| 13:E:139:VAL:HG11 | 13:E:142:GLU:HB2  | 2.03                     | 0.41              |
| 21:M:123:MET:SD   | 21:M:128:LYS:NZ   | 2.94                     | 0.41              |
| 26:R:93:VAL:HG13  | 26:R:94:LYS:N     | 2.35                     | 0.41              |
| 1:1:1445:U:O2     | 34:Z:26:ARG:NH1   | 2.53                     | 0.41              |
| 1:1:1353:A:H2'    | 1:1:1354:C:O4'    | 2.20                     | 0.41              |
| 1:1:1611:A:OP2    | 1:1:1611:A:H8     | 2.03                     | 0.41              |
| 1:1:1617:C:H2'    | 1:1:1619:C:C5     | 2.55                     | 0.41              |
| 1:1:491:A:C2      | 1:1:644:G:N2      | 2.88                     | 0.41              |
| 1:1:512:U:OP2     | 1:1:513:C:N4      | 2.53                     | 0.41              |
| 1:1:658:G:OP2     | 1:1:658:G:H8      | 2.04                     | 0.41              |
| 2:2:602:A:N1      | 2:2:1422:C:H5     | 2.18                     | 0.41              |
| 2:2:4:C:H2'       | 2:2:5:A:C8        | 2.55                     | 0.41              |
| 3:3:208:G:C6      | 3:3:209:G:C6      | 3.08                     | 0.41              |
| 4:4:90:G:H2'      | 4:4:91:U:O4'      | 2.20                     | 0.41              |
| 6:6:13:C:C2'      | 6:6:14:A:H2'      | 2.46                     | 0.41              |
| 8:8:77:G:N2       | 8:8:101:G:H2'     | 2.36                     | 0.41              |
| 10:B:102:ILE:HG13 | 10:B:153:PHE:HE1  | 1.86                     | 0.41              |
| 10:B:97:VAL:HG23  | 10:B:100:LYS:HE2  | 2.02                     | 0.41              |
| 11:C:93:ASN:ND2   | 11:C:101:PHE:HB2  | 2.35                     | 0.41              |
| 11:C:40:HIS:CD2   | 11:C:236:LEU:HA   | 2.55                     | 0.41              |
| 11:C:272:LYS:HB3  | 11:C:275:PHE:HB3  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 13:E:27:VAL:HG11 | 13:E:80:ILE:HA      | 2.03                     | 0.41              |
| 16:H:108:ARG:HG3 | 16:H:109:TYR:CD2    | 2.54                     | 0.41              |
| 16:H:75:TYR:CE2  | 16:H:90:HIS:HD2     | 2.38                     | 0.41              |
| 17:I:33:GLN:N    | 17:I:34:PRO:HD2     | 2.35                     | 0.41              |
| 18:J:28:ALA:HB2  | 18:J:82:ARG:HH22    | 1.84                     | 0.41              |
| 16:H:148:TYR:CB  | 19:K:59:MET:CB      | 2.97                     | 0.41              |
| 11:C:113:LYS:HG3 | 21:M:203:LYS:HB3    | 2.01                     | 0.41              |
| 21:M:36:VAL:HG22 | 21:M:64:VAL:HG22    | 2.02                     | 0.41              |
| 23:O:201:HIS:O   | 23:O:205:ILE:N      | 2.52                     | 0.41              |
| 3:3:114:C:OP2    | 25:Q:110:ARG:NH1    | 2.53                     | 0.41              |
| 26:R:87:CYS:O    | 26:R:90:THR:HG23    | 2.20                     | 0.41              |
| 27:S:102:GLN:O   | 27:S:106:LYS:HG2    | 2.20                     | 0.41              |
| 1:1:1614:G:N2    | 28:T:129:THR:OG1    | 2.52                     | 0.41              |
| 28:T:41:LEU:HD21 | 28:T:99:GLU:CG      | 2.46                     | 0.41              |
| 31:W:53:VAL:HG12 | 31:W:103:ILE:HA     | 2.02                     | 0.41              |
| 33:Y:10:VAL:CG1  | 33:Y:85:TYR:HB2     | 2.51                     | 0.41              |
| 33:Y:44:ALA:HA   | 33:Y:71:PHE:O       | 2.19                     | 0.41              |
| 1:1:1146:A:H61   | 1:1:1147:A:N6       | 2.18                     | 0.41              |
| 1:1:1393:A:P     | 1:1:1393:A:H3'      | 2.60                     | 0.41              |
| 1:1:490:C:HO2'   | 6:6:54:A:H2         | 1.49                     | 0.41              |
| 1:1:491:A:N6     | 1:1:644:G:H1        | 2.13                     | 0.41              |
| 1:1:7:C:O2'      | 1:1:8:U:H5'         | 2.20                     | 0.41              |
| 2:2:1323:C:H2'   | 2:2:1324:C:C6       | 2.55                     | 0.41              |
| 2:2:372:A:H61    | 2:2:573:U:H3        | 1.68                     | 0.41              |
| 2:2:667:OMU:C6   | 2:2:667:OMU:H5'     | 2.36                     | 0.41              |
| 2:2:68:A:HO2'    | 2:2:69:A:P          | 2.39                     | 0.41              |
| 3:3:194:A:H1'    | 3:3:196:A:C8        | 2.55                     | 0.41              |
| 6:6:28:A:C1'     | 6:6:29:G:N7         | 2.77                     | 0.41              |
| 9:A:134:CYS:SG   | 9:A:150:LEU:HA      | 2.61                     | 0.41              |
| 2:2:403:G:C4     | 9:A:150:LEU:HD13    | 2.55                     | 0.41              |
| 10:B:193:VAL:O   | 10:B:197:ILE:HD12   | 2.21                     | 0.41              |
| 11:C:121:PHE:CE1 | 11:C:278[B]:PRO:HG2 | 2.55                     | 0.41              |
| 13:E:117:GLU:HG3 | 13:E:119:ARG:HG2    | 2.02                     | 0.41              |
| 1:1:139:C:H5''   | 15:G:191:ARG:NH2    | 2.36                     | 0.41              |
| 1:1:120:G:H1     | 15:G:222:GLN:NE2    | 2.18                     | 0.41              |
| 16:H:25:ILE:HG23 | 16:H:51:ILE:HG13    | 2.02                     | 0.41              |
| 1:1:87:A:O2'     | 20:L:60:HIS:O       | 2.36                     | 0.41              |
| 29:U:29:ASP:CG   | 29:U:30:CYS:H       | 2.23                     | 0.41              |
| 30:V:72:THR:H    | 30:V:75:ALA:HB3     | 1.85                     | 0.41              |
| 30:V:91:SER:HA   | 30:V:123:LYS:HB2    | 2.01                     | 0.41              |
| 31:W:13:ARG:O    | 31:W:17:PHE:HD2     | 2.02                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:W:37:ARG:HG3  | 31:W:38:ALA:H     | 1.86                     | 0.41              |
| 31:W:37:ARG:HH12 | 31:W:43:ARG:NH2   | 2.18                     | 0.41              |
| 1:1:1062:A:H4'   | 22:N:40:ARG:HA    | 2.00                     | 0.41              |
| 1:1:1224:A:H2'   | 1:1:1225:U:O4'    | 2.21                     | 0.41              |
| 1:1:12:U:H1'     | 1:1:13:G:H5'      | 2.01                     | 0.41              |
| 1:1:240:U:O2'    | 1:1:241:G:O5'     | 2.33                     | 0.41              |
| 1:1:98:A:H1'     | 1:1:318:G:N7      | 2.35                     | 0.41              |
| 1:1:537:G:N3     | 1:1:537:G:H2'     | 2.35                     | 0.41              |
| 1:1:679:A:H3'    | 1:1:680:C:H5''    | 2.01                     | 0.41              |
| 1:1:894:G:O2'    | 1:1:895:G:H5'     | 2.21                     | 0.41              |
| 2:2:519:G:H1'    | 2:2:520:U:H5      | 1.85                     | 0.41              |
| 2:2:608:C:C2     | 2:2:609:A:H1'     | 2.56                     | 0.41              |
| 2:2:749:G:O3'    | 2:2:749:G:P       | 2.79                     | 0.41              |
| 2:2:790:U:H2'    | 2:2:791:A:O4'     | 2.19                     | 0.41              |
| 6:6:34:C:C5      | 6:6:35:U:C4       | 3.08                     | 0.41              |
| 8:8:7:A:N6       | 8:8:117:A:C6      | 2.89                     | 0.41              |
| 9:A:104:LEU:HD12 | 9:A:107:ILE:HD12  | 2.03                     | 0.41              |
| 9:A:114:CYS:HB2  | 9:A:169:ILE:HG12  | 2.01                     | 0.41              |
| 9:A:209:HIS:NE2  | 9:A:235:VAL:HG21  | 2.35                     | 0.41              |
| 9:A:234:LYS:HG2  | 9:A:238:ILE:HG12  | 2.01                     | 0.41              |
| 9:A:74:GLU:HG3   | 9:A:76:MET:HG3    | 2.02                     | 0.41              |
| 10:B:122:TRP:CG  | 10:B:122:TRP:O    | 2.74                     | 0.41              |
| 10:B:219:ALA:HA  | 10:B:286:LYS:HA   | 2.02                     | 0.41              |
| 11:C:268:ALA:HA  | 11:C:276:THR:HG22 | 2.02                     | 0.41              |
| 4:4:52:A:C8      | 13:E:174:PHE:HB2  | 2.55                     | 0.41              |
| 16:H:28:ASP:N    | 16:H:137:VAL:O    | 2.53                     | 0.41              |
| 22:N:76:MET:HA   | 22:N:147:GLN:NE2  | 2.35                     | 0.41              |
| 33:Y:9:LYS:NZ    | 33:Y:86:ASN:HD21  | 2.19                     | 0.41              |
| 1:1:1043:C:O2'   | 1:1:1044:G:H5'    | 2.20                     | 0.41              |
| 1:1:1549:U:O2'   | 1:1:1550:C:H6     | 2.04                     | 0.41              |
| 1:1:1605:G:H2'   | 1:1:1606:U:C6     | 2.56                     | 0.41              |
| 1:1:281:G:H3'    | 1:1:282:C:H5''    | 2.02                     | 0.41              |
| 1:1:388:A:H4'    | 1:1:407:A:H61     | 1.82                     | 0.41              |
| 1:1:486:C:H1'    | 1:1:487:G:N7      | 2.36                     | 0.41              |
| 1:1:566:G:H2'    | 1:1:567:G:C8      | 2.56                     | 0.41              |
| 1:1:569:G:N2     | 1:1:570:A:C4      | 2.88                     | 0.41              |
| 1:1:661:G:H2'    | 1:1:662:C:C6      | 2.55                     | 0.41              |
| 1:1:682:C:H2'    | 1:1:683:G:C8      | 2.54                     | 0.41              |
| 1:1:728:C:H1'    | 1:1:730:G:C5      | 2.56                     | 0.41              |
| 1:1:770:G:OP1    | 1:1:770:G:H2'     | 2.20                     | 0.41              |
| 2:2:1248:C:O5'   | 2:2:1248:C:H6     | 2.04                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:2:1387:C:H4'   | 10:B:247:THR:HG23 | 2.02                     | 0.41              |
| 2:2:1426:A:H2'   | 2:2:1427:C:O4'    | 2.20                     | 0.41              |
| 2:2:424:U:H1'    | 2:2:426:G:C5      | 2.56                     | 0.41              |
| 1:1:922:U:H1'    | 2:2:570:A:H1'     | 2.02                     | 0.41              |
| 2:2:742:U:H2'    | 2:2:743:C:O4'     | 2.21                     | 0.41              |
| 2:2:972:A:O4'    | 15:G:123:GLN:NE2  | 2.53                     | 0.41              |
| 4:4:96:C:OP1     | 25:Q:58:HIS:HA    | 2.21                     | 0.41              |
| 5:5:26:A:O3'     | 5:5:27:U:H4'      | 2.21                     | 0.41              |
| 6:6:31:U:C3'     | 6:6:31:U:C6       | 3.04                     | 0.41              |
| 6:6:40:C:H5''    | 6:6:41:G:N7       | 2.35                     | 0.41              |
| 6:6:59:C:C5'     | 6:6:59:C:H6       | 2.32                     | 0.41              |
| 7:7:122:A:H3'    | 7:7:123:G:C8      | 2.56                     | 0.41              |
| 10:B:224:SER:OG  | 10:B:336:SER:HB2  | 2.20                     | 0.41              |
| 14:F:29:LEU:HG   | 14:F:56:GLN:OE1   | 2.20                     | 0.41              |
| 19:K:40:TYR:HD2  | 19:K:42:VAL:HG13  | 1.86                     | 0.41              |
| 20:L:109:LEU:HG  | 20:L:121:VAL:HG21 | 2.03                     | 0.41              |
| 20:L:56:LEU:HD23 | 24:P:180:THR:HG23 | 2.02                     | 0.41              |
| 20:L:61:TYR:OH   | 22:N:38:ARG:NH1   | 111.25                   | 0.41              |
| 21:M:19:MET:O    | 21:M:23:GLN:HG2   | 2.20                     | 0.41              |
| 22:N:184:LEU:O   | 22:N:188:GLY:N    | 2.54                     | 0.41              |
| 3:3:112:C:OP1    | 25:Q:118:HIS:HB2  | 2.20                     | 0.41              |
| 27:S:48:VAL:O    | 27:S:49:ARG:HG2   | 2.21                     | 0.41              |
| 28:T:3:HIS:HD2   | 28:T:4:TYR:HB2    | 1.84                     | 0.41              |
| 28:T:24:CYS:HB3  | 28:T:86:LYS:HE2   | 2.03                     | 0.41              |
| 1:1:1525:A:O2'   | 1:1:1526:OMG:P    | 2.79                     | 0.41              |
| 1:1:685:A:H5'    | 2:2:606:G:H2'     | 2.02                     | 0.41              |
| 1:1:841:U:H2'    | 1:1:842:G:H8      | 1.86                     | 0.41              |
| 1:1:882:A:H2'    | 1:1:883:G:O4'     | 2.20                     | 0.41              |
| 2:2:1001:U:H2'   | 2:2:1002:C:C6     | 2.56                     | 0.41              |
| 2:2:686:G:H2'    | 2:2:687:C:C6      | 2.56                     | 0.41              |
| 2:2:70:A:C2'     | 2:2:71:OMG:C5'    | 2.86                     | 0.41              |
| 2:2:756:C:H2'    | 2:2:757:A:C8      | 2.55                     | 0.41              |
| 2:2:775:C:OP1    | 15:G:332:ARG:NH1  | 2.47                     | 0.41              |
| 3:3:57:U:C6      | 3:3:58:C:N4       | 2.89                     | 0.41              |
| 3:3:63:C:H5''    | 25:Q:58:HIS:O     | 2.20                     | 0.41              |
| 6:6:13:C:C4      | 6:6:14:A:C6       | 3.09                     | 0.41              |
| 6:6:4:U:C2'      | 6:6:4:U:O2        | 2.68                     | 0.41              |
| 6:6:8:A:O2'      | 6:6:9:U:P         | 2.78                     | 0.41              |
| 7:7:7:OMU:HM22   | 7:7:7:OMU:H4'     | 2.02                     | 0.41              |
| 8:8:67:G:H3'     | 8:8:68:G:H8       | 1.86                     | 0.41              |
| 8:8:7:A:O2'      | 8:8:8:C:P         | 2.79                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:63:PHE:HE2    | 9:A:76:MET:HE3    | 1.85                     | 0.41              |
| 10:B:199:LEU:HG   | 10:B:203:LEU:HD22 | 2.03                     | 0.41              |
| 10:B:49:PHE:CD1   | 10:B:342:VAL:CG2  | 3.04                     | 0.41              |
| 4:4:66:C:H4'      | 10:B:64:GLY:HA3   | 2.02                     | 0.41              |
| 11:C:178:ASP:HA   | 11:C:181:ARG:HG2  | 2.03                     | 0.41              |
| 11:C:250:TRP:CH2  | 11:C:258:LEU:HD11 | 2.56                     | 0.41              |
| 11:C:32:ARG:NH2   | 11:C:34:ASP:OD2   | 2.52                     | 0.41              |
| 15:G:237:VAL:HG12 | 15:G:271:LEU:HD21 | 2.01                     | 0.41              |
| 15:G:296:LEU:O    | 15:G:300:ILE:HD12 | 2.20                     | 0.41              |
| 1:1:1369:G:C4     | 16:H:78:LYS:HD3   | 2.55                     | 0.41              |
| 17:I:32:ASN:O     | 17:I:36:GLN:HG2   | 2.20                     | 0.41              |
| 17:I:61:PRO:HB3   | 17:I:80:PHE:CD2   | 2.55                     | 0.41              |
| 19:K:115:GLU:HA   | 19:K:116:PRO:HD3  | 1.93                     | 0.41              |
| 19:K:73:ILE:HG23  | 19:K:113:ASN:O    | 2.20                     | 0.41              |
| 22:N:22:PHE:HD2   | 22:N:23:CYS:HG    | 1.68                     | 0.41              |
| 27:S:29:THR:HA    | 27:S:32:THR:HG23  | 2.03                     | 0.41              |
| 28:T:31:GLU:HG2   | 28:T:61:LYS:H     | 1.85                     | 0.41              |
| 28:T:6:ARG:HH21   | 28:T:116:HIS:CG   | 2.38                     | 0.41              |
| 29:U:49:GLN:O     | 29:U:53:ASP:N     | 2.28                     | 0.41              |
| 30:V:130:SER:C    | 30:V:132:ALA:H    | 2.22                     | 0.41              |
| 1:1:552:G:H3'     | 1:1:553:A:O4'     | 2.21                     | 0.41              |
| 1:1:688:A:H2'     | 1:1:689:A:C8      | 2.56                     | 0.41              |
| 1:1:819:C:H2'     | 1:1:820:U:C4'     | 2.51                     | 0.41              |
| 2:2:1317:G:H2'    | 2:2:1317:G:N3     | 2.36                     | 0.41              |
| 2:2:1333:C:H2'    | 2:2:1334:G:O4'    | 2.21                     | 0.41              |
| 2:2:1409:C:H5''   | 2:2:1410:A:C6     | 2.56                     | 0.41              |
| 2:2:69:A:N1       | 2:2:636:A:O2'     | 2.54                     | 0.41              |
| 2:2:707:A:O2'     | 2:2:708:G:H5''    | 2.21                     | 0.41              |
| 3:3:23:C:H42      | 3:3:208:G:H1      | 1.69                     | 0.41              |
| 5:5:3:C:H2'       | 5:5:4:G:O4'       | 2.20                     | 0.41              |
| 6:6:28:A:O3'      | 6:6:29:G:H2'      | 2.21                     | 0.41              |
| 6:6:8:A:O2'       | 6:6:9:U:OP1       | 2.35                     | 0.41              |
| 7:7:27:U:H2'      | 7:7:28:C:O4'      | 2.21                     | 0.41              |
| 11:C:142:ARG:HG3  | 11:C:181:ARG:HD2  | 2.02                     | 0.41              |
| 4:4:52:A:H2'      | 13:E:96:ALA:HB3   | 2.02                     | 0.41              |
| 7:7:166:U:OP1     | 15:G:148:ARG:NE   | 2.54                     | 0.41              |
| 16:H:65:GLU:OE2   | 16:H:163:HIS:ND1  | 2.53                     | 0.41              |
| 18:J:22:GLY:HA2   | 18:J:37:TYR:CZ    | 2.56                     | 0.41              |
| 21:M:14:LYS:HD3   | 21:M:120:TRP:CZ3  | 2.55                     | 0.41              |
| 28:T:61:LYS:HG2   | 28:T:78:GLN:HE22  | 1.85                     | 0.41              |
| 1:1:1380:A:H62    | 16:H:36:ARG:HD3   | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:248:A:C8      | 11:C:223:PHE:HB2  | 2.56                     | 0.41              |
| 1:1:480:U:H2'     | 1:1:481:U:C6      | 2.56                     | 0.41              |
| 1:1:491:A:H2'     | 1:1:492:G:H8      | 1.86                     | 0.41              |
| 1:1:694:U:C6      | 1:1:694:U:OP2     | 2.74                     | 0.41              |
| 1:1:716:A:H2'     | 1:1:717:G:O4'     | 2.20                     | 0.41              |
| 2:2:1160:OMC:H1'  | 2:2:1160:OMC:HM23 | 1.84                     | 0.41              |
| 2:2:1340:G:H5''   | 2:2:1341:A:OP2    | 2.20                     | 0.41              |
| 2:2:1436:A:H2     | 4:4:173:C:OP2     | 2.03                     | 0.41              |
| 2:2:382:A2M:H1'   | 2:2:382:A2M:HM'3  | 1.79                     | 0.41              |
| 2:2:411:C:H2'     | 2:2:413:A:OP2     | 2.21                     | 0.41              |
| 2:2:439:U:H1'     | 2:2:561:G:N2      | 2.35                     | 0.41              |
| 2:2:663:U:H5''    | 9:A:221:HIS:CE1   | 2.56                     | 0.41              |
| 2:2:870:C:N4      | 2:2:940:G:O6      | 2.54                     | 0.41              |
| 2:2:982:C:H2'     | 2:2:983:G:C8      | 2.56                     | 0.41              |
| 3:3:55:U:O2'      | 3:3:58:C:N4       | 2.53                     | 0.41              |
| 4:4:174:A:N3      | 4:4:174:A:H2'     | 2.36                     | 0.41              |
| 5:5:107:G:H2'     | 5:5:108:C:O4'     | 2.21                     | 0.41              |
| 6:6:17:U:H1'      | 6:6:18:A:C4       | 2.55                     | 0.41              |
| 9:A:42:ARG:NH1    | 9:A:87:SER:OG     | 2.53                     | 0.41              |
| 10:B:84:MET:HE2   | 10:B:164:ALA:HB3  | 2.02                     | 0.41              |
| 10:B:261:HIS:HA   | 10:B:262:PRO:C    | 2.40                     | 0.41              |
| 16:H:106:LEU:HD12 | 16:H:107:PRO:HD2  | 2.03                     | 0.41              |
| 16:H:55:ARG:HG2   | 16:H:125:GLY:HA2  | 2.03                     | 0.41              |
| 21:M:101:VAL:O    | 21:M:105:ARG:HG2  | 2.21                     | 0.41              |
| 21:M:124:ASP:OD1  | 21:M:127:PHE:N    | 2.25                     | 0.41              |
| 2:2:1268:U:OP1    | 22:N:5:PRO:HD3    | 2.20                     | 0.41              |
| 23:O:21:ARG:O     | 23:O:21:ARG:HD3   | 2.21                     | 0.41              |
| 24:P:153:ARG:HG2  | 24:P:155:SER:H    | 1.86                     | 0.41              |
| 24:P:79:ALA:C     | 24:P:81:SER:H     | 2.24                     | 0.41              |
| 25:Q:50:ILE:HG22  | 25:Q:50:ILE:O     | 2.21                     | 0.41              |
| 1:1:1114:A:H4'    | 1:1:1115:C:H5'    | 2.02                     | 0.41              |
| 1:1:1157:U:H2'    | 1:1:1158:U:C6     | 2.56                     | 0.41              |
| 1:1:1169:A:H3'    | 1:1:1170:G:H8     | 1.86                     | 0.41              |
| 1:1:1417:G:H2'    | 1:1:1418:G:O4'    | 2.20                     | 0.41              |
| 1:1:1583:U:H2'    | 1:1:1584:A:O4'    | 2.21                     | 0.41              |
| 1:1:175:G:O6      | 1:1:176:C:N4      | 2.54                     | 0.41              |
| 1:1:181:G:N1      | 1:1:273:A:N6      | 2.69                     | 0.41              |
| 1:1:203:C:H2'     | 1:1:204:A:O4'     | 2.21                     | 0.41              |
| 1:1:226:C:N4      | 1:1:227:U:C2      | 2.89                     | 0.41              |
| 1:1:159:U:H1'     | 1:1:297:A:C2      | 2.56                     | 0.41              |
| 1:1:685:A:H5''    | 2:2:607:A:H5'     | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:745:U:H5''    | 1:1:830:G:H1'     | 2.02                     | 0.41              |
| 1:1:905:G:H4'     | 25:Q:130:ASN:ND2  | 2.34                     | 0.41              |
| 1:1:959:OMG:N2    | 21:M:76:HIS:CB    | 2.84                     | 0.41              |
| 2:2:1446:A:H3'    | 16:H:129:ASN:HD22 | 1.86                     | 0.41              |
| 2:2:83:G:O2'      | 2:2:580:U:O4      | 2.21                     | 0.41              |
| 2:2:739:C:C2'     | 2:2:740:A:H5'     | 2.51                     | 0.41              |
| 6:6:5:C:N4        | 6:6:6:G:N1        | 2.69                     | 0.41              |
| 7:7:91:A:H5''     | 7:7:92:C:OP2      | 2.21                     | 0.41              |
| 2:2:424:U:H5''    | 9:A:151:PRO:HG2   | 2.03                     | 0.41              |
| 11:C:290:ILE:HB   | 24:P:135:MET:HE1  | 2.03                     | 0.41              |
| 13:E:159:VAL:O    | 13:E:163:MET:N    | 2.52                     | 0.41              |
| 13:E:23:ARG:HH22  | 13:E:45:LEU:HD13  | 1.86                     | 0.41              |
| 13:E:54:PHE:CD2   | 13:E:76:VAL:HG21  | 2.56                     | 0.41              |
| 18:J:111:MET:SD   | 18:J:111:MET:O    | 2.79                     | 0.41              |
| 18:J:118:GLY:O    | 18:J:136:PRO:HD2  | 2.21                     | 0.41              |
| 16:H:146:VAL:CG1  | 19:K:55:ALA:HB3   | 2.34                     | 0.41              |
| 27:S:28:SER:O     | 27:S:32:THR:HG23  | 2.20                     | 0.41              |
| 31:W:37:ARG:HB2   | 31:W:42:VAL:O     | 2.21                     | 0.41              |
| 1:1:1392:G:O2'    | 1:1:1393:A:P      | 2.79                     | 0.41              |
| 1:1:1773:U:H2'    | 1:1:1774:G:H8     | 1.84                     | 0.41              |
| 1:1:187:A:N6      | 1:1:266:G:H2'     | 2.36                     | 0.41              |
| 1:1:458:A:H3'     | 1:1:459:A:H4'     | 2.02                     | 0.41              |
| 1:1:898:A:H2'     | 1:1:899:A:N7      | 2.35                     | 0.41              |
| 2:2:1078:OMU:HM22 | 2:2:1079:OMG:O4'  | 2.20                     | 0.41              |
| 2:2:1228:C:C2'    | 2:2:1229:A:H5'    | 2.51                     | 0.41              |
| 2:2:443:OMC:HN42  | 2:2:488:A:P       | 2.43                     | 0.41              |
| 2:2:496:G:N2      | 2:2:514:U:O4'     | 2.55                     | 0.41              |
| 2:2:534:OMG:H2'   | 2:2:535:U:C5      | 2.57                     | 0.41              |
| 1:1:967:G:O6      | 2:2:660:G:O2'     | 2.39                     | 0.41              |
| 3:3:93:G:O5'      | 3:3:93:G:H8       | 2.04                     | 0.41              |
| 4:4:60:A:N3       | 4:4:60:A:H2'      | 2.36                     | 0.41              |
| 5:5:112:A:H3'     | 5:5:114:A:O4'     | 2.21                     | 0.41              |
| 6:6:42:A:H1'      | 6:6:43:A:C8       | 2.56                     | 0.41              |
| 7:7:67:U:O2'      | 7:7:68:A:H8       | 2.04                     | 0.41              |
| 8:8:12:C:O2       | 8:8:15:A:N1       | 2.54                     | 0.41              |
| 8:8:20:A:H2'      | 8:8:21:G:C8       | 2.56                     | 0.41              |
| 9:A:146:THR:N     | 9:A:158:VAL:O     | 2.54                     | 0.41              |
| 10:B:171:LEU:HA   | 10:B:326:ASN:HD21 | 1.86                     | 0.41              |
| 11:C:43:MET:CB    | 11:C:236:LEU:HD11 | 2.50                     | 0.41              |
| 14:F:182:PHE:CZ   | 14:F:195:TRP:HH2  | 2.38                     | 0.41              |
| 15:G:228:ILE:HG23 | 15:G:260:ILE:HD13 | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:H:25:ILE:O     | 16:H:25:ILE:HG23  | 2.21                     | 0.41              |
| 20:L:19:TYR:CB    | 20:L:25:HIS:HB2   | 2.51                     | 0.41              |
| 27:S:92:ARG:HB2   | 27:S:94:GLU:OE2   | 2.21                     | 0.41              |
| 1:1:12:U:H4'      | 30:V:42:ARG:CD    | 2.50                     | 0.41              |
| 34:Z:108:PHE:O    | 34:Z:112:ARG:HG3  | 2.21                     | 0.41              |
| 1:1:1039:U:H2'    | 1:1:1040:G:O4'    | 2.20                     | 0.40              |
| 1:1:17:C:H2'      | 1:1:18:A:C8       | 2.56                     | 0.40              |
| 1:1:292:A:C6      | 1:1:293:C:H1'     | 2.56                     | 0.40              |
| 1:1:487:G:H5''    | 1:1:488:G:OP2     | 2.21                     | 0.40              |
| 1:1:838:G:H5'     | 24:P:154:GLU:CD   | 2.42                     | 0.40              |
| 1:1:911:G:O2'     | 1:1:946:G:H4'     | 2.21                     | 0.40              |
| 1:1:36:OMU:HM23   | 1:1:94:A:O2'      | 2.15                     | 0.40              |
| 2:2:1078:OMU:O2'  | 2:2:1079:OMG:H5'  | 2.21                     | 0.40              |
| 2:2:1158:U:P      | 24:P:164:VAL:HG13 | 2.61                     | 0.40              |
| 2:2:1271:C:H2'    | 2:2:1272:G:H8     | 1.87                     | 0.40              |
| 2:2:382:A2M:O5'   | 2:2:382:A2M:H8    | 2.21                     | 0.40              |
| 2:2:536:C:O2      | 2:2:548:G:N2      | 2.41                     | 0.40              |
| 2:2:747:A:C6      | 2:2:749:G:C5      | 3.09                     | 0.40              |
| 2:2:779:U:H1'     | 15:G:332:ARG:HD3  | 2.02                     | 0.40              |
| 2:2:867:G:N2      | 2:2:942:G:O6      | 2.48                     | 0.40              |
| 3:3:117:G:O2'     | 3:3:118:U:OP1     | 2.36                     | 0.40              |
| 3:3:3:G:H2'       | 3:3:4:U:H6        | 1.87                     | 0.40              |
| 8:8:113:C:H2'     | 8:8:114:C:C6      | 2.56                     | 0.40              |
| 2:2:419:G:H5''    | 9:A:18:VAL:H      | 1.86                     | 0.40              |
| 13:E:114:PHE:CE2  | 13:E:115:LEU:HD23 | 2.56                     | 0.40              |
| 17:I:125:MET:HA   | 17:I:125:MET:HE2  | 2.03                     | 0.40              |
| 17:I:94:TYR:O     | 17:I:97:THR:HG22  | 2.20                     | 0.40              |
| 17:I:71:ASN:OD1   | 20:L:124:ARG:NH2  | 2.54                     | 0.40              |
| 21:M:177:LYS:HG2  | 21:M:185:ARG:NH2  | 2.36                     | 0.40              |
| 26:R:29:PHE:CE1   | 26:R:43:PHE:HD1   | 2.39                     | 0.40              |
| 30:V:75:ALA:HB1   | 30:V:86:THR:OG1   | 2.21                     | 0.40              |
| 1:1:1542:OMG:HM23 | 1:1:1542:OMG:H1'  | 1.87                     | 0.40              |
| 1:1:278:U:C2      | 1:1:279:G:N7      | 2.89                     | 0.40              |
| 1:1:450:G:N2      | 1:1:1534:U:H4'    | 2.36                     | 0.40              |
| 1:1:508:A:H2'     | 1:1:509:U:C6      | 2.56                     | 0.40              |
| 2:2:1078:OMU:H4'  | 2:2:1186:A2M:C2   | 2.51                     | 0.40              |
| 2:2:114:A:C8      | 2:2:116:A:H1'     | 2.57                     | 0.40              |
| 2:2:1167:A:H2'    | 2:2:1168:G:C8     | 2.57                     | 0.40              |
| 2:2:1369:A:H2'    | 2:2:1370:C:C6     | 2.56                     | 0.40              |
| 2:2:364:G:H2'     | 2:2:365:G:O4'     | 2.22                     | 0.40              |
| 3:3:104:U:OP1     | 33:Y:76:ASN:ND2   | 2.46                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:208:G:O6      | 3:3:209:G:C6      | 2.75                     | 0.40              |
| 4:4:113:G:OP1     | 32:X:38:PRO:HG2   | 2.21                     | 0.40              |
| 8:8:3:G:C6        | 8:8:4:A:C4        | 3.09                     | 0.40              |
| 9:A:14:SER:OG     | 9:A:15:VAL:N      | 2.55                     | 0.40              |
| 10:B:310:LYS:HE2  | 10:B:368:THR:HG23 | 2.03                     | 0.40              |
| 10:B:93:ARG:O     | 10:B:99:LEU:HA    | 2.22                     | 0.40              |
| 11:C:58:GLY:O     | 11:C:91:PHE:HB3   | 2.21                     | 0.40              |
| 14:F:53:ILE:HG13  | 14:F:65:VAL:HG12  | 2.03                     | 0.40              |
| 15:G:129:ARG:O    | 15:G:131:LEU:HD12 | 2.22                     | 0.40              |
| 1:1:147:G:N7      | 15:G:222:GLN:HG2  | 2.37                     | 0.40              |
| 15:G:235:MET:HG2  | 15:G:300:ILE:HG13 | 2.03                     | 0.40              |
| 15:G:312:ASP:O    | 15:G:316:ARG:HG2  | 2.22                     | 0.40              |
| 17:I:128:LEU:CD2  | 17:I:130:LEU:HB2  | 2.50                     | 0.40              |
| 17:I:65:CYS:HA    | 17:I:66:PRO:HD3   | 1.90                     | 0.40              |
| 2:2:1156:A:C2     | 20:L:43:ILE:HG23  | 2.56                     | 0.40              |
| 1:1:1445:U:C2     | 34:Z:26:ARG:NH1   | 2.89                     | 0.40              |
| 1:1:1102:U:HO2'   | 1:1:1103:U:P      | 2.43                     | 0.40              |
| 1:1:1422:A:H2'    | 1:1:1422:A:N3     | 2.35                     | 0.40              |
| 1:1:1466:G:N3     | 1:1:1466:G:H2'    | 2.36                     | 0.40              |
| 1:1:1677:A:P      | 1:1:1677:A:H8     | 2.44                     | 0.40              |
| 1:1:435:G:H2'     | 1:1:437:A:H2      | 1.87                     | 0.40              |
| 1:1:478:C:H2'     | 1:1:479:A:H8      | 1.85                     | 0.40              |
| 1:1:53:G:H4'      | 21:M:108:LYS:NZ   | 2.36                     | 0.40              |
| 1:1:927:A2M:H1'   | 1:1:927:A2M:HM'3  | 1.84                     | 0.40              |
| 2:2:740:A:H8      | 2:2:740:A:OP2     | 2.03                     | 0.40              |
| 3:3:134:C:H2'     | 3:3:135:U:O4'     | 2.21                     | 0.40              |
| 8:8:37:C:N3       | 8:8:48:G:C1'      | 2.84                     | 0.40              |
| 10:B:203:LEU:HD12 | 10:B:208:VAL:HG22 | 2.04                     | 0.40              |
| 1:1:856:OMG:OP1   | 11:C:76:PRO:HD3   | 2.21                     | 0.40              |
| 13:E:42:GLN:HB3   | 13:E:58:ARG:HB2   | 2.03                     | 0.40              |
| 14:F:75:PRO:HA    | 14:F:154:GLN:HE22 | 1.86                     | 0.40              |
| 15:G:158:PRO:HD3  | 15:G:318:TRP:CE2  | 2.56                     | 0.40              |
| 16:H:53:VAL:HG21  | 16:H:98:PHE:CE2   | 2.56                     | 0.40              |
| 17:I:16:HIS:CD2   | 17:I:23:GLN:HG3   | 2.57                     | 0.40              |
| 17:I:52:PHE:CG    | 17:I:53:PRO:HA    | 2.57                     | 0.40              |
| 20:L:53:PHE:O     | 24:P:182:ARG:HB3  | 2.21                     | 0.40              |
| 21:M:135:VAL:HG21 | 21:M:148:ILE:HD11 | 2.03                     | 0.40              |
| 7:7:146:U:H4'     | 30:V:51:ASN:HB2   | 2.03                     | 0.40              |
| 1:1:801:G:H21     | 1:1:1027:U:H4'    | 1.86                     | 0.40              |
| 1:1:11:G:C6       | 1:1:12:U:O4       | 2.74                     | 0.40              |
| 1:1:140:U:OP2     | 15:G:188:LYS:HD3  | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:1548:A:N6     | 1:1:1584:A:O2'    | 2.53                     | 0.40              |
| 1:1:184:G:C6      | 1:1:185:C:C4      | 3.09                     | 0.40              |
| 1:1:708:A:C5      | 24:P:94:LEU:HD21  | 2.57                     | 0.40              |
| 1:1:841:U:H2'     | 1:1:842:G:C8      | 2.57                     | 0.40              |
| 2:2:1286:A:O2'    | 2:2:1345:C:H4'    | 2.22                     | 0.40              |
| 2:2:1329:C:O2'    | 2:2:1372:G:N3     | 2.54                     | 0.40              |
| 2:2:449:U:H4'     | 9:A:241:ARG:CB    | 2.50                     | 0.40              |
| 2:2:476:C:N4      | 2:2:477:G:C2      | 2.90                     | 0.40              |
| 2:2:490:A:O4'     | 9:A:243:THR:CG2   | 2.67                     | 0.40              |
| 2:2:556:U:O5'     | 2:2:556:U:H6      | 2.04                     | 0.40              |
| 2:2:666:C:H6      | 2:2:666:C:OP2     | 2.05                     | 0.40              |
| 2:2:677:C:O2      | 2:2:1026:G:N2     | 2.46                     | 0.40              |
| 7:7:67:U:O2'      | 7:7:68:A:H5'      | 2.21                     | 0.40              |
| 8:8:45:U:C4       | 8:8:46:U:C4       | 3.09                     | 0.40              |
| 11:C:153:VAL:HG11 | 11:C:169:PHE:HZ   | 1.87                     | 0.40              |
| 13:E:18:VAL:HG12  | 13:E:47:VAL:HG21  | 2.03                     | 0.40              |
| 16:H:65:GLU:HA    | 16:H:155:THR:HG21 | 2.03                     | 0.40              |
| 17:I:114:MET:O    | 17:I:118:VAL:HG23 | 2.21                     | 0.40              |
| 18:J:98:GLU:HG2   | 32:X:23:PRO:HA    | 2.02                     | 0.40              |
| 2:2:1276:A:H4'    | 22:N:154:ARG:NH1  | 2.36                     | 0.40              |
| 22:N:50:ILE:HG22  | 22:N:167:MET:HA   | 2.03                     | 0.40              |
| 30:V:118:ARG:C    | 30:V:120:ASP:H    | 2.25                     | 0.40              |
| 32:X:46:ARG:HD2   | 32:X:48:LYS:HE2   | 2.03                     | 0.40              |
| 1:1:1149:G:H5'    | 1:1:1150:A:OP2    | 2.22                     | 0.40              |
| 1:1:130:U:H3'     | 1:1:131:U:C5'     | 2.50                     | 0.40              |
| 1:1:136:G:H3'     | 1:1:136:G:P       | 2.61                     | 0.40              |
| 1:1:1394:U:C2'    | 1:1:1395:U:H5'    | 2.47                     | 0.40              |
| 1:1:1529:OMC:H1'  | 1:1:1529:OMC:HM23 | 1.83                     | 0.40              |
| 1:1:183:G:N3      | 1:1:272:U:H1'     | 2.36                     | 0.40              |
| 1:1:262:C:O3'     | 31:W:29:SER:OG    | 2.39                     | 0.40              |
| 1:1:693:G:H2'     | 20:L:8:CYS:SG     | 2.61                     | 0.40              |
| 1:1:708:A:O2'     | 1:1:837:A:N1      | 2.49                     | 0.40              |
| 1:1:87:A:H2'      | 1:1:88:G:O4'      | 2.21                     | 0.40              |
| 2:2:1152:U:H2'    | 2:2:1153:OMU:O4'  | 2.21                     | 0.40              |
| 2:2:531:C:OP2     | 2:2:532:U:O2'     | 2.30                     | 0.40              |
| 2:2:611:U:O2      | 2:2:628:A2M:H2    | 2.22                     | 0.40              |
| 3:3:202:A:H2'     | 3:3:203:A:O4'     | 2.22                     | 0.40              |
| 4:4:116:G:H2'     | 4:4:117:C:O4'     | 2.21                     | 0.40              |
| 4:4:135:C:H2'     | 4:4:136:G:C8      | 2.56                     | 0.40              |
| 6:6:49:C:O2'      | 6:6:49:C:O2       | 2.29                     | 0.40              |
| 7:7:164:U:H6      | 7:7:164:U:H2'     | 1.65                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 12:D:21:ILE:HA   | 12:D:128:ASP:O  | 2.21                     | 0.40              |
| 16:H:201:ARG:HG3 | 19:K:178:ARG:CD | 2.50                     | 0.40              |
| 19:K:106:ARG:NH1 | 26:R:71:LEU:O   | 2.54                     | 0.40              |
| 22:N:59:GLN:HG2  | 22:N:128:ARG:HA | 2.04                     | 0.40              |
| 26:R:11:VAL:HG21 | 26:R:39:ALA:HB1 | 2.04                     | 0.40              |
| 28:T:21:ASP:O    | 28:T:23:ARG:N   | 2.54                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 9   | A     | 245/260 (94%) | 220 (90%) | 25 (10%) | 0        | 100         | 100 |
| 10  | B     | 396/419 (94%) | 352 (89%) | 43 (11%) | 1 (0%)   | 46          | 79  |
| 11  | C     | 300/373 (80%) | 269 (90%) | 31 (10%) | 0        | 100         | 100 |
| 12  | D     | 159/188 (85%) | 136 (86%) | 23 (14%) | 0        | 100         | 100 |
| 13  | E     | 188/190 (99%) | 160 (85%) | 28 (15%) | 0        | 100         | 100 |
| 14  | F     | 134/195 (69%) | 112 (84%) | 22 (16%) | 0        | 100         | 100 |
| 15  | G     | 225/348 (65%) | 205 (91%) | 18 (8%)  | 2 (1%)   | 21          | 55  |
| 16  | H     | 200/222 (90%) | 175 (88%) | 24 (12%) | 1 (0%)   | 34          | 69  |
| 17  | I     | 130/220 (59%) | 120 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 18  | J     | 126/139 (91%) | 115 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 19  | K     | 154/233 (66%) | 136 (88%) | 17 (11%) | 1 (1%)   | 30          | 65  |
| 20  | L     | 142/145 (98%) | 127 (89%) | 15 (11%) | 0        | 100         | 100 |
| 21  | M     | 201/204 (98%) | 187 (93%) | 14 (7%)  | 0        | 100         | 100 |
| 22  | N     | 211/213 (99%) | 186 (88%) | 25 (12%) | 0        | 100         | 100 |
| 23  | O     | 229/305 (75%) | 205 (90%) | 24 (10%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 24  | P     | 194/198 (98%)   | 179 (92%)  | 15 (8%)   | 0        | 100         | 100 |
| 25  | Q     | 154/245 (63%)   | 141 (92%)  | 13 (8%)   | 0        | 100         | 100 |
| 26  | R     | 130/179 (73%)   | 104 (80%)  | 25 (19%)  | 1 (1%)   | 24          | 58  |
| 27  | S     | 149/159 (94%)   | 125 (84%)  | 22 (15%)  | 2 (1%)   | 15          | 44  |
| 28  | T     | 154/166 (93%)   | 127 (82%)  | 27 (18%)  | 0        | 100         | 100 |
| 29  | U     | 98/129 (76%)    | 81 (83%)   | 17 (17%)  | 0        | 100         | 100 |
| 30  | V     | 116/145 (80%)   | 99 (85%)   | 17 (15%)  | 0        | 100         | 100 |
| 31  | W     | 116/143 (81%)   | 106 (91%)  | 10 (9%)   | 0        | 100         | 100 |
| 32  | X     | 62/124 (50%)    | 59 (95%)   | 3 (5%)    | 0        | 100         | 100 |
| 33  | Y     | 130/134 (97%)   | 111 (85%)  | 19 (15%)  | 0        | 100         | 100 |
| 34  | Z     | 75/147 (51%)    | 65 (87%)   | 10 (13%)  | 0        | 100         | 100 |
| 35  | a     | 122/127 (96%)   | 105 (86%)  | 17 (14%)  | 0        | 100         | 100 |
| 36  | b     | 63/70 (90%)     | 53 (84%)   | 10 (16%)  | 0        | 100         | 100 |
| 37  | c     | 220/252 (87%)   | 190 (86%)  | 30 (14%)  | 0        | 100         | 100 |
| 38  | d     | 71/104 (68%)    | 63 (89%)   | 8 (11%)   | 0        | 100         | 100 |
| 39  | e     | 111/183 (61%)   | 92 (83%)   | 19 (17%)  | 0        | 100         | 100 |
| 40  | f     | 124/133 (93%)   | 110 (89%)  | 14 (11%)  | 0        | 100         | 100 |
| 41  | g     | 123/144 (85%)   | 112 (91%)  | 11 (9%)   | 0        | 100         | 100 |
| 42  | h     | 106/168 (63%)   | 91 (86%)   | 15 (14%)  | 0        | 100         | 100 |
| 43  | i     | 62/105 (59%)    | 57 (92%)   | 5 (8%)    | 0        | 100         | 100 |
| 44  | j     | 76/83 (92%)     | 68 (90%)   | 8 (10%)   | 0        | 100         | 100 |
| 45  | k     | 56/83 (68%)     | 52 (93%)   | 4 (7%)    | 0        | 100         | 100 |
| 46  | l     | 49/51 (96%)     | 46 (94%)   | 2 (4%)    | 1 (2%)   | 9           | 30  |
| 47  | m     | 88/92 (96%)     | 71 (81%)   | 16 (18%)  | 1 (1%)   | 17          | 50  |
| 48  | n     | 82/106 (77%)    | 66 (80%)   | 16 (20%)  | 0        | 100         | 100 |
| All | All   | 5771/7124 (81%) | 5078 (88%) | 683 (12%) | 10 (0%)  | 56          | 84  |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | G     | 132 | SER  |
| 26  | R     | 22  | PRO  |
| 27  | S     | 101 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | m     | 40  | SER  |
| 10  | B     | 380 | LYS  |
| 46  | l     | 46  | ARG  |
| 19  | K     | 46  | PRO  |
| 15  | G     | 116 | PRO  |
| 27  | S     | 80  | VAL  |
| 16  | H     | 94  | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 9   | A     | 188/204 (92%)  | 181 (96%)  | 7 (4%)   | 41          | 76  |
| 10  | B     | 296/352 (84%)  | 288 (97%)  | 8 (3%)   | 52          | 85  |
| 11  | C     | 222/302 (74%)  | 221 (100%) | 1 (0%)   | 92          | 98  |
| 12  | D     | 4/163 (2%)     | 4 (100%)   | 0        | 100         | 100 |
| 13  | E     | 172/172 (100%) | 169 (98%)  | 3 (2%)   | 68          | 92  |
| 14  | F     | 92/154 (60%)   | 91 (99%)   | 1 (1%)   | 80          | 95  |
| 15  | G     | 179/292 (61%)  | 173 (97%)  | 6 (3%)   | 44          | 78  |
| 16  | H     | 166/188 (88%)  | 164 (99%)  | 2 (1%)   | 78          | 95  |
| 17  | I     | 114/181 (63%)  | 110 (96%)  | 4 (4%)   | 43          | 77  |
| 18  | J     | 91/111 (82%)   | 88 (97%)   | 3 (3%)   | 45          | 79  |
| 19  | K     | 79/195 (40%)   | 68 (86%)   | 11 (14%) | 4           | 13  |
| 20  | L     | 105/115 (91%)  | 103 (98%)  | 2 (2%)   | 65          | 91  |
| 21  | M     | 179/180 (99%)  | 176 (98%)  | 3 (2%)   | 68          | 92  |
| 22  | N     | 178/179 (99%)  | 175 (98%)  | 3 (2%)   | 68          | 92  |
| 23  | O     | 103/242 (43%)  | 100 (97%)  | 3 (3%)   | 50          | 83  |
| 24  | P     | 149/164 (91%)  | 145 (97%)  | 4 (3%)   | 52          | 85  |
| 25  | Q     | 100/196 (51%)  | 98 (98%)   | 2 (2%)   | 63          | 90  |
| 26  | R     | 98/158 (62%)   | 96 (98%)   | 2 (2%)   | 63          | 90  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 27  | S     | 100/133 (75%)   | 100 (100%) | 0        | 100         | 100 |
| 28  | T     | 125/144 (87%)   | 125 (100%) | 0        | 100         | 100 |
| 29  | U     | 13/114 (11%)    | 13 (100%)  | 0        | 100         | 100 |
| 30  | V     | 86/124 (69%)    | 84 (98%)   | 2 (2%)   | 58          | 88  |
| 31  | W     | 87/122 (71%)    | 87 (100%)  | 0        | 100         | 100 |
| 32  | X     | 48/104 (46%)    | 46 (96%)   | 2 (4%)   | 36          | 71  |
| 33  | Y     | 70/115 (61%)    | 69 (99%)   | 1 (1%)   | 74          | 94  |
| 34  | Z     | 44/119 (37%)    | 44 (100%)  | 0        | 100         | 100 |
| 35  | a     | 99/117 (85%)    | 92 (93%)   | 7 (7%)   | 18          | 46  |
| 36  | b     | 48/58 (83%)     | 44 (92%)   | 4 (8%)   | 14          | 38  |
| 37  | c     | 168/209 (80%)   | 164 (98%)  | 4 (2%)   | 57          | 87  |
| 38  | d     | 47/90 (52%)     | 44 (94%)   | 3 (6%)   | 22          | 52  |
| 39  | e     | 79/156 (51%)    | 79 (100%)  | 0        | 100         | 100 |
| 40  | f     | 97/114 (85%)    | 95 (98%)   | 2 (2%)   | 61          | 90  |
| 41  | g     | 98/121 (81%)    | 96 (98%)   | 2 (2%)   | 63          | 90  |
| 42  | h     | 85/145 (59%)    | 84 (99%)   | 1 (1%)   | 78          | 95  |
| 43  | i     | 47/89 (53%)     | 44 (94%)   | 3 (6%)   | 22          | 52  |
| 44  | j     | 63/70 (90%)     | 60 (95%)   | 3 (5%)   | 31          | 66  |
| 45  | k     | 26/74 (35%)     | 25 (96%)   | 1 (4%)   | 40          | 74  |
| 46  | l     | 46/47 (98%)     | 44 (96%)   | 2 (4%)   | 35          | 70  |
| 47  | m     | 63/74 (85%)     | 58 (92%)   | 5 (8%)   | 15          | 40  |
| 48  | n     | 64/92 (70%)     | 63 (98%)   | 1 (2%)   | 70          | 93  |
| All | All   | 4118/5979 (69%) | 4010 (97%) | 108 (3%) | 57          | 86  |

All (108) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | A     | 16  | TYR  |
| 9   | A     | 30  | ARG  |
| 9   | A     | 42  | ARG  |
| 9   | A     | 73  | LYS  |
| 9   | A     | 115 | ASN  |
| 9   | A     | 190 | ARG  |
| 9   | A     | 193 | ARG  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 10  | B     | 10     | ARG  |
| 10  | B     | 173    | ASN  |
| 10  | B     | 174[A] | HIS  |
| 10  | B     | 174[B] | HIS  |
| 10  | B     | 227[A] | LYS  |
| 10  | B     | 227[B] | LYS  |
| 10  | B     | 249    | ARG  |
| 10  | B     | 339    | ARG  |
| 11  | C     | 139    | ARG  |
| 13  | E     | 23     | ARG  |
| 13  | E     | 58     | ARG  |
| 13  | E     | 172    | ARG  |
| 14  | F     | 192    | ARG  |
| 15  | G     | 133    | ARG  |
| 15  | G     | 161    | ASN  |
| 15  | G     | 240    | ASN  |
| 15  | G     | 253    | ASN  |
| 15  | G     | 256    | ARG  |
| 15  | G     | 334    | LYS  |
| 16  | H     | 103    | ARG  |
| 16  | H     | 108    | ARG  |
| 17  | I     | 18     | ASN  |
| 17  | I     | 39     | ARG  |
| 17  | I     | 72     | MET  |
| 17  | I     | 78     | ARG  |
| 18  | J     | 84     | ARG  |
| 18  | J     | 88     | ARG  |
| 18  | J     | 112    | LYS  |
| 19  | K     | 44     | LEU  |
| 19  | K     | 45     | SER  |
| 19  | K     | 50     | CYS  |
| 19  | K     | 72     | ARG  |
| 19  | K     | 74     | LEU  |
| 19  | K     | 78     | ARG  |
| 19  | K     | 95     | LEU  |
| 19  | K     | 106    | ARG  |
| 19  | K     | 107    | HIS  |
| 19  | K     | 180    | HIS  |
| 19  | K     | 185    | VAL  |
| 20  | L     | 4      | ARG  |
| 20  | L     | 112    | ASN  |
| 21  | M     | 60     | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | M     | 71  | ARG  |
| 21  | M     | 122 | ASN  |
| 22  | N     | 33  | ASN  |
| 22  | N     | 73  | ASN  |
| 22  | N     | 116 | ARG  |
| 23  | O     | 21  | ARG  |
| 23  | O     | 23  | ARG  |
| 23  | O     | 94  | ASN  |
| 24  | P     | 56  | ARG  |
| 24  | P     | 142 | ASN  |
| 24  | P     | 147 | ARG  |
| 24  | P     | 182 | ARG  |
| 25  | Q     | 47  | ASP  |
| 25  | Q     | 51  | ILE  |
| 26  | R     | 91  | ARG  |
| 26  | R     | 119 | ARG  |
| 30  | V     | 57  | SER  |
| 30  | V     | 92  | ARG  |
| 32  | X     | 37  | ARG  |
| 32  | X     | 60  | ARG  |
| 33  | Y     | 113 | ARG  |
| 35  | a     | 49  | ARG  |
| 35  | a     | 72  | MET  |
| 35  | a     | 88  | ARG  |
| 35  | a     | 107 | LYS  |
| 35  | a     | 110 | ARG  |
| 35  | a     | 111 | GLN  |
| 35  | a     | 112 | MET  |
| 36  | b     | 11  | ASN  |
| 36  | b     | 18  | ARG  |
| 36  | b     | 34  | ARG  |
| 36  | b     | 62  | ARG  |
| 37  | c     | 138 | ARG  |
| 37  | c     | 167 | ASN  |
| 37  | c     | 196 | ASN  |
| 37  | c     | 229 | ARG  |
| 38  | d     | 40  | ARG  |
| 38  | d     | 42  | LYS  |
| 38  | d     | 54  | ARG  |
| 40  | f     | 23  | TYR  |
| 40  | f     | 46  | ARG  |
| 41  | g     | 65  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | g     | 96  | ARG  |
| 42  | h     | 30  | LYS  |
| 43  | i     | 59  | ARG  |
| 43  | i     | 71  | ARG  |
| 43  | i     | 93  | MET  |
| 44  | j     | 22  | CYS  |
| 44  | j     | 33  | ARG  |
| 44  | j     | 73  | ARG  |
| 45  | k     | 40  | ARG  |
| 46  | l     | 5   | LYS  |
| 46  | l     | 34  | ARG  |
| 47  | m     | 28  | LYS  |
| 47  | m     | 44  | LYS  |
| 47  | m     | 56  | ARG  |
| 47  | m     | 58  | ASP  |
| 47  | m     | 60  | CYS  |
| 48  | n     | 45  | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | A     | 19  | HIS  |
| 9   | A     | 21  | HIS  |
| 9   | A     | 65  | HIS  |
| 9   | A     | 92  | GLN  |
| 9   | A     | 115 | ASN  |
| 9   | A     | 140 | ASN  |
| 9   | A     | 194 | ASN  |
| 9   | A     | 205 | ASN  |
| 10  | B     | 55  | HIS  |
| 10  | B     | 109 | HIS  |
| 10  | B     | 165 | HIS  |
| 10  | B     | 173 | ASN  |
| 10  | B     | 279 | HIS  |
| 10  | B     | 282 | GLN  |
| 10  | B     | 326 | ASN  |
| 10  | B     | 378 | GLN  |
| 11  | C     | 49  | GLN  |
| 11  | C     | 197 | ASN  |
| 11  | C     | 237 | HIS  |
| 13  | E     | 42  | GLN  |
| 13  | E     | 51  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | E     | 70  | ASN  |
| 13  | E     | 78  | ASN  |
| 13  | E     | 97  | HIS  |
| 13  | E     | 123 | GLN  |
| 13  | E     | 161 | HIS  |
| 14  | F     | 72  | ASN  |
| 14  | F     | 154 | GLN  |
| 15  | G     | 161 | ASN  |
| 15  | G     | 222 | GLN  |
| 16  | H     | 74  | GLN  |
| 16  | H     | 90  | HIS  |
| 16  | H     | 190 | GLN  |
| 17  | I     | 12  | HIS  |
| 17  | I     | 13  | GLN  |
| 17  | I     | 33  | GLN  |
| 17  | I     | 70  | HIS  |
| 17  | I     | 108 | ASN  |
| 18  | J     | 77  | ASN  |
| 18  | J     | 134 | HIS  |
| 19  | K     | 52  | GLN  |
| 19  | K     | 92  | ASN  |
| 19  | K     | 107 | HIS  |
| 19  | K     | 180 | HIS  |
| 20  | L     | 28  | HIS  |
| 20  | L     | 60  | HIS  |
| 20  | L     | 112 | ASN  |
| 21  | M     | 57  | GLN  |
| 21  | M     | 76  | HIS  |
| 21  | M     | 122 | ASN  |
| 22  | N     | 33  | ASN  |
| 22  | N     | 59  | GLN  |
| 22  | N     | 71  | GLN  |
| 22  | N     | 100 | ASN  |
| 22  | N     | 163 | GLN  |
| 22  | N     | 196 | HIS  |
| 23  | O     | 17  | GLN  |
| 23  | O     | 31  | HIS  |
| 23  | O     | 39  | GLN  |
| 23  | O     | 94  | ASN  |
| 24  | P     | 58  | ASN  |
| 24  | P     | 142 | ASN  |
| 24  | P     | 197 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | Q     | 58  | HIS  |
| 25  | Q     | 118 | HIS  |
| 25  | Q     | 130 | ASN  |
| 25  | Q     | 137 | ASN  |
| 26  | R     | 8   | HIS  |
| 26  | R     | 107 | GLN  |
| 26  | R     | 122 | ASN  |
| 27  | S     | 54  | HIS  |
| 27  | S     | 58  | HIS  |
| 27  | S     | 77  | ASN  |
| 27  | S     | 95  | HIS  |
| 28  | T     | 3   | HIS  |
| 28  | T     | 78  | GLN  |
| 28  | T     | 97  | ASN  |
| 28  | T     | 110 | ASN  |
| 30  | V     | 34  | GLN  |
| 30  | V     | 114 | ASN  |
| 30  | V     | 133 | HIS  |
| 31  | W     | 18  | GLN  |
| 31  | W     | 110 | HIS  |
| 33  | Y     | 79  | HIS  |
| 33  | Y     | 86  | ASN  |
| 33  | Y     | 121 | ASN  |
| 34  | Z     | 3   | HIS  |
| 34  | Z     | 14  | GLN  |
| 35  | a     | 116 | HIS  |
| 36  | b     | 7   | HIS  |
| 36  | b     | 11  | ASN  |
| 36  | b     | 16  | ASN  |
| 36  | b     | 30  | HIS  |
| 36  | b     | 43  | ASN  |
| 37  | c     | 120 | GLN  |
| 37  | c     | 123 | ASN  |
| 37  | c     | 135 | ASN  |
| 37  | c     | 167 | ASN  |
| 37  | c     | 176 | ASN  |
| 37  | c     | 196 | ASN  |
| 37  | c     | 245 | ASN  |
| 38  | d     | 71  | HIS  |
| 39  | e     | 120 | ASN  |
| 40  | f     | 122 | ASN  |
| 41  | g     | 52  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | g     | 80  | HIS  |
| 42  | h     | 13  | HIS  |
| 42  | h     | 51  | HIS  |
| 42  | h     | 62  | HIS  |
| 44  | j     | 12  | HIS  |
| 44  | j     | 16  | HIS  |
| 45  | k     | 27  | HIS  |
| 46  | l     | 33  | ASN  |
| 46  | l     | 43  | HIS  |
| 47  | m     | 33  | GLN  |
| 48  | n     | 3   | ASN  |
| 48  | n     | 82  | GLN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1     | 1535/1782 (86%) | 588 (38%)         | 57 (3%)         |
| 2   | 2     | 1106/1527 (72%) | 445 (40%)         | 28 (2%)         |
| 3   | 3     | 177/213 (83%)   | 83 (46%)          | 10 (5%)         |
| 4   | 4     | 146/183 (79%)   | 48 (32%)          | 5 (3%)          |
| 5   | 5     | 78/133 (58%)    | 30 (38%)          | 4 (5%)          |
| 6   | 6     | 60/76 (78%)     | 48 (80%)          | 15 (25%)        |
| 7   | 7     | 150/171 (87%)   | 50 (33%)          | 2 (1%)          |
| 8   | 8     | 118/121 (97%)   | 54 (45%)          | 5 (4%)          |
| All | All   | 3370/4206 (80%) | 1346 (39%)        | 126 (3%)        |

All (1346) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 4   | G    |
| 1   | 1     | 10  | A    |
| 1   | 1     | 13  | G    |
| 1   | 1     | 23  | U    |
| 1   | 1     | 24  | A    |
| 1   | 1     | 32  | A    |
| 1   | 1     | 36  | OMU  |
| 1   | 1     | 38  | A    |
| 1   | 1     | 41  | A    |
| 1   | 1     | 47  | C    |
| 1   | 1     | 48  | OMU  |
| 1   | 1     | 49  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 51  | G    |
| 1   | 1     | 54  | G    |
| 1   | 1     | 57  | G    |
| 1   | 1     | 58  | A    |
| 1   | 1     | 64  | A    |
| 1   | 1     | 66  | A    |
| 1   | 1     | 83  | A    |
| 1   | 1     | 85  | U    |
| 1   | 1     | 86  | G    |
| 1   | 1     | 87  | A    |
| 1   | 1     | 91  | G    |
| 1   | 1     | 92  | C    |
| 1   | 1     | 104 | G    |
| 1   | 1     | 109 | A    |
| 1   | 1     | 110 | A    |
| 1   | 1     | 119 | C    |
| 1   | 1     | 121 | A    |
| 1   | 1     | 126 | G    |
| 1   | 1     | 127 | G    |
| 1   | 1     | 130 | U    |
| 1   | 1     | 131 | U    |
| 1   | 1     | 132 | A    |
| 1   | 1     | 133 | C    |
| 1   | 1     | 134 | A    |
| 1   | 1     | 135 | A    |
| 1   | 1     | 136 | G    |
| 1   | 1     | 137 | G    |
| 1   | 1     | 139 | C    |
| 1   | 1     | 141 | U    |
| 1   | 1     | 142 | G    |
| 1   | 1     | 145 | U    |
| 1   | 1     | 153 | C    |
| 1   | 1     | 154 | A    |
| 1   | 1     | 155 | A    |
| 1   | 1     | 156 | A    |
| 1   | 1     | 158 | A    |
| 1   | 1     | 159 | U    |
| 1   | 1     | 160 | C    |
| 1   | 1     | 165 | C    |
| 1   | 1     | 168 | G    |
| 1   | 1     | 169 | G    |
| 1   | 1     | 170 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 171 | U    |
| 1   | 1     | 172 | G    |
| 1   | 1     | 174 | U    |
| 1   | 1     | 175 | G    |
| 1   | 1     | 177 | A    |
| 1   | 1     | 178 | G    |
| 1   | 1     | 180 | A    |
| 1   | 1     | 184 | G    |
| 1   | 1     | 187 | A    |
| 1   | 1     | 188 | A    |
| 1   | 1     | 189 | A    |
| 1   | 1     | 191 | U    |
| 1   | 1     | 192 | C    |
| 1   | 1     | 193 | A    |
| 1   | 1     | 195 | G    |
| 1   | 1     | 196 | C    |
| 1   | 1     | 197 | G    |
| 1   | 1     | 198 | C    |
| 1   | 1     | 199 | A    |
| 1   | 1     | 202 | G    |
| 1   | 1     | 204 | A    |
| 1   | 1     | 206 | A    |
| 1   | 1     | 207 | C    |
| 1   | 1     | 209 | C    |
| 1   | 1     | 210 | G    |
| 1   | 1     | 211 | U    |
| 1   | 1     | 214 | C    |
| 1   | 1     | 216 | G    |
| 1   | 1     | 217 | A    |
| 1   | 1     | 218 | A    |
| 1   | 1     | 221 | C    |
| 1   | 1     | 222 | A    |
| 1   | 1     | 227 | U    |
| 1   | 1     | 228 | U    |
| 1   | 1     | 230 | A    |
| 1   | 1     | 231 | U    |
| 1   | 1     | 232 | G    |
| 1   | 1     | 233 | U    |
| 1   | 1     | 236 | G    |
| 1   | 1     | 237 | U    |
| 1   | 1     | 239 | U    |
| 1   | 1     | 240 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 242 | A    |
| 1   | 1     | 243 | G    |
| 1   | 1     | 248 | A    |
| 1   | 1     | 249 | G    |
| 1   | 1     | 250 | A    |
| 1   | 1     | 251 | A    |
| 1   | 1     | 252 | G    |
| 1   | 1     | 255 | G    |
| 1   | 1     | 256 | U    |
| 1   | 1     | 260 | C    |
| 1   | 1     | 261 | C    |
| 1   | 1     | 264 | U    |
| 1   | 1     | 267 | A    |
| 1   | 1     | 268 | G    |
| 1   | 1     | 270 | C    |
| 1   | 1     | 271 | A    |
| 1   | 1     | 273 | A    |
| 1   | 1     | 275 | A    |
| 1   | 1     | 278 | U    |
| 1   | 1     | 279 | G    |
| 1   | 1     | 280 | A    |
| 1   | 1     | 282 | C    |
| 1   | 1     | 283 | G    |
| 1   | 1     | 284 | C    |
| 1   | 1     | 286 | U    |
| 1   | 1     | 288 | A    |
| 1   | 1     | 291 | A    |
| 1   | 1     | 293 | C    |
| 1   | 1     | 294 | U    |
| 1   | 1     | 299 | U    |
| 1   | 1     | 301 | A    |
| 1   | 1     | 303 | C    |
| 1   | 1     | 305 | A    |
| 1   | 1     | 306 | G    |
| 1   | 1     | 313 | U    |
| 1   | 1     | 314 | G    |
| 1   | 1     | 320 | G    |
| 1   | 1     | 323 | U    |
| 1   | 1     | 332 | A    |
| 1   | 1     | 333 | A    |
| 1   | 1     | 334 | G    |
| 1   | 1     | 335 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 336 | U    |
| 1   | 1     | 337 | G    |
| 1   | 1     | 341 | G    |
| 1   | 1     | 343 | U    |
| 1   | 1     | 344 | A    |
| 1   | 1     | 348 | G    |
| 1   | 1     | 361 | A    |
| 1   | 1     | 367 | A    |
| 1   | 1     | 368 | G    |
| 1   | 1     | 370 | G    |
| 1   | 1     | 371 | U    |
| 1   | 1     | 374 | G    |
| 1   | 1     | 377 | G    |
| 1   | 1     | 378 | A    |
| 1   | 1     | 380 | C    |
| 1   | 1     | 383 | U    |
| 1   | 1     | 409 | U    |
| 1   | 1     | 410 | U    |
| 1   | 1     | 411 | U    |
| 1   | 1     | 416 | A    |
| 1   | 1     | 417 | G    |
| 1   | 1     | 428 | A    |
| 1   | 1     | 431 | G    |
| 1   | 1     | 438 | A    |
| 1   | 1     | 440 | A    |
| 1   | 1     | 442 | A    |
| 1   | 1     | 443 | A    |
| 1   | 1     | 444 | C    |
| 1   | 1     | 448 | A    |
| 1   | 1     | 454 | U    |
| 1   | 1     | 455 | G    |
| 1   | 1     | 458 | A    |
| 1   | 1     | 459 | A    |
| 1   | 1     | 460 | A    |
| 1   | 1     | 462 | A    |
| 1   | 1     | 463 | C    |
| 1   | 1     | 464 | A    |
| 1   | 1     | 475 | C    |
| 1   | 1     | 476 | U    |
| 1   | 1     | 477 | C    |
| 1   | 1     | 478 | C    |
| 1   | 1     | 483 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 484 | A    |
| 1   | 1     | 486 | C    |
| 1   | 1     | 487 | G    |
| 1   | 1     | 490 | C    |
| 1   | 1     | 494 | A    |
| 1   | 1     | 495 | C    |
| 1   | 1     | 498 | G    |
| 1   | 1     | 500 | C    |
| 1   | 1     | 501 | C    |
| 1   | 1     | 502 | U    |
| 1   | 1     | 505 | U    |
| 1   | 1     | 508 | A    |
| 1   | 1     | 510 | U    |
| 1   | 1     | 512 | U    |
| 1   | 1     | 513 | C    |
| 1   | 1     | 515 | U    |
| 1   | 1     | 516 | G    |
| 1   | 1     | 519 | G    |
| 1   | 1     | 520 | G    |
| 1   | 1     | 532 | C    |
| 1   | 1     | 533 | G    |
| 1   | 1     | 534 | G    |
| 1   | 1     | 537 | G    |
| 1   | 1     | 539 | C    |
| 1   | 1     | 540 | A    |
| 1   | 1     | 541 | A    |
| 1   | 1     | 543 | G    |
| 1   | 1     | 544 | A    |
| 1   | 1     | 545 | A    |
| 1   | 1     | 547 | U    |
| 1   | 1     | 548 | G    |
| 1   | 1     | 549 | C    |
| 1   | 1     | 551 | A    |
| 1   | 1     | 553 | A    |
| 1   | 1     | 554 | A    |
| 1   | 1     | 558 | U    |
| 1   | 1     | 559 | G    |
| 1   | 1     | 560 | G    |
| 1   | 1     | 561 | G    |
| 1   | 1     | 563 | C    |
| 1   | 1     | 566 | G    |
| 1   | 1     | 567 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 569 | G    |
| 1   | 1     | 570 | A    |
| 1   | 1     | 634 | G    |
| 1   | 1     | 636 | U    |
| 1   | 1     | 638 | C    |
| 1   | 1     | 648 | A    |
| 1   | 1     | 650 | G    |
| 1   | 1     | 651 | G    |
| 1   | 1     | 652 | A    |
| 1   | 1     | 653 | A    |
| 1   | 1     | 654 | A    |
| 1   | 1     | 658 | G    |
| 1   | 1     | 659 | G    |
| 1   | 1     | 665 | C    |
| 1   | 1     | 666 | C    |
| 1   | 1     | 669 | C    |
| 1   | 1     | 670 | C    |
| 1   | 1     | 677 | A    |
| 1   | 1     | 679 | A    |
| 1   | 1     | 680 | C    |
| 1   | 1     | 681 | A2M  |
| 1   | 1     | 693 | G    |
| 1   | 1     | 694 | U    |
| 1   | 1     | 695 | OMC  |
| 1   | 1     | 696 | A    |
| 1   | 1     | 698 | A    |
| 1   | 1     | 709 | A    |
| 1   | 1     | 713 | A    |
| 1   | 1     | 728 | C    |
| 1   | 1     | 729 | A    |
| 1   | 1     | 730 | G    |
| 1   | 1     | 735 | U    |
| 1   | 1     | 737 | U    |
| 1   | 1     | 741 | G    |
| 1   | 1     | 742 | U    |
| 1   | 1     | 750 | G    |
| 1   | 1     | 753 | A    |
| 1   | 1     | 767 | U    |
| 1   | 1     | 768 | C    |
| 1   | 1     | 769 | U    |
| 1   | 1     | 770 | G    |
| 1   | 1     | 771 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 779 | A    |
| 1   | 1     | 780 | C    |
| 1   | 1     | 782 | C    |
| 1   | 1     | 783 | G    |
| 1   | 1     | 785 | C    |
| 1   | 1     | 787 | A    |
| 1   | 1     | 788 | A    |
| 1   | 1     | 789 | U    |
| 1   | 1     | 790 | C    |
| 1   | 1     | 793 | U    |
| 1   | 1     | 795 | U    |
| 1   | 1     | 799 | U    |
| 1   | 1     | 801 | G    |
| 1   | 1     | 802 | C    |
| 1   | 1     | 807 | C    |
| 1   | 1     | 817 | C    |
| 1   | 1     | 818 | C    |
| 1   | 1     | 820 | U    |
| 1   | 1     | 821 | C    |
| 1   | 1     | 823 | G    |
| 1   | 1     | 824 | U    |
| 1   | 1     | 826 | G    |
| 1   | 1     | 829 | U    |
| 1   | 1     | 830 | G    |
| 1   | 1     | 831 | C    |
| 1   | 1     | 832 | G    |
| 1   | 1     | 836 | G    |
| 1   | 1     | 837 | A    |
| 1   | 1     | 838 | G    |
| 1   | 1     | 846 | G    |
| 1   | 1     | 847 | OMU  |
| 1   | 1     | 848 | U    |
| 1   | 1     | 849 | U    |
| 1   | 1     | 850 | G    |
| 1   | 1     | 855 | C    |
| 1   | 1     | 857 | A    |
| 1   | 1     | 860 | G    |
| 1   | 1     | 867 | A    |
| 1   | 1     | 868 | A    |
| 1   | 1     | 878 | A    |
| 1   | 1     | 883 | G    |
| 1   | 1     | 887 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 892  | C    |
| 1   | 1     | 894  | G    |
| 1   | 1     | 895  | G    |
| 1   | 1     | 900  | C    |
| 1   | 1     | 901  | C    |
| 1   | 1     | 902  | C    |
| 1   | 1     | 903  | A    |
| 1   | 1     | 907  | G    |
| 1   | 1     | 908  | G    |
| 1   | 1     | 912  | C    |
| 1   | 1     | 922  | U    |
| 1   | 1     | 925  | U    |
| 1   | 1     | 926  | G    |
| 1   | 1     | 927  | A2M  |
| 1   | 1     | 931  | G    |
| 1   | 1     | 932  | C    |
| 1   | 1     | 945  | U    |
| 1   | 1     | 947  | A    |
| 1   | 1     | 956  | U    |
| 1   | 1     | 957  | C    |
| 1   | 1     | 959  | OMG  |
| 1   | 1     | 960  | A    |
| 1   | 1     | 963  | G    |
| 1   | 1     | 965  | A    |
| 1   | 1     | 967  | G    |
| 1   | 1     | 972  | A    |
| 1   | 1     | 974  | C    |
| 1   | 1     | 975  | G    |
| 1   | 1     | 977  | A    |
| 1   | 1     | 985  | G    |
| 1   | 1     | 988  | G    |
| 1   | 1     | 995  | C    |
| 1   | 1     | 1000 | C    |
| 1   | 1     | 1010 | C    |
| 1   | 1     | 1011 | U    |
| 1   | 1     | 1013 | A    |
| 1   | 1     | 1021 | U    |
| 1   | 1     | 1025 | G    |
| 1   | 1     | 1028 | A    |
| 1   | 1     | 1029 | G    |
| 1   | 1     | 1030 | U    |
| 1   | 1     | 1031 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1032 | G    |
| 1   | 1     | 1036 | U    |
| 1   | 1     | 1042 | G    |
| 1   | 1     | 1044 | G    |
| 1   | 1     | 1046 | U    |
| 1   | 1     | 1051 | C    |
| 1   | 1     | 1055 | U    |
| 1   | 1     | 1056 | G    |
| 1   | 1     | 1057 | A    |
| 1   | 1     | 1058 | U    |
| 1   | 1     | 1059 | U    |
| 1   | 1     | 1063 | G    |
| 1   | 1     | 1073 | U    |
| 1   | 1     | 1081 | A    |
| 1   | 1     | 1083 | A    |
| 1   | 1     | 1085 | C    |
| 1   | 1     | 1086 | G    |
| 1   | 1     | 1088 | C    |
| 1   | 1     | 1092 | U    |
| 1   | 1     | 1097 | A    |
| 1   | 1     | 1102 | U    |
| 1   | 1     | 1103 | U    |
| 1   | 1     | 1104 | A    |
| 1   | 1     | 1105 | A    |
| 1   | 1     | 1108 | G    |
| 1   | 1     | 1110 | G    |
| 1   | 1     | 1114 | A    |
| 1   | 1     | 1117 | A    |
| 1   | 1     | 1118 | A    |
| 1   | 1     | 1120 | C    |
| 1   | 1     | 1123 | G    |
| 1   | 1     | 1124 | C    |
| 1   | 1     | 1127 | U    |
| 1   | 1     | 1128 | A    |
| 1   | 1     | 1131 | C    |
| 1   | 1     | 1142 | C    |
| 1   | 1     | 1146 | A    |
| 1   | 1     | 1147 | A    |
| 1   | 1     | 1149 | G    |
| 1   | 1     | 1150 | A    |
| 1   | 1     | 1156 | A    |
| 1   | 1     | 1159 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1160 | G    |
| 1   | 1     | 1161 | A    |
| 1   | 1     | 1162 | G    |
| 1   | 1     | 1164 | C    |
| 1   | 1     | 1169 | A    |
| 1   | 1     | 1174 | G    |
| 1   | 1     | 1181 | U    |
| 1   | 1     | 1182 | C    |
| 1   | 1     | 1188 | G    |
| 1   | 1     | 1200 | A    |
| 1   | 1     | 1201 | U    |
| 1   | 1     | 1206 | A    |
| 1   | 1     | 1210 | A    |
| 1   | 1     | 1211 | A    |
| 1   | 1     | 1212 | C    |
| 1   | 1     | 1213 | C    |
| 1   | 1     | 1216 | U    |
| 1   | 1     | 1218 | A    |
| 1   | 1     | 1231 | G    |
| 1   | 1     | 1234 | A    |
| 1   | 1     | 1235 | A    |
| 1   | 1     | 1239 | U    |
| 1   | 1     | 1240 | U    |
| 1   | 1     | 1242 | U    |
| 1   | 1     | 1243 | G    |
| 1   | 1     | 1249 | A    |
| 1   | 1     | 1254 | C    |
| 1   | 1     | 1255 | G    |
| 1   | 1     | 1257 | U    |
| 1   | 1     | 1258 | A    |
| 1   | 1     | 1259 | C    |
| 1   | 1     | 1260 | G    |
| 1   | 1     | 1261 | U    |
| 1   | 1     | 1263 | A    |
| 1   | 1     | 1264 | A    |
| 1   | 1     | 1265 | A    |
| 1   | 1     | 1266 | A    |
| 1   | 1     | 1268 | G    |
| 1   | 1     | 1270 | U    |
| 1   | 1     | 1271 | G    |
| 1   | 1     | 1273 | U    |
| 1   | 1     | 1276 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1281 | A    |
| 1   | 1     | 1349 | A    |
| 1   | 1     | 1357 | G    |
| 1   | 1     | 1364 | A    |
| 1   | 1     | 1365 | A    |
| 1   | 1     | 1366 | A    |
| 1   | 1     | 1367 | U    |
| 1   | 1     | 1369 | G    |
| 1   | 1     | 1370 | A    |
| 1   | 1     | 1371 | U    |
| 1   | 1     | 1372 | G    |
| 1   | 1     | 1375 | G    |
| 1   | 1     | 1379 | A    |
| 1   | 1     | 1383 | C    |
| 1   | 1     | 1385 | A    |
| 1   | 1     | 1386 | A    |
| 1   | 1     | 1389 | A    |
| 1   | 1     | 1390 | G    |
| 1   | 1     | 1392 | G    |
| 1   | 1     | 1393 | A    |
| 1   | 1     | 1394 | U    |
| 1   | 1     | 1395 | U    |
| 1   | 1     | 1396 | G    |
| 1   | 1     | 1399 | C    |
| 1   | 1     | 1400 | A    |
| 1   | 1     | 1402 | U    |
| 1   | 1     | 1407 | C    |
| 1   | 1     | 1413 | U    |
| 1   | 1     | 1414 | A    |
| 1   | 1     | 1415 | A    |
| 1   | 1     | 1416 | G    |
| 1   | 1     | 1418 | G    |
| 1   | 1     | 1420 | G    |
| 1   | 1     | 1421 | G    |
| 1   | 1     | 1423 | A    |
| 1   | 1     | 1424 | A    |
| 1   | 1     | 1433 | U    |
| 1   | 1     | 1434 | U    |
| 1   | 1     | 1435 | G    |
| 1   | 1     | 1436 | G    |
| 1   | 1     | 1437 | A    |
| 1   | 1     | 1438 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1439 | A    |
| 1   | 1     | 1440 | A    |
| 1   | 1     | 1443 | U    |
| 1   | 1     | 1445 | U    |
| 1   | 1     | 1446 | A    |
| 1   | 1     | 1447 | G    |
| 1   | 1     | 1448 | C    |
| 1   | 1     | 1449 | C    |
| 1   | 1     | 1450 | C    |
| 1   | 1     | 1451 | U    |
| 1   | 1     | 1452 | U    |
| 1   | 1     | 1453 | C    |
| 1   | 1     | 1466 | G    |
| 1   | 1     | 1467 | G    |
| 1   | 1     | 1468 | C    |
| 1   | 1     | 1478 | A    |
| 1   | 1     | 1479 | G    |
| 1   | 1     | 1489 | U    |
| 1   | 1     | 1490 | A    |
| 1   | 1     | 1491 | U    |
| 1   | 1     | 1492 | G    |
| 1   | 1     | 1494 | C    |
| 1   | 1     | 1495 | G    |
| 1   | 1     | 1504 | A    |
| 1   | 1     | 1505 | G    |
| 1   | 1     | 1506 | A    |
| 1   | 1     | 1507 | U    |
| 1   | 1     | 1509 | G    |
| 1   | 1     | 1510 | A    |
| 1   | 1     | 1511 | C    |
| 1   | 1     | 1521 | G    |
| 1   | 1     | 1522 | U    |
| 1   | 1     | 1523 | G    |
| 1   | 1     | 1524 | C    |
| 1   | 1     | 1526 | OMG  |
| 1   | 1     | 1527 | A    |
| 1   | 1     | 1529 | OMC  |
| 1   | 1     | 1530 | U    |
| 1   | 1     | 1540 | U    |
| 1   | 1     | 1541 | A2M  |
| 1   | 1     | 1542 | OMG  |
| 1   | 1     | 1544 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1547 | G    |
| 1   | 1     | 1548 | A    |
| 1   | 1     | 1549 | U    |
| 1   | 1     | 1550 | C    |
| 1   | 1     | 1553 | A    |
| 1   | 1     | 1554 | C    |
| 1   | 1     | 1576 | C    |
| 1   | 1     | 1577 | G    |
| 1   | 1     | 1584 | A    |
| 1   | 1     | 1588 | G    |
| 1   | 1     | 1589 | A    |
| 1   | 1     | 1590 | G    |
| 1   | 1     | 1591 | C    |
| 1   | 1     | 1592 | G    |
| 1   | 1     | 1593 | G    |
| 1   | 1     | 1595 | G    |
| 1   | 1     | 1601 | U    |
| 1   | 1     | 1602 | U    |
| 1   | 1     | 1607 | G    |
| 1   | 1     | 1609 | C    |
| 1   | 1     | 1611 | A    |
| 1   | 1     | 1612 | C    |
| 1   | 1     | 1614 | G    |
| 1   | 1     | 1615 | C    |
| 1   | 1     | 1621 | U    |
| 1   | 1     | 1627 | A    |
| 1   | 1     | 1629 | U    |
| 1   | 1     | 1633 | U    |
| 1   | 1     | 1639 | A    |
| 1   | 1     | 1644 | G    |
| 1   | 1     | 1648 | A    |
| 1   | 1     | 1656 | A    |
| 1   | 1     | 1657 | U    |
| 1   | 1     | 1658 | C    |
| 1   | 1     | 1662 | U    |
| 1   | 1     | 1663 | U    |
| 1   | 1     | 1664 | G    |
| 1   | 1     | 1665 | U    |
| 1   | 1     | 1667 | A    |
| 1   | 1     | 1668 | G    |
| 1   | 1     | 1669 | G    |
| 1   | 1     | 1670 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1671 | A    |
| 1   | 1     | 1679 | G    |
| 1   | 1     | 1683 | G    |
| 1   | 1     | 1719 | G    |
| 1   | 1     | 1720 | C    |
| 1   | 1     | 1721 | C    |
| 1   | 1     | 1723 | U    |
| 1   | 1     | 1725 | A    |
| 1   | 1     | 1728 | G    |
| 1   | 1     | 1729 | A    |
| 1   | 1     | 1732 | A    |
| 1   | 1     | 1735 | G    |
| 1   | 1     | 1737 | C    |
| 1   | 1     | 1739 | A    |
| 1   | 1     | 1740 | C    |
| 1   | 1     | 1741 | A    |
| 1   | 1     | 1746 | A    |
| 1   | 1     | 1749 | U    |
| 1   | 1     | 1752 | G    |
| 1   | 1     | 1755 | U    |
| 1   | 1     | 1761 | C    |
| 1   | 1     | 1763 | A    |
| 1   | 1     | 1764 | A    |
| 1   | 1     | 1765 | A    |
| 1   | 1     | 1766 | A    |
| 1   | 1     | 1767 | A    |
| 1   | 1     | 1768 | G    |
| 1   | 1     | 1771 | A    |
| 1   | 1     | 1777 | U    |
| 1   | 1     | 1778 | G    |
| 2   | 2     | 9    | G    |
| 2   | 2     | 13   | A    |
| 2   | 2     | 22   | A    |
| 2   | 2     | 26   | C    |
| 2   | 2     | 29   | C    |
| 2   | 2     | 30   | A    |
| 2   | 2     | 33   | A    |
| 2   | 2     | 34   | G    |
| 2   | 2     | 36   | U    |
| 2   | 2     | 41   | A    |
| 2   | 2     | 44   | C    |
| 2   | 2     | 49   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 54  | U    |
| 2   | 2     | 61  | C    |
| 2   | 2     | 63  | U    |
| 2   | 2     | 67  | G    |
| 2   | 2     | 68  | A    |
| 2   | 2     | 69  | A    |
| 2   | 2     | 70  | A    |
| 2   | 2     | 75  | C    |
| 2   | 2     | 78  | U    |
| 2   | 2     | 89  | G    |
| 2   | 2     | 90  | G    |
| 2   | 2     | 92  | A    |
| 2   | 2     | 98  | G    |
| 2   | 2     | 99  | A    |
| 2   | 2     | 103 | G    |
| 2   | 2     | 109 | U    |
| 2   | 2     | 110 | C    |
| 2   | 2     | 111 | G    |
| 2   | 2     | 116 | A    |
| 2   | 2     | 119 | C    |
| 2   | 2     | 122 | U    |
| 2   | 2     | 123 | G    |
| 2   | 2     | 127 | C    |
| 2   | 2     | 130 | A    |
| 2   | 2     | 131 | G    |
| 2   | 2     | 133 | G    |
| 2   | 2     | 134 | C    |
| 2   | 2     | 135 | A    |
| 2   | 2     | 343 | U    |
| 2   | 2     | 344 | G    |
| 2   | 2     | 345 | C    |
| 2   | 2     | 346 | C    |
| 2   | 2     | 349 | C    |
| 2   | 2     | 350 | U    |
| 2   | 2     | 355 | A    |
| 2   | 2     | 358 | G    |
| 2   | 2     | 359 | C    |
| 2   | 2     | 360 | U    |
| 2   | 2     | 361 | U    |
| 2   | 2     | 362 | A    |
| 2   | 2     | 363 | C    |
| 2   | 2     | 368 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 372 | A    |
| 2   | 2     | 377 | A    |
| 2   | 2     | 380 | G    |
| 2   | 2     | 385 | A    |
| 2   | 2     | 388 | A    |
| 2   | 2     | 390 | A    |
| 2   | 2     | 394 | U    |
| 2   | 2     | 401 | G    |
| 2   | 2     | 404 | A    |
| 2   | 2     | 405 | U    |
| 2   | 2     | 413 | A    |
| 2   | 2     | 414 | G    |
| 2   | 2     | 415 | U    |
| 2   | 2     | 416 | G    |
| 2   | 2     | 424 | U    |
| 2   | 2     | 425 | C    |
| 2   | 2     | 429 | A    |
| 2   | 2     | 434 | A    |
| 2   | 2     | 435 | U    |
| 2   | 2     | 438 | C    |
| 2   | 2     | 444 | A    |
| 2   | 2     | 446 | U    |
| 2   | 2     | 447 | G    |
| 2   | 2     | 448 | C    |
| 2   | 2     | 451 | U    |
| 2   | 2     | 452 | G    |
| 2   | 2     | 453 | A    |
| 2   | 2     | 454 | A    |
| 2   | 2     | 455 | U    |
| 2   | 2     | 456 | G    |
| 2   | 2     | 458 | C    |
| 2   | 2     | 459 | A    |
| 2   | 2     | 464 | G    |
| 2   | 2     | 469 | G    |
| 2   | 2     | 470 | A    |
| 2   | 2     | 471 | U    |
| 2   | 2     | 473 | C    |
| 2   | 2     | 477 | G    |
| 2   | 2     | 478 | A    |
| 2   | 2     | 482 | G    |
| 2   | 2     | 483 | C    |
| 2   | 2     | 484 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 489 | A    |
| 2   | 2     | 490 | A    |
| 2   | 2     | 495 | G    |
| 2   | 2     | 497 | G    |
| 2   | 2     | 498 | A    |
| 2   | 2     | 509 | C    |
| 2   | 2     | 511 | C    |
| 2   | 2     | 512 | U    |
| 2   | 2     | 513 | C    |
| 2   | 2     | 515 | U    |
| 2   | 2     | 518 | G    |
| 2   | 2     | 519 | G    |
| 2   | 2     | 522 | G    |
| 2   | 2     | 525 | A    |
| 2   | 2     | 526 | A    |
| 2   | 2     | 527 | A2M  |
| 2   | 2     | 528 | U    |
| 2   | 2     | 529 | G    |
| 2   | 2     | 530 | C    |
| 2   | 2     | 534 | OMG  |
| 2   | 2     | 535 | U    |
| 2   | 2     | 541 | A    |
| 2   | 2     | 543 | U    |
| 2   | 2     | 544 | U    |
| 2   | 2     | 547 | A    |
| 2   | 2     | 549 | A    |
| 2   | 2     | 553 | G    |
| 2   | 2     | 554 | OMC  |
| 2   | 2     | 555 | A    |
| 2   | 2     | 556 | U    |
| 2   | 2     | 559 | A    |
| 2   | 2     | 560 | U    |
| 2   | 2     | 561 | G    |
| 2   | 2     | 570 | A    |
| 2   | 2     | 571 | OMG  |
| 2   | 2     | 572 | A2M  |
| 2   | 2     | 580 | U    |
| 2   | 2     | 582 | U    |
| 2   | 2     | 583 | OMC  |
| 2   | 2     | 584 | C    |
| 2   | 2     | 591 | A2M  |
| 2   | 2     | 592 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 609 | A    |
| 2   | 2     | 611 | U    |
| 2   | 2     | 620 | C    |
| 2   | 2     | 621 | G    |
| 2   | 2     | 623 | A    |
| 2   | 2     | 624 | C    |
| 2   | 2     | 629 | A    |
| 2   | 2     | 633 | C    |
| 2   | 2     | 635 | A    |
| 2   | 2     | 640 | G    |
| 2   | 2     | 643 | A    |
| 2   | 2     | 647 | A    |
| 2   | 2     | 648 | A    |
| 2   | 2     | 649 | G    |
| 2   | 2     | 650 | A    |
| 2   | 2     | 656 | OMU  |
| 2   | 2     | 657 | U    |
| 2   | 2     | 658 | G    |
| 2   | 2     | 664 | G    |
| 2   | 2     | 666 | C    |
| 2   | 2     | 668 | C    |
| 2   | 2     | 675 | G    |
| 2   | 2     | 681 | G    |
| 2   | 2     | 683 | G    |
| 2   | 2     | 694 | U    |
| 2   | 2     | 696 | A    |
| 2   | 2     | 697 | G    |
| 2   | 2     | 699 | U    |
| 2   | 2     | 700 | G    |
| 2   | 2     | 701 | U    |
| 2   | 2     | 702 | A    |
| 2   | 2     | 704 | U    |
| 2   | 2     | 705 | A    |
| 2   | 2     | 706 | U    |
| 2   | 2     | 707 | A    |
| 2   | 2     | 709 | G    |
| 2   | 2     | 711 | G    |
| 2   | 2     | 713 | A    |
| 2   | 2     | 714 | A    |
| 2   | 2     | 715 | G    |
| 2   | 2     | 718 | C    |
| 2   | 2     | 720 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 721 | G    |
| 2   | 2     | 725 | A    |
| 2   | 2     | 726 | A    |
| 2   | 2     | 727 | A    |
| 2   | 2     | 728 | U    |
| 2   | 2     | 729 | G    |
| 2   | 2     | 730 | A    |
| 2   | 2     | 731 | A    |
| 2   | 2     | 732 | A    |
| 2   | 2     | 733 | U    |
| 2   | 2     | 734 | A    |
| 2   | 2     | 735 | C    |
| 2   | 2     | 736 | C    |
| 2   | 2     | 737 | A    |
| 2   | 2     | 739 | C    |
| 2   | 2     | 741 | C    |
| 2   | 2     | 742 | U    |
| 2   | 2     | 750 | U    |
| 2   | 2     | 756 | C    |
| 2   | 2     | 758 | C    |
| 2   | 2     | 759 | U    |
| 2   | 2     | 760 | U    |
| 2   | 2     | 761 | A    |
| 2   | 2     | 768 | G    |
| 2   | 2     | 769 | A    |
| 2   | 2     | 774 | A    |
| 2   | 2     | 775 | C    |
| 2   | 2     | 776 | C    |
| 2   | 2     | 777 | A    |
| 2   | 2     | 778 | A    |
| 2   | 2     | 779 | U    |
| 2   | 2     | 780 | G    |
| 2   | 2     | 782 | G    |
| 2   | 2     | 783 | U    |
| 2   | 2     | 784 | U    |
| 2   | 2     | 785 | U    |
| 2   | 2     | 786 | A    |
| 2   | 2     | 789 | G    |
| 2   | 2     | 790 | U    |
| 2   | 2     | 791 | A    |
| 2   | 2     | 794 | C    |
| 2   | 2     | 795 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 800 | G    |
| 2   | 2     | 801 | C    |
| 2   | 2     | 802 | U    |
| 2   | 2     | 803 | A    |
| 2   | 2     | 807 | A    |
| 2   | 2     | 808 | C    |
| 2   | 2     | 809 | C    |
| 2   | 2     | 810 | G    |
| 2   | 2     | 811 | U    |
| 2   | 2     | 812 | C    |
| 2   | 2     | 813 | U    |
| 2   | 2     | 814 | A    |
| 2   | 2     | 816 | G    |
| 2   | 2     | 817 | U    |
| 2   | 2     | 818 | U    |
| 2   | 2     | 824 | G    |
| 2   | 2     | 825 | U    |
| 2   | 2     | 827 | A    |
| 2   | 2     | 828 | U    |
| 2   | 2     | 829 | U    |
| 2   | 2     | 830 | U    |
| 2   | 2     | 831 | U    |
| 2   | 2     | 833 | U    |
| 2   | 2     | 834 | G    |
| 2   | 2     | 835 | G    |
| 2   | 2     | 836 | C    |
| 2   | 2     | 837 | G    |
| 2   | 2     | 868 | U    |
| 2   | 2     | 869 | G    |
| 2   | 2     | 870 | C    |
| 2   | 2     | 872 | U    |
| 2   | 2     | 940 | G    |
| 2   | 2     | 941 | C    |
| 2   | 2     | 948 | C    |
| 2   | 2     | 949 | G    |
| 2   | 2     | 950 | U    |
| 2   | 2     | 951 | G    |
| 2   | 2     | 952 | G    |
| 2   | 2     | 954 | U    |
| 2   | 2     | 956 | C    |
| 2   | 2     | 957 | C    |
| 2   | 2     | 958 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 2     | 959  | A    |
| 2   | 2     | 960  | A    |
| 2   | 2     | 961  | C    |
| 2   | 2     | 962  | C    |
| 2   | 2     | 967  | U    |
| 2   | 2     | 968  | G    |
| 2   | 2     | 969  | U    |
| 2   | 2     | 970  | A    |
| 2   | 2     | 971  | A    |
| 2   | 2     | 972  | A    |
| 2   | 2     | 973  | C    |
| 2   | 2     | 974  | U    |
| 2   | 2     | 975  | G    |
| 2   | 2     | 976  | A    |
| 2   | 2     | 977  | A    |
| 2   | 2     | 979  | C    |
| 2   | 2     | 981  | A    |
| 2   | 2     | 982  | C    |
| 2   | 2     | 983  | G    |
| 2   | 2     | 989  | G    |
| 2   | 2     | 991  | C    |
| 2   | 2     | 992  | U    |
| 2   | 2     | 993  | C    |
| 2   | 2     | 996  | G    |
| 2   | 2     | 997  | C    |
| 2   | 2     | 1010 | U    |
| 2   | 2     | 1011 | U    |
| 2   | 2     | 1012 | G    |
| 2   | 2     | 1013 | U    |
| 2   | 2     | 1014 | U    |
| 2   | 2     | 1016 | C    |
| 2   | 2     | 1020 | A    |
| 2   | 2     | 1024 | C    |
| 2   | 2     | 1025 | U    |
| 2   | 2     | 1028 | C    |
| 2   | 2     | 1034 | G    |
| 2   | 2     | 1035 | G    |
| 2   | 2     | 1037 | A    |
| 2   | 2     | 1042 | G    |
| 2   | 2     | 1045 | U    |
| 2   | 2     | 1050 | C    |
| 2   | 2     | 1057 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 2     | 1063 | A    |
| 2   | 2     | 1066 | C    |
| 2   | 2     | 1067 | G    |
| 2   | 2     | 1072 | C    |
| 2   | 2     | 1073 | G    |
| 2   | 2     | 1076 | G    |
| 2   | 2     | 1077 | G    |
| 2   | 2     | 1079 | OMG  |
| 2   | 2     | 1080 | U    |
| 2   | 2     | 1084 | A    |
| 2   | 2     | 1086 | G    |
| 2   | 2     | 1093 | U    |
| 2   | 2     | 1096 | G    |
| 2   | 2     | 1097 | U    |
| 2   | 2     | 1101 | A    |
| 2   | 2     | 1102 | A    |
| 2   | 2     | 1104 | A    |
| 2   | 2     | 1109 | U    |
| 2   | 2     | 1111 | U    |
| 2   | 2     | 1112 | C    |
| 2   | 2     | 1114 | C    |
| 2   | 2     | 1116 | U    |
| 2   | 2     | 1117 | A    |
| 2   | 2     | 1118 | G    |
| 2   | 2     | 1119 | A    |
| 2   | 2     | 1122 | A    |
| 2   | 2     | 1124 | A    |
| 2   | 2     | 1131 | A    |
| 2   | 2     | 1132 | A    |
| 2   | 2     | 1133 | A    |
| 2   | 2     | 1134 | G    |
| 2   | 2     | 1142 | G    |
| 2   | 2     | 1144 | U    |
| 2   | 2     | 1147 | A    |
| 2   | 2     | 1148 | C    |
| 2   | 2     | 1149 | G    |
| 2   | 2     | 1152 | U    |
| 2   | 2     | 1154 | C    |
| 2   | 2     | 1156 | A    |
| 2   | 2     | 1157 | G    |
| 2   | 2     | 1158 | U    |
| 2   | 2     | 1161 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 2     | 1166 | G    |
| 2   | 2     | 1169 | A    |
| 2   | 2     | 1171 | U    |
| 2   | 2     | 1182 | G    |
| 2   | 2     | 1184 | C    |
| 2   | 2     | 1185 | C    |
| 2   | 2     | 1186 | A2M  |
| 2   | 2     | 1187 | G    |
| 2   | 2     | 1189 | G    |
| 2   | 2     | 1190 | A    |
| 2   | 2     | 1199 | G    |
| 2   | 2     | 1216 | A    |
| 2   | 2     | 1217 | A    |
| 2   | 2     | 1218 | C    |
| 2   | 2     | 1229 | A    |
| 2   | 2     | 1230 | OMG  |
| 2   | 2     | 1231 | A    |
| 2   | 2     | 1238 | A    |
| 2   | 2     | 1239 | G    |
| 2   | 2     | 1240 | A    |
| 2   | 2     | 1242 | U    |
| 2   | 2     | 1243 | A    |
| 2   | 2     | 1248 | C    |
| 2   | 2     | 1249 | OMC  |
| 2   | 2     | 1253 | G    |
| 2   | 2     | 1254 | OMG  |
| 2   | 2     | 1255 | G    |
| 2   | 2     | 1256 | A    |
| 2   | 2     | 1257 | U    |
| 2   | 2     | 1266 | U    |
| 2   | 2     | 1267 | G    |
| 2   | 2     | 1275 | C    |
| 2   | 2     | 1276 | A    |
| 2   | 2     | 1277 | A    |
| 2   | 2     | 1278 | G    |
| 2   | 2     | 1288 | C    |
| 2   | 2     | 1290 | A    |
| 2   | 2     | 1292 | G    |
| 2   | 2     | 1295 | G    |
| 2   | 2     | 1296 | C    |
| 2   | 2     | 1298 | U    |
| 2   | 2     | 1299 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 2     | 1302 | G    |
| 2   | 2     | 1303 | A    |
| 2   | 2     | 1305 | C    |
| 2   | 2     | 1306 | C    |
| 2   | 2     | 1310 | G    |
| 2   | 2     | 1312 | U    |
| 2   | 2     | 1317 | G    |
| 2   | 2     | 1318 | OMC  |
| 2   | 2     | 1325 | U    |
| 2   | 2     | 1326 | A    |
| 2   | 2     | 1329 | C    |
| 2   | 2     | 1333 | C    |
| 2   | 2     | 1338 | C    |
| 2   | 2     | 1339 | A    |
| 2   | 2     | 1341 | A    |
| 2   | 2     | 1343 | G    |
| 2   | 2     | 1346 | G    |
| 2   | 2     | 1347 | C    |
| 2   | 2     | 1348 | U    |
| 2   | 2     | 1349 | A    |
| 2   | 2     | 1350 | A    |
| 2   | 2     | 1351 | G    |
| 2   | 2     | 1361 | G    |
| 2   | 2     | 1362 | U    |
| 2   | 2     | 1367 | C    |
| 2   | 2     | 1372 | G    |
| 2   | 2     | 1374 | C    |
| 2   | 2     | 1375 | A    |
| 2   | 2     | 1380 | A    |
| 2   | 2     | 1381 | C    |
| 2   | 2     | 1384 | G    |
| 2   | 2     | 1385 | A    |
| 2   | 2     | 1386 | G    |
| 2   | 2     | 1389 | G    |
| 2   | 2     | 1390 | G    |
| 2   | 2     | 1393 | U    |
| 2   | 2     | 1394 | U    |
| 2   | 2     | 1410 | A    |
| 2   | 2     | 1415 | G    |
| 2   | 2     | 1417 | U    |
| 2   | 2     | 1418 | U    |
| 2   | 2     | 1422 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 2     | 1423 | C    |
| 2   | 2     | 1429 | U    |
| 2   | 2     | 1435 | G    |
| 2   | 2     | 1437 | A    |
| 2   | 2     | 1438 | A    |
| 2   | 2     | 1440 | U    |
| 2   | 2     | 1441 | G    |
| 2   | 2     | 1442 | C    |
| 2   | 2     | 1443 | G    |
| 2   | 2     | 1444 | A    |
| 2   | 2     | 1446 | A    |
| 2   | 2     | 1448 | A    |
| 2   | 2     | 1449 | A    |
| 3   | 3     | 10   | U    |
| 3   | 3     | 14   | A    |
| 3   | 3     | 21   | U    |
| 3   | 3     | 22   | G    |
| 3   | 3     | 23   | C    |
| 3   | 3     | 29   | A    |
| 3   | 3     | 30   | A    |
| 3   | 3     | 32   | A    |
| 3   | 3     | 33   | A    |
| 3   | 3     | 37   | A    |
| 3   | 3     | 38   | A    |
| 3   | 3     | 47   | C    |
| 3   | 3     | 48   | G    |
| 3   | 3     | 50   | U    |
| 3   | 3     | 54   | C    |
| 3   | 3     | 55   | U    |
| 3   | 3     | 56   | U    |
| 3   | 3     | 58   | C    |
| 3   | 3     | 61   | U    |
| 3   | 3     | 62   | U    |
| 3   | 3     | 63   | C    |
| 3   | 3     | 69   | A    |
| 3   | 3     | 70   | A    |
| 3   | 3     | 78   | C    |
| 3   | 3     | 79   | U    |
| 3   | 3     | 81   | C    |
| 3   | 3     | 82   | G    |
| 3   | 3     | 83   | G    |
| 3   | 3     | 84   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 3     | 86  | U    |
| 3   | 3     | 87  | U    |
| 3   | 3     | 88  | G    |
| 3   | 3     | 90  | U    |
| 3   | 3     | 92  | G    |
| 3   | 3     | 95  | C    |
| 3   | 3     | 96  | U    |
| 3   | 3     | 97  | U    |
| 3   | 3     | 98  | G    |
| 3   | 3     | 99  | G    |
| 3   | 3     | 101 | C    |
| 3   | 3     | 105 | U    |
| 3   | 3     | 107 | U    |
| 3   | 3     | 108 | A    |
| 3   | 3     | 109 | C    |
| 3   | 3     | 110 | U    |
| 3   | 3     | 111 | U    |
| 3   | 3     | 112 | C    |
| 3   | 3     | 114 | C    |
| 3   | 3     | 118 | U    |
| 3   | 3     | 119 | U    |
| 3   | 3     | 120 | G    |
| 3   | 3     | 122 | U    |
| 3   | 3     | 133 | G    |
| 3   | 3     | 135 | U    |
| 3   | 3     | 138 | A    |
| 3   | 3     | 142 | U    |
| 3   | 3     | 146 | A    |
| 3   | 3     | 147 | A    |
| 3   | 3     | 148 | A    |
| 3   | 3     | 149 | U    |
| 3   | 3     | 150 | G    |
| 3   | 3     | 152 | A    |
| 3   | 3     | 153 | G    |
| 3   | 3     | 156 | C    |
| 3   | 3     | 157 | U    |
| 3   | 3     | 164 | G    |
| 3   | 3     | 165 | U    |
| 3   | 3     | 166 | A    |
| 3   | 3     | 167 | C    |
| 3   | 3     | 168 | U    |
| 3   | 3     | 169 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 3     | 170 | U    |
| 3   | 3     | 176 | U    |
| 3   | 3     | 181 | A    |
| 3   | 3     | 182 | G    |
| 3   | 3     | 185 | C    |
| 3   | 3     | 186 | U    |
| 3   | 3     | 194 | A    |
| 3   | 3     | 195 | A    |
| 3   | 3     | 196 | A    |
| 3   | 3     | 198 | C    |
| 3   | 3     | 199 | A    |
| 3   | 3     | 210 | G    |
| 4   | 4     | 31  | G    |
| 4   | 4     | 40  | G    |
| 4   | 4     | 46  | G    |
| 4   | 4     | 50  | G    |
| 4   | 4     | 51  | U    |
| 4   | 4     | 52  | A    |
| 4   | 4     | 62  | C    |
| 4   | 4     | 63  | U    |
| 4   | 4     | 64  | C    |
| 4   | 4     | 65  | C    |
| 4   | 4     | 67  | A    |
| 4   | 4     | 73  | U    |
| 4   | 4     | 86  | U    |
| 4   | 4     | 93  | U    |
| 4   | 4     | 96  | C    |
| 4   | 4     | 97  | G    |
| 4   | 4     | 100 | C    |
| 4   | 4     | 102 | G    |
| 4   | 4     | 106 | G    |
| 4   | 4     | 107 | U    |
| 4   | 4     | 114 | A    |
| 4   | 4     | 119 | A    |
| 4   | 4     | 120 | U    |
| 4   | 4     | 121 | C    |
| 4   | 4     | 127 | G    |
| 4   | 4     | 128 | U    |
| 4   | 4     | 129 | G    |
| 4   | 4     | 131 | U    |
| 4   | 4     | 132 | U    |
| 4   | 4     | 139 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 4     | 140 | G    |
| 4   | 4     | 141 | A    |
| 4   | 4     | 147 | U    |
| 4   | 4     | 148 | C    |
| 4   | 4     | 150 | A    |
| 4   | 4     | 151 | A    |
| 4   | 4     | 153 | C    |
| 4   | 4     | 154 | C    |
| 4   | 4     | 157 | A    |
| 4   | 4     | 158 | A    |
| 4   | 4     | 162 | A    |
| 4   | 4     | 169 | A    |
| 4   | 4     | 171 | A    |
| 4   | 4     | 172 | C    |
| 4   | 4     | 174 | A    |
| 4   | 4     | 175 | G    |
| 4   | 4     | 180 | C    |
| 4   | 4     | 182 | A    |
| 5   | 5     | 4   | G    |
| 5   | 5     | 12  | C    |
| 5   | 5     | 13  | C    |
| 5   | 5     | 14  | A    |
| 5   | 5     | 15  | A    |
| 5   | 5     | 22  | G    |
| 5   | 5     | 25  | C    |
| 5   | 5     | 26  | A    |
| 5   | 5     | 27  | U    |
| 5   | 5     | 28  | G    |
| 5   | 5     | 38  | G    |
| 5   | 5     | 40  | A    |
| 5   | 5     | 42  | G    |
| 5   | 5     | 43  | A    |
| 5   | 5     | 101 | C    |
| 5   | 5     | 102 | U    |
| 5   | 5     | 105 | A    |
| 5   | 5     | 112 | A    |
| 5   | 5     | 113 | A    |
| 5   | 5     | 114 | A    |
| 5   | 5     | 115 | U    |
| 5   | 5     | 119 | A    |
| 5   | 5     | 120 | U    |
| 5   | 5     | 122 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 5     | 123 | U    |
| 5   | 5     | 126 | G    |
| 5   | 5     | 127 | G    |
| 5   | 5     | 131 | A    |
| 5   | 5     | 132 | C    |
| 5   | 5     | 133 | A    |
| 6   | 6     | 2   | C    |
| 6   | 6     | 3   | A    |
| 6   | 6     | 4   | U    |
| 6   | 6     | 5   | C    |
| 6   | 6     | 7   | A    |
| 6   | 6     | 8   | A    |
| 6   | 6     | 9   | U    |
| 6   | 6     | 12  | C    |
| 6   | 6     | 13  | C    |
| 6   | 6     | 14  | A    |
| 6   | 6     | 15  | C    |
| 6   | 6     | 16  | C    |
| 6   | 6     | 17  | U    |
| 6   | 6     | 18  | A    |
| 6   | 6     | 19  | C    |
| 6   | 6     | 20  | A    |
| 6   | 6     | 21  | A    |
| 6   | 6     | 22  | G    |
| 6   | 6     | 23  | A    |
| 6   | 6     | 24  | C    |
| 6   | 6     | 25  | U    |
| 6   | 6     | 26  | G    |
| 6   | 6     | 27  | G    |
| 6   | 6     | 28  | A    |
| 6   | 6     | 29  | G    |
| 6   | 6     | 30  | C    |
| 6   | 6     | 31  | U    |
| 6   | 6     | 32  | U    |
| 6   | 6     | 33  | G    |
| 6   | 6     | 35  | U    |
| 6   | 6     | 37  | C    |
| 6   | 6     | 39  | U    |
| 6   | 6     | 40  | C    |
| 6   | 6     | 41  | G    |
| 6   | 6     | 42  | A    |
| 6   | 6     | 44  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 6     | 49  | C    |
| 6   | 6     | 50  | A    |
| 6   | 6     | 51  | A    |
| 6   | 6     | 52  | G    |
| 6   | 6     | 53  | U    |
| 6   | 6     | 54  | A    |
| 6   | 6     | 55  | U    |
| 6   | 6     | 56  | A    |
| 6   | 6     | 57  | U    |
| 6   | 6     | 58  | U    |
| 6   | 6     | 59  | C    |
| 6   | 6     | 61  | U    |
| 7   | 7     | 2   | A    |
| 7   | 7     | 5   | U    |
| 7   | 7     | 6   | G    |
| 7   | 7     | 7   | OMU  |
| 7   | 7     | 8   | C    |
| 7   | 7     | 22  | U    |
| 7   | 7     | 34  | U    |
| 7   | 7     | 35  | C    |
| 7   | 7     | 38  | U    |
| 7   | 7     | 40  | A    |
| 7   | 7     | 44  | A    |
| 7   | 7     | 48  | A    |
| 7   | 7     | 49  | G    |
| 7   | 7     | 52  | A    |
| 7   | 7     | 59  | A    |
| 7   | 7     | 60  | U    |
| 7   | 7     | 62  | A    |
| 7   | 7     | 63  | G    |
| 7   | 7     | 68  | A    |
| 7   | 7     | 69  | U    |
| 7   | 7     | 71  | A    |
| 7   | 7     | 77  | A    |
| 7   | 7     | 78  | G    |
| 7   | 7     | 89  | U    |
| 7   | 7     | 92  | C    |
| 7   | 7     | 103 | A    |
| 7   | 7     | 104 | A    |
| 7   | 7     | 105 | C    |
| 7   | 7     | 107 | C    |
| 7   | 7     | 109 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | 7     | 110 | A    |
| 7   | 7     | 111 | C    |
| 7   | 7     | 115 | G    |
| 7   | 7     | 119 | G    |
| 7   | 7     | 120 | G    |
| 7   | 7     | 121 | G    |
| 7   | 7     | 122 | A    |
| 7   | 7     | 124 | A    |
| 7   | 7     | 125 | A    |
| 7   | 7     | 126 | G    |
| 7   | 7     | 127 | C    |
| 7   | 7     | 137 | U    |
| 7   | 7     | 138 | C    |
| 7   | 7     | 139 | A    |
| 7   | 7     | 140 | U    |
| 7   | 7     | 142 | C    |
| 7   | 7     | 157 | U    |
| 7   | 7     | 158 | U    |
| 7   | 7     | 159 | C    |
| 7   | 7     | 161 | C    |
| 8   | 8     | 2   | C    |
| 8   | 8     | 3   | G    |
| 8   | 8     | 4   | A    |
| 8   | 8     | 5   | G    |
| 8   | 8     | 7   | A    |
| 8   | 8     | 8   | C    |
| 8   | 8     | 9   | G    |
| 8   | 8     | 12  | C    |
| 8   | 8     | 13  | A    |
| 8   | 8     | 15  | A    |
| 8   | 8     | 17  | U    |
| 8   | 8     | 18  | U    |
| 8   | 8     | 24  | A    |
| 8   | 8     | 27  | A    |
| 8   | 8     | 36  | C    |
| 8   | 8     | 39  | G    |
| 8   | 8     | 40  | U    |
| 8   | 8     | 41  | C    |
| 8   | 8     | 43  | G    |
| 8   | 8     | 44  | A    |
| 8   | 8     | 45  | U    |
| 8   | 8     | 47  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 8     | 48  | G    |
| 8   | 8     | 51  | A    |
| 8   | 8     | 52  | A    |
| 8   | 8     | 53  | G    |
| 8   | 8     | 55  | U    |
| 8   | 8     | 56  | A    |
| 8   | 8     | 57  | A    |
| 8   | 8     | 61  | C    |
| 8   | 8     | 63  | C    |
| 8   | 8     | 64  | A    |
| 8   | 8     | 67  | G    |
| 8   | 8     | 73  | G    |
| 8   | 8     | 74  | U    |
| 8   | 8     | 78  | U    |
| 8   | 8     | 82  | G    |
| 8   | 8     | 85  | G    |
| 8   | 8     | 86  | U    |
| 8   | 8     | 87  | C    |
| 8   | 8     | 88  | A    |
| 8   | 8     | 89  | G    |
| 8   | 8     | 91  | G    |
| 8   | 8     | 92  | A    |
| 8   | 8     | 94  | G    |
| 8   | 8     | 102 | A    |
| 8   | 8     | 108 | G    |
| 8   | 8     | 110 | G    |
| 8   | 8     | 111 | U    |
| 8   | 8     | 112 | G    |
| 8   | 8     | 115 | G    |
| 8   | 8     | 116 | U    |
| 8   | 8     | 119 | U    |
| 8   | 8     | 120 | C    |

All (126) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 23  | U    |
| 1   | 1     | 132 | A    |
| 1   | 1     | 136 | G    |
| 1   | 1     | 141 | U    |
| 1   | 1     | 153 | C    |
| 1   | 1     | 154 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 155  | A    |
| 1   | 1     | 167  | U    |
| 1   | 1     | 170  | U    |
| 1   | 1     | 171  | U    |
| 1   | 1     | 191  | U    |
| 1   | 1     | 195  | G    |
| 1   | 1     | 203  | C    |
| 1   | 1     | 205  | A    |
| 1   | 1     | 229  | C    |
| 1   | 1     | 232  | G    |
| 1   | 1     | 333  | A    |
| 1   | 1     | 334  | G    |
| 1   | 1     | 367  | A    |
| 1   | 1     | 409  | U    |
| 1   | 1     | 415  | A    |
| 1   | 1     | 477  | C    |
| 1   | 1     | 559  | G    |
| 1   | 1     | 560  | G    |
| 1   | 1     | 669  | C    |
| 1   | 1     | 693  | G    |
| 1   | 1     | 786  | A    |
| 1   | 1     | 822  | C    |
| 1   | 1     | 959  | OMG  |
| 1   | 1     | 1029 | G    |
| 1   | 1     | 1109 | U    |
| 1   | 1     | 1239 | U    |
| 1   | 1     | 1253 | U    |
| 1   | 1     | 1257 | U    |
| 1   | 1     | 1263 | A    |
| 1   | 1     | 1270 | U    |
| 1   | 1     | 1369 | G    |
| 1   | 1     | 1388 | U    |
| 1   | 1     | 1389 | A    |
| 1   | 1     | 1392 | G    |
| 1   | 1     | 1413 | U    |
| 1   | 1     | 1420 | G    |
| 1   | 1     | 1423 | A    |
| 1   | 1     | 1432 | C    |
| 1   | 1     | 1436 | G    |
| 1   | 1     | 1439 | A    |
| 1   | 1     | 1442 | G    |
| 1   | 1     | 1452 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1466 | G    |
| 1   | 1     | 1506 | A    |
| 1   | 1     | 1526 | OMG  |
| 1   | 1     | 1529 | OMC  |
| 1   | 1     | 1542 | OMG  |
| 1   | 1     | 1591 | C    |
| 1   | 1     | 1662 | U    |
| 1   | 1     | 1751 | G    |
| 1   | 1     | 1763 | A    |
| 2   | 2     | 29   | C    |
| 2   | 2     | 68   | A    |
| 2   | 2     | 349  | C    |
| 2   | 2     | 360  | U    |
| 2   | 2     | 443  | OMC  |
| 2   | 2     | 468  | A    |
| 2   | 2     | 512  | U    |
| 2   | 2     | 552  | C    |
| 2   | 2     | 646  | G    |
| 2   | 2     | 749  | G    |
| 2   | 2     | 755  | U    |
| 2   | 2     | 775  | C    |
| 2   | 2     | 776  | C    |
| 2   | 2     | 782  | G    |
| 2   | 2     | 815  | G    |
| 2   | 2     | 827  | A    |
| 2   | 2     | 832  | A    |
| 2   | 2     | 835  | G    |
| 2   | 2     | 948  | C    |
| 2   | 2     | 957  | C    |
| 2   | 2     | 973  | C    |
| 2   | 2     | 981  | A    |
| 2   | 2     | 996  | G    |
| 2   | 2     | 1184 | C    |
| 2   | 2     | 1318 | OMC  |
| 2   | 2     | 1393 | U    |
| 2   | 2     | 1437 | A    |
| 2   | 2     | 1443 | G    |
| 3   | 3     | 22   | G    |
| 3   | 3     | 31   | C    |
| 3   | 3     | 32   | A    |
| 3   | 3     | 77   | U    |
| 3   | 3     | 78   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 3     | 108 | A    |
| 3   | 3     | 117 | G    |
| 3   | 3     | 132 | G    |
| 3   | 3     | 141 | U    |
| 3   | 3     | 195 | A    |
| 4   | 4     | 50  | G    |
| 4   | 4     | 64  | C    |
| 4   | 4     | 149 | U    |
| 4   | 4     | 157 | A    |
| 4   | 4     | 174 | A    |
| 5   | 5     | 113 | A    |
| 5   | 5     | 125 | A    |
| 5   | 5     | 126 | G    |
| 5   | 5     | 130 | C    |
| 6   | 6     | 2   | C    |
| 6   | 6     | 4   | U    |
| 6   | 6     | 8   | A    |
| 6   | 6     | 14  | A    |
| 6   | 6     | 21  | A    |
| 6   | 6     | 24  | C    |
| 6   | 6     | 29  | G    |
| 6   | 6     | 30  | C    |
| 6   | 6     | 31  | U    |
| 6   | 6     | 32  | U    |
| 6   | 6     | 38  | C    |
| 6   | 6     | 40  | C    |
| 6   | 6     | 41  | G    |
| 6   | 6     | 50  | A    |
| 6   | 6     | 58  | U    |
| 7   | 7     | 88  | A    |
| 7   | 7     | 139 | A    |
| 8   | 8     | 43  | G    |
| 8   | 8     | 48  | G    |
| 8   | 8     | 66  | A    |
| 8   | 8     | 85  | G    |
| 8   | 8     | 91  | G    |

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

44 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | OMG  | 1     | 1526 | 1    | 18,26,27     | 1.11 | 2 (11%)  | 21,38,41    | 2.07 | 5 (23%)  |
| 1   | OMC  | 1     | 1529 | 1    | 15,22,23     | 0.86 | 0        | 20,31,34    | 1.65 | 2 (10%)  |
| 1   | A2M  | 1     | 1541 | 1,2  | 18,25,26     | 0.98 | 1 (5%)   | 18,36,39    | 1.77 | 1 (5%)   |
| 1   | OMG  | 1     | 1542 | 1,2  | 18,26,27     | 1.12 | 2 (11%)  | 21,38,41    | 2.06 | 4 (19%)  |
| 1   | OMG  | 1     | 1628 | 1    | 18,26,27     | 1.14 | 2 (11%)  | 21,38,41    | 2.22 | 6 (28%)  |
| 1   | OMU  | 1     | 36   | 1    | 14,22,23     | 0.92 | 1 (7%)   | 19,31,34    | 1.58 | 2 (10%)  |
| 1   | OMU  | 1     | 48   | 1    | 14,22,23     | 1.02 | 1 (7%)   | 19,31,34    | 1.68 | 1 (5%)   |
| 1   | A2M  | 1     | 678  | 1,2  | 18,25,26     | 0.98 | 1 (5%)   | 18,36,39    | 1.82 | 1 (5%)   |
| 1   | A2M  | 1     | 681  | 1    | 18,25,26     | 0.96 | 1 (5%)   | 18,36,39    | 1.82 | 1 (5%)   |
| 1   | OMC  | 1     | 695  | 1    | 15,22,23     | 0.95 | 1 (6%)   | 20,31,34    | 1.61 | 4 (20%)  |
| 1   | OMU  | 1     | 845  | 1    | 14,22,23     | 1.03 | 2 (14%)  | 19,31,34    | 1.64 | 2 (10%)  |
| 1   | OMU  | 1     | 847  | 1    | 14,22,23     | 0.93 | 1 (7%)   | 19,31,34    | 1.56 | 1 (5%)   |
| 1   | OMG  | 1     | 856  | 1    | 18,26,27     | 1.06 | 2 (11%)  | 21,38,41    | 2.23 | 6 (28%)  |
| 1   | A2M  | 1     | 927  | 1    | 18,25,26     | 1.04 | 1 (5%)   | 18,36,39    | 1.94 | 1 (5%)   |
| 1   | A2M  | 1     | 955  | 1    | 18,25,26     | 0.97 | 1 (5%)   | 18,36,39    | 1.92 | 2 (11%)  |
| 1   | OMG  | 1     | 959  | 1    | 18,26,27     | 1.22 | 2 (11%)  | 21,38,41    | 2.02 | 5 (23%)  |
| 2   | OMU  | 2     | 1078 | 2    | 14,22,23     | 0.87 | 1 (7%)   | 19,31,34    | 1.63 | 1 (5%)   |
| 2   | OMG  | 2     | 1079 | 2    | 18,26,27     | 1.21 | 2 (11%)  | 21,38,41    | 2.13 | 6 (28%)  |
| 2   | OMU  | 2     | 1153 | 2    | 14,22,23     | 0.97 | 1 (7%)   | 19,31,34    | 1.73 | 2 (10%)  |
| 2   | OMC  | 2     | 1160 | 2    | 15,22,23     | 0.84 | 0        | 20,31,34    | 1.69 | 2 (10%)  |
| 2   | A2M  | 2     | 1186 | 2    | 18,25,26     | 0.97 | 1 (5%)   | 18,36,39    | 1.82 | 2 (11%)  |
| 2   | OMG  | 2     | 1230 | 2    | 18,26,27     | 1.17 | 2 (11%)  | 21,38,41    | 2.04 | 5 (23%)  |
| 2   | OMC  | 2     | 1249 | 2    | 15,22,23     | 0.81 | 0        | 20,31,34    | 1.64 | 3 (15%)  |
| 2   | OMG  | 2     | 1254 | 2    | 18,26,27     | 1.13 | 2 (11%)  | 21,38,41    | 1.94 | 4 (19%)  |
| 2   | OMC  | 2     | 1318 | 2    | 15,22,23     | 0.82 | 0        | 20,31,34    | 1.52 | 2 (10%)  |
| 2   | OMC  | 2     | 1398 | 2    | 15,22,23     | 0.86 | 0        | 20,31,34    | 1.55 | 2 (10%)  |
| 2   | H2U  | 2     | 1404 | 2    | 17,21,22     | 1.10 | 2 (11%)  | 23,30,33    | 1.79 | 4 (17%)  |
| 2   | A2M  | 2     | 382  | 2    | 18,25,26     | 0.95 | 1 (5%)   | 18,36,39    | 1.73 | 1 (5%)   |
| 2   | OMC  | 2     | 443  | 2    | 15,22,23     | 0.84 | 0        | 20,31,34    | 1.61 | 1 (5%)   |
| 2   | A2M  | 2     | 527  | 2    | 18,25,26     | 0.97 | 1 (5%)   | 18,36,39    | 2.01 | 2 (11%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | OMG  | 2     | 534 | 2    | 18,26,27     | 1.19 | 2 (11%)  | 21,38,41    | 2.14 | 6 (28%)  |
| 2   | OMC  | 2     | 554 | 2    | 15,22,23     | 0.81 | 0        | 20,31,34    | 1.67 | 2 (10%)  |
| 2   | OMG  | 2     | 571 | 2    | 18,26,27     | 1.15 | 2 (11%)  | 21,38,41    | 2.21 | 6 (28%)  |
| 2   | A2M  | 2     | 572 | 2    | 18,25,26     | 1.00 | 1 (5%)   | 18,36,39    | 1.71 | 1 (5%)   |
| 2   | OMC  | 2     | 583 | 2    | 15,22,23     | 0.89 | 0        | 20,31,34    | 1.66 | 1 (5%)   |
| 2   | A2M  | 2     | 591 | 2    | 18,25,26     | 0.98 | 1 (5%)   | 18,36,39    | 1.86 | 1 (5%)   |
| 2   | A2M  | 2     | 628 | 2    | 18,25,26     | 0.97 | 1 (5%)   | 18,36,39    | 1.91 | 2 (11%)  |
| 2   | OMG  | 2     | 641 | 2    | 18,26,27     | 1.13 | 2 (11%)  | 21,38,41    | 2.15 | 6 (28%)  |
| 2   | OMG  | 2     | 655 | 2    | 18,26,27     | 1.16 | 2 (11%)  | 21,38,41    | 1.94 | 4 (19%)  |
| 2   | OMU  | 2     | 656 | 2    | 14,22,23     | 0.89 | 1 (7%)   | 19,31,34    | 1.64 | 2 (10%)  |
| 2   | OMU  | 2     | 667 | 2    | 14,22,23     | 0.88 | 1 (7%)   | 19,31,34    | 1.70 | 1 (5%)   |
| 2   | OMG  | 2     | 71  | 2    | 18,26,27     | 1.15 | 2 (11%)  | 21,38,41    | 1.98 | 5 (23%)  |
| 7   | A2M  | 7     | 162 | 1,7  | 18,25,26     | 1.03 | 1 (5%)   | 18,36,39    | 2.06 | 3 (16%)  |
| 7   | OMU  | 7     | 7   | 1,7  | 14,22,23     | 0.94 | 1 (7%)   | 19,31,34    | 1.79 | 2 (10%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | OMG  | 1     | 1526 | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | OMC  | 1     | 1529 | 1    | -       | 0/5/27/28 | 0/2/2/2 |
| 1   | A2M  | 1     | 1541 | 1,2  | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | OMG  | 1     | 1542 | 1,2  | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | OMG  | 1     | 1628 | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | OMU  | 1     | 36   | 1    | -       | 0/5/27/28 | 0/2/2/2 |
| 1   | OMU  | 1     | 48   | 1    | -       | 0/5/27/28 | 0/2/2/2 |
| 1   | A2M  | 1     | 678  | 1,2  | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | A2M  | 1     | 681  | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | OMC  | 1     | 695  | 1    | -       | 0/5/27/28 | 0/2/2/2 |
| 1   | OMU  | 1     | 845  | 1    | -       | 0/5/27/28 | 0/2/2/2 |
| 1   | OMU  | 1     | 847  | 1    | -       | 0/5/27/28 | 0/2/2/2 |
| 1   | OMG  | 1     | 856  | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | A2M  | 1     | 927  | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | A2M  | 1     | 955  | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | OMG  | 1     | 959  | 1    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | OMU  | 2     | 1078 | 2    | -       | 0/5/27/28 | 0/2/2/2 |
| 2   | OMG  | 2     | 1079 | 2    | -       | 0/5/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 2   | OMU  | 2     | 1153 | 2    | -       | 0/5/27/28 | 0/2/2/2 |
| 2   | OMC  | 2     | 1160 | 2    | -       | 0/5/27/28 | 0/2/2/2 |
| 2   | A2M  | 2     | 1186 | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | OMG  | 2     | 1230 | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | OMC  | 2     | 1249 | 2    | -       | 0/5/27/28 | 0/2/2/2 |
| 2   | OMG  | 2     | 1254 | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | OMC  | 2     | 1318 | 2    | -       | 0/5/27/28 | 0/2/2/2 |
| 2   | OMC  | 2     | 1398 | 2    | -       | 0/5/27/28 | 0/2/2/2 |
| 2   | H2U  | 2     | 1404 | 2    | -       | 0/7/38/39 | 0/2/2/2 |
| 2   | A2M  | 2     | 382  | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | OMC  | 2     | 443  | 2    | -       | 0/5/27/28 | 0/2/2/2 |
| 2   | A2M  | 2     | 527  | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | OMG  | 2     | 534  | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | OMC  | 2     | 554  | 2    | -       | 0/5/27/28 | 0/2/2/2 |
| 2   | OMG  | 2     | 571  | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | A2M  | 2     | 572  | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | OMC  | 2     | 583  | 2    | -       | 0/5/27/28 | 0/2/2/2 |
| 2   | A2M  | 2     | 591  | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | A2M  | 2     | 628  | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | OMG  | 2     | 641  | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | OMG  | 2     | 655  | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 2   | OMU  | 2     | 656  | 2    | -       | 0/5/27/28 | 0/2/2/2 |
| 2   | OMU  | 2     | 667  | 2    | -       | 0/5/27/28 | 0/2/2/2 |
| 2   | OMG  | 2     | 71   | 2    | -       | 0/5/27/28 | 0/3/3/3 |
| 7   | A2M  | 7     | 162  | 1,7  | -       | 0/5/27/28 | 0/3/3/3 |
| 7   | OMU  | 7     | 7    | 1,7  | -       | 0/5/27/28 | 0/2/2/2 |

All (51) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | 2     | 1404 | H2U  | C4-N3 | -2.68 | 1.33        | 1.37     |
| 2   | 2     | 1404 | H2U  | C2-N3 | -2.57 | 1.33        | 1.38     |
| 1   | 1     | 845  | OMU  | C2-N3 | -2.37 | 1.33        | 1.38     |
| 1   | 1     | 48   | OMU  | C2-N3 | -2.32 | 1.33        | 1.38     |
| 1   | 1     | 36   | OMU  | C2-N3 | -2.21 | 1.33        | 1.38     |
| 1   | 1     | 847  | OMU  | C2-N3 | -2.21 | 1.33        | 1.38     |
| 2   | 2     | 1153 | OMU  | C2-N3 | -2.17 | 1.33        | 1.38     |
| 2   | 2     | 667  | OMU  | C2-N3 | -2.11 | 1.33        | 1.38     |
| 2   | 2     | 1078 | OMU  | C2-N3 | -2.09 | 1.33        | 1.38     |
| 1   | 1     | 845  | OMU  | C6-N1 | -2.05 | 1.33        | 1.35     |
| 2   | 2     | 656  | OMU  | C2-N3 | -2.02 | 1.34        | 1.38     |
| 7   | 7     | 7    | OMU  | C2-N3 | -2.01 | 1.34        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 1   | 1     | 695  | OMC  | O4'-C1' | 2.00 | 1.44        | 1.41     |
| 1   | 1     | 1628 | OMG  | C5-C4   | 2.54 | 1.46        | 1.40     |
| 1   | 1     | 856  | OMG  | C5-C4   | 2.57 | 1.46        | 1.40     |
| 1   | 1     | 1542 | OMG  | C5-C4   | 2.64 | 1.46        | 1.40     |
| 2   | 2     | 641  | OMG  | C5-C4   | 2.70 | 1.46        | 1.40     |
| 2   | 2     | 1254 | OMG  | C5-C4   | 2.71 | 1.46        | 1.40     |
| 1   | 1     | 681  | A2M  | C5-C4   | 2.74 | 1.46        | 1.40     |
| 2   | 2     | 655  | OMG  | C5-C4   | 2.74 | 1.46        | 1.40     |
| 2   | 2     | 71   | OMG  | C5-C4   | 2.74 | 1.46        | 1.40     |
| 1   | 1     | 1526 | OMG  | C5-C4   | 2.77 | 1.46        | 1.40     |
| 1   | 1     | 955  | A2M  | C5-C4   | 2.77 | 1.46        | 1.40     |
| 1   | 1     | 1541 | A2M  | C5-C4   | 2.79 | 1.46        | 1.40     |
| 2   | 2     | 382  | A2M  | C5-C4   | 2.79 | 1.46        | 1.40     |
| 2   | 2     | 527  | A2M  | C5-C4   | 2.80 | 1.46        | 1.40     |
| 2   | 2     | 1230 | OMG  | C5-C4   | 2.80 | 1.46        | 1.40     |
| 2   | 2     | 1079 | OMG  | C5-C4   | 2.80 | 1.46        | 1.40     |
| 2   | 2     | 571  | OMG  | C5-C4   | 2.81 | 1.46        | 1.40     |
| 2   | 2     | 628  | A2M  | C5-C4   | 2.82 | 1.46        | 1.40     |
| 1   | 1     | 678  | A2M  | C5-C4   | 2.84 | 1.46        | 1.40     |
| 2   | 2     | 534  | OMG  | C5-C4   | 2.85 | 1.46        | 1.40     |
| 2   | 2     | 591  | A2M  | C5-C4   | 2.87 | 1.47        | 1.40     |
| 1   | 1     | 927  | A2M  | C5-C4   | 2.88 | 1.47        | 1.40     |
| 2   | 2     | 1186 | A2M  | C5-C4   | 2.89 | 1.47        | 1.40     |
| 2   | 2     | 572  | A2M  | C5-C4   | 2.96 | 1.47        | 1.40     |
| 1   | 1     | 856  | OMG  | C6-C5   | 3.05 | 1.47        | 1.41     |
| 1   | 1     | 959  | OMG  | C5-C4   | 3.06 | 1.47        | 1.40     |
| 7   | 7     | 162  | A2M  | C5-C4   | 3.07 | 1.47        | 1.40     |
| 2   | 2     | 641  | OMG  | C6-C5   | 3.10 | 1.47        | 1.41     |
| 2   | 2     | 1254 | OMG  | C6-C5   | 3.20 | 1.47        | 1.41     |
| 1   | 1     | 1542 | OMG  | C6-C5   | 3.22 | 1.47        | 1.41     |
| 1   | 1     | 1526 | OMG  | C6-C5   | 3.23 | 1.47        | 1.41     |
| 1   | 1     | 1628 | OMG  | C6-C5   | 3.26 | 1.47        | 1.41     |
| 2   | 2     | 1230 | OMG  | C6-C5   | 3.35 | 1.48        | 1.41     |
| 2   | 2     | 71   | OMG  | C6-C5   | 3.35 | 1.48        | 1.41     |
| 1   | 1     | 959  | OMG  | C6-C5   | 3.39 | 1.48        | 1.41     |
| 2   | 2     | 655  | OMG  | C6-C5   | 3.40 | 1.48        | 1.41     |
| 2   | 2     | 571  | OMG  | C6-C5   | 3.44 | 1.48        | 1.41     |
| 2   | 2     | 534  | OMG  | C6-C5   | 3.46 | 1.48        | 1.41     |
| 2   | 2     | 1079 | OMG  | C6-C5   | 3.57 | 1.48        | 1.41     |

All (123) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | 1     | 927  | A2M  | N3-C2-N1   | -7.00 | 123.37      | 128.87   |
| 1   | 1     | 678  | A2M  | N3-C2-N1   | -6.92 | 123.43      | 128.87   |
| 1   | 1     | 955  | A2M  | N3-C2-N1   | -6.88 | 123.47      | 128.87   |
| 2   | 2     | 628  | A2M  | N3-C2-N1   | -6.83 | 123.50      | 128.87   |
| 2   | 2     | 591  | A2M  | N3-C2-N1   | -6.72 | 123.59      | 128.87   |
| 1   | 1     | 681  | A2M  | N3-C2-N1   | -6.71 | 123.60      | 128.87   |
| 1   | 1     | 1541 | A2M  | N3-C2-N1   | -6.65 | 123.65      | 128.87   |
| 2   | 2     | 527  | A2M  | N3-C2-N1   | -6.58 | 123.70      | 128.87   |
| 2   | 2     | 1186 | A2M  | N3-C2-N1   | -6.41 | 123.83      | 128.87   |
| 7   | 7     | 162  | A2M  | N3-C2-N1   | -6.34 | 123.89      | 128.87   |
| 2   | 2     | 382  | A2M  | N3-C2-N1   | -6.33 | 123.89      | 128.87   |
| 2   | 2     | 572  | A2M  | N3-C2-N1   | -6.21 | 123.99      | 128.87   |
| 2   | 2     | 1404 | H2U  | C4-N3-C2   | -5.59 | 120.71      | 125.77   |
| 2   | 2     | 534  | OMG  | C5-C6-N1   | -4.43 | 117.73      | 123.52   |
| 1   | 1     | 1526 | OMG  | C5-C6-N1   | -4.30 | 117.91      | 123.52   |
| 2   | 2     | 641  | OMG  | C5-C6-N1   | -4.24 | 117.97      | 123.52   |
| 2   | 2     | 71   | OMG  | C5-C6-N1   | -4.22 | 118.00      | 123.52   |
| 2   | 2     | 571  | OMG  | C5-C6-N1   | -4.20 | 118.03      | 123.52   |
| 2   | 2     | 1079 | OMG  | C5-C6-N1   | -4.19 | 118.04      | 123.52   |
| 1   | 1     | 856  | OMG  | C5-C6-N1   | -4.13 | 118.13      | 123.52   |
| 2   | 2     | 1230 | OMG  | C5-C6-N1   | -4.12 | 118.14      | 123.52   |
| 2   | 2     | 1254 | OMG  | C5-C6-N1   | -4.08 | 118.19      | 123.52   |
| 2   | 2     | 655  | OMG  | C5-C6-N1   | -4.08 | 118.19      | 123.52   |
| 1   | 1     | 1542 | OMG  | C5-C6-N1   | -4.03 | 118.26      | 123.52   |
| 1   | 1     | 1628 | OMG  | C5-C6-N1   | -3.97 | 118.34      | 123.52   |
| 1   | 1     | 959  | OMG  | C5-C6-N1   | -3.95 | 118.36      | 123.52   |
| 1   | 1     | 1628 | OMG  | C6-C5-C4   | -3.89 | 116.42      | 120.86   |
| 1   | 1     | 1628 | OMG  | N3-C2-N1   | -3.83 | 122.35      | 127.56   |
| 2   | 2     | 641  | OMG  | N3-C2-N1   | -3.78 | 122.42      | 127.56   |
| 2   | 2     | 1404 | H2U  | C5-C6-N1   | -3.74 | 106.66      | 110.76   |
| 1   | 1     | 856  | OMG  | C2'-C1'-N9 | -3.73 | 102.82      | 113.48   |
| 1   | 1     | 856  | OMG  | N3-C2-N1   | -3.71 | 122.51      | 127.56   |
| 2   | 2     | 1079 | OMG  | C6-C5-C4   | -3.65 | 116.68      | 120.86   |
| 2   | 2     | 641  | OMG  | C6-C5-C4   | -3.64 | 116.70      | 120.86   |
| 2   | 2     | 1079 | OMG  | N3-C2-N1   | -3.62 | 122.63      | 127.56   |
| 2   | 2     | 571  | OMG  | C6-C5-C4   | -3.60 | 116.75      | 120.86   |
| 1   | 1     | 856  | OMG  | C6-C5-C4   | -3.59 | 116.75      | 120.86   |
| 2   | 2     | 1254 | OMG  | N3-C2-N1   | -3.59 | 122.67      | 127.56   |
| 2   | 2     | 571  | OMG  | N3-C2-N1   | -3.56 | 122.72      | 127.56   |
| 1   | 1     | 1542 | OMG  | C6-C5-C4   | -3.55 | 116.80      | 120.86   |
| 1   | 1     | 1542 | OMG  | N3-C2-N1   | -3.54 | 122.74      | 127.56   |
| 2   | 2     | 1230 | OMG  | N3-C2-N1   | -3.51 | 122.78      | 127.56   |
| 2   | 2     | 534  | OMG  | N3-C2-N1   | -3.50 | 122.79      | 127.56   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | 2     | 1230 | OMG  | C6-C5-C4    | -3.48 | 116.88      | 120.86   |
| 7   | 7     | 7    | OMU  | C2'-C1'-N1  | -3.46 | 103.60      | 113.48   |
| 1   | 1     | 1526 | OMG  | N3-C2-N1    | -3.43 | 122.90      | 127.56   |
| 1   | 1     | 959  | OMG  | N3-C2-N1    | -3.37 | 122.97      | 127.56   |
| 2   | 2     | 655  | OMG  | C6-C5-C4    | -3.36 | 117.02      | 120.86   |
| 2   | 2     | 655  | OMG  | N3-C2-N1    | -3.35 | 122.99      | 127.56   |
| 2   | 2     | 534  | OMG  | C6-C5-C4    | -3.28 | 117.11      | 120.86   |
| 2   | 2     | 71   | OMG  | N3-C2-N1    | -3.26 | 123.12      | 127.56   |
| 2   | 2     | 71   | OMG  | C6-C5-C4    | -3.21 | 117.19      | 120.86   |
| 2   | 2     | 1254 | OMG  | C6-C5-C4    | -3.20 | 117.20      | 120.86   |
| 1   | 1     | 1526 | OMG  | C6-C5-C4    | -3.16 | 117.24      | 120.86   |
| 1   | 1     | 959  | OMG  | C6-C5-C4    | -3.10 | 117.32      | 120.86   |
| 2   | 2     | 571  | OMG  | C2'-C1'-N9  | -3.07 | 104.71      | 113.48   |
| 1   | 1     | 1628 | OMG  | C1'-N9-C4   | -3.05 | 123.40      | 126.81   |
| 2   | 2     | 1079 | OMG  | C1'-N9-C4   | -2.92 | 123.55      | 126.81   |
| 7   | 7     | 162  | A2M  | C4'-O4'-C1' | -2.92 | 106.55      | 109.64   |
| 2   | 2     | 71   | OMG  | C2'-C1'-N9  | -2.78 | 105.55      | 113.48   |
| 2   | 2     | 571  | OMG  | C1'-N9-C4   | -2.69 | 123.80      | 126.81   |
| 1   | 1     | 1628 | OMG  | C2'-C1'-N9  | -2.63 | 105.95      | 113.48   |
| 2   | 2     | 534  | OMG  | C2'-C1'-N9  | -2.55 | 106.19      | 113.48   |
| 1   | 1     | 845  | OMU  | C2'-C1'-N1  | -2.53 | 106.23      | 113.48   |
| 2   | 2     | 1230 | OMG  | C2'-C1'-N9  | -2.50 | 106.33      | 113.48   |
| 2   | 2     | 641  | OMG  | C2'-C1'-N9  | -2.49 | 106.37      | 113.48   |
| 2   | 2     | 1398 | OMC  | C2'-C1'-N1  | -2.48 | 106.38      | 113.48   |
| 2   | 2     | 1153 | OMU  | C2'-C1'-N1  | -2.47 | 106.43      | 113.48   |
| 2   | 2     | 656  | OMU  | C2'-C1'-N1  | -2.46 | 106.43      | 113.48   |
| 1   | 1     | 856  | OMG  | C1'-N9-C4   | -2.38 | 124.14      | 126.81   |
| 1   | 1     | 695  | OMC  | C2'-C1'-N1  | -2.15 | 107.34      | 113.48   |
| 2   | 2     | 641  | OMG  | C1'-N9-C4   | -2.15 | 124.41      | 126.81   |
| 2   | 2     | 628  | A2M  | C2'-C1'-N9  | -2.11 | 107.45      | 113.48   |
| 1   | 1     | 36   | OMU  | C2'-C1'-N1  | -2.11 | 107.46      | 113.48   |
| 2   | 2     | 534  | OMG  | C1'-N9-C4   | -2.09 | 124.47      | 126.81   |
| 2   | 2     | 1249 | OMC  | C2'-C1'-N1  | -2.05 | 107.61      | 113.48   |
| 1   | 1     | 695  | OMC  | C5'-C4'-C3' | -2.05 | 107.28      | 115.20   |
| 1   | 1     | 955  | A2M  | C1'-N9-C4   | -2.03 | 124.54      | 126.81   |
| 2   | 2     | 1318 | OMC  | N4-C4-N3    | 2.03  | 120.05      | 116.50   |
| 1   | 1     | 959  | OMG  | C4'-O4'-C1' | 2.04  | 111.81      | 109.64   |
| 1   | 1     | 695  | OMC  | N4-C4-N3    | 2.04  | 120.07      | 116.50   |
| 2   | 2     | 1079 | OMG  | O4'-C1'-N9  | 2.05  | 111.97      | 108.11   |
| 2   | 2     | 554  | OMC  | N4-C4-N3    | 2.07  | 120.11      | 116.50   |
| 2   | 2     | 1186 | A2M  | C4'-O4'-C1' | 2.09  | 111.86      | 109.64   |
| 2   | 2     | 1160 | OMC  | O4'-C1'-N1  | 2.09  | 112.08      | 108.10   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 1   | 1     | 1526 | OMG  | O4'-C1'-N9 | 2.10 | 112.07      | 108.11   |
| 1   | 1     | 1529 | OMC  | N4-C4-N3   | 2.11 | 120.18      | 116.50   |
| 2   | 2     | 1249 | OMC  | N4-C4-N3   | 2.22 | 120.38      | 116.50   |
| 2   | 2     | 1404 | H2U  | C6-N1-C2   | 2.29 | 125.70      | 122.16   |
| 2   | 2     | 527  | A2M  | O4'-C1'-N9 | 2.66 | 113.14      | 108.11   |
| 7   | 7     | 162  | A2M  | O4'-C1'-N9 | 3.37 | 114.48      | 108.11   |
| 2   | 2     | 1404 | H2U  | C1'-N1-C2  | 3.53 | 123.13      | 118.19   |
| 1   | 1     | 695  | OMC  | C6-C5-C4   | 4.75 | 119.30      | 117.44   |
| 2   | 2     | 1318 | OMC  | C6-C5-C4   | 4.83 | 119.33      | 117.44   |
| 1   | 1     | 959  | OMG  | C6-N1-C2   | 5.23 | 122.01      | 115.88   |
| 2   | 2     | 655  | OMG  | C6-N1-C2   | 5.34 | 122.14      | 115.88   |
| 2   | 2     | 71   | OMG  | C6-N1-C2   | 5.43 | 122.25      | 115.88   |
| 1   | 1     | 1542 | OMG  | C6-N1-C2   | 5.46 | 122.28      | 115.88   |
| 2   | 2     | 1398 | OMC  | C6-C5-C4   | 5.47 | 119.58      | 117.44   |
| 2   | 2     | 1254 | OMG  | C6-N1-C2   | 5.51 | 122.34      | 115.88   |
| 2   | 2     | 1230 | OMG  | C6-N1-C2   | 5.54 | 122.37      | 115.88   |
| 1   | 1     | 1526 | OMG  | C6-N1-C2   | 5.55 | 122.39      | 115.88   |
| 1   | 1     | 1628 | OMG  | C6-N1-C2   | 5.60 | 122.44      | 115.88   |
| 2   | 2     | 1079 | OMG  | C6-N1-C2   | 5.64 | 122.48      | 115.88   |
| 1   | 1     | 1529 | OMC  | C6-C5-C4   | 5.70 | 119.67      | 117.44   |
| 2   | 2     | 571  | OMG  | C6-N1-C2   | 5.70 | 122.56      | 115.88   |
| 2   | 2     | 554  | OMC  | C6-C5-C4   | 5.70 | 119.67      | 117.44   |
| 2   | 2     | 534  | OMG  | C6-N1-C2   | 5.72 | 122.59      | 115.88   |
| 2   | 2     | 1249 | OMC  | C6-C5-C4   | 5.74 | 119.69      | 117.44   |
| 7   | 7     | 7    | OMU  | C4-N3-C2   | 5.74 | 120.26      | 114.21   |
| 1   | 1     | 856  | OMG  | C6-N1-C2   | 5.76 | 122.63      | 115.88   |
| 2   | 2     | 656  | OMU  | C4-N3-C2   | 5.79 | 120.31      | 114.21   |
| 1   | 1     | 845  | OMU  | C4-N3-C2   | 5.79 | 120.31      | 114.21   |
| 2   | 2     | 1078 | OMU  | C4-N3-C2   | 5.85 | 120.37      | 114.21   |
| 1   | 1     | 36   | OMU  | C4-N3-C2   | 5.87 | 120.39      | 114.21   |
| 2   | 2     | 1153 | OMU  | C4-N3-C2   | 5.87 | 120.40      | 114.21   |
| 1   | 1     | 847  | OMU  | C4-N3-C2   | 5.88 | 120.40      | 114.21   |
| 2   | 2     | 641  | OMG  | C6-N1-C2   | 5.90 | 122.80      | 115.88   |
| 2   | 2     | 443  | OMC  | C6-C5-C4   | 6.04 | 119.80      | 117.44   |
| 1   | 1     | 48   | OMU  | C4-N3-C2   | 6.05 | 120.58      | 114.21   |
| 2   | 2     | 583  | OMC  | C6-C5-C4   | 6.08 | 119.82      | 117.44   |
| 2   | 2     | 667  | OMU  | C4-N3-C2   | 6.20 | 120.74      | 114.21   |
| 2   | 2     | 1160 | OMC  | C6-C5-C4   | 6.36 | 119.93      | 117.44   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

41 monomers are involved in 186 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 1     | 1526 | OMG  | 2       | 0            |
| 1   | 1     | 1529 | OMC  | 6       | 0            |
| 1   | 1     | 1541 | A2M  | 3       | 0            |
| 1   | 1     | 1542 | OMG  | 2       | 0            |
| 1   | 1     | 1628 | OMG  | 1       | 0            |
| 1   | 1     | 36   | OMU  | 14      | 0            |
| 1   | 1     | 48   | OMU  | 4       | 0            |
| 1   | 1     | 678  | A2M  | 2       | 0            |
| 1   | 1     | 681  | A2M  | 2       | 0            |
| 1   | 1     | 695  | OMC  | 3       | 0            |
| 1   | 1     | 845  | OMU  | 2       | 0            |
| 1   | 1     | 847  | OMU  | 3       | 0            |
| 1   | 1     | 856  | OMG  | 2       | 0            |
| 1   | 1     | 927  | A2M  | 3       | 0            |
| 1   | 1     | 955  | A2M  | 2       | 0            |
| 1   | 1     | 959  | OMG  | 9       | 0            |
| 2   | 2     | 1078 | OMU  | 11      | 0            |
| 2   | 2     | 1079 | OMG  | 9       | 0            |
| 2   | 2     | 1153 | OMU  | 6       | 0            |
| 2   | 2     | 1160 | OMC  | 3       | 0            |
| 2   | 2     | 1186 | A2M  | 3       | 0            |
| 2   | 2     | 1230 | OMG  | 2       | 0            |
| 2   | 2     | 1249 | OMC  | 1       | 0            |
| 2   | 2     | 1254 | OMG  | 10      | 0            |
| 2   | 2     | 1318 | OMC  | 7       | 0            |
| 2   | 2     | 1398 | OMC  | 4       | 0            |
| 2   | 2     | 1404 | H2U  | 2       | 0            |
| 2   | 2     | 382  | A2M  | 2       | 0            |
| 2   | 2     | 443  | OMC  | 7       | 0            |
| 2   | 2     | 527  | A2M  | 13      | 0            |
| 2   | 2     | 534  | OMG  | 4       | 0            |
| 2   | 2     | 554  | OMC  | 3       | 0            |
| 2   | 2     | 571  | OMG  | 1       | 0            |
| 2   | 2     | 572  | A2M  | 2       | 0            |
| 2   | 2     | 583  | OMC  | 1       | 0            |
| 2   | 2     | 591  | A2M  | 7       | 0            |
| 2   | 2     | 628  | A2M  | 4       | 0            |
| 2   | 2     | 655  | OMG  | 7       | 0            |
| 2   | 2     | 667  | OMU  | 5       | 0            |
| 2   | 2     | 71   | OMG  | 11      | 0            |
| 7   | 7     | 7    | OMU  | 10      | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 109 ligands modelled in this entry, 109 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.